



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:16 PM UTC

PDB ID : 1LKR / pdb\_00001lkr  
Title : MONOCLINIC HEN EGG WHITE LYSOZYME IODIDE  
Authors : Steinrauf, L.K.  
Deposited on : 1998-01-20  
Resolution : 1.60 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)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

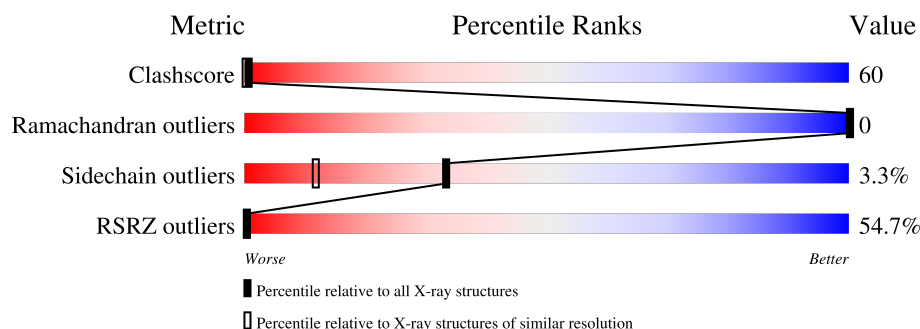
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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                      | 4931 (1.60-1.60)                                      |
| Ramachandran outliers | 187476                      | 4831 (1.60-1.60)                                      |
| Sidechain outliers    | 187428                      | 4830 (1.60-1.60)                                      |
| RSRZ outliers         | 180081                      | 4672 (1.60-1.60)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | A     | 129    | <div> <div>53%</div> <div> <div></div> <div>62%</div> <div>34%</div> </div> </div> |
| 1   | B     | 129    | <div> <div>57%</div> <div> <div></div> <div>75%</div> <div>22%</div> </div> </div> |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2330 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 LYSOZYME.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 1   | A     | 129      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1001  | 613 | 193 | 185 | 10 |         |         |       |
| 1   | B     | 129      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1001  | 613 | 193 | 185 | 10 |         |         |       |

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 11       | Total | I  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 2   | B     | 6        | Total | I  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |

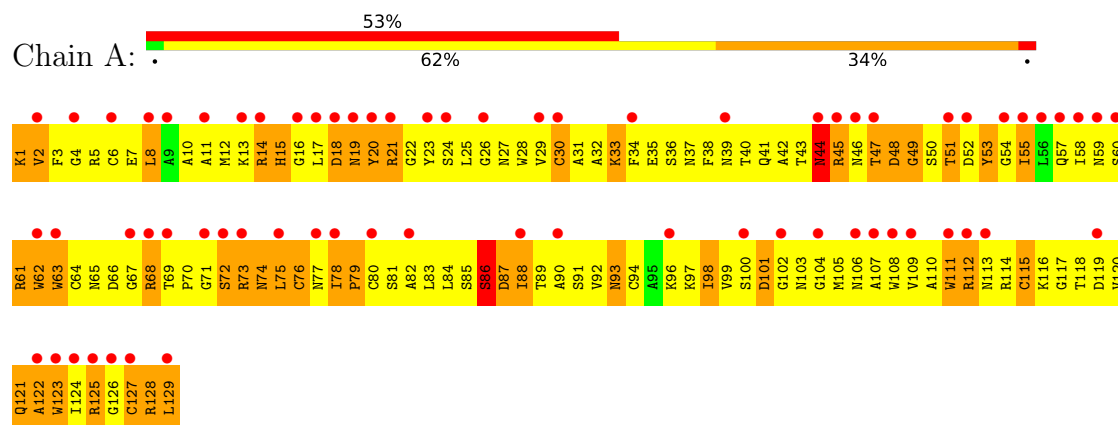
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 143      | Total | O   | 0       | 0       |
|     |       |          | 143   | 143 |         |         |
| 3   | B     | 168      | Total | O   | 0       | 0       |
|     |       |          | 168   | 168 |         |         |

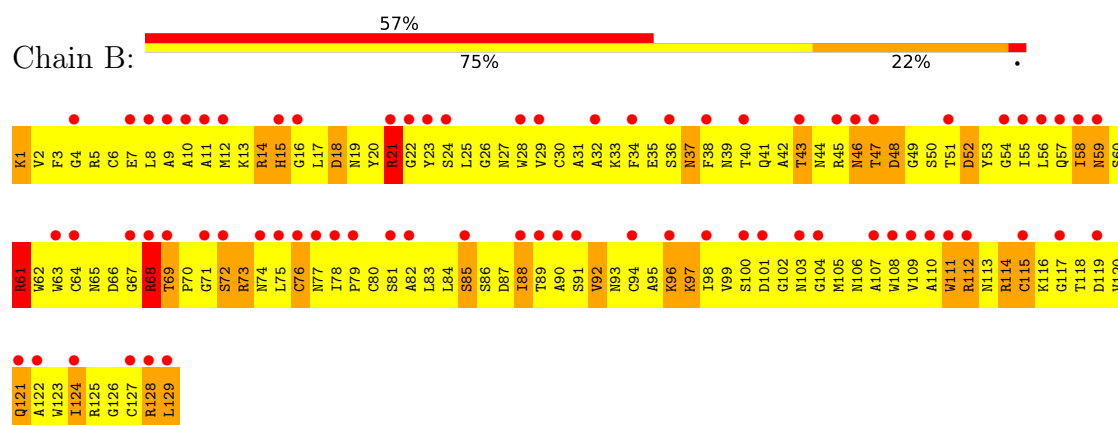
### 3 Residue-property plots

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

#### • Molecule 1: LYSOZYME



#### • Molecule 1: LYSOZYME



## 4 Data and refinement statistics

| Property                                                                | Value                                                                            | Source           |
|-------------------------------------------------------------------------|----------------------------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 27.89Å 63.15Å 60.23Å<br>90.00° 90.12° 90.00°                                     | Depositor        |
| Resolution (Å)                                                          | 8.00 – 1.60<br>8.00 – 1.60                                                       | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 63.0 (8.00-1.60)<br>41.5 (8.00-1.60)                                             | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                                  | Depositor        |
| $\langle I/\sigma(I) \rangle$                                           | -                                                                                | Xtrriage         |
| Refinement program                                                      | X-PLOR                                                                           | Depositor        |
| R, $R_{free}$                                                           | 0.106 , 0.140<br>0.531 , (Not available)                                         | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                                           | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | (Not available)                                                                  | Xtrriage         |
| Anisotropy                                                              | (Not available)                                                                  | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.39 , 127.0                                                                     | EDS              |
| L-test for twinning <sup>1</sup>                                        | $\langle  L  \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available) | Xtrriage         |
| Estimated twinning fraction                                             | No twinning to report.                                                           | Xtrriage         |
| $F_o, F_c$ correlation                                                  | 0.52                                                                             | EDS              |
| Total number of atoms                                                   | 2330                                                                             | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 4.0                                                                              | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IOD

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     | 8.03         | 429/1021 (42.0%) | 6.96        | 480/1379 (34.8%) |
| 1   | B     | 8.10         | 404/1021 (39.6%) | 6.97        | 494/1379 (35.8%) |
| All | All   | 8.06         | 833/2042 (40.8%) | 6.96        | 974/2758 (35.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | B     | 0                   | 3                   |

All (833) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | B     | 21  | ARG  | NE-CZ  | -91.13 | 0.32        | 1.33     |
| 1   | B     | 61  | ARG  | CZ-NH1 | 61.16  | 2.18        | 1.32     |
| 1   | A     | 45  | ARG  | CZ-NH1 | 49.11  | 2.01        | 1.32     |
| 1   | B     | 128 | ARG  | NE-CZ  | 45.86  | 1.83        | 1.33     |
| 1   | A     | 47  | THR  | N-CA   | 45.41  | 2.06        | 1.46     |
| 1   | B     | 114 | ARG  | NE-CZ  | 44.26  | 1.81        | 1.33     |
| 1   | B     | 45  | ARG  | CZ-NH1 | 38.11  | 1.86        | 1.32     |
| 1   | A     | 45  | ARG  | NE-CZ  | 37.52  | 1.74        | 1.33     |
| 1   | B     | 14  | ARG  | CD-NE  | -36.52 | 0.95        | 1.46     |
| 1   | A     | 48  | ASP  | C-N    | 35.98  | 1.86        | 1.33     |
| 1   | B     | 128 | ARG  | CZ-NH2 | 35.66  | 1.79        | 1.33     |
| 1   | A     | 112 | ARG  | CZ-NH1 | -30.87 | 0.89        | 1.32     |
| 1   | B     | 73  | ARG  | CZ-NH1 | 29.74  | 1.74        | 1.32     |
| 1   | A     | 87  | ASP  | CA-CB  | 29.66  | 1.95        | 1.53     |
| 1   | A     | 112 | ARG  | CZ-NH2 | 29.14  | 1.71        | 1.33     |
| 1   | B     | 5   | ARG  | C-O    | -28.85 | 0.91        | 1.24     |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 2   | VAL  | CA-CB  | -28.79 | 1.21        | 1.53     |
| 1   | A     | 125 | ARG  | CZ-NH1 | 28.28  | 1.72        | 1.32     |
| 1   | A     | 68  | ARG  | NE-CZ  | -28.14 | 1.02        | 1.33     |
| 1   | A     | 78  | ILE  | CA-CB  | 27.67  | 1.89        | 1.54     |
| 1   | B     | 44  | ASN  | C-O    | -27.18 | 0.93        | 1.23     |
| 1   | B     | 45  | ARG  | NE-CZ  | -27.03 | 1.03        | 1.33     |
| 1   | A     | 14  | ARG  | CD-NE  | 27.00  | 1.84        | 1.46     |
| 1   | A     | 69  | THR  | C-O    | -26.89 | 0.95        | 1.24     |
| 1   | B     | 47  | THR  | CB-OG1 | 26.63  | 1.86        | 1.43     |
| 1   | B     | 61  | ARG  | CZ-NH2 | 26.38  | 1.67        | 1.33     |
| 1   | A     | 45  | ARG  | CB-CG  | 26.18  | 2.31        | 1.52     |
| 1   | A     | 15  | HIS  | CG-ND1 | -25.77 | 1.09        | 1.38     |
| 1   | A     | 122 | ALA  | CA-C   | 25.64  | 1.87        | 1.52     |
| 1   | A     | 2   | VAL  | CA-C   | 25.12  | 1.82        | 1.52     |
| 1   | A     | 72  | SER  | C-O    | 24.85  | 1.53        | 1.23     |
| 1   | B     | 68  | ARG  | CD-NE  | -24.79 | 1.11        | 1.46     |
| 1   | A     | 87  | ASP  | CB-CG  | 24.77  | 2.13        | 1.52     |
| 1   | A     | 21  | ARG  | NE-CZ  | 24.58  | 1.60        | 1.33     |
| 1   | B     | 114 | ARG  | CZ-NH2 | 24.02  | 1.64        | 1.33     |
| 1   | A     | 62  | TRP  | CA-CB  | 24.00  | 1.87        | 1.54     |
| 1   | A     | 45  | ARG  | CD-NE  | -23.67 | 1.13        | 1.46     |
| 1   | A     | 129 | LEU  | CA-CB  | 23.19  | 1.99        | 1.53     |
| 1   | A     | 128 | ARG  | N-CA   | 22.69  | 1.75        | 1.46     |
| 1   | A     | 14  | ARG  | CZ-NH1 | -22.52 | 1.01        | 1.32     |
| 1   | A     | 62  | TRP  | CG-CD2 | -22.33 | 1.03        | 1.43     |
| 1   | B     | 46  | ASN  | N-CA   | -22.05 | 1.17        | 1.46     |
| 1   | A     | 112 | ARG  | CD-NE  | 22.04  | 1.77        | 1.46     |
| 1   | B     | 15  | HIS  | CB-CG  | 21.83  | 1.80        | 1.50     |
| 1   | A     | 128 | ARG  | CA-C   | 21.66  | 1.79        | 1.52     |
| 1   | A     | 48  | ASP  | CA-CB  | 21.35  | 1.85        | 1.53     |
| 1   | B     | 61  | ARG  | CD-NE  | -21.00 | 1.16        | 1.46     |
| 1   | A     | 121 | GLN  | CB-CG  | 20.91  | 2.15        | 1.52     |
| 1   | A     | 127 | CYS  | CA-C   | 20.79  | 1.80        | 1.52     |
| 1   | A     | 48  | ASP  | CG-OD1 | -20.69 | 0.86        | 1.25     |
| 1   | A     | 47  | THR  | CA-CB  | -20.04 | 1.18        | 1.53     |
| 1   | B     | 19  | ASN  | CG-OD1 | 19.72  | 1.61        | 1.23     |
| 1   | A     | 68  | ARG  | CD-NE  | 19.55  | 1.73        | 1.46     |
| 1   | A     | 13  | LYS  | CA-C   | -19.39 | 1.27        | 1.52     |
| 1   | A     | 5   | ARG  | CZ-NH2 | 19.26  | 1.58        | 1.33     |
| 1   | B     | 15  | HIS  | CG-ND1 | 19.17  | 1.59        | 1.38     |
| 1   | B     | 42  | ALA  | C-N    | -19.04 | 1.06        | 1.33     |
| 1   | A     | 47  | THR  | C-O    | -19.02 | 0.99        | 1.24     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | B     | 14  | ARG  | NE-CZ   | 18.98  | 1.53        | 1.33     |
| 1   | B     | 43  | THR  | C-O     | 18.91  | 1.46        | 1.23     |
| 1   | B     | 50  | SER  | C-O     | 18.87  | 1.48        | 1.23     |
| 1   | B     | 21  | ARG  | C-O     | 18.72  | 1.47        | 1.23     |
| 1   | B     | 69  | THR  | CB-OG1  | 18.67  | 1.73        | 1.43     |
| 1   | B     | 21  | ARG  | CZ-NH2  | 18.57  | 1.57        | 1.33     |
| 1   | A     | 15  | HIS  | CE1-NE2 | -18.32 | 1.14        | 1.32     |
| 1   | B     | 44  | ASN  | CG-ND2  | -18.14 | 0.95        | 1.33     |
| 1   | A     | 41  | GLN  | CD-OE1  | 18.09  | 1.57        | 1.23     |
| 1   | B     | 73  | ARG  | NE-CZ   | -18.08 | 1.13        | 1.33     |
| 1   | A     | 57  | GLN  | CD-OE1  | 18.02  | 1.57        | 1.23     |
| 1   | B     | 85  | SER  | CA-C    | 17.83  | 1.76        | 1.52     |
| 1   | B     | 37  | ASN  | CA-C    | 17.74  | 1.75        | 1.53     |
| 1   | A     | 115 | CYS  | N-CA    | -17.56 | 1.22        | 1.46     |
| 1   | A     | 121 | GLN  | CD-OE1  | 17.49  | 1.56        | 1.23     |
| 1   | A     | 125 | ARG  | CD-NE   | -17.48 | 1.21        | 1.46     |
| 1   | B     | 88  | ILE  | CA-C    | -17.46 | 1.32        | 1.52     |
| 1   | A     | 72  | SER  | CA-CB   | 17.39  | 1.82        | 1.53     |
| 1   | A     | 114 | ARG  | CZ-NH1  | -17.35 | 1.08        | 1.32     |
| 1   | A     | 66  | ASP  | CA-CB   | -17.17 | 1.27        | 1.54     |
| 1   | B     | 121 | GLN  | CD-NE2  | 17.08  | 1.69        | 1.33     |
| 1   | A     | 45  | ARG  | CG-CD   | 17.07  | 2.03        | 1.52     |
| 1   | A     | 48  | ASP  | C-O     | -16.84 | 1.01        | 1.24     |
| 1   | B     | 19  | ASN  | CB-CG   | -16.82 | 1.09        | 1.52     |
| 1   | A     | 66  | ASP  | CA-C    | -16.62 | 1.31        | 1.52     |
| 1   | B     | 49  | GLY  | C-N     | -16.57 | 1.10        | 1.33     |
| 1   | A     | 74  | ASN  | C-N     | 16.54  | 1.56        | 1.33     |
| 1   | B     | 108 | TRP  | CA-C    | 16.48  | 1.73        | 1.52     |
| 1   | A     | 21  | ARG  | N-CA    | 16.20  | 1.69        | 1.46     |
| 1   | B     | 129 | LEU  | CB-CG   | -16.15 | 1.21        | 1.53     |
| 1   | B     | 80  | CYS  | CA-C    | -16.15 | 1.30        | 1.52     |
| 1   | B     | 123 | TRP  | NE1-CE2 | -16.08 | 1.19        | 1.37     |
| 1   | B     | 45  | ARG  | C-N     | -16.02 | 1.11        | 1.33     |
| 1   | A     | 62  | TRP  | CZ2-CH2 | 15.91  | 1.67        | 1.37     |
| 1   | B     | 50  | SER  | N-CA    | -15.78 | 1.27        | 1.45     |
| 1   | A     | 124 | ILE  | CA-CB   | -15.53 | 1.33        | 1.54     |
| 1   | B     | 21  | ARG  | CZ-NH1  | 15.49  | 1.54        | 1.32     |
| 1   | A     | 119 | ASP  | C-O     | -15.46 | 1.06        | 1.23     |
| 1   | A     | 113 | ASN  | N-CA    | -15.40 | 1.26        | 1.46     |
| 1   | B     | 69  | THR  | C-N     | 15.29  | 1.53        | 1.33     |
| 1   | B     | 112 | ARG  | CB-CG   | -15.28 | 1.06        | 1.52     |
| 1   | A     | 45  | ARG  | CZ-NH2  | -15.21 | 1.13        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 46  | ASN  | CG-ND2  | -15.17 | 1.01        | 1.33     |
| 1   | B     | 127 | CYS  | N-CA    | -15.16 | 1.26        | 1.46     |
| 1   | A     | 2   | VAL  | N-CA    | 15.15  | 1.63        | 1.46     |
| 1   | B     | 21  | ARG  | CA-CB   | 15.11  | 1.77        | 1.53     |
| 1   | A     | 51  | THR  | C-O     | -15.06 | 1.04        | 1.23     |
| 1   | B     | 20  | TYR  | C-O     | -15.02 | 1.05        | 1.24     |
| 1   | A     | 119 | ASP  | CA-C    | 14.96  | 1.71        | 1.53     |
| 1   | A     | 128 | ARG  | CZ-NH2  | -14.89 | 1.14        | 1.33     |
| 1   | A     | 118 | THR  | C-O     | -14.82 | 1.03        | 1.23     |
| 1   | A     | 41  | GLN  | CA-C    | -14.71 | 1.31        | 1.52     |
| 1   | B     | 114 | ARG  | CD-NE   | 14.55  | 1.66        | 1.46     |
| 1   | A     | 112 | ARG  | CA-C    | -14.48 | 1.34        | 1.52     |
| 1   | B     | 21  | ARG  | CA-C    | 14.43  | 1.72        | 1.53     |
| 1   | A     | 68  | ARG  | CA-C    | 14.38  | 1.70        | 1.52     |
| 1   | B     | 48  | ASP  | C-O     | 14.32  | 1.45        | 1.24     |
| 1   | A     | 45  | ARG  | CA-CB   | 14.29  | 1.74        | 1.53     |
| 1   | A     | 66  | ASP  | C-O     | 14.22  | 1.42        | 1.24     |
| 1   | A     | 4   | GLY  | C-N     | -14.21 | 1.16        | 1.33     |
| 1   | A     | 97  | LYS  | C-O     | 14.11  | 1.40        | 1.24     |
| 1   | B     | 116 | LYS  | C-O     | -14.04 | 1.06        | 1.23     |
| 1   | A     | 42  | ALA  | CA-C    | 14.01  | 1.71        | 1.52     |
| 1   | A     | 109 | VAL  | CA-CB   | 13.98  | 1.72        | 1.54     |
| 1   | A     | 110 | ALA  | C-O     | 13.90  | 1.42        | 1.24     |
| 1   | B     | 47  | THR  | CA-C    | 13.88  | 1.71        | 1.52     |
| 1   | B     | 72  | SER  | N-CA    | -13.86 | 1.28        | 1.45     |
| 1   | B     | 19  | ASN  | CG-ND2  | 13.68  | 1.61        | 1.33     |
| 1   | A     | 123 | TRP  | NE1-CE2 | -13.68 | 1.22        | 1.37     |
| 1   | B     | 58  | ILE  | N-CA    | 13.66  | 1.63        | 1.46     |
| 1   | B     | 122 | ALA  | C-N     | 13.59  | 1.52        | 1.33     |
| 1   | A     | 87  | ASP  | CG-OD2  | -13.48 | 0.99        | 1.25     |
| 1   | B     | 68  | ARG  | C-O     | 13.44  | 1.42        | 1.24     |
| 1   | B     | 2   | VAL  | CA-CB   | -13.37 | 1.37        | 1.53     |
| 1   | B     | 55  | ILE  | CA-C    | 13.36  | 1.71        | 1.52     |
| 1   | B     | 42  | ALA  | N-CA    | -13.27 | 1.28        | 1.46     |
| 1   | B     | 91  | SER  | N-CA    | 13.26  | 1.62        | 1.46     |
| 1   | B     | 112 | ARG  | CD-NE   | -13.20 | 1.27        | 1.46     |
| 1   | A     | 71  | GLY  | CA-C    | 13.16  | 1.70        | 1.51     |
| 1   | A     | 63  | TRP  | C-N     | 13.11  | 1.50        | 1.33     |
| 1   | A     | 15  | HIS  | CG-CD2  | -13.05 | 1.21        | 1.35     |
| 1   | A     | 94  | CYS  | N-CA    | 13.03  | 1.62        | 1.46     |
| 1   | B     | 69  | THR  | C-O     | -13.01 | 1.07        | 1.24     |
| 1   | A     | 62  | TRP  | CD1-NE1 | 12.94  | 1.65        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 101 | ASP  | CA-C    | -12.90 | 1.33        | 1.52     |
| 1   | B     | 6   | CYS  | CA-CB   | 12.87  | 1.74        | 1.53     |
| 1   | A     | 14  | ARG  | NE-CZ   | 12.87  | 1.47        | 1.33     |
| 1   | B     | 47  | THR  | C-O     | 12.86  | 1.40        | 1.24     |
| 1   | B     | 110 | ALA  | C-O     | 12.86  | 1.40        | 1.24     |
| 1   | A     | 120 | VAL  | C-O     | -12.86 | 1.06        | 1.24     |
| 1   | B     | 17  | LEU  | C-O     | 12.86  | 1.41        | 1.24     |
| 1   | B     | 121 | GLN  | CA-C    | -12.86 | 1.34        | 1.52     |
| 1   | A     | 33  | LYS  | CA-C    | 12.82  | 1.69        | 1.52     |
| 1   | B     | 67  | GLY  | N-CA    | 12.79  | 1.64        | 1.45     |
| 1   | A     | 125 | ARG  | CZ-NH2  | -12.78 | 1.16        | 1.33     |
| 1   | B     | 21  | ARG  | C-N     | 12.71  | 1.52        | 1.33     |
| 1   | A     | 48  | ASP  | N-CA    | 12.70  | 1.61        | 1.46     |
| 1   | A     | 107 | ALA  | C-N     | -12.66 | 1.15        | 1.33     |
| 1   | A     | 39  | ASN  | CG-OD1  | 12.66  | 1.47        | 1.23     |
| 1   | A     | 21  | ARG  | CZ-NH2  | -12.65 | 1.17        | 1.33     |
| 1   | A     | 108 | TRP  | C-N     | 12.64  | 1.49        | 1.33     |
| 1   | B     | 105 | MET  | C-N     | 12.61  | 1.50        | 1.33     |
| 1   | A     | 77  | ASN  | C-O     | -12.54 | 1.07        | 1.23     |
| 1   | B     | 67  | GLY  | CA-C    | 12.53  | 1.68        | 1.51     |
| 1   | B     | 5   | ARG  | CA-CB   | 12.52  | 1.72        | 1.53     |
| 1   | B     | 44  | ASN  | CG-OD1  | 12.50  | 1.47        | 1.23     |
| 1   | B     | 46  | ASN  | C-O     | 12.48  | 1.39        | 1.23     |
| 1   | B     | 21  | ARG  | CD-NE   | -12.48 | 1.28        | 1.46     |
| 1   | A     | 15  | HIS  | ND1-CE1 | 12.47  | 1.45        | 1.32     |
| 1   | A     | 121 | GLN  | N-CA    | -12.47 | 1.30        | 1.46     |
| 1   | A     | 86  | SER  | N-CA    | 12.46  | 1.62        | 1.46     |
| 1   | A     | 5   | ARG  | C-N     | -12.36 | 1.17        | 1.34     |
| 1   | A     | 23  | TYR  | C-O     | 12.35  | 1.38        | 1.24     |
| 1   | A     | 24  | SER  | C-O     | 12.33  | 1.41        | 1.23     |
| 1   | B     | 125 | ARG  | CA-C    | 12.30  | 1.68        | 1.52     |
| 1   | A     | 28  | TRP  | CA-C    | -12.28 | 1.36        | 1.52     |
| 1   | B     | 68  | ARG  | N-CA    | 12.25  | 1.62        | 1.46     |
| 1   | B     | 33  | LYS  | CA-C    | -12.22 | 1.37        | 1.52     |
| 1   | A     | 122 | ALA  | N-CA    | -12.20 | 1.31        | 1.46     |
| 1   | A     | 114 | ARG  | CZ-NH2  | 12.19  | 1.49        | 1.33     |
| 1   | B     | 19  | ASN  | CA-C    | -12.15 | 1.36        | 1.52     |
| 1   | B     | 88  | ILE  | C-N     | -12.10 | 1.18        | 1.33     |
| 1   | B     | 99  | VAL  | C-N     | -12.08 | 1.17        | 1.33     |
| 1   | B     | 121 | GLN  | C-O     | 12.05  | 1.39        | 1.24     |
| 1   | B     | 76  | CYS  | N-CA    | -12.05 | 1.30        | 1.46     |
| 1   | B     | 61  | ARG  | NE-CZ   | -12.02 | 1.19        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 3   | PHE  | N-CA    | -12.01 | 1.31        | 1.45     |
| 1   | A     | 15  | HIS  | C-N     | -12.00 | 1.16        | 1.33     |
| 1   | A     | 40  | THR  | CA-C    | -12.00 | 1.35        | 1.52     |
| 1   | A     | 110 | ALA  | N-CA    | -11.98 | 1.30        | 1.46     |
| 1   | A     | 109 | VAL  | CA-C    | -11.98 | 1.37        | 1.52     |
| 1   | B     | 78  | ILE  | CA-CB   | 11.98  | 1.69        | 1.54     |
| 1   | B     | 53  | TYR  | CE1-CZ  | -11.97 | 1.09        | 1.38     |
| 1   | A     | 20  | TYR  | N-CA    | 11.90  | 1.60        | 1.46     |
| 1   | B     | 79  | PRO  | N-CA    | -11.86 | 1.32        | 1.47     |
| 1   | A     | 76  | CYS  | CA-CB   | 11.86  | 1.74        | 1.53     |
| 1   | B     | 76  | CYS  | CA-CB   | 11.83  | 1.74        | 1.53     |
| 1   | A     | 72  | SER  | N-CA    | 11.83  | 1.60        | 1.46     |
| 1   | A     | 2   | VAL  | C-N     | -11.80 | 1.16        | 1.33     |
| 1   | A     | 100 | SER  | C-O     | 11.76  | 1.39        | 1.24     |
| 1   | A     | 21  | ARG  | CZ-NH1  | 11.76  | 1.49        | 1.32     |
| 1   | B     | 128 | ARG  | CG-CD   | 11.73  | 1.87        | 1.52     |
| 1   | B     | 9   | ALA  | C-N     | 11.70  | 1.49        | 1.33     |
| 1   | B     | 43  | THR  | CB-CG2  | 11.70  | 1.91        | 1.52     |
| 1   | B     | 87  | ASP  | C-O     | 11.70  | 1.38        | 1.24     |
| 1   | A     | 128 | ARG  | C-N     | -11.67 | 1.17        | 1.33     |
| 1   | A     | 83  | LEU  | C-O     | 11.58  | 1.39        | 1.24     |
| 1   | A     | 29  | VAL  | N-CA    | 11.55  | 1.60        | 1.46     |
| 1   | A     | 61  | ARG  | CG-CD   | 11.53  | 1.87        | 1.52     |
| 1   | B     | 68  | ARG  | NE-CZ   | 11.50  | 1.45        | 1.33     |
| 1   | B     | 22  | GLY  | C-N     | -11.45 | 1.18        | 1.33     |
| 1   | B     | 40  | THR  | CA-C    | -11.44 | 1.36        | 1.52     |
| 1   | A     | 101 | ASP  | CB-CG   | 11.39  | 1.80        | 1.52     |
| 1   | B     | 53  | TYR  | N-CA    | -11.38 | 1.32        | 1.46     |
| 1   | B     | 122 | ALA  | C-O     | -11.32 | 1.09        | 1.24     |
| 1   | B     | 45  | ARG  | C-O     | 11.29  | 1.37        | 1.23     |
| 1   | B     | 23  | TYR  | CZ-OH   | 11.27  | 1.61        | 1.38     |
| 1   | B     | 43  | THR  | C-N     | -11.25 | 1.19        | 1.33     |
| 1   | A     | 63  | TRP  | NE1-CE2 | -11.24 | 1.25        | 1.37     |
| 1   | B     | 63  | TRP  | CE2-CZ2 | -11.23 | 1.16        | 1.39     |
| 1   | A     | 73  | ARG  | C-O     | 11.23  | 1.38        | 1.24     |
| 1   | B     | 60  | SER  | CA-CB   | 11.22  | 1.73        | 1.53     |
| 1   | A     | 61  | ARG  | CZ-NH2  | -11.19 | 1.19        | 1.33     |
| 1   | A     | 73  | ARG  | C-N     | -11.18 | 1.19        | 1.33     |
| 1   | B     | 119 | ASP  | CA-C    | -11.18 | 1.37        | 1.52     |
| 1   | B     | 22  | GLY  | C-O     | 11.17  | 1.39        | 1.24     |
| 1   | B     | 87  | ASP  | CA-CB   | 11.16  | 1.68        | 1.53     |
| 1   | B     | 78  | ILE  | C-O     | 11.15  | 1.38        | 1.24     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 108 | TRP  | CD2-CE2 | 11.11  | 1.60        | 1.41     |
| 1   | B     | 3   | PHE  | CA-CB   | 11.11  | 1.71        | 1.53     |
| 1   | A     | 98  | ILE  | N-CA    | -11.09 | 1.33        | 1.46     |
| 1   | A     | 67  | GLY  | C-O     | 11.09  | 1.38        | 1.23     |
| 1   | B     | 124 | ILE  | N-CA    | -11.08 | 1.31        | 1.46     |
| 1   | A     | 88  | ILE  | CA-C    | -11.06 | 1.38        | 1.52     |
| 1   | B     | 63  | TRP  | C-O     | -11.03 | 1.09        | 1.24     |
| 1   | B     | 84  | LEU  | C-N     | -11.03 | 1.19        | 1.33     |
| 1   | A     | 33  | LYS  | CD-CE   | 11.02  | 1.85        | 1.52     |
| 1   | A     | 68  | ARG  | N-CA    | -11.01 | 1.34        | 1.46     |
| 1   | B     | 61  | ARG  | C-O     | 11.00  | 1.36        | 1.24     |
| 1   | B     | 121 | GLN  | CG-CD   | 10.99  | 1.79        | 1.52     |
| 1   | A     | 102 | GLY  | N-CA    | 10.93  | 1.61        | 1.45     |
| 1   | A     | 61  | ARG  | CD-NE   | 10.92  | 1.61        | 1.46     |
| 1   | B     | 45  | ARG  | N-CA    | -10.90 | 1.31        | 1.46     |
| 1   | B     | 39  | ASN  | CG-OD1  | -10.85 | 1.02        | 1.23     |
| 1   | A     | 34  | PHE  | CG-CD2  | -10.85 | 1.16        | 1.38     |
| 1   | A     | 124 | ILE  | CB-CG1  | -10.85 | 1.31        | 1.53     |
| 1   | A     | 43  | THR  | C-O     | 10.83  | 1.37        | 1.23     |
| 1   | A     | 78  | ILE  | CA-C    | -10.80 | 1.41        | 1.52     |
| 1   | B     | 7   | GLU  | CA-CB   | 10.78  | 1.70        | 1.53     |
| 1   | A     | 39  | ASN  | C-O     | -10.77 | 1.11        | 1.24     |
| 1   | A     | 75  | LEU  | C-N     | -10.76 | 1.17        | 1.33     |
| 1   | A     | 97  | LYS  | CA-C    | 10.72  | 1.66        | 1.52     |
| 1   | A     | 47  | THR  | CB-CG2  | 10.72  | 1.88        | 1.52     |
| 1   | A     | 90  | ALA  | CA-C    | 10.70  | 1.66        | 1.52     |
| 1   | B     | 42  | ALA  | C-O     | 10.70  | 1.36        | 1.23     |
| 1   | B     | 66  | ASP  | CA-C    | -10.70 | 1.37        | 1.52     |
| 1   | B     | 74  | ASN  | CA-C    | -10.69 | 1.39        | 1.53     |
| 1   | B     | 81  | SER  | N-CA    | 10.70  | 1.60        | 1.46     |
| 1   | A     | 55  | ILE  | CA-CB   | 10.64  | 1.70        | 1.54     |
| 1   | B     | 126 | GLY  | CA-C    | 10.64  | 1.67        | 1.51     |
| 1   | B     | 129 | LEU  | CA-C    | -10.62 | 1.30        | 1.52     |
| 1   | B     | 15  | HIS  | CE1-NE2 | 10.62  | 1.43        | 1.32     |
| 1   | B     | 41  | GLN  | CD-NE2  | 10.60  | 1.55        | 1.33     |
| 1   | A     | 115 | CYS  | C-O     | 10.55  | 1.40        | 1.23     |
| 1   | A     | 60  | SER  | N-CA    | -10.55 | 1.31        | 1.46     |
| 1   | B     | 45  | ARG  | CD-NE   | 10.54  | 1.61        | 1.46     |
| 1   | B     | 72  | SER  | CA-CB   | 10.54  | 1.75        | 1.54     |
| 1   | B     | 116 | LYS  | N-CA    | 10.54  | 1.59        | 1.46     |
| 1   | A     | 41  | GLN  | C-O     | 10.50  | 1.38        | 1.24     |
| 1   | B     | 102 | GLY  | C-N     | -10.49 | 1.19        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 70  | PRO  | CA-C    | 10.48  | 1.65        | 1.52     |
| 1   | A     | 18  | ASP  | N-CA    | 10.47  | 1.59        | 1.46     |
| 1   | B     | 67  | GLY  | C-O     | 10.47  | 1.37        | 1.24     |
| 1   | A     | 108 | TRP  | CG-CD2  | -10.43 | 1.25        | 1.43     |
| 1   | B     | 93  | ASN  | CB-CG   | -10.42 | 1.25        | 1.52     |
| 1   | B     | 116 | LYS  | CA-C    | 10.40  | 1.66        | 1.52     |
| 1   | B     | 61  | ARG  | CG-CD   | 10.38  | 1.83        | 1.52     |
| 1   | B     | 71  | GLY  | N-CA    | 10.34  | 1.60        | 1.45     |
| 1   | A     | 22  | GLY  | C-O     | -10.33 | 1.09        | 1.24     |
| 1   | A     | 65  | ASN  | CA-C    | -10.29 | 1.40        | 1.52     |
| 1   | B     | 70  | PRO  | CA-C    | 10.29  | 1.66        | 1.52     |
| 1   | A     | 59  | ASN  | C-N     | 10.24  | 1.48        | 1.33     |
| 1   | A     | 104 | GLY  | CA-C    | 10.24  | 1.64        | 1.51     |
| 1   | A     | 62  | TRP  | NE1-CE2 | 10.24  | 1.48        | 1.37     |
| 1   | A     | 2   | VAL  | C-O     | 10.23  | 1.35        | 1.23     |
| 1   | B     | 29  | VAL  | CA-C    | -10.23 | 1.39        | 1.52     |
| 1   | A     | 11  | ALA  | CA-C    | 10.21  | 1.65        | 1.52     |
| 1   | B     | 66  | ASP  | CA-CB   | -10.17 | 1.35        | 1.53     |
| 1   | A     | 121 | GLN  | C-O     | 10.14  | 1.37        | 1.24     |
| 1   | B     | 44  | ASN  | CA-C    | 10.11  | 1.64        | 1.52     |
| 1   | A     | 70  | PRO  | N-CA    | -10.10 | 1.34        | 1.47     |
| 1   | A     | 75  | LEU  | C-O     | -10.10 | 1.10        | 1.24     |
| 1   | B     | 14  | ARG  | C-O     | 10.09  | 1.35        | 1.24     |
| 1   | A     | 65  | ASN  | C-O     | 10.07  | 1.36        | 1.24     |
| 1   | B     | 12  | MET  | N-CA    | 10.07  | 1.59        | 1.46     |
| 1   | A     | 71  | GLY  | C-N     | -10.07 | 1.19        | 1.33     |
| 1   | A     | 7   | GLU  | C-O     | 10.03  | 1.35        | 1.24     |
| 1   | A     | 115 | CYS  | CA-CB   | 10.03  | 1.74        | 1.54     |
| 1   | B     | 43  | THR  | CA-C    | -10.02 | 1.40        | 1.52     |
| 1   | B     | 63  | TRP  | CD2-CE3 | -10.02 | 1.24        | 1.40     |
| 1   | A     | 7   | GLU  | CG-CD   | -10.00 | 1.27        | 1.52     |
| 1   | A     | 39  | ASN  | C-N     | 9.92   | 1.47        | 1.33     |
| 1   | A     | 125 | ARG  | CA-C    | -9.89  | 1.40        | 1.52     |
| 1   | A     | 57  | GLN  | CD-NE2  | -9.87  | 1.12        | 1.33     |
| 1   | A     | 36  | SER  | C-N     | 9.86   | 1.48        | 1.33     |
| 1   | B     | 21  | ARG  | CB-CG   | 9.86   | 1.82        | 1.52     |
| 1   | A     | 114 | ARG  | NE-CZ   | 9.84   | 1.43        | 1.33     |
| 1   | A     | 73  | ARG  | CA-C    | 9.80   | 1.66        | 1.52     |
| 1   | A     | 16  | GLY  | N-CA    | 9.80   | 1.60        | 1.45     |
| 1   | B     | 1   | LYS  | CD-CE   | 9.77   | 1.81        | 1.52     |
| 1   | A     | 83  | LEU  | C-N     | -9.74  | 1.21        | 1.33     |
| 1   | A     | 42  | ALA  | C-O     | -9.71  | 1.12        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 93  | ASN  | CB-CG   | 9.68  | 1.76        | 1.52     |
| 1   | A     | 112 | ARG  | CG-CD   | 9.68  | 1.81        | 1.52     |
| 1   | A     | 26  | GLY  | C-O     | 9.67  | 1.36        | 1.23     |
| 1   | B     | 30  | CYS  | C-N     | 9.62  | 1.46        | 1.33     |
| 1   | B     | 69  | THR  | N-CA    | -9.62 | 1.32        | 1.46     |
| 1   | A     | 128 | ARG  | NE-CZ   | -9.60 | 1.22        | 1.33     |
| 1   | B     | 60  | SER  | CB-OG   | -9.60 | 1.23        | 1.42     |
| 1   | B     | 14  | ARG  | CZ-NH1  | 9.59  | 1.46        | 1.32     |
| 1   | A     | 90  | ALA  | C-N     | 9.58  | 1.46        | 1.33     |
| 1   | A     | 68  | ARG  | CZ-NH1  | 9.58  | 1.46        | 1.32     |
| 1   | A     | 39  | ASN  | CB-CG   | -9.56 | 1.28        | 1.52     |
| 1   | A     | 68  | ARG  | CG-CD   | 9.54  | 1.81        | 1.52     |
| 1   | A     | 105 | MET  | N-CA    | -9.53 | 1.33        | 1.46     |
| 1   | A     | 129 | LEU  | CA-C    | -9.52 | 1.32        | 1.52     |
| 1   | A     | 4   | GLY  | N-CA    | 9.52  | 1.61        | 1.45     |
| 1   | A     | 50  | SER  | N-CA    | -9.47 | 1.34        | 1.45     |
| 1   | B     | 69  | THR  | CA-C    | 9.43  | 1.64        | 1.52     |
| 1   | A     | 51  | THR  | CB-OG1  | 9.42  | 1.58        | 1.43     |
| 1   | A     | 50  | SER  | C-N     | 9.42  | 1.47        | 1.33     |
| 1   | B     | 120 | VAL  | CA-CB   | 9.41  | 1.66        | 1.54     |
| 1   | A     | 87  | ASP  | N-CA    | 9.40  | 1.57        | 1.46     |
| 1   | B     | 41  | GLN  | CB-CG   | -9.39 | 1.24        | 1.52     |
| 1   | B     | 100 | SER  | CA-C    | 9.37  | 1.66        | 1.52     |
| 1   | B     | 12  | MET  | C-O     | 9.37  | 1.35        | 1.24     |
| 1   | B     | 68  | ARG  | C-N     | -9.35 | 1.14        | 1.33     |
| 1   | A     | 126 | GLY  | C-O     | 9.35  | 1.37        | 1.24     |
| 1   | B     | 24  | SER  | C-O     | -9.34 | 1.11        | 1.23     |
| 1   | A     | 44  | ASN  | CB-CG   | 9.33  | 1.75        | 1.52     |
| 1   | A     | 70  | PRO  | CA-CB   | -9.31 | 1.41        | 1.53     |
| 1   | A     | 112 | ARG  | C-N     | 9.31  | 1.47        | 1.33     |
| 1   | A     | 93  | ASN  | CG-OD1  | 9.31  | 1.41        | 1.23     |
| 1   | A     | 123 | TRP  | CA-CB   | 9.29  | 1.69        | 1.53     |
| 1   | B     | 80  | CYS  | CA-CB   | -9.28 | 1.38        | 1.53     |
| 1   | A     | 86  | SER  | CB-OG   | 9.27  | 1.60        | 1.42     |
| 1   | B     | 63  | TRP  | NE1-CE2 | -9.26 | 1.27        | 1.37     |
| 1   | A     | 14  | ARG  | N-CA    | 9.26  | 1.57        | 1.46     |
| 1   | A     | 60  | SER  | C-N     | -9.25 | 1.20        | 1.33     |
| 1   | A     | 91  | SER  | C-N     | 9.22  | 1.45        | 1.33     |
| 1   | A     | 113 | ASN  | CA-C    | 9.22  | 1.65        | 1.52     |
| 1   | A     | 51  | THR  | CA-C    | 9.22  | 1.63        | 1.52     |
| 1   | A     | 46  | ASN  | CB-CG   | -9.21 | 1.29        | 1.52     |
| 1   | A     | 101 | ASP  | C-O     | 9.20  | 1.35        | 1.24     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 121 | GLN  | CA-CB   | -9.20 | 1.37        | 1.53     |
| 1   | A     | 73  | ARG  | NE-CZ   | -9.18 | 1.23        | 1.33     |
| 1   | B     | 55  | ILE  | N-CA    | 9.18  | 1.58        | 1.46     |
| 1   | A     | 25  | LEU  | C-O     | -9.17 | 1.13        | 1.24     |
| 1   | B     | 83  | LEU  | C-N     | -9.17 | 1.21        | 1.33     |
| 1   | A     | 58  | ILE  | CA-CB   | -9.14 | 1.42        | 1.54     |
| 1   | A     | 16  | GLY  | CA-C    | -9.13 | 1.39        | 1.51     |
| 1   | B     | 123 | TRP  | C-O     | 9.13  | 1.35        | 1.24     |
| 1   | A     | 72  | SER  | CA-C    | -9.10 | 1.41        | 1.52     |
| 1   | B     | 43  | THR  | CA-CB   | -9.08 | 1.35        | 1.53     |
| 1   | A     | 51  | THR  | CB-CG2  | -9.04 | 1.22        | 1.52     |
| 1   | A     | 90  | ALA  | N-CA    | -9.04 | 1.35        | 1.46     |
| 1   | A     | 67  | GLY  | CA-C    | -9.04 | 1.39        | 1.51     |
| 1   | A     | 93  | ASN  | N-CA    | -9.04 | 1.35        | 1.46     |
| 1   | A     | 85  | SER  | CA-CB   | 9.03  | 1.67        | 1.53     |
| 1   | B     | 36  | SER  | CA-C    | -9.03 | 1.40        | 1.52     |
| 1   | B     | 104 | GLY  | CA-C    | 9.02  | 1.65        | 1.51     |
| 1   | B     | 46  | ASN  | CB-CG   | 8.99  | 1.74        | 1.52     |
| 1   | A     | 111 | TRP  | CD2-CE3 | 8.98  | 1.54        | 1.40     |
| 1   | B     | 5   | ARG  | N-CA    | 8.98  | 1.57        | 1.46     |
| 1   | B     | 37  | ASN  | C-O     | 8.96  | 1.35        | 1.23     |
| 1   | B     | 87  | ASP  | C-N     | -8.96 | 1.25        | 1.34     |
| 1   | B     | 94  | CYS  | N-CA    | -8.96 | 1.35        | 1.46     |
| 1   | A     | 123 | TRP  | CA-C    | 8.95  | 1.65        | 1.52     |
| 1   | A     | 121 | GLN  | CA-C    | -8.94 | 1.40        | 1.52     |
| 1   | B     | 18  | ASP  | C-N     | -8.93 | 1.21        | 1.33     |
| 1   | B     | 50  | SER  | CA-C    | 8.91  | 1.65        | 1.53     |
| 1   | B     | 77  | ASN  | C-N     | -8.90 | 1.23        | 1.33     |
| 1   | A     | 34  | PHE  | CG-CD1  | 8.90  | 1.57        | 1.38     |
| 1   | B     | 34  | PHE  | CG-CD2  | -8.89 | 1.20        | 1.38     |
| 1   | A     | 86  | SER  | CA-CB   | 8.87  | 1.69        | 1.53     |
| 1   | A     | 30  | CYS  | C-O     | -8.86 | 1.13        | 1.24     |
| 1   | A     | 112 | ARG  | N-CA    | -8.83 | 1.35        | 1.46     |
| 1   | B     | 9   | ALA  | N-CA    | 8.83  | 1.57        | 1.46     |
| 1   | A     | 98  | ILE  | CA-C    | -8.81 | 1.41        | 1.52     |
| 1   | A     | 3   | PHE  | CG-CD2  | -8.80 | 1.20        | 1.38     |
| 1   | A     | 63  | TRP  | CZ3-CH2 | -8.79 | 1.18        | 1.40     |
| 1   | B     | 45  | ARG  | CZ-NH2  | 8.78  | 1.44        | 1.33     |
| 1   | A     | 14  | ARG  | CG-CD   | 8.76  | 1.78        | 1.52     |
| 1   | A     | 14  | ARG  | CA-CB   | 8.76  | 1.67        | 1.53     |
| 1   | B     | 124 | ILE  | CA-CB   | -8.74 | 1.44        | 1.54     |
| 1   | B     | 59  | ASN  | CA-CB   | 8.72  | 1.66        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 74  | ASN  | C-N     | -8.66 | 1.22        | 1.34     |
| 1   | A     | 63  | TRP  | CG-CD2  | 8.65  | 1.59        | 1.43     |
| 1   | B     | 13  | LYS  | CA-CB   | 8.64  | 1.67        | 1.53     |
| 1   | A     | 99  | VAL  | C-O     | -8.64 | 1.12        | 1.24     |
| 1   | A     | 129 | LEU  | CB-CG   | -8.61 | 1.36        | 1.53     |
| 1   | B     | 114 | ARG  | C-N     | -8.61 | 1.18        | 1.33     |
| 1   | A     | 108 | TRP  | NE1-CE2 | 8.60  | 1.47        | 1.37     |
| 1   | B     | 40  | THR  | N-CA    | 8.56  | 1.57        | 1.46     |
| 1   | B     | 77  | ASN  | CG-OD1  | 8.56  | 1.39        | 1.23     |
| 1   | A     | 80  | CYS  | N-CA    | -8.55 | 1.35        | 1.46     |
| 1   | B     | 114 | ARG  | CA-C    | -8.55 | 1.41        | 1.52     |
| 1   | A     | 125 | ARG  | C-O     | 8.55  | 1.34        | 1.23     |
| 1   | B     | 62  | TRP  | CA-C    | 8.54  | 1.63        | 1.52     |
| 1   | B     | 39  | ASN  | CG-ND2  | 8.53  | 1.51        | 1.33     |
| 1   | B     | 31  | ALA  | CA-C    | -8.50 | 1.42        | 1.52     |
| 1   | B     | 50  | SER  | CB-OG   | 8.50  | 1.59        | 1.42     |
| 1   | B     | 124 | ILE  | C-N     | 8.49  | 1.44        | 1.33     |
| 1   | A     | 59  | ASN  | C-O     | -8.49 | 1.13        | 1.23     |
| 1   | A     | 30  | CYS  | CB-SG   | 8.48  | 2.09        | 1.81     |
| 1   | A     | 116 | LYS  | N-CA    | -8.47 | 1.35        | 1.46     |
| 1   | B     | 10  | ALA  | N-CA    | 8.46  | 1.56        | 1.46     |
| 1   | A     | 128 | ARG  | CA-CB   | -8.46 | 1.41        | 1.52     |
| 1   | A     | 7   | GLU  | CA-CB   | 8.45  | 1.66        | 1.53     |
| 1   | A     | 78  | ILE  | CB-CG2  | -8.44 | 1.24        | 1.52     |
| 1   | A     | 118 | THR  | CA-CB   | 8.44  | 1.66        | 1.53     |
| 1   | A     | 123 | TRP  | C-N     | 8.43  | 1.43        | 1.33     |
| 1   | A     | 15  | HIS  | CB-CG   | 8.43  | 1.61        | 1.50     |
| 1   | B     | 70  | PRO  | N-CA    | 8.43  | 1.57        | 1.47     |
| 1   | B     | 18  | ASP  | CB-CG   | 8.41  | 1.73        | 1.52     |
| 1   | B     | 90  | ALA  | C-O     | -8.40 | 1.14        | 1.24     |
| 1   | B     | 62  | TRP  | CG-CD1  | -8.37 | 1.16        | 1.36     |
| 1   | B     | 52  | ASP  | N-CA    | 8.34  | 1.56        | 1.46     |
| 1   | B     | 71  | GLY  | C-N     | -8.34 | 1.22        | 1.33     |
| 1   | B     | 63  | TRP  | CA-CB   | 8.34  | 1.68        | 1.53     |
| 1   | B     | 78  | ILE  | CA-C    | -8.34 | 1.44        | 1.52     |
| 1   | B     | 41  | GLN  | C-O     | -8.32 | 1.12        | 1.24     |
| 1   | B     | 15  | HIS  | C-O     | -8.31 | 1.11        | 1.24     |
| 1   | B     | 27  | ASN  | C-O     | -8.31 | 1.14        | 1.24     |
| 1   | A     | 98  | ILE  | CA-CB   | -8.30 | 1.44        | 1.54     |
| 1   | A     | 93  | ASN  | C-N     | -8.29 | 1.22        | 1.33     |
| 1   | B     | 86  | SER  | CA-CB   | 8.28  | 1.68        | 1.53     |
| 1   | A     | 63  | TRP  | CE3-CZ3 | 8.27  | 1.63        | 1.38     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 83  | LEU  | CA-C   | 8.26  | 1.64        | 1.52     |
| 1   | A     | 107 | ALA  | CA-CB  | 8.26  | 1.67        | 1.53     |
| 1   | B     | 66  | ASP  | CG-OD2 | 8.25  | 1.41        | 1.25     |
| 1   | B     | 46  | ASN  | CG-ND2 | 8.24  | 1.50        | 1.33     |
| 1   | B     | 42  | ALA  | CA-CB  | -8.22 | 1.40        | 1.53     |
| 1   | B     | 78  | ILE  | N-CA   | -8.21 | 1.36        | 1.46     |
| 1   | A     | 32  | ALA  | CA-CB  | 8.13  | 1.66        | 1.53     |
| 1   | B     | 87  | ASP  | CG-OD2 | -8.12 | 1.09        | 1.25     |
| 1   | A     | 68  | ARG  | CB-CG  | -8.11 | 1.28        | 1.52     |
| 1   | B     | 18  | ASP  | C-O    | 8.10  | 1.34        | 1.24     |
| 1   | B     | 128 | ARG  | CA-C   | -8.09 | 1.42        | 1.53     |
| 1   | A     | 8   | LEU  | CA-C   | -8.08 | 1.42        | 1.52     |
| 1   | B     | 27  | ASN  | N-CA   | 8.07  | 1.55        | 1.46     |
| 1   | B     | 5   | ARG  | CZ-NH2 | 8.07  | 1.44        | 1.33     |
| 1   | A     | 14  | ARG  | CZ-NH2 | 8.06  | 1.44        | 1.33     |
| 1   | B     | 96  | LYS  | C-O    | 8.06  | 1.34        | 1.24     |
| 1   | B     | 105 | MET  | N-CA   | -8.05 | 1.35        | 1.46     |
| 1   | A     | 68  | ARG  | CA-CB  | 8.05  | 1.65        | 1.53     |
| 1   | A     | 78  | ILE  | C-N    | 8.02  | 1.44        | 1.33     |
| 1   | A     | 105 | MET  | C-N    | -8.01 | 1.23        | 1.33     |
| 1   | A     | 82  | ALA  | N-CA   | 8.00  | 1.56        | 1.46     |
| 1   | B     | 128 | ARG  | C-N    | -7.99 | 1.22        | 1.33     |
| 1   | A     | 44  | ASN  | N-CA   | -7.99 | 1.36        | 1.46     |
| 1   | A     | 55  | ILE  | N-CA   | -7.98 | 1.36        | 1.46     |
| 1   | B     | 99  | VAL  | CA-C   | 7.98  | 1.62        | 1.52     |
| 1   | A     | 103 | ASN  | CG-OD1 | -7.96 | 1.08        | 1.23     |
| 1   | A     | 116 | LYS  | CA-C   | 7.95  | 1.63        | 1.52     |
| 1   | A     | 124 | ILE  | C-O    | -7.95 | 1.12        | 1.24     |
| 1   | B     | 17  | LEU  | CB-CG  | -7.94 | 1.37        | 1.53     |
| 1   | A     | 28  | TRP  | N-CA   | 7.93  | 1.56        | 1.46     |
| 1   | A     | 114 | ARG  | C-O    | 7.92  | 1.33        | 1.23     |
| 1   | B     | 44  | ASN  | N-CA   | 7.92  | 1.55        | 1.46     |
| 1   | A     | 99  | VAL  | C-N    | -7.89 | 1.23        | 1.33     |
| 1   | B     | 52  | ASP  | CG-OD2 | 7.87  | 1.40        | 1.25     |
| 1   | B     | 75  | LEU  | CA-CB  | -7.87 | 1.40        | 1.53     |
| 1   | B     | 32  | ALA  | N-CA   | 7.83  | 1.55        | 1.46     |
| 1   | B     | 84  | LEU  | CA-C   | -7.83 | 1.42        | 1.52     |
| 1   | B     | 96  | LYS  | C-N    | -7.79 | 1.22        | 1.33     |
| 1   | A     | 112 | ARG  | NE-CZ  | 7.77  | 1.41        | 1.33     |
| 1   | B     | 129 | LEU  | C-OXT  | 7.76  | 1.39        | 1.23     |
| 1   | B     | 124 | ILE  | CB-CG1 | -7.76 | 1.38        | 1.53     |
| 1   | B     | 64  | CYS  | C-N    | 7.74  | 1.44        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 18  | ASP  | CG-OD2  | 7.74  | 1.40        | 1.25     |
| 1   | A     | 52  | ASP  | CA-C    | 7.74  | 1.61        | 1.52     |
| 1   | B     | 129 | LEU  | C-O     | 7.74  | 1.39        | 1.23     |
| 1   | B     | 113 | ASN  | CA-CB   | -7.72 | 1.40        | 1.53     |
| 1   | B     | 70  | PRO  | C-O     | -7.72 | 1.15        | 1.23     |
| 1   | A     | 37  | ASN  | CA-CB   | 7.71  | 1.65        | 1.53     |
| 1   | B     | 125 | ARG  | N-CA    | 7.71  | 1.56        | 1.46     |
| 1   | B     | 47  | THR  | C-N     | -7.71 | 1.21        | 1.33     |
| 1   | B     | 68  | ARG  | CZ-NH1  | 7.69  | 1.43        | 1.32     |
| 1   | B     | 38  | PHE  | C-N     | -7.69 | 1.22        | 1.33     |
| 1   | B     | 115 | CYS  | N-CA    | -7.68 | 1.35        | 1.46     |
| 1   | A     | 106 | ASN  | CA-CB   | 7.68  | 1.67        | 1.53     |
| 1   | B     | 92  | VAL  | C-O     | 7.68  | 1.33        | 1.24     |
| 1   | B     | 46  | ASN  | CG-OD1  | 7.66  | 1.38        | 1.23     |
| 1   | B     | 95  | ALA  | CA-C    | 7.64  | 1.62        | 1.52     |
| 1   | A     | 118 | THR  | CA-C    | 7.63  | 1.63        | 1.53     |
| 1   | A     | 8   | LEU  | N-CA    | 7.63  | 1.55        | 1.46     |
| 1   | A     | 63  | TRP  | CE2-CZ2 | -7.63 | 1.23        | 1.39     |
| 1   | B     | 107 | ALA  | C-O     | -7.63 | 1.14        | 1.24     |
| 1   | A     | 29  | VAL  | CA-C    | -7.61 | 1.43        | 1.52     |
| 1   | B     | 59  | ASN  | C-O     | -7.61 | 1.14        | 1.23     |
| 1   | A     | 34  | PHE  | CA-CB   | 7.61  | 1.67        | 1.53     |
| 1   | B     | 107 | ALA  | N-CA    | 7.60  | 1.56        | 1.46     |
| 1   | B     | 74  | ASN  | N-CA    | -7.60 | 1.35        | 1.46     |
| 1   | A     | 7   | GLU  | C-N     | -7.60 | 1.24        | 1.33     |
| 1   | B     | 66  | ASP  | CG-OD1  | 7.59  | 1.39        | 1.25     |
| 1   | A     | 80  | CYS  | CA-C    | 7.58  | 1.63        | 1.52     |
| 1   | B     | 109 | VAL  | CA-CB   | -7.55 | 1.45        | 1.54     |
| 1   | A     | 5   | ARG  | NE-CZ   | -7.55 | 1.24        | 1.33     |
| 1   | B     | 2   | VAL  | C-O     | -7.53 | 1.16        | 1.24     |
| 1   | B     | 51  | THR  | CB-OG1  | 7.53  | 1.55        | 1.43     |
| 1   | B     | 111 | TRP  | CA-CB   | -7.51 | 1.41        | 1.53     |
| 1   | A     | 21  | ARG  | C-N     | -7.50 | 1.22        | 1.33     |
| 1   | B     | 31  | ALA  | C-O     | 7.50  | 1.32        | 1.24     |
| 1   | B     | 3   | PHE  | N-CA    | -7.49 | 1.36        | 1.45     |
| 1   | A     | 53  | TYR  | CG-CD2  | -7.48 | 1.23        | 1.39     |
| 1   | A     | 77  | ASN  | CG-ND2  | -7.47 | 1.17        | 1.33     |
| 1   | A     | 77  | ASN  | C-N     | -7.46 | 1.25        | 1.33     |
| 1   | A     | 45  | ARG  | C-N     | 7.45  | 1.43        | 1.33     |
| 1   | A     | 75  | LEU  | N-CA    | 7.43  | 1.56        | 1.46     |
| 1   | B     | 77  | ASN  | CB-CG   | 7.41  | 1.70        | 1.52     |
| 1   | A     | 113 | ASN  | CA-CB   | 7.39  | 1.65        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 86  | SER  | CA-C    | -7.37 | 1.42        | 1.52     |
| 1   | A     | 5   | ARG  | CA-CB   | 7.36  | 1.65        | 1.53     |
| 1   | A     | 52  | ASP  | C-N     | 7.36  | 1.43        | 1.33     |
| 1   | A     | 52  | ASP  | CB-CG   | -7.35 | 1.33        | 1.52     |
| 1   | B     | 34  | PHE  | CA-CB   | 7.35  | 1.65        | 1.53     |
| 1   | B     | 100 | SER  | CA-CB   | 7.34  | 1.65        | 1.53     |
| 1   | B     | 3   | PHE  | C-O     | -7.34 | 1.14        | 1.23     |
| 1   | B     | 94  | CYS  | C-N     | 7.33  | 1.43        | 1.33     |
| 1   | B     | 15  | HIS  | N-CA    | 7.33  | 1.56        | 1.46     |
| 1   | A     | 113 | ASN  | CG-ND2  | -7.32 | 1.17        | 1.33     |
| 1   | B     | 26  | GLY  | CA-C    | 7.32  | 1.60        | 1.52     |
| 1   | B     | 35  | GLU  | CG-CD   | -7.32 | 1.33        | 1.52     |
| 1   | B     | 115 | CYS  | C-N     | -7.32 | 1.23        | 1.33     |
| 1   | B     | 66  | ASP  | C-N     | -7.29 | 1.23        | 1.33     |
| 1   | B     | 22  | GLY  | CA-C    | 7.29  | 1.61        | 1.51     |
| 1   | B     | 69  | THR  | CA-CB   | -7.26 | 1.42        | 1.53     |
| 1   | A     | 96  | LYS  | CA-C    | -7.23 | 1.43        | 1.52     |
| 1   | A     | 96  | LYS  | C-N     | 7.22  | 1.43        | 1.33     |
| 1   | B     | 40  | THR  | C-O     | -7.22 | 1.14        | 1.24     |
| 1   | A     | 38  | PHE  | CD2-CE2 | -7.20 | 1.17        | 1.38     |
| 1   | B     | 50  | SER  | CA-CB   | 7.20  | 1.65        | 1.53     |
| 1   | B     | 14  | ARG  | CG-CD   | -7.18 | 1.30        | 1.52     |
| 1   | B     | 100 | SER  | C-N     | -7.18 | 1.22        | 1.33     |
| 1   | A     | 60  | SER  | CA-CB   | 7.17  | 1.66        | 1.53     |
| 1   | A     | 69  | THR  | CB-OG1  | 7.17  | 1.55        | 1.43     |
| 1   | A     | 108 | TRP  | CD2-CE3 | 7.16  | 1.51        | 1.40     |
| 1   | A     | 55  | ILE  | C-N     | -7.15 | 1.24        | 1.33     |
| 1   | B     | 60  | SER  | C-N     | -7.12 | 1.24        | 1.33     |
| 1   | B     | 111 | TRP  | CE2-CZ2 | -7.12 | 1.24        | 1.39     |
| 1   | A     | 23  | TYR  | CA-C    | -7.12 | 1.43        | 1.52     |
| 1   | A     | 53  | TYR  | CG-CD1  | -7.11 | 1.24        | 1.39     |
| 1   | B     | 111 | TRP  | C-O     | 7.11  | 1.32        | 1.24     |
| 1   | B     | 89  | THR  | CA-C    | -7.11 | 1.42        | 1.52     |
| 1   | B     | 110 | ALA  | C-N     | -7.09 | 1.24        | 1.33     |
| 1   | A     | 40  | THR  | N-CA    | 7.07  | 1.55        | 1.46     |
| 1   | A     | 34  | PHE  | N-CA    | -7.07 | 1.36        | 1.46     |
| 1   | A     | 103 | ASN  | C-O     | 7.06  | 1.34        | 1.24     |
| 1   | A     | 74  | ASN  | CA-C    | -7.05 | 1.43        | 1.53     |
| 1   | A     | 15  | HIS  | CA-C    | 7.04  | 1.62        | 1.52     |
| 1   | B     | 39  | ASN  | C-O     | -7.03 | 1.15        | 1.24     |
| 1   | B     | 33  | LYS  | CD-CE   | 7.02  | 1.73        | 1.52     |
| 1   | A     | 58  | ILE  | C-N     | 7.00  | 1.43        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 14  | ARG  | CA-C    | 6.99  | 1.62        | 1.52     |
| 1   | B     | 45  | ARG  | CA-C    | 6.98  | 1.61        | 1.52     |
| 1   | A     | 1   | LYS  | CA-CB   | -6.97 | 1.39        | 1.53     |
| 1   | B     | 39  | ASN  | CA-CB   | -6.96 | 1.44        | 1.53     |
| 1   | A     | 128 | ARG  | C-O     | 6.95  | 1.33        | 1.23     |
| 1   | A     | 32  | ALA  | N-CA    | 6.94  | 1.54        | 1.46     |
| 1   | A     | 123 | TRP  | C-O     | -6.92 | 1.14        | 1.24     |
| 1   | B     | 113 | ASN  | N-CA    | -6.92 | 1.37        | 1.46     |
| 1   | A     | 13  | LYS  | C-N     | 6.91  | 1.43        | 1.33     |
| 1   | B     | 16  | GLY  | CA-C    | 6.90  | 1.60        | 1.51     |
| 1   | B     | 89  | THR  | C-O     | -6.86 | 1.16        | 1.24     |
| 1   | B     | 93  | ASN  | CA-CB   | -6.85 | 1.42        | 1.53     |
| 1   | B     | 19  | ASN  | N-CA    | -6.85 | 1.37        | 1.46     |
| 1   | A     | 113 | ASN  | CG-OD1  | -6.85 | 1.10        | 1.23     |
| 1   | B     | 106 | ASN  | CG-OD1  | -6.84 | 1.10        | 1.23     |
| 1   | A     | 49  | GLY  | CA-C    | 6.84  | 1.61        | 1.51     |
| 1   | A     | 79  | PRO  | N-CA    | -6.81 | 1.39        | 1.47     |
| 1   | B     | 38  | PHE  | CA-CB   | 6.81  | 1.63        | 1.53     |
| 1   | A     | 111 | TRP  | CZ2-CH2 | -6.81 | 1.24        | 1.37     |
| 1   | A     | 37  | ASN  | C-O     | 6.79  | 1.32        | 1.23     |
| 1   | B     | 28  | TRP  | CD2-CE2 | 6.78  | 1.52        | 1.41     |
| 1   | B     | 106 | ASN  | CA-C    | 6.77  | 1.62        | 1.52     |
| 1   | B     | 16  | GLY  | C-N     | 6.77  | 1.44        | 1.33     |
| 1   | B     | 94  | CYS  | C-O     | -6.77 | 1.16        | 1.24     |
| 1   | B     | 106 | ASN  | CG-ND2  | 6.76  | 1.47        | 1.33     |
| 1   | B     | 91  | SER  | C-N     | 6.76  | 1.42        | 1.33     |
| 1   | B     | 71  | GLY  | CA-C    | 6.75  | 1.60        | 1.51     |
| 1   | A     | 45  | ARG  | C-O     | -6.72 | 1.15        | 1.24     |
| 1   | A     | 54  | GLY  | C-N     | 6.71  | 1.42        | 1.34     |
| 1   | A     | 1   | LYS  | N-CA    | 6.71  | 1.58        | 1.46     |
| 1   | B     | 8   | LEU  | CA-CB   | 6.70  | 1.63        | 1.53     |
| 1   | B     | 65  | ASN  | CB-CG   | -6.69 | 1.35        | 1.52     |
| 1   | B     | 58  | ILE  | CB-CG2  | 6.69  | 1.74        | 1.52     |
| 1   | B     | 88  | ILE  | N-CA    | 6.69  | 1.53        | 1.46     |
| 1   | A     | 117 | GLY  | N-CA    | 6.68  | 1.55        | 1.45     |
| 1   | B     | 4   | GLY  | C-N     | -6.67 | 1.25        | 1.33     |
| 1   | B     | 1   | LYS  | CB-CG   | -6.67 | 1.32        | 1.52     |
| 1   | A     | 109 | VAL  | CB-CG1  | -6.67 | 1.30        | 1.52     |
| 1   | A     | 19  | ASN  | CB-CG   | 6.67  | 1.68        | 1.52     |
| 1   | B     | 1   | LYS  | CE-NZ   | -6.66 | 1.29        | 1.49     |
| 1   | A     | 106 | ASN  | C-N     | -6.65 | 1.24        | 1.33     |
| 1   | A     | 124 | ILE  | CA-C    | 6.65  | 1.61        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 123 | TRP  | CG-CD2  | 6.64  | 1.55        | 1.43     |
| 1   | A     | 42  | ALA  | N-CA    | -6.63 | 1.37        | 1.46     |
| 1   | A     | 102 | GLY  | CA-C    | 6.62  | 1.61        | 1.51     |
| 1   | A     | 88  | ILE  | N-CA    | 6.61  | 1.54        | 1.46     |
| 1   | A     | 34  | PHE  | CA-C    | -6.59 | 1.43        | 1.52     |
| 1   | B     | 56  | LEU  | CG-CD2  | 6.59  | 1.74        | 1.52     |
| 1   | B     | 82  | ALA  | C-N     | 6.58  | 1.43        | 1.33     |
| 1   | A     | 62  | TRP  | CD2-CE3 | 6.58  | 1.50        | 1.40     |
| 1   | A     | 5   | ARG  | CA-C    | -6.57 | 1.44        | 1.52     |
| 1   | B     | 17  | LEU  | C-N     | -6.56 | 1.24        | 1.33     |
| 1   | A     | 92  | VAL  | CA-CB   | 6.54  | 1.62        | 1.54     |
| 1   | B     | 72  | SER  | CA-C    | 6.53  | 1.60        | 1.52     |
| 1   | A     | 42  | ALA  | C-N     | 6.52  | 1.43        | 1.33     |
| 1   | B     | 116 | LYS  | C-N     | 6.51  | 1.43        | 1.33     |
| 1   | A     | 7   | GLU  | CD-OE1  | 6.50  | 1.37        | 1.25     |
| 1   | A     | 10  | ALA  | C-N     | -6.50 | 1.25        | 1.33     |
| 1   | A     | 102 | GLY  | C-N     | 6.49  | 1.44        | 1.34     |
| 1   | A     | 111 | TRP  | CZ3-CH2 | -6.48 | 1.24        | 1.40     |
| 1   | B     | 107 | ALA  | CA-C    | 6.47  | 1.61        | 1.52     |
| 1   | B     | 81  | SER  | CB-OG   | 6.47  | 1.55        | 1.42     |
| 1   | B     | 49  | GLY  | N-CA    | -6.46 | 1.35        | 1.45     |
| 1   | A     | 72  | SER  | CB-OG   | 6.46  | 1.55        | 1.42     |
| 1   | A     | 116 | LYS  | C-O     | -6.46 | 1.16        | 1.23     |
| 1   | B     | 7   | GLU  | C-O     | -6.43 | 1.16        | 1.24     |
| 1   | B     | 122 | ALA  | CA-C    | 6.43  | 1.61        | 1.52     |
| 1   | B     | 51  | THR  | N-CA    | -6.42 | 1.38        | 1.46     |
| 1   | A     | 63  | TRP  | CD2-CE2 | 6.42  | 1.52        | 1.41     |
| 1   | B     | 4   | GLY  | C-O     | -6.42 | 1.12        | 1.23     |
| 1   | A     | 127 | CYS  | N-CA    | 6.42  | 1.54        | 1.46     |
| 1   | B     | 23  | TYR  | C-O     | -6.41 | 1.16        | 1.24     |
| 1   | A     | 73  | ARG  | CD-NE   | 6.40  | 1.55        | 1.46     |
| 1   | A     | 87  | ASP  | CA-C    | 6.38  | 1.60        | 1.52     |
| 1   | A     | 49  | GLY  | C-O     | -6.38 | 1.15        | 1.23     |
| 1   | A     | 64  | CYS  | CA-C    | 6.37  | 1.60        | 1.52     |
| 1   | B     | 24  | SER  | CA-CB   | 6.37  | 1.63        | 1.53     |
| 1   | B     | 29  | VAL  | CB-CG1  | 6.36  | 1.73        | 1.52     |
| 1   | B     | 121 | GLN  | N-CA    | 6.35  | 1.54        | 1.46     |
| 1   | A     | 93  | ASN  | CG-ND2  | -6.34 | 1.20        | 1.33     |
| 1   | B     | 57  | GLN  | C-N     | -6.34 | 1.22        | 1.33     |
| 1   | B     | 89  | THR  | N-CA    | 6.33  | 1.54        | 1.46     |
| 1   | A     | 73  | ARG  | CA-CB   | -6.32 | 1.45        | 1.54     |
| 1   | B     | 92  | VAL  | N-CA    | -6.32 | 1.38        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 103 | ASN  | CG-ND2  | -6.32 | 1.20        | 1.33     |
| 1   | A     | 30  | CYS  | C-N     | 6.31  | 1.42        | 1.33     |
| 1   | B     | 114 | ARG  | CZ-NH1  | 6.30  | 1.41        | 1.32     |
| 1   | B     | 104 | GLY  | C-N     | -6.28 | 1.24        | 1.33     |
| 1   | A     | 101 | ASP  | CG-OD2  | -6.28 | 1.13        | 1.25     |
| 1   | A     | 46  | ASN  | C-O     | -6.28 | 1.16        | 1.23     |
| 1   | A     | 120 | VAL  | N-CA    | 6.26  | 1.55        | 1.46     |
| 1   | A     | 125 | ARG  | N-CA    | 6.25  | 1.53        | 1.46     |
| 1   | B     | 44  | ASN  | C-N     | 6.25  | 1.42        | 1.33     |
| 1   | A     | 63  | TRP  | CA-C    | -6.25 | 1.44        | 1.52     |
| 1   | A     | 53  | TYR  | N-CA    | -6.25 | 1.38        | 1.46     |
| 1   | B     | 103 | ASN  | N-CA    | -6.24 | 1.38        | 1.46     |
| 1   | A     | 85  | SER  | N-CA    | -6.23 | 1.37        | 1.45     |
| 1   | B     | 93  | ASN  | CG-OD1  | 6.23  | 1.35        | 1.23     |
| 1   | A     | 69  | THR  | CA-CB   | 6.22  | 1.64        | 1.53     |
| 1   | A     | 46  | ASN  | N-CA    | 6.22  | 1.53        | 1.45     |
| 1   | A     | 84  | LEU  | CA-C    | -6.20 | 1.43        | 1.52     |
| 1   | B     | 112 | ARG  | CA-C    | -6.19 | 1.44        | 1.52     |
| 1   | A     | 5   | ARG  | C-O     | 6.19  | 1.31        | 1.24     |
| 1   | A     | 119 | ASP  | CB-CG   | 6.19  | 1.67        | 1.52     |
| 1   | A     | 99  | VAL  | CA-CB   | 6.18  | 1.63        | 1.54     |
| 1   | B     | 73  | ARG  | C-O     | 6.17  | 1.31        | 1.24     |
| 1   | B     | 23  | TYR  | CA-C    | 6.17  | 1.60        | 1.52     |
| 1   | B     | 124 | ILE  | CG1-CD1 | 6.17  | 1.75        | 1.51     |
| 1   | A     | 36  | SER  | C-O     | -6.16 | 1.16        | 1.24     |
| 1   | A     | 123 | TRP  | CD2-CE3 | -6.16 | 1.30        | 1.40     |
| 1   | A     | 34  | PHE  | CE2-CZ  | -6.15 | 1.20        | 1.38     |
| 1   | B     | 30  | CYS  | CA-C    | -6.15 | 1.44        | 1.52     |
| 1   | A     | 46  | ASN  | CA-CB   | -6.15 | 1.43        | 1.53     |
| 1   | B     | 56  | LEU  | C-N     | 6.14  | 1.41        | 1.33     |
| 1   | B     | 50  | SER  | C-N     | -6.13 | 1.24        | 1.33     |
| 1   | B     | 105 | MET  | CA-C    | -6.11 | 1.44        | 1.52     |
| 1   | B     | 96  | LYS  | CD-CE   | -6.10 | 1.34        | 1.52     |
| 1   | B     | 27  | ASN  | CA-C    | 6.09  | 1.60        | 1.52     |
| 1   | B     | 86  | SER  | CB-OG   | 6.08  | 1.54        | 1.42     |
| 1   | B     | 28  | TRP  | NE1-CE2 | -6.07 | 1.30        | 1.37     |
| 1   | A     | 43  | THR  | CB-OG1  | -6.06 | 1.34        | 1.43     |
| 1   | B     | 80  | CYS  | N-CA    | 6.06  | 1.53        | 1.46     |
| 1   | A     | 82  | ALA  | C-O     | 6.02  | 1.31        | 1.24     |
| 1   | B     | 66  | ASP  | N-CA    | 6.01  | 1.53        | 1.46     |
| 1   | B     | 37  | ASN  | N-CA    | -5.99 | 1.37        | 1.46     |
| 1   | B     | 47  | THR  | CB-CG2  | 5.99  | 1.72        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 22  | GLY  | C-N     | 5.99  | 1.43        | 1.33     |
| 1   | B     | 61  | ARG  | N-CA    | 5.99  | 1.53        | 1.46     |
| 1   | A     | 91  | SER  | N-CA    | 5.98  | 1.53        | 1.46     |
| 1   | A     | 109 | VAL  | C-N     | 5.97  | 1.42        | 1.33     |
| 1   | A     | 78  | ILE  | C-O     | 5.96  | 1.31        | 1.24     |
| 1   | A     | 79  | PRO  | N-CD    | -5.96 | 1.39        | 1.47     |
| 1   | A     | 61  | ARG  | CB-CG   | 5.94  | 1.70        | 1.52     |
| 1   | B     | 25  | LEU  | CA-C    | -5.93 | 1.44        | 1.52     |
| 1   | A     | 47  | THR  | C-N     | -5.93 | 1.25        | 1.33     |
| 1   | B     | 35  | GLU  | CA-C    | 5.93  | 1.60        | 1.52     |
| 1   | B     | 58  | ILE  | CA-CB   | -5.92 | 1.47        | 1.54     |
| 1   | A     | 80  | CYS  | CA-CB   | 5.91  | 1.63        | 1.53     |
| 1   | B     | 72  | SER  | C-N     | 5.89  | 1.42        | 1.33     |
| 1   | A     | 128 | ARG  | CZ-NH1  | -5.89 | 1.24        | 1.32     |
| 1   | B     | 57  | GLN  | CA-C    | 5.88  | 1.60        | 1.53     |
| 1   | B     | 111 | TRP  | CD2-CE3 | 5.88  | 1.49        | 1.40     |
| 1   | A     | 29  | VAL  | CA-CB   | -5.87 | 1.47        | 1.54     |
| 1   | A     | 35  | GLU  | CD-OE1  | 5.87  | 1.36        | 1.25     |
| 1   | A     | 37  | ASN  | CA-C    | -5.86 | 1.45        | 1.53     |
| 1   | B     | 63  | TRP  | N-CA    | 5.86  | 1.53        | 1.46     |
| 1   | B     | 37  | ASN  | CA-CB   | -5.86 | 1.44        | 1.53     |
| 1   | B     | 55  | ILE  | CA-CB   | -5.83 | 1.46        | 1.54     |
| 1   | B     | 35  | GLU  | C-O     | 5.83  | 1.31        | 1.24     |
| 1   | A     | 76  | CYS  | C-N     | 5.81  | 1.42        | 1.33     |
| 1   | B     | 70  | PRO  | C-N     | 5.81  | 1.41        | 1.33     |
| 1   | A     | 89  | THR  | CA-C    | -5.80 | 1.45        | 1.52     |
| 1   | A     | 78  | ILE  | CB-CG1  | -5.80 | 1.41        | 1.53     |
| 1   | A     | 25  | LEU  | CB-CG   | 5.78  | 1.65        | 1.53     |
| 1   | A     | 122 | ALA  | C-N     | -5.78 | 1.24        | 1.33     |
| 1   | A     | 73  | ARG  | CZ-NH2  | 5.77  | 1.41        | 1.33     |
| 1   | B     | 20  | TYR  | CE1-CZ  | 5.77  | 1.52        | 1.38     |
| 1   | A     | 11  | ALA  | N-CA    | -5.76 | 1.39        | 1.46     |
| 1   | B     | 97  | LYS  | CE-NZ   | 5.75  | 1.66        | 1.49     |
| 1   | A     | 43  | THR  | CB-CG2  | -5.74 | 1.33        | 1.52     |
| 1   | A     | 33  | LYS  | CE-NZ   | 5.72  | 1.66        | 1.49     |
| 1   | B     | 41  | GLN  | CG-CD   | -5.71 | 1.37        | 1.52     |
| 1   | B     | 14  | ARG  | N-CA    | 5.69  | 1.53        | 1.46     |
| 1   | B     | 10  | ALA  | C-N     | -5.69 | 1.26        | 1.33     |
| 1   | A     | 83  | LEU  | N-CA    | 5.68  | 1.53        | 1.46     |
| 1   | A     | 65  | ASN  | C-N     | -5.67 | 1.25        | 1.33     |
| 1   | B     | 11  | ALA  | N-CA    | 5.66  | 1.53        | 1.46     |
| 1   | B     | 72  | SER  | CB-OG   | -5.66 | 1.30        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 113 | ASN  | CB-CG   | -5.65 | 1.38        | 1.52     |
| 1   | A     | 8   | LEU  | CB-CG   | -5.64 | 1.42        | 1.53     |
| 1   | A     | 63  | TRP  | CG-CD1  | -5.63 | 1.22        | 1.36     |
| 1   | B     | 11  | ALA  | C-N     | -5.62 | 1.26        | 1.34     |
| 1   | A     | 105 | MET  | SD-CE   | -5.62 | 1.65        | 1.79     |
| 1   | A     | 93  | ASN  | CA-CB   | 5.62  | 1.62        | 1.53     |
| 1   | B     | 51  | THR  | CA-CB   | -5.61 | 1.40        | 1.53     |
| 1   | B     | 101 | ASP  | CA-C    | -5.61 | 1.44        | 1.52     |
| 1   | B     | 15  | HIS  | CG-CD2  | 5.61  | 1.42        | 1.35     |
| 1   | B     | 73  | ARG  | CB-CG   | 5.60  | 1.69        | 1.52     |
| 1   | A     | 13  | LYS  | C-O     | 5.59  | 1.30        | 1.24     |
| 1   | B     | 20  | TYR  | CD2-CE2 | -5.59 | 1.21        | 1.38     |
| 1   | A     | 94  | CYS  | CA-CB   | -5.58 | 1.44        | 1.53     |
| 1   | A     | 3   | PHE  | CA-C    | -5.58 | 1.45        | 1.53     |
| 1   | A     | 64  | CYS  | N-CA    | 5.58  | 1.53        | 1.45     |
| 1   | B     | 62  | TRP  | CB-CG   | 5.56  | 1.67        | 1.50     |
| 1   | B     | 93  | ASN  | C-O     | -5.56 | 1.17        | 1.24     |
| 1   | B     | 8   | LEU  | C-O     | -5.55 | 1.17        | 1.24     |
| 1   | B     | 21  | ARG  | CG-CD   | -5.55 | 1.35        | 1.52     |
| 1   | B     | 28  | TRP  | N-CA    | 5.55  | 1.53        | 1.46     |
| 1   | A     | 129 | LEU  | CG-CD2  | -5.54 | 1.34        | 1.52     |
| 1   | A     | 105 | MET  | CA-CB   | 5.53  | 1.63        | 1.53     |
| 1   | B     | 101 | ASP  | N-CA    | 5.53  | 1.53        | 1.46     |
| 1   | A     | 122 | ALA  | CA-CB   | 5.52  | 1.62        | 1.53     |
| 1   | B     | 20  | TYR  | CG-CD1  | 5.52  | 1.50        | 1.39     |
| 1   | A     | 17  | LEU  | C-O     | 5.51  | 1.31        | 1.24     |
| 1   | B     | 83  | LEU  | N-CA    | 5.51  | 1.53        | 1.46     |
| 1   | B     | 90  | ALA  | CA-C    | 5.51  | 1.59        | 1.52     |
| 1   | A     | 21  | ARG  | CD-NE   | 5.51  | 1.53        | 1.46     |
| 1   | A     | 58  | ILE  | CB-CG1  | 5.51  | 1.64        | 1.53     |
| 1   | A     | 73  | ARG  | N-CA    | -5.51 | 1.38        | 1.45     |
| 1   | B     | 76  | CYS  | C-O     | 5.50  | 1.31        | 1.24     |
| 1   | B     | 62  | TRP  | CA-CB   | 5.50  | 1.61        | 1.53     |
| 1   | A     | 97  | LYS  | CD-CE   | 5.49  | 1.69        | 1.52     |
| 1   | A     | 62  | TRP  | CE3-CZ3 | 5.49  | 1.55        | 1.38     |
| 1   | A     | 66  | ASP  | C-N     | -5.48 | 1.25        | 1.33     |
| 1   | B     | 38  | PHE  | CG-CD2  | -5.47 | 1.27        | 1.38     |
| 1   | B     | 10  | ALA  | CA-C    | 5.46  | 1.59        | 1.52     |
| 1   | A     | 1   | LYS  | C-N     | 5.45  | 1.39        | 1.33     |
| 1   | B     | 123 | TRP  | N-CA    | -5.44 | 1.39        | 1.46     |
| 1   | A     | 1   | LYS  | CB-CG   | -5.44 | 1.36        | 1.52     |
| 1   | A     | 62  | TRP  | CE2-CZ2 | -5.44 | 1.28        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 15  | HIS  | CA-CB   | 5.43  | 1.62        | 1.53     |
| 1   | B     | 75  | LEU  | N-CA    | 5.42  | 1.53        | 1.46     |
| 1   | B     | 68  | ARG  | CB-CG   | -5.42 | 1.36        | 1.52     |
| 1   | B     | 23  | TYR  | CA-CB   | 5.42  | 1.61        | 1.53     |
| 1   | A     | 77  | ASN  | CA-CB   | -5.41 | 1.45        | 1.53     |
| 1   | B     | 23  | TYR  | C-N     | 5.40  | 1.40        | 1.33     |
| 1   | A     | 123 | TRP  | CE3-CZ3 | 5.38  | 1.54        | 1.38     |
| 1   | B     | 52  | ASP  | C-O     | 5.38  | 1.30        | 1.24     |
| 1   | A     | 30  | CYS  | CA-C    | -5.37 | 1.45        | 1.52     |
| 1   | A     | 18  | ASP  | CG-OD2  | 5.36  | 1.35        | 1.25     |
| 1   | B     | 109 | VAL  | C-O     | 5.36  | 1.30        | 1.24     |
| 1   | B     | 109 | VAL  | CA-C    | -5.36 | 1.46        | 1.52     |
| 1   | A     | 48  | ASP  | CB-CG   | 5.34  | 1.65        | 1.52     |
| 1   | B     | 25  | LEU  | C-N     | 5.34  | 1.41        | 1.33     |
| 1   | B     | 41  | GLN  | C-N     | 5.33  | 1.40        | 1.33     |
| 1   | A     | 38  | PHE  | C-N     | -5.33 | 1.25        | 1.33     |
| 1   | B     | 125 | ARG  | CD-NE   | -5.33 | 1.38        | 1.46     |
| 1   | A     | 62  | TRP  | CB-CG   | 5.32  | 1.66        | 1.50     |
| 1   | B     | 19  | ASN  | C-O     | 5.31  | 1.33        | 1.24     |
| 1   | B     | 60  | SER  | CA-C    | -5.30 | 1.45        | 1.52     |
| 1   | A     | 8   | LEU  | CA-CB   | 5.30  | 1.61        | 1.53     |
| 1   | A     | 96  | LYS  | N-CA    | 5.29  | 1.53        | 1.46     |
| 1   | A     | 98  | ILE  | CB-CG1  | 5.27  | 1.64        | 1.53     |
| 1   | B     | 46  | ASN  | CA-C    | 5.27  | 1.59        | 1.52     |
| 1   | A     | 106 | ASN  | CG-OD1  | 5.27  | 1.33        | 1.23     |
| 1   | A     | 53  | TYR  | CA-CB   | 5.26  | 1.61        | 1.53     |
| 1   | B     | 86  | SER  | N-CA    | -5.26 | 1.39        | 1.46     |
| 1   | B     | 116 | LYS  | CD-CE   | -5.23 | 1.36        | 1.52     |
| 1   | B     | 108 | TRP  | CZ2-CH2 | 5.21  | 1.47        | 1.37     |
| 1   | A     | 33  | LYS  | C-N     | 5.18  | 1.41        | 1.33     |
| 1   | B     | 129 | LEU  | CG-CD2  | -5.18 | 1.35        | 1.52     |
| 1   | A     | 58  | ILE  | CG1-CD1 | 5.17  | 1.72        | 1.51     |
| 1   | B     | 56  | LEU  | N-CA    | -5.17 | 1.39        | 1.46     |
| 1   | A     | 107 | ALA  | C-O     | 5.17  | 1.30        | 1.24     |
| 1   | A     | 87  | ASP  | CG-OD1  | -5.17 | 1.15        | 1.25     |
| 1   | B     | 37  | ASN  | C-N     | -5.16 | 1.26        | 1.33     |
| 1   | B     | 45  | ARG  | CA-CB   | 5.16  | 1.61        | 1.53     |
| 1   | A     | 50  | SER  | CA-CB   | 5.15  | 1.61        | 1.53     |
| 1   | B     | 108 | TRP  | CG-CD1  | 5.14  | 1.49        | 1.36     |
| 1   | B     | 44  | ASN  | CA-CB   | 5.12  | 1.61        | 1.53     |
| 1   | A     | 15  | HIS  | N-CA    | 5.11  | 1.52        | 1.46     |
| 1   | B     | 38  | PHE  | CG-CD1  | -5.11 | 1.28        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 117 | GLY  | CA-C    | -5.10 | 1.44        | 1.51     |
| 1   | A     | 1   | LYS  | CA-C    | -5.08 | 1.42        | 1.52     |
| 1   | A     | 101 | ASP  | N-CA    | -5.08 | 1.40        | 1.46     |
| 1   | A     | 17  | LEU  | CA-C    | -5.07 | 1.45        | 1.52     |
| 1   | B     | 44  | ASN  | CB-CG   | 5.07  | 1.64        | 1.52     |
| 1   | B     | 123 | TRP  | CD2-CE3 | -5.07 | 1.32        | 1.40     |
| 1   | B     | 59  | ASN  | CG-OD1  | -5.07 | 1.14        | 1.23     |
| 1   | A     | 110 | ALA  | C-N     | -5.07 | 1.27        | 1.33     |
| 1   | A     | 5   | ARG  | CZ-NH1  | 5.04  | 1.39        | 1.32     |
| 1   | B     | 20  | TYR  | CB-CG   | 5.03  | 1.62        | 1.51     |
| 1   | A     | 3   | PHE  | C-O     | -5.02 | 1.17        | 1.23     |
| 1   | B     | 96  | LYS  | CG-CD   | 5.02  | 1.67        | 1.52     |
| 1   | A     | 81  | SER  | CA-C    | 5.02  | 1.59        | 1.52     |
| 1   | A     | 74  | ASN  | CG-OD1  | -5.02 | 1.14        | 1.23     |
| 1   | A     | 81  | SER  | C-N     | -5.02 | 1.27        | 1.33     |
| 1   | A     | 23  | TYR  | CG-CD2  | -5.01 | 1.28        | 1.39     |
| 1   | B     | 111 | TRP  | CD1-NE1 | 5.00  | 1.48        | 1.37     |
| 1   | B     | 127 | CYS  | CA-CB   | 5.00  | 1.61        | 1.53     |
| 1   | A     | 3   | PHE  | CB-CG   | -5.00 | 1.39        | 1.50     |

All (974) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | B     | 128 | ARG  | NE-CZ-NH2  | -44.41 | 79.23       | 119.20   |
| 1   | B     | 128 | ARG  | NH1-CZ-NH2 | 39.64  | 170.84      | 119.30   |
| 1   | A     | 125 | ARG  | NE-CZ-NH2  | -39.09 | 84.01       | 119.20   |
| 1   | B     | 121 | GLN  | OE1-CD-NE2 | 38.65  | 161.25      | 122.60   |
| 1   | B     | 21  | ARG  | CD-NE-CZ   | 38.56  | 178.38      | 124.40   |
| 1   | B     | 19  | ASN  | OD1-CG-ND2 | -37.33 | 85.27       | 122.60   |
| 1   | A     | 125 | ARG  | NE-CZ-NH1  | 35.97  | 157.47      | 121.50   |
| 1   | B     | 61  | ARG  | NE-CZ-NH2  | 35.79  | 151.41      | 119.20   |
| 1   | B     | 114 | ARG  | NE-CZ-NH2  | -35.51 | 87.25       | 119.20   |
| 1   | B     | 45  | ARG  | NE-CZ-NH2  | 33.06  | 148.96      | 119.20   |
| 1   | B     | 21  | ARG  | NH1-CZ-NH2 | -33.04 | 76.35       | 119.30   |
| 1   | B     | 73  | ARG  | NE-CZ-NH2  | 31.15  | 147.24      | 119.20   |
| 1   | B     | 61  | ARG  | CD-NE-CZ   | 30.94  | 167.72      | 124.40   |
| 1   | A     | 128 | ARG  | CA-C-O     | -30.35 | 87.58       | 121.58   |
| 1   | A     | 125 | ARG  | CD-NE-CZ   | -30.32 | 81.95       | 124.40   |
| 1   | B     | 128 | ARG  | NE-CZ-NH1  | -29.64 | 91.86       | 121.50   |
| 1   | B     | 14  | ARG  | CD-NE-CZ   | 29.44  | 165.61      | 124.40   |
| 1   | A     | 127 | CYS  | O-C-N      | 29.04  | 157.02      | 123.04   |
| 1   | A     | 39  | ASN  | OD1-CG-ND2 | -27.26 | 95.34       | 122.60   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | A     | 75  | LEU  | O-C-N       | 27.21  | 158.89      | 122.43   |
| 1   | A     | 14  | ARG  | NE-CZ-NH2   | -27.21 | 94.72       | 119.20   |
| 1   | B     | 68  | ARG  | CA-C-O      | -26.53 | 88.91       | 119.15   |
| 1   | A     | 21  | ARG  | CD-NE-CZ    | -26.43 | 87.40       | 124.40   |
| 1   | A     | 14  | ARG  | CD-NE-CZ    | -25.31 | 88.97       | 124.40   |
| 1   | A     | 112 | ARG  | NE-CZ-NH1   | 25.24  | 146.74      | 121.50   |
| 1   | B     | 114 | ARG  | CD-NE-CZ    | -25.12 | 89.23       | 124.40   |
| 1   | B     | 93  | ASN  | OD1-CG-ND2  | -24.63 | 97.97       | 122.60   |
| 1   | A     | 47  | THR  | CA-C-O      | -24.04 | 89.81       | 119.38   |
| 1   | A     | 39  | ASN  | CA-C-O      | 23.65  | 146.34      | 120.32   |
| 1   | B     | 21  | ARG  | NE-CZ-NH1   | 23.59  | 145.09      | 121.50   |
| 1   | A     | 121 | GLN  | CB-CG-CD    | -23.04 | 73.43       | 112.60   |
| 1   | A     | 87  | ASP  | CB-CG-OD2   | -22.85 | 65.83       | 118.40   |
| 1   | A     | 75  | LEU  | CA-C-O      | -22.82 | 91.32       | 119.38   |
| 1   | A     | 47  | THR  | O-C-N       | 22.67  | 152.81      | 122.43   |
| 1   | A     | 123 | TRP  | CE2-CD2-CE3 | 22.50  | 141.30      | 118.80   |
| 1   | B     | 5   | ARG  | O-C-N       | 22.36  | 145.10      | 122.07   |
| 1   | B     | 61  | ARG  | NH1-CZ-NH2  | -22.06 | 90.62       | 119.30   |
| 1   | A     | 114 | ARG  | NE-CZ-NH2   | -21.89 | 99.50       | 119.20   |
| 1   | A     | 112 | ARG  | NE-CZ-NH2   | -21.03 | 100.28      | 119.20   |
| 1   | B     | 59  | ASN  | OD1-CG-ND2  | 20.61  | 143.21      | 122.60   |
| 1   | A     | 62  | TRP  | CZ3-CH2-CZ2 | -20.36 | 95.04       | 121.50   |
| 1   | B     | 69  | THR  | CA-C-O      | 20.26  | 147.91      | 120.16   |
| 1   | A     | 14  | ARG  | NE-CZ-NH1   | 20.07  | 141.57      | 121.50   |
| 1   | B     | 15  | HIS  | ND1-CE1-NE2 | 20.05  | 128.45      | 108.40   |
| 1   | A     | 129 | LEU  | N-CA-CB     | -19.96 | 76.57       | 110.50   |
| 1   | B     | 63  | TRP  | CE3-CZ3-CH2 | -19.87 | 95.27       | 121.10   |
| 1   | A     | 68  | ARG  | CA-C-O      | -19.75 | 96.88       | 119.78   |
| 1   | A     | 15  | HIS  | ND1-CG-CD2  | 19.68  | 125.78      | 106.10   |
| 1   | B     | 128 | ARG  | CD-NE-CZ    | -19.54 | 97.04       | 124.40   |
| 1   | A     | 72  | SER  | CA-C-N      | 19.54  | 152.91      | 122.24   |
| 1   | A     | 72  | SER  | C-N-CA      | 19.54  | 152.91      | 122.24   |
| 1   | B     | 45  | ARG  | NE-CZ-NH1   | -19.51 | 101.99      | 121.50   |
| 1   | B     | 19  | ASN  | CB-CG-ND2   | 19.50  | 145.65      | 116.40   |
| 1   | B     | 47  | THR  | CA-CB-OG1   | -19.32 | 80.61       | 109.60   |
| 1   | A     | 46  | ASN  | OD1-CG-ND2  | -19.13 | 103.47      | 122.60   |
| 1   | B     | 65  | ASN  | OD1-CG-ND2  | -19.01 | 103.59      | 122.60   |
| 1   | A     | 87  | ASP  | OD1-CG-OD2  | 18.85  | 168.15      | 122.90   |
| 1   | A     | 72  | SER  | O-C-N       | -18.77 | 98.80       | 122.82   |
| 1   | A     | 70  | PRO  | N-CA-CB     | 18.64  | 119.90      | 103.31   |
| 1   | B     | 78  | ILE  | O-C-N       | -18.56 | 99.94       | 121.10   |
| 1   | B     | 114 | ARG  | NE-CZ-NH1   | 18.55  | 140.05      | 121.50   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | A     | 127 | CYS  | CA-C-O      | -18.49 | 99.61       | 120.69   |
| 1   | A     | 68  | ARG  | O-C-N       | 18.38  | 147.44      | 122.26   |
| 1   | B     | 20  | TYR  | CA-C-O      | 18.33  | 141.59      | 120.69   |
| 1   | A     | 108 | TRP  | CE2-CD2-CE3 | -18.05 | 100.75      | 118.80   |
| 1   | A     | 87  | ASP  | CA-CB-CG    | -17.98 | 94.62       | 112.60   |
| 1   | B     | 14  | ARG  | NH1-CZ-NH2  | -17.98 | 95.93       | 119.30   |
| 1   | A     | 13  | LYS  | CA-C-O      | 17.88  | 139.50      | 120.55   |
| 1   | A     | 112 | ARG  | O-C-N       | -17.87 | 103.66      | 122.07   |
| 1   | A     | 18  | ASP  | CA-CB-CG    | -17.86 | 94.74       | 112.60   |
| 1   | A     | 100 | SER  | O-C-N       | -17.85 | 100.39      | 122.35   |
| 1   | B     | 78  | ILE  | CA-C-N      | 17.48  | 137.24      | 119.76   |
| 1   | B     | 78  | ILE  | C-N-CA      | 17.48  | 137.24      | 119.76   |
| 1   | B     | 73  | ARG  | NE-CZ-NH1   | -17.44 | 104.06      | 121.50   |
| 1   | A     | 114 | ARG  | CA-C-O      | -17.26 | 100.50      | 118.97   |
| 1   | B     | 15  | HIS  | ND1-CG-CD2  | 17.21  | 123.31      | 106.10   |
| 1   | B     | 102 | GLY  | CA-C-O      | -17.20 | 99.42       | 119.03   |
| 1   | B     | 37  | ASN  | OD1-CG-ND2  | -17.13 | 105.47      | 122.60   |
| 1   | A     | 12  | MET  | O-C-N       | 17.07  | 140.22      | 122.12   |
| 1   | A     | 48  | ASP  | CA-CB-CG    | -16.96 | 95.64       | 112.60   |
| 1   | A     | 15  | HIS  | CG-CD2-NE2  | -16.94 | 90.26       | 107.20   |
| 1   | A     | 127 | CYS  | CA-C-N      | -16.84 | 95.39       | 122.34   |
| 1   | A     | 127 | CYS  | C-N-CA      | -16.84 | 95.39       | 122.34   |
| 1   | A     | 13  | LYS  | O-C-N       | -16.83 | 104.28      | 122.12   |
| 1   | B     | 42  | ALA  | CA-C-O      | -16.76 | 102.69      | 120.96   |
| 1   | A     | 122 | ALA  | O-C-N       | 16.76  | 141.82      | 122.22   |
| 1   | B     | 39  | ASN  | CA-CB-CG    | -16.57 | 96.03       | 112.60   |
| 1   | A     | 63  | TRP  | CG-CD1-NE1  | 16.48  | 131.63      | 110.20   |
| 1   | A     | 112 | ARG  | CG-CD-NE    | -16.48 | 75.75       | 112.00   |
| 1   | A     | 43  | THR  | O-C-N       | -16.36 | 103.30      | 123.27   |
| 1   | B     | 22  | GLY  | CA-C-O      | -16.30 | 100.92      | 119.02   |
| 1   | B     | 119 | ASP  | CA-CB-CG    | -16.26 | 96.34       | 112.60   |
| 1   | A     | 93  | ASN  | CA-CB-CG    | -16.24 | 96.36       | 112.60   |
| 1   | A     | 44  | ASN  | CB-CG-ND2   | 16.24  | 140.76      | 116.40   |
| 1   | B     | 86  | SER  | CA-CB-OG    | -16.18 | 78.73       | 111.10   |
| 1   | A     | 43  | THR  | CA-C-N      | 16.15  | 145.54      | 122.77   |
| 1   | A     | 43  | THR  | C-N-CA      | 16.15  | 145.54      | 122.77   |
| 1   | A     | 86  | SER  | N-CA-C      | -15.89 | 93.89       | 113.28   |
| 1   | B     | 68  | ARG  | CD-NE-CZ    | -15.88 | 102.17      | 124.40   |
| 1   | A     | 15  | HIS  | O-C-N       | 15.86  | 145.86      | 122.39   |
| 1   | B     | 70  | PRO  | N-CA-CB     | 15.82  | 118.06      | 103.34   |
| 1   | A     | 62  | TRP  | CB-CG-CD1   | -15.75 | 103.27      | 126.90   |
| 1   | A     | 44  | ASN  | CB-CG-OD1   | -15.74 | 89.32       | 120.80   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | A     | 45  | ARG  | NE-CZ-NH2   | -15.70 | 105.07      | 119.20   |
| 1   | B     | 121 | GLN  | CG-CD-NE2   | -15.65 | 92.93       | 116.40   |
| 1   | B     | 125 | ARG  | O-C-N       | 15.63  | 141.81      | 123.06   |
| 1   | A     | 73  | ARG  | NE-CZ-NH1   | 15.60  | 137.10      | 121.50   |
| 1   | A     | 108 | TRP  | CD2-CE3-CZ3 | 15.49  | 138.74      | 118.60   |
| 1   | B     | 123 | TRP  | CE2-CD2-CE3 | 15.44  | 134.24      | 118.80   |
| 1   | A     | 41  | GLN  | CG-CD-NE2   | 15.38  | 139.48      | 116.40   |
| 1   | A     | 48  | ASP  | CA-C-N      | -15.29 | 91.44       | 121.41   |
| 1   | A     | 48  | ASP  | C-N-CA      | -15.29 | 91.44       | 121.41   |
| 1   | B     | 123 | TRP  | CD2-CE2-CZ2 | -15.21 | 107.19      | 122.40   |
| 1   | A     | 123 | TRP  | CZ3-CH2-CZ2 | 15.15  | 141.20      | 121.50   |
| 1   | A     | 107 | ALA  | O-C-N       | 15.10  | 142.66      | 122.43   |
| 1   | B     | 41  | GLN  | OE1-CD-NE2  | -15.05 | 107.55      | 122.60   |
| 1   | B     | 105 | MET  | CA-C-O      | 14.97  | 138.73      | 119.12   |
| 1   | A     | 47  | THR  | OG1-CB-CG2  | -14.97 | 79.37       | 109.30   |
| 1   | A     | 15  | HIS  | CA-C-O      | -14.94 | 99.54       | 119.12   |
| 1   | B     | 15  | HIS  | CG-ND1-CE1  | -14.88 | 84.00       | 109.30   |
| 1   | A     | 15  | HIS  | CB-CG-CD2   | -14.87 | 111.87      | 131.20   |
| 1   | A     | 107 | ALA  | CA-C-O      | -14.87 | 101.10      | 119.38   |
| 1   | A     | 53  | TYR  | CA-C-O      | -14.85 | 104.19      | 120.38   |
| 1   | B     | 43  | THR  | OG1-CB-CG2  | -14.80 | 79.69       | 109.30   |
| 1   | B     | 112 | ARG  | NE-CZ-NH2   | -14.75 | 105.93      | 119.20   |
| 1   | A     | 2   | VAL  | CA-C-O      | -14.72 | 102.80      | 120.75   |
| 1   | B     | 44  | ASN  | CA-C-N      | -14.69 | 100.35      | 122.09   |
| 1   | B     | 44  | ASN  | C-N-CA      | -14.69 | 100.35      | 122.09   |
| 1   | A     | 118 | THR  | O-C-N       | 14.69  | 140.72      | 122.65   |
| 1   | A     | 38  | PHE  | CA-CB-CG    | 14.65  | 128.45      | 113.80   |
| 1   | A     | 61  | ARG  | CA-C-N      | -14.63 | 99.27       | 122.24   |
| 1   | A     | 61  | ARG  | C-N-CA      | -14.63 | 99.27       | 122.24   |
| 1   | B     | 68  | ARG  | N-CA-C      | -14.56 | 95.47       | 113.38   |
| 1   | B     | 50  | SER  | CA-C-O      | -14.54 | 103.42      | 121.89   |
| 1   | B     | 111 | TRP  | CE2-CD2-CG  | 14.51  | 124.61      | 107.20   |
| 1   | A     | 15  | HIS  | CE1-NE2-CD2 | 14.34  | 123.34      | 109.00   |
| 1   | A     | 63  | TRP  | CA-C-O      | 14.33  | 135.60      | 119.41   |
| 1   | B     | 65  | ASN  | CB-CG-OD1   | 14.32  | 149.44      | 120.80   |
| 1   | A     | 74  | ASN  | CA-C-O      | 14.30  | 138.76      | 122.03   |
| 1   | B     | 5   | ARG  | N-CA-C      | 14.29  | 126.36      | 111.07   |
| 1   | A     | 47  | THR  | N-CA-C      | -14.20 | 95.22       | 112.54   |
| 1   | A     | 123 | TRP  | CG-CD2-CE3  | -14.20 | 119.70      | 133.90   |
| 1   | A     | 62  | TRP  | CE3-CZ3-CH2 | 14.16  | 139.51      | 121.10   |
| 1   | A     | 19  | ASN  | CA-CB-CG    | -14.10 | 98.50       | 112.60   |
| 1   | A     | 59  | ASN  | OD1-CG-ND2  | -13.99 | 108.61      | 122.60   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | B     | 21  | ARG  | CB-CA-C     | -13.98 | 92.04       | 111.89   |
| 1   | B     | 45  | ARG  | CA-C-N      | 13.95  | 141.37      | 121.42   |
| 1   | B     | 45  | ARG  | C-N-CA      | 13.95  | 141.37      | 121.42   |
| 1   | A     | 78  | ILE  | CA-CB-CG2   | 13.92  | 134.17      | 110.50   |
| 1   | B     | 46  | ASN  | CA-C-O      | -13.92 | 105.19      | 121.05   |
| 1   | A     | 59  | ASN  | CA-C-O      | 13.91  | 136.92      | 120.92   |
| 1   | A     | 47  | THR  | CA-CB-CG2   | 13.89  | 134.12      | 110.50   |
| 1   | B     | 27  | ASN  | O-C-N       | 13.88  | 136.36      | 122.07   |
| 1   | A     | 51  | THR  | O-C-N       | 13.86  | 140.29      | 123.24   |
| 1   | A     | 78  | ILE  | N-CA-CB     | -13.86 | 91.81       | 111.21   |
| 1   | B     | 108 | TRP  | CG-CD1-NE1  | -13.84 | 92.21       | 110.20   |
| 1   | A     | 39  | ASN  | O-C-N       | -13.77 | 107.03      | 123.27   |
| 1   | A     | 66  | ASP  | O-C-N       | -13.74 | 105.44      | 122.35   |
| 1   | B     | 63  | TRP  | CE2-CD2-CE3 | 13.74  | 132.54      | 118.80   |
| 1   | A     | 38  | PHE  | CA-C-O      | -13.73 | 104.33      | 120.12   |
| 1   | A     | 112 | ARG  | CA-C-O      | 13.65  | 135.15      | 120.82   |
| 1   | B     | 21  | ARG  | NE-CZ-NH2   | -13.64 | 106.93      | 119.20   |
| 1   | A     | 41  | GLN  | OE1-CD-NE2  | -13.62 | 108.98      | 122.60   |
| 1   | A     | 69  | THR  | CA-C-O      | 13.58  | 132.59      | 119.55   |
| 1   | A     | 63  | TRP  | N-CA-C      | 13.51  | 129.89      | 113.41   |
| 1   | B     | 71  | GLY  | O-C-N       | 13.45  | 139.22      | 122.41   |
| 1   | A     | 39  | ASN  | CB-CG-ND2   | 13.41  | 136.51      | 116.40   |
| 1   | B     | 113 | ASN  | OD1-CG-ND2  | -13.40 | 109.20      | 122.60   |
| 1   | B     | 55  | ILE  | O-C-N       | 13.35  | 135.35      | 121.87   |
| 1   | A     | 62  | TRP  | CD1-CG-CD2  | 13.33  | 127.62      | 106.30   |
| 1   | A     | 108 | TRP  | CG-CD2-CE3  | 13.27  | 147.17      | 133.90   |
| 1   | A     | 83  | LEU  | CA-C-O      | -13.22 | 101.80      | 119.12   |
| 1   | A     | 78  | ILE  | O-C-N       | -13.22 | 106.03      | 121.10   |
| 1   | A     | 48  | ASP  | CB-CG-OD2   | -13.21 | 88.01       | 118.40   |
| 1   | B     | 18  | ASP  | CA-C-O      | -13.14 | 101.72      | 120.51   |
| 1   | B     | 21  | ARG  | CA-CB-CG    | -13.13 | 87.83       | 114.10   |
| 1   | B     | 10  | ALA  | CA-C-O      | -13.12 | 106.52      | 120.42   |
| 1   | A     | 63  | TRP  | CB-CG-CD1   | 13.10  | 146.55      | 126.90   |
| 1   | A     | 123 | TRP  | CG-CD1-NE1  | -13.08 | 93.20       | 110.20   |
| 1   | B     | 3   | PHE  | CA-C-O      | 13.04  | 137.10      | 121.72   |
| 1   | A     | 15  | HIS  | ND1-CE1-NE2 | -12.93 | 95.47       | 108.40   |
| 1   | B     | 70  | PRO  | CA-C-O      | 12.93  | 136.82      | 121.31   |
| 1   | A     | 53  | TYR  | O-C-N       | 12.92  | 138.54      | 123.29   |
| 1   | A     | 63  | TRP  | CH2-CZ2-CE2 | 12.91  | 134.29      | 117.50   |
| 1   | A     | 47  | THR  | CA-CB-OG1   | 12.87  | 128.90      | 109.60   |
| 1   | B     | 50  | SER  | CB-CA-C     | -12.79 | 88.33       | 110.45   |
| 1   | A     | 114 | ARG  | NE-CZ-NH1   | 12.66  | 134.16      | 121.50   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | B     | 95  | ALA  | O-C-N       | 12.65  | 135.53      | 122.12   |
| 1   | A     | 86  | SER  | CA-C-O      | -12.63 | 104.15      | 119.18   |
| 1   | A     | 21  | ARG  | CA-C-O      | -12.58 | 105.47      | 120.32   |
| 1   | B     | 14  | ARG  | N-CA-CB     | 12.55  | 128.57      | 110.12   |
| 1   | B     | 14  | ARG  | NE-CZ-NH2   | 12.53  | 130.48      | 119.20   |
| 1   | B     | 43  | THR  | O-C-N       | -12.51 | 108.20      | 123.33   |
| 1   | A     | 87  | ASP  | CB-CA-C     | -12.49 | 89.14       | 109.75   |
| 1   | B     | 123 | TRP  | CG-CD2-CE3  | -12.46 | 121.44      | 133.90   |
| 1   | A     | 45  | ARG  | CA-CB-CG    | -12.46 | 89.18       | 114.10   |
| 1   | B     | 87  | ASP  | CA-CB-CG    | 12.45  | 125.05      | 112.60   |
| 1   | B     | 29  | VAL  | O-C-N       | -12.43 | 109.03      | 121.83   |
| 1   | A     | 85  | SER  | CA-C-O      | -12.37 | 107.52      | 121.87   |
| 1   | A     | 61  | ARG  | CD-NE-CZ    | -12.35 | 107.11      | 124.40   |
| 1   | B     | 39  | ASN  | CB-CG-ND2   | -12.31 | 97.93       | 116.40   |
| 1   | B     | 12  | MET  | CA-C-O      | -12.29 | 105.83      | 119.97   |
| 1   | B     | 104 | GLY  | CA-C-O      | -12.28 | 106.21      | 121.56   |
| 1   | B     | 39  | ASN  | CB-CG-OD1   | 12.27  | 145.33      | 120.80   |
| 1   | B     | 125 | ARG  | NE-CZ-NH2   | 12.21  | 130.19      | 119.20   |
| 1   | A     | 108 | TRP  | NE1-CE2-CD2 | -12.18 | 91.56       | 107.40   |
| 1   | B     | 68  | ARG  | NE-CZ-NH2   | -12.12 | 108.29      | 119.20   |
| 1   | B     | 63  | TRP  | N-CA-C      | 12.07  | 128.23      | 113.38   |
| 1   | A     | 37  | ASN  | CA-CB-CG    | -12.06 | 100.54      | 112.60   |
| 1   | A     | 103 | ASN  | OD1-CG-ND2  | 12.02  | 134.62      | 122.60   |
| 1   | B     | 69  | THR  | CB-CA-C     | -12.00 | 86.52       | 110.17   |
| 1   | B     | 129 | LEU  | CB-CA-C     | 11.99  | 132.88      | 110.10   |
| 1   | A     | 74  | ASN  | O-C-N       | -11.94 | 107.64      | 122.57   |
| 1   | A     | 125 | ARG  | CA-C-O      | 11.92  | 134.18      | 121.55   |
| 1   | B     | 44  | ASN  | O-C-N       | 11.89  | 138.50      | 123.28   |
| 1   | A     | 1   | LYS  | O-C-N       | -11.89 | 103.98      | 123.00   |
| 1   | B     | 61  | ARG  | NE-CZ-NH1   | -11.88 | 109.62      | 121.50   |
| 1   | A     | 57  | GLN  | CG-CD-NE2   | 11.84  | 134.15      | 116.40   |
| 1   | B     | 128 | ARG  | CA-C-O      | -11.81 | 108.14      | 121.84   |
| 1   | A     | 86  | SER  | CA-CB-OG    | -11.78 | 87.54       | 111.10   |
| 1   | B     | 63  | TRP  | CZ3-CH2-CZ2 | 11.75  | 136.78      | 121.50   |
| 1   | B     | 88  | ILE  | CA-CB-CG2   | 11.69  | 130.38      | 110.50   |
| 1   | A     | 124 | ILE  | CB-CG1-CD1  | 11.66  | 138.28      | 113.80   |
| 1   | B     | 48  | ASP  | O-C-N       | -11.64 | 103.68      | 122.42   |
| 1   | B     | 67  | GLY  | N-CA-C      | -11.64 | 99.13       | 115.30   |
| 1   | A     | 118 | THR  | N-CA-CB     | 11.62  | 127.05      | 110.44   |
| 1   | B     | 125 | ARG  | NE-CZ-NH1   | -11.62 | 109.88      | 121.50   |
| 1   | B     | 41  | GLN  | CA-C-O      | 11.59  | 133.12      | 119.56   |
| 1   | A     | 47  | THR  | CA-C-N      | -11.58 | 103.42      | 122.65   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 47  | THR  | C-N-CA     | -11.58 | 103.42      | 122.65   |
| 1   | B     | 106 | ASN  | CB-CG-ND2  | -11.57 | 99.05       | 116.40   |
| 1   | A     | 31  | ALA  | O-C-N      | 11.56  | 133.97      | 122.07   |
| 1   | B     | 68  | ARG  | N-CA-CB    | -11.52 | 93.36       | 110.53   |
| 1   | A     | 65  | ASN  | CA-CB-CG   | -11.51 | 101.09      | 112.60   |
| 1   | B     | 118 | THR  | CA-C-O     | -11.48 | 108.13      | 121.68   |
| 1   | A     | 61  | ARG  | NE-CZ-NH1  | -11.41 | 110.09      | 121.50   |
| 1   | B     | 93  | ASN  | CB-CG-ND2  | 11.39  | 133.48      | 116.40   |
| 1   | B     | 3   | PHE  | O-C-N      | -11.31 | 110.27      | 122.94   |
| 1   | B     | 69  | THR  | OG1-CB-CG2 | -11.30 | 86.70       | 109.30   |
| 1   | B     | 68  | ARG  | CA-CB-CG   | 11.28  | 136.66      | 114.10   |
| 1   | B     | 99  | VAL  | CA-C-O     | -11.24 | 104.81      | 119.53   |
| 1   | B     | 17  | LEU  | CA-C-O     | -11.18 | 105.87      | 119.18   |
| 1   | A     | 128 | ARG  | NH1-CZ-NH2 | -11.15 | 104.80      | 119.30   |
| 1   | A     | 62  | TRP  | N-CA-CB    | -11.15 | 96.07       | 110.90   |
| 1   | B     | 85  | SER  | CA-C-O     | -11.12 | 109.44      | 121.56   |
| 1   | B     | 20  | TYR  | CA-C-N     | 11.07  | 138.09      | 122.36   |
| 1   | B     | 20  | TYR  | C-N-CA     | 11.07  | 138.09      | 122.36   |
| 1   | B     | 41  | GLN  | N-CA-C     | 11.07  | 126.54      | 112.92   |
| 1   | A     | 115 | CYS  | CA-C-O     | -11.06 | 106.48      | 119.64   |
| 1   | B     | 55  | ILE  | CA-C-O     | -11.06 | 108.74      | 120.57   |
| 1   | A     | 66  | ASP  | CA-C-N     | 11.05  | 143.07      | 121.41   |
| 1   | A     | 66  | ASP  | C-N-CA     | 11.05  | 143.07      | 121.41   |
| 1   | B     | 46  | ASN  | N-CA-CB    | 11.03  | 126.72      | 110.06   |
| 1   | A     | 84  | LEU  | O-C-N      | -10.96 | 108.87      | 122.35   |
| 1   | A     | 46  | ASN  | CA-C-O     | 10.95  | 135.02      | 121.66   |
| 1   | B     | 108 | TRP  | CD1-CG-CD2 | 10.88  | 123.72      | 106.30   |
| 1   | A     | 65  | ASN  | CB-CG-OD1  | 10.88  | 142.56      | 120.80   |
| 1   | A     | 65  | ASN  | CB-CG-ND2  | -10.86 | 100.11      | 116.40   |
| 1   | A     | 93  | ASN  | CB-CG-OD1  | -10.85 | 99.10       | 120.80   |
| 1   | A     | 62  | TRP  | CG-CD1-NE1 | -10.81 | 96.15       | 110.20   |
| 1   | A     | 75  | LEU  | CA-C-N     | -10.80 | 102.83      | 122.38   |
| 1   | A     | 75  | LEU  | C-N-CA     | -10.80 | 102.83      | 122.38   |
| 1   | A     | 11  | ALA  | O-C-N      | 10.76  | 133.16      | 122.07   |
| 1   | A     | 128 | ARG  | NE-CZ-NH1  | 10.76  | 132.26      | 121.50   |
| 1   | B     | 12  | MET  | O-C-N      | 10.75  | 135.49      | 122.27   |
| 1   | B     | 62  | TRP  | CA-C-N     | -10.72 | 103.72      | 122.26   |
| 1   | B     | 62  | TRP  | C-N-CA     | -10.72 | 103.72      | 122.26   |
| 1   | A     | 70  | PRO  | CA-C-O     | 10.71  | 133.55      | 121.34   |
| 1   | A     | 78  | ILE  | CA-CB-CG1  | -10.68 | 92.24       | 110.40   |
| 1   | B     | 74  | ASN  | CA-C-N     | 10.68  | 135.97      | 120.38   |
| 1   | B     | 74  | ASN  | C-N-CA     | 10.68  | 135.97      | 120.38   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | A     | 72  | SER  | CA-CB-OG    | -10.67 | 89.77       | 111.10   |
| 1   | A     | 78  | ILE  | CB-CA-C     | -10.65 | 91.97       | 111.36   |
| 1   | B     | 65  | ASN  | CA-CB-CG    | -10.65 | 101.95      | 112.60   |
| 1   | A     | 48  | ASP  | CB-CG-OD1   | 10.59  | 142.75      | 118.40   |
| 1   | B     | 86  | SER  | O-C-N       | -10.59 | 107.85      | 122.46   |
| 1   | B     | 23  | TYR  | CB-CG-CD1   | -10.56 | 104.95      | 120.80   |
| 1   | A     | 45  | ARG  | NE-CZ-NH1   | 10.56  | 132.06      | 121.50   |
| 1   | B     | 63  | TRP  | CD2-CE2-CZ2 | -10.54 | 111.86      | 122.40   |
| 1   | B     | 59  | ASN  | CA-CB-CG    | 10.53  | 123.13      | 112.60   |
| 1   | A     | 63  | TRP  | CD1-CG-CD2  | -10.51 | 89.49       | 106.30   |
| 1   | B     | 103 | ASN  | OD1-CG-ND2  | 10.51  | 133.11      | 122.60   |
| 1   | B     | 125 | ARG  | CA-C-N      | -10.51 | 104.33      | 122.09   |
| 1   | B     | 125 | ARG  | C-N-CA      | -10.51 | 104.33      | 122.09   |
| 1   | B     | 25  | LEU  | CA-C-N      | 10.49  | 131.78      | 120.03   |
| 1   | B     | 25  | LEU  | C-N-CA      | 10.49  | 131.78      | 120.03   |
| 1   | B     | 23  | TYR  | CD1-CG-CD2  | 10.48  | 133.83      | 118.10   |
| 1   | B     | 125 | ARG  | CA-C-O      | -10.45 | 109.56      | 120.96   |
| 1   | A     | 124 | ILE  | CA-C-N      | -10.45 | 104.97      | 120.75   |
| 1   | A     | 124 | ILE  | C-N-CA      | -10.45 | 104.97      | 120.75   |
| 1   | A     | 62  | TRP  | CH2-CZ2-CE2 | 10.42  | 131.05      | 117.50   |
| 1   | A     | 12  | MET  | CA-C-O      | -10.39 | 109.54      | 120.55   |
| 1   | A     | 21  | ARG  | N-CA-C      | -10.38 | 100.19      | 112.86   |
| 1   | B     | 96  | LYS  | CA-C-O      | -10.38 | 106.62      | 119.38   |
| 1   | A     | 93  | ASN  | OD1-CG-ND2  | 10.37  | 132.97      | 122.60   |
| 1   | A     | 14  | ARG  | CA-C-O      | 10.34  | 131.79      | 120.63   |
| 1   | B     | 114 | ARG  | NH1-CZ-NH2  | 10.30  | 132.69      | 119.30   |
| 1   | A     | 1   | LYS  | CA-C-N      | 10.29  | 135.40      | 122.43   |
| 1   | A     | 1   | LYS  | C-N-CA      | 10.29  | 135.40      | 122.43   |
| 1   | A     | 108 | TRP  | O-C-N       | -10.29 | 111.49      | 123.22   |
| 1   | B     | 5   | ARG  | N-CA-CB     | -10.28 | 95.10       | 110.01   |
| 1   | A     | 108 | TRP  | CE3-CZ3-CH2 | -10.28 | 107.74      | 121.10   |
| 1   | A     | 41  | GLN  | O-C-N       | -10.24 | 108.24      | 122.37   |
| 1   | A     | 12  | MET  | CA-C-N      | -10.23 | 106.58      | 120.28   |
| 1   | A     | 12  | MET  | C-N-CA      | -10.23 | 106.58      | 120.28   |
| 1   | A     | 21  | ARG  | NE-CZ-NH1   | 10.19  | 131.69      | 121.50   |
| 1   | A     | 4   | GLY  | CA-C-O      | -10.19 | 109.82      | 121.94   |
| 1   | A     | 21  | ARG  | CB-CA-C     | 10.19  | 127.97      | 111.36   |
| 1   | A     | 51  | THR  | CA-CB-CG2   | 10.17  | 127.78      | 110.50   |
| 1   | B     | 77  | ASN  | CA-C-O      | -10.16 | 109.77      | 121.65   |
| 1   | A     | 128 | ARG  | CB-CA-C     | 10.14  | 128.72      | 111.68   |
| 1   | A     | 129 | LEU  | CD1-CG-CD2  | -10.12 | 88.55       | 110.80   |
| 1   | A     | 109 | VAL  | O-C-N       | -10.09 | 111.44      | 121.83   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | A     | 23  | TYR  | CD1-CG-CD2  | 10.08  | 133.22      | 118.10   |
| 1   | A     | 34  | PHE  | CB-CG-CD2   | 10.07  | 137.82      | 120.70   |
| 1   | A     | 63  | TRP  | CA-C-N      | -10.07 | 105.90      | 122.21   |
| 1   | A     | 63  | TRP  | C-N-CA      | -10.07 | 105.90      | 122.21   |
| 1   | B     | 111 | TRP  | CH2-CZ2-CE2 | 10.07  | 130.59      | 117.50   |
| 1   | B     | 112 | ARG  | NE-CZ-NH1   | 10.05  | 131.55      | 121.50   |
| 1   | B     | 108 | TRP  | CG-CD2-CE3  | 10.04  | 143.94      | 133.90   |
| 1   | A     | 33  | LYS  | O-C-N       | 10.04  | 132.41      | 122.07   |
| 1   | B     | 14  | ARG  | N-CA-C      | -10.03 | 100.35      | 111.28   |
| 1   | A     | 18  | ASP  | CB-CG-OD1   | 10.00  | 141.40      | 118.40   |
| 1   | A     | 125 | ARG  | CA-CB-CG    | 9.98   | 134.05      | 114.10   |
| 1   | B     | 61  | ARG  | CA-C-O      | -9.97  | 110.35      | 120.82   |
| 1   | B     | 67  | GLY  | CA-C-O      | -9.96  | 106.98      | 119.13   |
| 1   | B     | 21  | ARG  | N-CA-C      | -9.92  | 97.70       | 111.39   |
| 1   | A     | 63  | TRP  | CD2-CE2-CZ2 | -9.88  | 112.52      | 122.40   |
| 1   | B     | 43  | THR  | N-CA-CB     | 9.87   | 128.79      | 111.13   |
| 1   | B     | 23  | TYR  | CG-CD1-CE1  | -9.86  | 106.41      | 121.20   |
| 1   | A     | 2   | VAL  | N-CA-CB     | 9.85   | 123.43      | 111.31   |
| 1   | A     | 53  | TYR  | N-CA-C      | 9.82   | 124.88      | 109.07   |
| 1   | B     | 95  | ALA  | CA-C-N      | -9.81  | 104.33      | 120.72   |
| 1   | B     | 95  | ALA  | C-N-CA      | -9.81  | 104.33      | 120.72   |
| 1   | A     | 125 | ARG  | O-C-N       | -9.81  | 110.75      | 122.81   |
| 1   | A     | 121 | GLN  | CA-C-O      | 9.80   | 131.35      | 119.49   |
| 1   | A     | 11  | ALA  | CA-C-O      | -9.79  | 110.53      | 120.82   |
| 1   | A     | 35  | GLU  | CA-C-O      | 9.72   | 131.03      | 120.24   |
| 1   | A     | 45  | ARG  | CB-CG-CD    | -9.71  | 88.96       | 111.30   |
| 1   | B     | 62  | TRP  | CZ3-CH2-CZ2 | 9.69   | 134.10      | 121.50   |
| 1   | B     | 23  | TYR  | CA-C-O      | 9.68   | 130.93      | 120.38   |
| 1   | A     | 84  | LEU  | N-CA-C      | -9.66  | 101.70      | 112.72   |
| 1   | A     | 66  | ASP  | CA-CB-CG    | 9.64   | 122.24      | 112.60   |
| 1   | B     | 31  | ALA  | O-C-N       | -9.63  | 112.15      | 122.07   |
| 1   | B     | 3   | PHE  | CE1-CZ-CE2  | 9.63   | 137.33      | 120.00   |
| 1   | B     | 15  | HIS  | CG-CD2-NE2  | -9.63  | 97.57       | 107.20   |
| 1   | B     | 8   | LEU  | CA-C-N      | -9.60  | 107.23      | 120.38   |
| 1   | B     | 8   | LEU  | C-N-CA      | -9.60  | 107.23      | 120.38   |
| 1   | A     | 61  | ARG  | NH1-CZ-NH2  | 9.59   | 131.76      | 119.30   |
| 1   | B     | 10  | ALA  | N-CA-C      | -9.57  | 100.93      | 111.36   |
| 1   | A     | 107 | ALA  | CA-C-N      | -9.56  | 110.05      | 122.77   |
| 1   | A     | 107 | ALA  | C-N-CA      | -9.56  | 110.05      | 122.77   |
| 1   | A     | 100 | SER  | CA-C-N      | 9.56   | 138.12      | 122.73   |
| 1   | A     | 100 | SER  | C-N-CA      | 9.56   | 138.12      | 122.73   |
| 1   | B     | 46  | ASN  | N-CA-C      | 9.56   | 125.30      | 110.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 123 | TRP  | CH2-CZ2-CE2 | -9.49 | 105.16      | 117.50   |
| 1   | A     | 67  | GLY  | CA-C-O      | -9.46 | 104.11      | 120.57   |
| 1   | B     | 61  | ARG  | O-C-N       | 9.46  | 131.81      | 122.07   |
| 1   | B     | 14  | ARG  | CG-CD-NE    | 9.45  | 132.80      | 112.00   |
| 1   | B     | 102 | GLY  | O-C-N       | 9.43  | 133.17      | 122.42   |
| 1   | A     | 21  | ARG  | CB-CG-CD    | 9.42  | 132.96      | 111.30   |
| 1   | A     | 97  | LYS  | CG-CD-CE    | -9.40 | 89.69       | 111.30   |
| 1   | A     | 37  | ASN  | OD1-CG-ND2  | -9.37 | 113.23      | 122.60   |
| 1   | A     | 3   | PHE  | CD1-CG-CD2  | -9.35 | 104.57      | 118.60   |
| 1   | A     | 71  | GLY  | CA-C-O      | -9.34 | 107.83      | 119.69   |
| 1   | A     | 1   | LYS  | CA-C-O      | 9.34  | 136.67      | 120.80   |
| 1   | B     | 15  | HIS  | CA-CB-CG    | -9.33 | 104.47      | 113.80   |
| 1   | A     | 112 | ARG  | CD-NE-CZ    | -9.33 | 111.34      | 124.40   |
| 1   | A     | 73  | ARG  | NH1-CZ-NH2  | -9.32 | 107.18      | 119.30   |
| 1   | B     | 66  | ASP  | OD1-CG-OD2  | -9.32 | 100.53      | 122.90   |
| 1   | A     | 92  | VAL  | CA-C-O      | 9.30  | 131.02      | 121.17   |
| 1   | B     | 129 | LEU  | CB-CG-CD2   | 9.29  | 138.58      | 110.70   |
| 1   | A     | 44  | ASN  | CB-CA-C     | 9.28  | 124.99      | 110.14   |
| 1   | A     | 33  | LYS  | CG-CD-CE    | -9.28 | 89.96       | 111.30   |
| 1   | B     | 89  | THR  | CA-C-O      | 9.28  | 131.31      | 120.92   |
| 1   | A     | 123 | TRP  | CE3-CZ3-CH2 | -9.27 | 109.05      | 121.10   |
| 1   | B     | 122 | ALA  | CA-C-O      | 9.26  | 130.56      | 120.10   |
| 1   | B     | 61  | ARG  | CG-CD-NE    | -9.23 | 91.70       | 112.00   |
| 1   | B     | 49  | GLY  | CA-C-O      | -9.18 | 109.09      | 119.10   |
| 1   | A     | 121 | GLN  | CG-CD-NE2   | -9.15 | 102.68      | 116.40   |
| 1   | B     | 13  | LYS  | CA-C-N      | 9.14  | 132.53      | 120.28   |
| 1   | B     | 13  | LYS  | C-N-CA      | 9.14  | 132.53      | 120.28   |
| 1   | B     | 45  | ARG  | CA-C-O      | -9.14 | 110.41      | 120.92   |
| 1   | B     | 66  | ASP  | CA-C-N      | 9.11  | 139.48      | 121.53   |
| 1   | B     | 66  | ASP  | C-N-CA      | 9.11  | 139.48      | 121.53   |
| 1   | B     | 52  | ASP  | CB-CG-OD2   | -9.11 | 97.45       | 118.40   |
| 1   | B     | 37  | ASN  | CA-C-O      | -9.09 | 110.46      | 121.28   |
| 1   | B     | 111 | TRP  | CA-C-O      | 9.09  | 130.37      | 120.82   |
| 1   | A     | 32  | ALA  | CA-C-O      | -9.07 | 110.80      | 120.42   |
| 1   | B     | 62  | TRP  | CG-CD1-NE1  | -9.05 | 98.43       | 110.20   |
| 1   | B     | 50  | SER  | N-CA-C      | 9.04  | 123.84      | 110.46   |
| 1   | B     | 68  | ARG  | CB-CG-CD    | 9.03  | 132.06      | 111.30   |
| 1   | B     | 21  | ARG  | CB-CG-CD    | 9.02  | 132.04      | 111.30   |
| 1   | B     | 110 | ALA  | CA-C-N      | 9.00  | 132.14      | 120.44   |
| 1   | B     | 110 | ALA  | C-N-CA      | 9.00  | 132.14      | 120.44   |
| 1   | B     | 63  | TRP  | CG-CD2-CE3  | -8.99 | 124.91      | 133.90   |
| 1   | B     | 3   | PHE  | CB-CA-C     | -8.98 | 94.11       | 109.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 51  | THR  | CA-CB-OG1   | -8.92 | 96.22       | 109.60   |
| 1   | A     | 101 | ASP  | CA-C-O      | 8.92  | 130.39      | 119.78   |
| 1   | A     | 72  | SER  | N-CA-CB     | -8.88 | 95.71       | 109.92   |
| 1   | B     | 43  | THR  | CA-CB-CG2   | -8.88 | 95.41       | 110.50   |
| 1   | B     | 62  | TRP  | CD1-CG-CD2  | 8.87  | 120.49      | 106.30   |
| 1   | A     | 122 | ALA  | CB-CA-C     | -8.87 | 94.23       | 110.63   |
| 1   | A     | 123 | TRP  | CD1-NE1-CE2 | 8.86  | 124.84      | 108.90   |
| 1   | B     | 125 | ARG  | CD-NE-CZ    | 8.84  | 136.77      | 124.40   |
| 1   | B     | 99  | VAL  | O-C-N       | 8.83  | 134.32      | 122.31   |
| 1   | B     | 116 | LYS  | CA-C-O      | 8.83  | 130.59      | 120.96   |
| 1   | B     | 108 | TRP  | CE2-CD2-CG  | -8.79 | 96.65       | 107.20   |
| 1   | A     | 3   | PHE  | CG-CD2-CE2  | 8.77  | 135.61      | 120.70   |
| 1   | B     | 76  | CYS  | CA-C-O      | 8.77  | 129.89      | 119.28   |
| 1   | A     | 28  | TRP  | CG-CD1-NE1  | 8.77  | 121.60      | 110.20   |
| 1   | A     | 44  | ASN  | O-C-N       | -8.77 | 113.01      | 123.27   |
| 1   | B     | 75  | LEU  | N-CA-CB     | 8.77  | 123.99      | 110.14   |
| 1   | B     | 11  | ALA  | O-C-N       | 8.75  | 131.39      | 122.12   |
| 1   | B     | 111 | TRP  | CG-CD2-CE3  | -8.75 | 125.15      | 133.90   |
| 1   | A     | 122 | ALA  | CA-C-N      | -8.74 | 104.45      | 121.94   |
| 1   | A     | 122 | ALA  | C-N-CA      | -8.74 | 104.45      | 121.94   |
| 1   | A     | 65  | ASN  | CA-C-N      | 8.73  | 136.14      | 122.26   |
| 1   | A     | 65  | ASN  | C-N-CA      | 8.73  | 136.14      | 122.26   |
| 1   | A     | 22  | GLY  | N-CA-C      | 8.72  | 127.35      | 115.32   |
| 1   | B     | 20  | TYR  | O-C-N       | -8.71 | 112.84      | 123.04   |
| 1   | A     | 78  | ILE  | CA-C-O      | 8.71  | 131.61      | 119.95   |
| 1   | A     | 63  | TRP  | NE1-CE2-CZ2 | 8.70  | 143.15      | 130.10   |
| 1   | A     | 122 | ALA  | CA-C-O      | -8.70 | 110.27      | 120.10   |
| 1   | A     | 117 | GLY  | CA-C-O      | 8.67  | 128.55      | 119.10   |
| 1   | B     | 127 | CYS  | CA-C-O      | 8.66  | 129.93      | 119.97   |
| 1   | A     | 40  | THR  | CA-CB-CG2   | 8.65  | 125.21      | 110.50   |
| 1   | B     | 9   | ALA  | CA-C-O      | 8.60  | 129.92      | 120.63   |
| 1   | A     | 74  | ASN  | CB-CG-ND2   | -8.58 | 103.53      | 116.40   |
| 1   | B     | 111 | TRP  | CE2-CD2-CE3 | -8.58 | 110.22      | 118.80   |
| 1   | B     | 121 | GLN  | O-C-N       | -8.56 | 110.95      | 122.43   |
| 1   | A     | 35  | GLU  | O-C-N       | -8.56 | 111.11      | 122.23   |
| 1   | B     | 3   | PHE  | CZ-CE2-CD2  | -8.54 | 104.62      | 120.00   |
| 1   | B     | 62  | TRP  | O-C-N       | 8.53  | 133.79      | 122.36   |
| 1   | B     | 62  | TRP  | CE3-CZ3-CH2 | -8.53 | 110.01      | 121.10   |
| 1   | B     | 43  | THR  | CB-CA-C     | -8.51 | 92.11       | 109.38   |
| 1   | B     | 59  | ASN  | CB-CG-ND2   | -8.47 | 103.69      | 116.40   |
| 1   | A     | 36  | SER  | N-CA-C      | 8.44  | 127.17      | 114.09   |
| 1   | B     | 18  | ASP  | CB-CG-OD2   | -8.43 | 99.01       | 118.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 43  | THR  | CA-C-N      | 8.41  | 134.83      | 122.39   |
| 1   | B     | 43  | THR  | C-N-CA      | 8.41  | 134.83      | 122.39   |
| 1   | A     | 77  | ASN  | O-C-N       | 8.40  | 133.67      | 122.41   |
| 1   | B     | 47  | THR  | CA-C-N      | -8.40 | 105.50      | 122.31   |
| 1   | B     | 47  | THR  | C-N-CA      | -8.40 | 105.50      | 122.31   |
| 1   | B     | 53  | TYR  | CD1-CG-CD2  | -8.40 | 105.50      | 118.10   |
| 1   | B     | 86  | SER  | CA-C-N      | 8.40  | 133.65      | 122.30   |
| 1   | B     | 86  | SER  | C-N-CA      | 8.40  | 133.65      | 122.30   |
| 1   | B     | 23  | TYR  | N-CA-CB     | -8.40 | 97.39       | 110.57   |
| 1   | B     | 70  | PRO  | N-CA-C      | -8.39 | 98.01       | 111.19   |
| 1   | A     | 99  | VAL  | O-C-N       | 8.38  | 133.03      | 122.05   |
| 1   | B     | 110 | ALA  | N-CA-C      | -8.38 | 101.67      | 112.23   |
| 1   | A     | 91  | SER  | N-CA-CB     | -8.38 | 97.81       | 110.12   |
| 1   | B     | 107 | ALA  | CA-C-N      | -8.38 | 111.22      | 123.11   |
| 1   | B     | 107 | ALA  | C-N-CA      | -8.38 | 111.22      | 123.11   |
| 1   | B     | 12  | MET  | CA-C-N      | -8.33 | 107.65      | 120.31   |
| 1   | B     | 12  | MET  | C-N-CA      | -8.33 | 107.65      | 120.31   |
| 1   | B     | 73  | ARG  | NH1-CZ-NH2  | -8.32 | 108.48      | 119.30   |
| 1   | B     | 14  | ARG  | O-C-N       | -8.31 | 113.31      | 122.12   |
| 1   | A     | 123 | TRP  | CD2-CE3-CZ3 | -8.30 | 107.81      | 118.60   |
| 1   | B     | 77  | ASN  | OD1-CG-ND2  | 8.29  | 130.89      | 122.60   |
| 1   | A     | 124 | ILE  | CA-CB-CG1   | 8.28  | 124.48      | 110.40   |
| 1   | B     | 3   | PHE  | CD1-CE1-CZ  | -8.27 | 105.11      | 120.00   |
| 1   | B     | 80  | CYS  | CA-C-O      | 8.27  | 129.44      | 120.10   |
| 1   | B     | 80  | CYS  | O-C-N       | -8.25 | 112.57      | 122.22   |
| 1   | A     | 46  | ASN  | N-CA-C      | -8.25 | 97.63       | 110.42   |
| 1   | A     | 68  | ARG  | NH1-CZ-NH2  | -8.25 | 108.58      | 119.30   |
| 1   | B     | 28  | TRP  | CG-CD1-NE1  | -8.24 | 99.48       | 110.20   |
| 1   | B     | 128 | ARG  | CB-CA-C     | 8.23  | 123.58      | 111.89   |
| 1   | A     | 122 | ALA  | N-CA-CB     | 8.22  | 122.88      | 110.22   |
| 1   | B     | 76  | CYS  | N-CA-C      | 8.22  | 123.35      | 113.16   |
| 1   | A     | 43  | THR  | CA-CB-OG1   | -8.22 | 97.28       | 109.60   |
| 1   | B     | 7   | GLU  | O-C-N       | -8.21 | 112.80      | 122.15   |
| 1   | B     | 33  | LYS  | N-CA-C      | 8.20  | 119.85      | 111.07   |
| 1   | A     | 83  | LEU  | N-CA-C      | -8.20 | 103.28      | 113.20   |
| 1   | A     | 97  | LYS  | CA-C-O      | -8.19 | 112.26      | 120.70   |
| 1   | B     | 53  | TYR  | CB-CG-CD1   | 8.16  | 133.04      | 120.80   |
| 1   | B     | 46  | ASN  | CA-CB-CG    | -8.15 | 104.45      | 112.60   |
| 1   | B     | 21  | ARG  | CG-CD-NE    | 8.15  | 129.93      | 112.00   |
| 1   | A     | 77  | ASN  | CA-C-O      | -8.14 | 111.60      | 121.28   |
| 1   | B     | 25  | LEU  | N-CA-C      | 8.10  | 124.73      | 111.37   |
| 1   | B     | 35  | GLU  | OE1-CD-OE2  | -8.09 | 103.49      | 122.90   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 77  | ASN  | CA-C-N      | -8.08 | 107.19      | 122.13   |
| 1   | A     | 77  | ASN  | C-N-CA      | -8.08 | 107.19      | 122.13   |
| 1   | A     | 94  | CYS  | N-CA-C      | -8.07 | 102.56      | 111.36   |
| 1   | A     | 46  | ASN  | CB-CG-ND2   | 8.06  | 128.49      | 116.40   |
| 1   | A     | 40  | THR  | N-CA-C      | 8.06  | 122.21      | 112.38   |
| 1   | A     | 5   | ARG  | NH1-CZ-NH2  | -8.05 | 108.83      | 119.30   |
| 1   | B     | 24  | SER  | O-C-N       | 8.05  | 131.97      | 122.79   |
| 1   | B     | 5   | ARG  | CA-C-N      | -8.04 | 107.01      | 120.68   |
| 1   | B     | 5   | ARG  | C-N-CA      | -8.04 | 107.01      | 120.68   |
| 1   | B     | 117 | GLY  | CA-C-O      | 8.02  | 128.04      | 119.06   |
| 1   | B     | 53  | TYR  | CZ-CE2-CD2  | -8.01 | 105.19      | 119.60   |
| 1   | A     | 108 | TRP  | NE1-CE2-CZ2 | 8.00  | 142.11      | 130.10   |
| 1   | A     | 118 | THR  | CA-CB-OG1   | -8.00 | 97.60       | 109.60   |
| 1   | B     | 29  | VAL  | CA-C-N      | 7.98  | 131.32      | 120.54   |
| 1   | B     | 29  | VAL  | C-N-CA      | 7.98  | 131.32      | 120.54   |
| 1   | A     | 26  | GLY  | CA-C-O      | -7.97 | 111.79      | 120.40   |
| 1   | A     | 22  | GLY  | CA-C-O      | 7.94  | 127.95      | 119.06   |
| 1   | B     | 8   | LEU  | O-C-N       | 7.93  | 130.24      | 122.07   |
| 1   | A     | 92  | VAL  | N-CA-C      | 7.92  | 118.02      | 110.42   |
| 1   | A     | 57  | GLN  | CG-CD-OE1   | -7.91 | 104.97      | 120.80   |
| 1   | A     | 34  | PHE  | CD1-CG-CD2  | -7.91 | 106.74      | 118.60   |
| 1   | A     | 51  | THR  | CA-C-N      | -7.90 | 111.47      | 122.93   |
| 1   | A     | 51  | THR  | C-N-CA      | -7.90 | 111.47      | 122.93   |
| 1   | A     | 23  | TYR  | CB-CG-CD2   | -7.89 | 108.96      | 120.80   |
| 1   | B     | 45  | ARG  | NH1-CZ-NH2  | -7.88 | 109.05      | 119.30   |
| 1   | A     | 93  | ASN  | N-CA-CB     | 7.85  | 121.40      | 110.01   |
| 1   | A     | 111 | TRP  | CE2-CD2-CE3 | -7.85 | 110.95      | 118.80   |
| 1   | A     | 41  | GLN  | CA-C-N      | 7.84  | 131.87      | 120.82   |
| 1   | A     | 41  | GLN  | C-N-CA      | 7.84  | 131.87      | 120.82   |
| 1   | B     | 60  | SER  | N-CA-CB     | -7.82 | 97.27       | 110.41   |
| 1   | A     | 32  | ALA  | O-C-N       | 7.80  | 131.04      | 122.15   |
| 1   | A     | 71  | GLY  | O-C-N       | 7.80  | 131.20      | 122.31   |
| 1   | B     | 58  | ILE  | CA-C-O      | 7.76  | 129.48      | 120.71   |
| 1   | B     | 106 | ASN  | CA-CB-CG    | -7.75 | 104.85      | 112.60   |
| 1   | B     | 27  | ASN  | CA-C-N      | -7.75 | 109.29      | 120.29   |
| 1   | B     | 27  | ASN  | C-N-CA      | -7.75 | 109.29      | 120.29   |
| 1   | B     | 37  | ASN  | N-CA-C      | -7.73 | 101.30      | 111.74   |
| 1   | B     | 66  | ASP  | CB-CA-C     | 7.72  | 122.98      | 110.09   |
| 1   | A     | 118 | THR  | CA-C-O      | -7.71 | 113.08      | 121.94   |
| 1   | B     | 35  | GLU  | N-CA-C      | -7.68 | 102.25      | 111.69   |
| 1   | B     | 73  | ARG  | CD-NE-CZ    | 7.66  | 135.13      | 124.40   |
| 1   | B     | 63  | TRP  | CG-CD1-NE1  | -7.66 | 100.25      | 110.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 23  | TYR  | CA-C-O      | 7.63  | 128.48      | 120.54   |
| 1   | A     | 61  | ARG  | O-C-N       | 7.62  | 132.13      | 122.23   |
| 1   | A     | 93  | ASN  | CB-CG-ND2   | 7.62  | 127.83      | 116.40   |
| 1   | A     | 108 | TRP  | CA-C-O      | 7.62  | 128.51      | 120.36   |
| 1   | B     | 46  | ASN  | CB-CG-ND2   | -7.61 | 104.98      | 116.40   |
| 1   | B     | 32  | ALA  | CA-C-N      | -7.60 | 110.56      | 120.44   |
| 1   | B     | 32  | ALA  | C-N-CA      | -7.60 | 110.56      | 120.44   |
| 1   | A     | 30  | CYS  | N-CA-CB     | -7.60 | 98.95       | 110.12   |
| 1   | A     | 3   | PHE  | CA-C-O      | 7.59  | 130.68      | 121.72   |
| 1   | B     | 98  | ILE  | N-CA-C      | 7.59  | 117.71      | 110.42   |
| 1   | B     | 110 | ALA  | CA-C-O      | -7.58 | 110.84      | 119.79   |
| 1   | B     | 8   | LEU  | CA-C-O      | 7.55  | 128.75      | 120.82   |
| 1   | B     | 128 | ARG  | CG-CD-NE    | -7.55 | 95.39       | 112.00   |
| 1   | B     | 69  | THR  | N-CA-CB     | 7.54  | 123.79      | 110.37   |
| 1   | A     | 100 | SER  | N-CA-C      | -7.54 | 104.13      | 112.72   |
| 1   | B     | 121 | GLN  | CG-CD-OE1   | -7.54 | 105.73      | 120.80   |
| 1   | A     | 105 | MET  | N-CA-C      | 7.53  | 122.32      | 113.20   |
| 1   | B     | 46  | ASN  | CB-CA-C     | -7.53 | 96.80       | 109.53   |
| 1   | A     | 23  | TYR  | O-C-N       | -7.53 | 114.09      | 123.05   |
| 1   | B     | 20  | TYR  | CB-CG-CD1   | -7.52 | 109.52      | 120.80   |
| 1   | B     | 89  | THR  | N-CA-C      | 7.51  | 123.77      | 111.37   |
| 1   | B     | 15  | HIS  | CB-CG-CD2   | -7.51 | 121.44      | 131.20   |
| 1   | B     | 36  | SER  | N-CA-CB     | -7.50 | 100.15      | 110.95   |
| 1   | A     | 34  | PHE  | CE1-CZ-CE2  | -7.50 | 106.51      | 120.00   |
| 1   | B     | 56  | LEU  | CA-C-O      | 7.49  | 128.32      | 119.48   |
| 1   | B     | 108 | TRP  | CB-CG-CD1   | -7.49 | 115.66      | 126.90   |
| 1   | A     | 128 | ARG  | O-C-N       | 7.49  | 132.17      | 122.43   |
| 1   | B     | 88  | ILE  | CA-C-O      | -7.45 | 109.93      | 119.39   |
| 1   | A     | 5   | ARG  | NE-CZ-NH1   | 7.44  | 128.94      | 121.50   |
| 1   | B     | 62  | TRP  | NE1-CE2-CD2 | -7.44 | 97.73       | 107.40   |
| 1   | B     | 116 | LYS  | CA-C-N      | -7.43 | 108.60      | 122.05   |
| 1   | B     | 116 | LYS  | C-N-CA      | -7.43 | 108.60      | 122.05   |
| 1   | A     | 39  | ASN  | CB-CA-C     | -7.40 | 98.06       | 110.19   |
| 1   | A     | 103 | ASN  | CB-CG-ND2   | -7.40 | 105.31      | 116.40   |
| 1   | B     | 119 | ASP  | CB-CG-OD2   | -7.39 | 101.41      | 118.40   |
| 1   | B     | 80  | CYS  | CA-CB-SG    | 7.37  | 131.34      | 114.40   |
| 1   | B     | 121 | GLN  | N-CA-C      | -7.36 | 103.56      | 112.54   |
| 1   | B     | 80  | CYS  | N-CA-CB     | -7.34 | 98.91       | 110.22   |
| 1   | A     | 3   | PHE  | CG-CD1-CE1  | 7.34  | 133.18      | 120.70   |
| 1   | A     | 66  | ASP  | CB-CA-C     | 7.34  | 121.88      | 109.55   |
| 1   | B     | 24  | SER  | N-CA-CB     | -7.34 | 99.87       | 110.36   |
| 1   | A     | 7   | GLU  | O-C-N       | -7.33 | 114.18      | 122.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 44  | ASN  | OD1-CG-ND2  | 7.32  | 129.92      | 122.60   |
| 1   | A     | 114 | ARG  | O-C-N       | 7.32  | 131.33      | 122.48   |
| 1   | B     | 65  | ASN  | O-C-N       | 7.31  | 131.56      | 123.22   |
| 1   | B     | 13  | LYS  | N-CA-CB     | -7.31 | 98.94       | 110.28   |
| 1   | B     | 129 | LEU  | CD1-CG-CD2  | -7.31 | 94.72       | 110.80   |
| 1   | A     | 74  | ASN  | CA-CB-CG    | -7.30 | 105.30      | 112.60   |
| 1   | A     | 25  | LEU  | CA-C-N      | -7.26 | 111.06      | 120.14   |
| 1   | A     | 25  | LEU  | C-N-CA      | -7.26 | 111.06      | 120.14   |
| 1   | A     | 70  | PRO  | CA-N-CD     | -7.25 | 101.85      | 112.00   |
| 1   | B     | 114 | ARG  | CA-C-O      | -7.24 | 110.93      | 118.90   |
| 1   | B     | 124 | ILE  | CA-C-N      | -7.24 | 110.69      | 121.05   |
| 1   | B     | 124 | ILE  | C-N-CA      | -7.24 | 110.69      | 121.05   |
| 1   | A     | 44  | ASN  | CA-C-O      | 7.24  | 127.91      | 120.24   |
| 1   | A     | 89  | THR  | N-CA-C      | 7.22  | 119.16      | 111.28   |
| 1   | B     | 123 | TRP  | NE1-CE2-CD2 | 7.22  | 116.79      | 107.40   |
| 1   | B     | 83  | LEU  | CA-C-O      | -7.21 | 109.68      | 119.12   |
| 1   | A     | 76  | CYS  | CA-C-N      | -7.20 | 112.04      | 122.19   |
| 1   | A     | 76  | CYS  | C-N-CA      | -7.20 | 112.04      | 122.19   |
| 1   | A     | 58  | ILE  | CA-C-O      | 7.16  | 129.02      | 120.85   |
| 1   | B     | 119 | ASP  | O-C-N       | -7.15 | 112.54      | 122.41   |
| 1   | B     | 111 | TRP  | NE1-CE2-CD2 | -7.15 | 98.11       | 107.40   |
| 1   | A     | 128 | ARG  | CA-C-N      | -7.15 | 108.83      | 121.70   |
| 1   | A     | 128 | ARG  | C-N-CA      | -7.15 | 108.83      | 121.70   |
| 1   | A     | 111 | TRP  | CE2-CD2-CG  | 7.13  | 115.75      | 107.20   |
| 1   | A     | 103 | ASN  | N-CA-C      | -7.11 | 102.63      | 112.30   |
| 1   | A     | 48  | ASP  | N-CA-C      | 7.09  | 120.87      | 112.93   |
| 1   | A     | 37  | ASN  | CB-CG-OD1   | 7.08  | 134.96      | 120.80   |
| 1   | B     | 88  | ILE  | CB-CG1-CD1  | 7.08  | 128.67      | 113.80   |
| 1   | A     | 63  | TRP  | N-CA-CB     | -7.08 | 100.13      | 110.47   |
| 1   | B     | 119 | ASP  | CA-C-O      | 7.08  | 129.94      | 121.66   |
| 1   | A     | 36  | SER  | O-C-N       | 7.07  | 129.80      | 122.09   |
| 1   | A     | 33  | LYS  | CA-C-N      | -7.07 | 108.91      | 122.06   |
| 1   | A     | 33  | LYS  | C-N-CA      | -7.07 | 108.91      | 122.06   |
| 1   | B     | 60  | SER  | N-CA-C      | 7.07  | 121.73      | 113.18   |
| 1   | B     | 21  | ARG  | CA-C-O      | 7.06  | 130.03      | 121.84   |
| 1   | A     | 123 | TRP  | O-C-N       | 7.05  | 132.82      | 122.39   |
| 1   | A     | 101 | ASP  | OD1-CG-OD2  | 7.04  | 139.80      | 122.90   |
| 1   | B     | 111 | TRP  | CB-CG-CD2   | 7.04  | 136.66      | 126.80   |
| 1   | A     | 104 | GLY  | O-C-N       | 7.03  | 129.91      | 122.60   |
| 1   | A     | 65  | ASN  | CA-C-O      | -7.02 | 112.77      | 120.43   |
| 1   | B     | 7   | GLU  | CG-CD-OE1   | 7.02  | 134.54      | 118.40   |
| 1   | A     | 73  | ARG  | CA-C-O      | -7.00 | 111.00      | 118.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 84  | LEU  | N-CA-C      | -6.99 | 103.93      | 113.30   |
| 1   | A     | 70  | PRO  | CB-CA-C     | -6.98 | 102.45      | 111.46   |
| 1   | A     | 91  | SER  | CA-C-O      | 6.97  | 127.94      | 120.55   |
| 1   | B     | 32  | ALA  | CA-C-O      | -6.97 | 113.17      | 120.55   |
| 1   | A     | 55  | ILE  | N-CA-C      | 6.96  | 119.75      | 111.05   |
| 1   | A     | 128 | ARG  | CD-NE-CZ    | -6.96 | 114.66      | 124.40   |
| 1   | B     | 70  | PRO  | CA-N-CD     | -6.95 | 102.27      | 112.00   |
| 1   | A     | 87  | ASP  | CB-CG-OD1   | -6.94 | 102.44      | 118.40   |
| 1   | B     | 20  | TYR  | CG-CD1-CE1  | -6.94 | 110.79      | 121.20   |
| 1   | A     | 123 | TRP  | CD2-CE2-CZ2 | -6.92 | 115.47      | 122.40   |
| 1   | B     | 56  | LEU  | O-C-N       | -6.92 | 113.82      | 122.19   |
| 1   | A     | 41  | GLN  | N-CA-CB     | 6.91  | 121.01      | 110.44   |
| 1   | A     | 23  | TYR  | CG-CD2-CE2  | -6.91 | 110.84      | 121.20   |
| 1   | B     | 89  | THR  | OG1-CB-CG2  | -6.90 | 95.50       | 109.30   |
| 1   | B     | 87  | ASP  | O-C-N       | -6.89 | 115.20      | 123.13   |
| 1   | B     | 37  | ASN  | CA-CB-CG    | -6.88 | 105.72      | 112.60   |
| 1   | A     | 73  | ARG  | N-CA-C      | -6.87 | 105.45      | 114.31   |
| 1   | B     | 53  | TYR  | CD1-CE1-CZ  | 6.86  | 131.94      | 119.60   |
| 1   | A     | 123 | TRP  | CE2-CD2-CG  | -6.84 | 98.99       | 107.20   |
| 1   | A     | 8   | LEU  | O-C-N       | -6.83 | 115.03      | 122.07   |
| 1   | A     | 121 | GLN  | OE1-CD-NE2  | 6.83  | 129.43      | 122.60   |
| 1   | B     | 108 | TRP  | CZ3-CH2-CZ2 | -6.82 | 112.64      | 121.50   |
| 1   | B     | 29  | VAL  | CG1-CB-CG2  | -6.81 | 95.82       | 110.80   |
| 1   | B     | 53  | TYR  | CG-CD2-CE2  | 6.81  | 131.41      | 121.20   |
| 1   | B     | 52  | ASP  | OD1-CG-OD2  | 6.81  | 139.24      | 122.90   |
| 1   | A     | 24  | SER  | N-CA-CB     | -6.80 | 100.53      | 110.26   |
| 1   | B     | 77  | ASN  | O-C-N       | 6.80  | 130.74      | 122.58   |
| 1   | A     | 38  | PHE  | CD1-CG-CD2  | -6.79 | 108.42      | 118.60   |
| 1   | B     | 34  | PHE  | CA-C-O      | -6.79 | 111.33      | 119.27   |
| 1   | A     | 72  | SER  | CA-C-O      | -6.78 | 114.11      | 121.44   |
| 1   | B     | 38  | PHE  | CA-C-O      | -6.78 | 110.71      | 119.59   |
| 1   | A     | 97  | LYS  | CB-CG-CD    | -6.76 | 95.75       | 111.30   |
| 1   | B     | 69  | THR  | CA-C-N      | -6.76 | 113.00      | 119.76   |
| 1   | B     | 69  | THR  | C-N-CA      | -6.76 | 113.00      | 119.76   |
| 1   | A     | 62  | TRP  | CD2-CE3-CZ3 | -6.76 | 109.81      | 118.60   |
| 1   | B     | 11  | ALA  | CA-C-O      | -6.76 | 113.39      | 120.55   |
| 1   | A     | 91  | SER  | O-C-N       | -6.75 | 114.96      | 122.12   |
| 1   | B     | 98  | ILE  | O-C-N       | 6.75  | 128.52      | 121.91   |
| 1   | A     | 66  | ASP  | N-CA-C      | -6.74 | 104.95      | 113.72   |
| 1   | A     | 38  | PHE  | CB-CA-C     | 6.74  | 122.52      | 111.26   |
| 1   | B     | 56  | LEU  | CD1-CG-CD2  | -6.72 | 96.00       | 110.80   |
| 1   | A     | 20  | TYR  | CG-CD1-CE1  | -6.68 | 111.18      | 121.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 74  | ASN  | CA-CB-CG    | 6.67  | 119.27      | 112.60   |
| 1   | B     | 63  | TRP  | NE1-CE2-CZ2 | 6.66  | 140.09      | 130.10   |
| 1   | B     | 24  | SER  | CA-C-N      | -6.66 | 110.84      | 120.82   |
| 1   | B     | 24  | SER  | C-N-CA      | -6.66 | 110.84      | 120.82   |
| 1   | B     | 6   | CYS  | CA-C-O      | 6.65  | 127.64      | 119.79   |
| 1   | A     | 123 | TRP  | N-CA-C      | 6.65  | 121.25      | 113.20   |
| 1   | A     | 32  | ALA  | CA-C-N      | -6.64 | 111.80      | 120.44   |
| 1   | A     | 32  | ALA  | C-N-CA      | -6.64 | 111.80      | 120.44   |
| 1   | B     | 50  | SER  | CA-C-N      | 6.64  | 133.49      | 122.73   |
| 1   | B     | 50  | SER  | C-N-CA      | 6.64  | 133.49      | 122.73   |
| 1   | A     | 2   | VAL  | O-C-N       | 6.60  | 130.95      | 122.77   |
| 1   | B     | 123 | TRP  | CH2-CZ2-CE2 | 6.60  | 126.08      | 117.50   |
| 1   | B     | 110 | ALA  | O-C-N       | -6.59 | 113.50      | 122.33   |
| 1   | A     | 125 | ARG  | CB-CG-CD    | 6.58  | 126.44      | 111.30   |
| 1   | A     | 31  | ALA  | N-CA-C      | 6.58  | 118.11      | 111.07   |
| 1   | B     | 47  | THR  | CB-CA-C     | 6.57  | 122.78      | 110.63   |
| 1   | A     | 25  | LEU  | N-CA-C      | 6.56  | 122.19      | 111.37   |
| 1   | A     | 98  | ILE  | N-CA-C      | 6.55  | 117.30      | 110.62   |
| 1   | B     | 86  | SER  | N-CA-C      | -6.55 | 105.15      | 113.01   |
| 1   | A     | 97  | LYS  | N-CA-C      | -6.54 | 104.07      | 111.14   |
| 1   | A     | 49  | GLY  | CA-C-O      | 6.54  | 131.95      | 120.57   |
| 1   | B     | 28  | TRP  | CD1-NE1-CE2 | 6.53  | 120.66      | 108.90   |
| 1   | A     | 18  | ASP  | CB-CG-OD2   | -6.51 | 103.42      | 118.40   |
| 1   | A     | 113 | ASN  | CA-CB-CG    | 6.50  | 119.10      | 112.60   |
| 1   | B     | 7   | GLU  | CA-C-N      | 6.50  | 128.89      | 120.44   |
| 1   | B     | 7   | GLU  | C-N-CA      | 6.50  | 128.89      | 120.44   |
| 1   | B     | 38  | PHE  | CE1-CZ-CE2  | -6.50 | 108.30      | 120.00   |
| 1   | B     | 47  | THR  | O-C-N       | 6.50  | 129.83      | 122.22   |
| 1   | B     | 12  | MET  | N-CA-CB     | -6.50 | 100.21      | 110.28   |
| 1   | A     | 7   | GLU  | N-CA-C      | -6.50 | 104.12      | 111.14   |
| 1   | B     | 34  | PHE  | CG-CD1-CE1  | 6.49  | 131.74      | 120.70   |
| 1   | B     | 119 | ASP  | CA-C-N      | 6.49  | 131.51      | 121.19   |
| 1   | B     | 119 | ASP  | C-N-CA      | 6.49  | 131.51      | 121.19   |
| 1   | B     | 106 | ASN  | CB-CG-OD1   | 6.49  | 133.77      | 120.80   |
| 1   | A     | 101 | ASP  | N-CA-C      | 6.47  | 120.10      | 112.72   |
| 1   | A     | 59  | ASN  | O-C-N       | -6.46 | 115.66      | 123.16   |
| 1   | B     | 15  | HIS  | CA-C-O      | 6.46  | 129.18      | 119.23   |
| 1   | A     | 84  | LEU  | CA-C-N      | 6.46  | 132.72      | 120.97   |
| 1   | A     | 84  | LEU  | C-N-CA      | 6.46  | 132.72      | 120.97   |
| 1   | B     | 86  | SER  | N-CA-CB     | -6.45 | 99.10       | 110.39   |
| 1   | B     | 111 | TRP  | CZ3-CH2-CZ2 | -6.44 | 113.12      | 121.50   |
| 1   | B     | 53  | TYR  | N-CA-C      | 6.44  | 119.40      | 108.90   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 18  | ASP  | CA-C-O      | -6.43 | 112.97      | 120.62   |
| 1   | A     | 86  | SER  | CB-CA-C     | -6.43 | 97.37       | 109.72   |
| 1   | A     | 85  | SER  | N-CA-C      | 6.42  | 119.01      | 110.53   |
| 1   | A     | 53  | TYR  | CB-CG-CD2   | -6.42 | 111.17      | 120.80   |
| 1   | A     | 74  | ASN  | N-CA-C      | 6.42  | 120.03      | 111.30   |
| 1   | A     | 48  | ASP  | CB-CA-C     | -6.41 | 99.72       | 110.81   |
| 1   | A     | 116 | LYS  | N-CA-CB     | -6.41 | 99.89       | 109.69   |
| 1   | A     | 113 | ASN  | CB-CG-OD1   | -6.40 | 108.01      | 120.80   |
| 1   | B     | 81  | SER  | CA-C-O      | -6.38 | 111.77      | 119.49   |
| 1   | B     | 78  | ILE  | CB-CA-C     | -6.36 | 99.78       | 111.36   |
| 1   | B     | 119 | ASP  | CB-CG-OD1   | 6.36  | 133.03      | 118.40   |
| 1   | A     | 109 | VAL  | N-CA-CB     | -6.36 | 101.04      | 110.58   |
| 1   | B     | 13  | LYS  | CA-C-O      | 6.36  | 127.28      | 119.97   |
| 1   | B     | 3   | PHE  | CG-CD2-CE2  | 6.35  | 131.50      | 120.70   |
| 1   | B     | 62  | TRP  | NE1-CE2-CZ2 | 6.33  | 139.60      | 130.10   |
| 1   | B     | 100 | SER  | CB-CA-C     | -6.33 | 99.86       | 110.56   |
| 1   | A     | 60  | SER  | O-C-N       | -6.33 | 113.72      | 122.46   |
| 1   | A     | 39  | ASN  | N-CA-CB     | -6.31 | 100.64      | 110.55   |
| 1   | A     | 119 | ASP  | CB-CA-C     | -6.30 | 101.75      | 111.83   |
| 1   | A     | 15  | HIS  | CA-C-N      | -6.30 | 110.77      | 121.85   |
| 1   | A     | 15  | HIS  | C-N-CA      | -6.30 | 110.77      | 121.85   |
| 1   | A     | 15  | HIS  | CA-CB-CG    | 6.30  | 120.10      | 113.80   |
| 1   | B     | 65  | ASN  | CB-CG-ND2   | -6.29 | 106.96      | 116.40   |
| 1   | B     | 103 | ASN  | CB-CG-ND2   | -6.29 | 106.96      | 116.40   |
| 1   | A     | 114 | ARG  | CD-NE-CZ    | -6.29 | 115.60      | 124.40   |
| 1   | B     | 28  | TRP  | NE1-CE2-CZ2 | 6.29  | 139.53      | 130.10   |
| 1   | A     | 124 | ILE  | O-C-N       | 6.28  | 128.65      | 122.05   |
| 1   | A     | 92  | VAL  | O-C-N       | -6.28 | 115.76      | 121.91   |
| 1   | A     | 73  | ARG  | CG-CD-NE    | -6.27 | 98.21       | 112.00   |
| 1   | B     | 66  | ASP  | CB-CG-OD2   | 6.26  | 132.81      | 118.40   |
| 1   | A     | 113 | ASN  | OD1-CG-ND2  | 6.26  | 128.86      | 122.60   |
| 1   | B     | 34  | PHE  | CD1-CE1-CZ  | -6.26 | 108.74      | 120.00   |
| 1   | B     | 25  | LEU  | CA-C-O      | 6.22  | 127.88      | 120.92   |
| 1   | B     | 62  | TRP  | CE2-CD2-CE3 | 6.21  | 125.01      | 118.80   |
| 1   | A     | 14  | ARG  | CG-CD-NE    | -6.21 | 98.35       | 112.00   |
| 1   | A     | 111 | TRP  | NE1-CE2-CZ2 | 6.19  | 139.39      | 130.10   |
| 1   | B     | 49  | GLY  | CA-C-N      | -6.19 | 111.97      | 122.67   |
| 1   | B     | 49  | GLY  | C-N-CA      | -6.19 | 111.97      | 122.67   |
| 1   | A     | 64  | CYS  | O-C-N       | -6.18 | 115.69      | 123.17   |
| 1   | A     | 6   | CYS  | CA-C-N      | 6.18  | 128.84      | 120.44   |
| 1   | A     | 6   | CYS  | C-N-CA      | 6.18  | 128.84      | 120.44   |
| 1   | A     | 28  | TRP  | CD1-NE1-CE2 | -6.18 | 97.78       | 108.90   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 73  | ARG  | CD-NE-CZ    | -6.16 | 115.77      | 124.40   |
| 1   | B     | 113 | ASN  | CB-CG-OD1   | 6.16  | 133.13      | 120.80   |
| 1   | B     | 41  | GLN  | CA-CB-CG    | 6.16  | 126.42      | 114.10   |
| 1   | B     | 45  | ARG  | CB-CA-C     | -6.16 | 99.37       | 109.53   |
| 1   | B     | 78  | ILE  | CA-C-O      | 6.15  | 128.19      | 119.95   |
| 1   | B     | 97  | LYS  | CD-CE-NZ    | -6.15 | 92.21       | 111.90   |
| 1   | A     | 14  | ARG  | CB-CG-CD    | -6.13 | 97.19       | 111.30   |
| 1   | A     | 52  | ASP  | OD1-CG-OD2  | -6.13 | 108.18      | 122.90   |
| 1   | A     | 34  | PHE  | N-CA-CB     | -6.13 | 100.83      | 110.46   |
| 1   | B     | 62  | TRP  | CD1-NE1-CE2 | 6.13  | 119.93      | 108.90   |
| 1   | B     | 112 | ARG  | CA-CB-CG    | 6.12  | 126.34      | 114.10   |
| 1   | A     | 30  | CYS  | CA-CB-SG    | -6.12 | 100.33      | 114.40   |
| 1   | B     | 72  | SER  | CA-CB-OG    | -6.12 | 98.87       | 111.10   |
| 1   | A     | 80  | CYS  | O-C-N       | 6.11  | 129.37      | 122.22   |
| 1   | B     | 123 | TRP  | CB-CG-CD2   | 6.10  | 135.35      | 126.80   |
| 1   | A     | 87  | ASP  | O-C-N       | -6.10 | 116.38      | 123.27   |
| 1   | A     | 54  | GLY  | O-C-N       | 6.09  | 128.70      | 122.91   |
| 1   | A     | 7   | GLU  | CB-CG-CD    | 6.09  | 122.95      | 112.60   |
| 1   | A     | 33  | LYS  | CA-C-O      | -6.08 | 114.43      | 120.82   |
| 1   | A     | 76  | CYS  | CA-C-O      | 6.07  | 126.63      | 119.28   |
| 1   | B     | 58  | ILE  | O-C-N       | -6.07 | 116.03      | 122.95   |
| 1   | B     | 50  | SER  | N-CA-CB     | 6.05  | 119.84      | 110.46   |
| 1   | B     | 73  | ARG  | CA-C-O      | -6.04 | 111.87      | 120.51   |
| 1   | B     | 3   | PHE  | CB-CG-CD1   | 6.04  | 130.97      | 120.70   |
| 1   | B     | 23  | TYR  | CA-C-N      | -6.04 | 109.98      | 120.97   |
| 1   | B     | 23  | TYR  | C-N-CA      | -6.04 | 109.98      | 120.97   |
| 1   | B     | 18  | ASP  | CB-CG-OD1   | 6.04  | 132.28      | 118.40   |
| 1   | B     | 27  | ASN  | CB-CG-ND2   | -6.03 | 107.36      | 116.40   |
| 1   | B     | 36  | SER  | CA-C-O      | -6.02 | 112.23      | 119.03   |
| 1   | B     | 7   | GLU  | N-CA-CB     | -6.02 | 101.26      | 110.16   |
| 1   | B     | 111 | TRP  | CD1-CG-CD2  | -6.01 | 96.68       | 106.30   |
| 1   | A     | 61  | ARG  | CA-C-O      | -6.01 | 113.57      | 120.24   |
| 1   | A     | 38  | PHE  | CB-CG-CD2   | 6.00  | 130.91      | 120.70   |
| 1   | A     | 43  | THR  | N-CA-C      | -6.00 | 99.22       | 109.24   |
| 1   | B     | 7   | GLU  | CB-CG-CD    | -5.99 | 102.42      | 112.60   |
| 1   | B     | 48  | ASP  | CA-C-N      | 5.98  | 131.71      | 122.20   |
| 1   | B     | 48  | ASP  | C-N-CA      | 5.98  | 131.71      | 122.20   |
| 1   | B     | 77  | ASN  | CA-C-N      | -5.98 | 111.07      | 122.13   |
| 1   | B     | 77  | ASN  | C-N-CA      | -5.98 | 111.07      | 122.13   |
| 1   | B     | 50  | SER  | O-C-N       | -5.97 | 115.91      | 122.84   |
| 1   | B     | 73  | ARG  | CA-CB-CG    | -5.97 | 102.16      | 114.10   |
| 1   | A     | 42  | ALA  | CA-C-N      | -5.96 | 113.07      | 122.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 42  | ALA  | C-N-CA      | -5.96 | 113.07      | 122.73   |
| 1   | A     | 86  | SER  | N-CA-CB     | -5.96 | 101.10      | 110.46   |
| 1   | B     | 18  | ASP  | O-C-N       | 5.96  | 130.52      | 122.59   |
| 1   | A     | 61  | ARG  | CB-CG-CD    | -5.96 | 97.60       | 111.30   |
| 1   | B     | 115 | CYS  | O-C-N       | 5.96  | 130.08      | 122.10   |
| 1   | B     | 62  | TRP  | CH2-CZ2-CE2 | -5.95 | 109.77      | 117.50   |
| 1   | B     | 51  | THR  | OG1-CB-CG2  | -5.94 | 97.42       | 109.30   |
| 1   | A     | 5   | ARG  | CA-C-O      | -5.94 | 114.77      | 121.00   |
| 1   | B     | 54  | GLY  | N-CA-C      | 5.93  | 123.71      | 112.62   |
| 1   | A     | 11  | ALA  | N-CA-CB     | 5.93  | 118.61      | 110.01   |
| 1   | A     | 34  | PHE  | CZ-CE2-CD2  | 5.93  | 130.67      | 120.00   |
| 1   | A     | 38  | PHE  | CG-CD1-CE1  | 5.91  | 130.75      | 120.70   |
| 1   | B     | 5   | ARG  | NE-CZ-NH1   | 5.91  | 127.41      | 121.50   |
| 1   | B     | 111 | TRP  | O-C-N       | -5.90 | 115.99      | 122.07   |
| 1   | B     | 106 | ASN  | N-CA-CB     | 5.90  | 120.35      | 110.32   |
| 1   | A     | 40  | THR  | CA-C-O      | 5.89  | 126.62      | 119.49   |
| 1   | A     | 89  | THR  | CA-CB-CG2   | 5.89  | 120.52      | 110.50   |
| 1   | B     | 39  | ASN  | OD1-CG-ND2  | -5.88 | 116.72      | 122.60   |
| 1   | A     | 65  | ASN  | O-C-N       | -5.87 | 116.64      | 123.27   |
| 1   | A     | 60  | SER  | N-CA-C      | 5.87  | 120.05      | 113.01   |
| 1   | B     | 123 | TRP  | CE3-CZ3-CH2 | -5.85 | 113.49      | 121.10   |
| 1   | B     | 33  | LYS  | CG-CD-CE    | -5.85 | 97.84       | 111.30   |
| 1   | B     | 28  | TRP  | NE1-CE2-CD2 | -5.85 | 99.80       | 107.40   |
| 1   | A     | 7   | GLU  | CA-C-N      | 5.83  | 128.03      | 120.44   |
| 1   | A     | 7   | GLU  | C-N-CA      | 5.83  | 128.03      | 120.44   |
| 1   | A     | 90  | ALA  | CA-C-O      | 5.83  | 126.60      | 120.42   |
| 1   | B     | 5   | ARG  | CB-CA-C     | 5.83  | 120.03      | 110.88   |
| 1   | B     | 65  | ASN  | CA-C-O      | -5.82 | 114.13      | 120.36   |
| 1   | B     | 85  | SER  | N-CA-C      | 5.82  | 118.70      | 110.50   |
| 1   | B     | 128 | ARG  | CA-C-N      | 5.82  | 132.17      | 121.70   |
| 1   | B     | 128 | ARG  | C-N-CA      | 5.82  | 132.17      | 121.70   |
| 1   | A     | 41  | GLN  | CA-CB-CG    | -5.81 | 102.48      | 114.10   |
| 1   | B     | 68  | ARG  | O-C-N       | 5.81  | 130.03      | 122.42   |
| 1   | B     | 40  | THR  | CA-CB-CG2   | 5.80  | 120.37      | 110.50   |
| 1   | A     | 3   | PHE  | CA-CB-CG    | 5.80  | 119.60      | 113.80   |
| 1   | A     | 34  | PHE  | N-CA-C      | 5.80  | 120.35      | 113.28   |
| 1   | A     | 21  | ARG  | NH1-CZ-NH2  | -5.79 | 111.77      | 119.30   |
| 1   | B     | 42  | ALA  | N-CA-C      | 5.79  | 118.75      | 110.24   |
| 1   | B     | 127 | CYS  | N-CA-C      | 5.78  | 118.53      | 111.82   |
| 1   | A     | 128 | ARG  | CG-CD-NE    | 5.78  | 124.72      | 112.00   |
| 1   | A     | 87  | ASP  | N-CA-CB     | -5.77 | 101.02      | 110.43   |
| 1   | B     | 100 | SER  | N-CA-C      | -5.77 | 105.82      | 112.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 68  | ARG  | NE-CZ-NH2   | 5.77  | 124.39      | 119.20   |
| 1   | A     | 13  | LYS  | CA-CB-CG    | -5.75 | 102.59      | 114.10   |
| 1   | B     | 99  | VAL  | CA-C-N      | -5.75 | 113.45      | 122.65   |
| 1   | B     | 99  | VAL  | C-N-CA      | -5.75 | 113.45      | 122.65   |
| 1   | B     | 68  | ARG  | NE-CZ-NH1   | 5.74  | 127.24      | 121.50   |
| 1   | B     | 35  | GLU  | CG-CD-OE1   | 5.73  | 131.59      | 118.40   |
| 1   | A     | 69  | THR  | O-C-N       | 5.73  | 128.15      | 121.10   |
| 1   | A     | 123 | TRP  | N-CA-CB     | -5.73 | 101.13      | 110.42   |
| 1   | A     | 87  | ASP  | N-CA-C      | -5.72 | 99.91       | 109.24   |
| 1   | A     | 16  | GLY  | CA-C-O      | -5.72 | 112.48      | 119.06   |
| 1   | A     | 62  | TRP  | CD1-NE1-CE2 | -5.72 | 98.61       | 108.90   |
| 1   | B     | 29  | VAL  | N-CA-CB     | -5.71 | 102.01      | 110.58   |
| 1   | B     | 83  | LEU  | N-CA-CB     | -5.71 | 101.17      | 110.42   |
| 1   | A     | 111 | TRP  | CH2-CZ2-CE2 | 5.71  | 124.92      | 117.50   |
| 1   | B     | 21  | ARG  | N-CA-CB     | -5.70 | 103.26      | 111.70   |
| 1   | B     | 6   | CYS  | N-CA-C      | 5.69  | 119.40      | 112.23   |
| 1   | A     | 44  | ASN  | CA-CB-CG    | -5.68 | 106.92      | 112.60   |
| 1   | A     | 77  | ASN  | CB-CA-C     | 5.67  | 119.78      | 111.73   |
| 1   | A     | 19  | ASN  | CB-CA-C     | -5.64 | 101.84      | 111.26   |
| 1   | B     | 60  | SER  | O-C-N       | 5.62  | 130.64      | 122.43   |
| 1   | B     | 28  | TRP  | CD1-CG-CD2  | 5.62  | 115.29      | 106.30   |
| 1   | A     | 66  | ASP  | CB-CG-OD2   | 5.62  | 131.31      | 118.40   |
| 1   | B     | 63  | TRP  | CD1-NE1-CE2 | 5.62  | 119.01      | 108.90   |
| 1   | B     | 108 | TRP  | CD1-NE1-CE2 | 5.61  | 119.00      | 108.90   |
| 1   | B     | 125 | ARG  | CB-CA-C     | 5.61  | 118.26      | 109.84   |
| 1   | A     | 100 | SER  | N-CA-CB     | -5.60 | 102.35      | 110.70   |
| 1   | A     | 116 | LYS  | O-C-N       | 5.60  | 129.89      | 122.95   |
| 1   | A     | 43  | THR  | CA-CB-CG2   | -5.59 | 100.99      | 110.50   |
| 1   | A     | 17  | LEU  | N-CA-C      | 5.58  | 119.93      | 113.18   |
| 1   | A     | 37  | ASN  | O-C-N       | -5.58 | 114.94      | 122.41   |
| 1   | B     | 11  | ALA  | CA-C-N      | -5.55 | 111.88      | 120.31   |
| 1   | B     | 11  | ALA  | C-N-CA      | -5.55 | 111.88      | 120.31   |
| 1   | B     | 60  | SER  | CA-C-O      | -5.54 | 112.02      | 119.11   |
| 1   | A     | 25  | LEU  | CA-C-O      | 5.54  | 127.12      | 120.92   |
| 1   | A     | 69  | THR  | N-CA-CB     | -5.54 | 99.86       | 110.27   |
| 1   | B     | 33  | LYS  | N-CA-CB     | -5.53 | 101.99      | 110.01   |
| 1   | B     | 91  | SER  | CA-C-N      | -5.53 | 112.56      | 120.42   |
| 1   | B     | 91  | SER  | C-N-CA      | -5.53 | 112.56      | 120.42   |
| 1   | A     | 106 | ASN  | OD1-CG-ND2  | 5.53  | 128.13      | 122.60   |
| 1   | B     | 7   | GLU  | CG-CD-OE2   | -5.51 | 105.72      | 118.40   |
| 1   | A     | 43  | THR  | N-CA-CB     | 5.50  | 120.96      | 111.00   |
| 1   | B     | 46  | ASN  | CA-C-N      | 5.50  | 128.20      | 120.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 46  | ASN  | C-N-CA      | 5.50  | 128.20      | 120.28   |
| 1   | B     | 80  | CYS  | CB-CA-C     | 5.50  | 120.81      | 110.63   |
| 1   | B     | 100 | SER  | CA-CB-OG    | -5.49 | 100.11      | 111.10   |
| 1   | B     | 1   | LYS  | CG-CD-CE    | 5.48  | 123.91      | 111.30   |
| 1   | A     | 120 | VAL  | CA-CB-CG2   | -5.48 | 101.08      | 110.40   |
| 1   | B     | 17  | LEU  | N-CA-C      | -5.48 | 106.59      | 113.28   |
| 1   | A     | 25  | LEU  | O-C-N       | 5.48  | 128.41      | 122.11   |
| 1   | A     | 38  | PHE  | O-C-N       | 5.48  | 130.85      | 122.03   |
| 1   | A     | 68  | ARG  | NE-CZ-NH1   | 5.48  | 126.98      | 121.50   |
| 1   | A     | 90  | ALA  | CB-CA-C     | -5.48 | 101.54      | 110.85   |
| 1   | B     | 92  | VAL  | N-CA-C      | 5.47  | 116.24      | 110.72   |
| 1   | B     | 117 | GLY  | N-CA-C      | 5.47  | 122.87      | 115.32   |
| 1   | A     | 106 | ASN  | O-C-N       | -5.47 | 115.28      | 122.39   |
| 1   | A     | 34  | PHE  | CG-CD2-CE2  | 5.46  | 129.99      | 120.70   |
| 1   | B     | 34  | PHE  | CG-CD2-CE2  | -5.45 | 111.43      | 120.70   |
| 1   | B     | 124 | ILE  | N-CA-CB     | 5.45  | 119.29      | 112.26   |
| 1   | B     | 21  | ARG  | CA-C-N      | -5.43 | 111.40      | 121.93   |
| 1   | B     | 21  | ARG  | C-N-CA      | -5.43 | 111.40      | 121.93   |
| 1   | B     | 1   | LYS  | CB-CG-CD    | 5.43  | 123.78      | 111.30   |
| 1   | B     | 105 | MET  | O-C-N       | -5.43 | 114.36      | 122.39   |
| 1   | B     | 41  | GLN  | O-C-N       | -5.41 | 115.85      | 122.34   |
| 1   | A     | 68  | ARG  | CD-NE-CZ    | -5.41 | 116.83      | 124.40   |
| 1   | B     | 47  | THR  | N-CA-CB     | 5.41  | 118.55      | 110.22   |
| 1   | A     | 114 | ARG  | NH1-CZ-NH2  | 5.40  | 126.32      | 119.30   |
| 1   | B     | 81  | SER  | O-C-N       | 5.40  | 129.41      | 122.39   |
| 1   | A     | 108 | TRP  | CZ3-CH2-CZ2 | 5.39  | 128.51      | 121.50   |
| 1   | A     | 23  | TYR  | N-CA-CB     | -5.37 | 101.51      | 110.37   |
| 1   | B     | 13  | LYS  | O-C-N       | -5.37 | 115.66      | 122.27   |
| 1   | A     | 68  | ARG  | CA-C-N      | -5.35 | 113.77      | 122.65   |
| 1   | A     | 68  | ARG  | C-N-CA      | -5.35 | 113.77      | 122.65   |
| 1   | B     | 116 | LYS  | N-CA-C      | -5.34 | 102.38      | 110.24   |
| 1   | A     | 55  | ILE  | CA-C-O      | -5.34 | 114.86      | 120.57   |
| 1   | A     | 65  | ASN  | OD1-CG-ND2  | -5.34 | 117.26      | 122.60   |
| 1   | B     | 5   | ARG  | CG-CD-NE    | 5.33  | 123.73      | 112.00   |
| 1   | B     | 67  | GLY  | O-C-N       | -5.33 | 115.75      | 122.41   |
| 1   | A     | 18  | ASP  | N-CA-CB     | -5.33 | 100.86      | 109.60   |
| 1   | B     | 97  | LYS  | CG-CD-CE    | 5.33  | 123.55      | 111.30   |
| 1   | B     | 115 | CYS  | CB-CA-C     | -5.31 | 100.72      | 109.65   |
| 1   | B     | 72  | SER  | CB-CA-C     | -5.31 | 97.77       | 109.56   |
| 1   | B     | 127 | CYS  | O-C-N       | -5.31 | 115.73      | 122.27   |
| 1   | A     | 78  | ILE  | CA-C-N      | 5.31  | 125.07      | 119.76   |
| 1   | A     | 78  | ILE  | C-N-CA      | 5.31  | 125.07      | 119.76   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 3   | PHE  | CG-CD1-CE1 | 5.31  | 129.72      | 120.70   |
| 1   | B     | 112 | ARG  | CB-CG-CD   | 5.30  | 123.50      | 111.30   |
| 1   | A     | 123 | TRP  | CA-C-N     | -5.30 | 114.44      | 122.76   |
| 1   | A     | 123 | TRP  | C-N-CA     | -5.30 | 114.44      | 122.76   |
| 1   | B     | 34  | PHE  | CZ-CE2-CD2 | 5.29  | 129.53      | 120.00   |
| 1   | A     | 47  | THR  | CB-CA-C    | 5.29  | 121.37      | 110.31   |
| 1   | B     | 104 | GLY  | O-C-N      | 5.29  | 128.86      | 122.67   |
| 1   | A     | 31  | ALA  | CA-C-N     | -5.29 | 112.78      | 120.29   |
| 1   | A     | 31  | ALA  | C-N-CA     | -5.29 | 112.78      | 120.29   |
| 1   | A     | 35  | GLU  | OE1-CD-OE2 | -5.28 | 110.24      | 122.90   |
| 1   | B     | 76  | CYS  | CB-CA-C    | -5.27 | 100.52      | 110.01   |
| 1   | B     | 5   | ARG  | CD-NE-CZ   | -5.27 | 117.03      | 124.40   |
| 1   | B     | 49  | GLY  | O-C-N      | 5.26  | 129.31      | 122.42   |
| 1   | B     | 7   | GLU  | N-CA-C     | -5.25 | 105.63      | 111.36   |
| 1   | B     | 23  | TYR  | CG-CD2-CE2 | -5.25 | 113.32      | 121.20   |
| 1   | A     | 27  | ASN  | CA-C-O     | 5.25  | 126.03      | 120.10   |
| 1   | B     | 100 | SER  | N-CA-CB    | -5.25 | 102.89      | 110.56   |
| 1   | B     | 55  | ILE  | CA-C-N     | -5.24 | 114.30      | 122.37   |
| 1   | B     | 55  | ILE  | C-N-CA     | -5.24 | 114.30      | 122.37   |
| 1   | B     | 41  | GLN  | CB-CG-CD   | 5.24  | 121.51      | 112.60   |
| 1   | B     | 77  | ASN  | CB-CA-C    | 5.23  | 118.87      | 111.86   |
| 1   | B     | 86  | SER  | CA-C-O     | 5.23  | 125.84      | 119.05   |
| 1   | B     | 112 | ARG  | CB-CA-C    | 5.22  | 120.30      | 110.63   |
| 1   | A     | 92  | VAL  | CA-C-N     | 5.22  | 127.22      | 120.44   |
| 1   | A     | 92  | VAL  | C-N-CA     | 5.22  | 127.22      | 120.44   |
| 1   | A     | 47  | THR  | N-CA-CB    | -5.21 | 101.73      | 110.39   |
| 1   | B     | 81  | SER  | CA-C-N     | -5.21 | 112.01      | 120.72   |
| 1   | B     | 81  | SER  | C-N-CA     | -5.21 | 112.01      | 120.72   |
| 1   | B     | 70  | PRO  | CA-CB-CG   | -5.21 | 94.60       | 104.50   |
| 1   | A     | 98  | ILE  | O-C-N      | -5.21 | 116.82      | 121.87   |
| 1   | B     | 53  | TYR  | OH-CZ-CE2  | -5.21 | 104.27      | 119.90   |
| 1   | A     | 34  | PHE  | CA-CB-CG   | 5.20  | 119.00      | 113.80   |
| 1   | A     | 103 | ASN  | CA-C-O     | -5.20 | 113.75      | 119.78   |
| 1   | A     | 108 | TRP  | CB-CG-CD1  | -5.20 | 119.10      | 126.90   |
| 1   | A     | 105 | MET  | CA-C-O     | 5.20  | 125.93      | 119.12   |
| 1   | A     | 125 | ARG  | N-CA-CB    | -5.19 | 102.41      | 110.04   |
| 1   | B     | 62  | TRP  | CB-CG-CD1  | -5.18 | 119.13      | 126.90   |
| 1   | A     | 76  | CYS  | CA-CB-SG   | -5.17 | 102.50      | 114.40   |
| 1   | B     | 20  | TYR  | N-CA-C     | -5.17 | 101.53      | 109.76   |
| 1   | B     | 81  | SER  | N-CA-C     | -5.17 | 106.07      | 112.38   |
| 1   | A     | 62  | TRP  | N-CA-C     | 5.17  | 120.97      | 114.31   |
| 1   | A     | 121 | GLN  | CA-CB-CG   | -5.16 | 103.78      | 114.10   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 32  | ALA  | N-CA-CB    | -5.16 | 102.54      | 110.12   |
| 1   | B     | 37  | ASN  | CB-CG-ND2  | 5.14  | 124.11      | 116.40   |
| 1   | B     | 34  | PHE  | CB-CG-CD1  | -5.13 | 111.98      | 120.70   |
| 1   | A     | 28  | TRP  | CB-CA-C    | 5.13  | 119.56      | 110.85   |
| 1   | B     | 33  | LYS  | CD-CE-NZ   | -5.12 | 95.51       | 111.90   |
| 1   | A     | 27  | ASN  | CB-CG-ND2  | -5.11 | 108.73      | 116.40   |
| 1   | B     | 38  | PHE  | CA-C-N     | 5.11  | 129.56      | 122.77   |
| 1   | B     | 38  | PHE  | C-N-CA     | 5.11  | 129.56      | 122.77   |
| 1   | B     | 123 | TRP  | CA-CB-CG   | -5.11 | 103.90      | 113.60   |
| 1   | B     | 79  | PRO  | N-CA-CB    | 5.10  | 108.09      | 103.34   |
| 1   | B     | 105 | MET  | N-CA-C     | 5.10  | 119.37      | 113.20   |
| 1   | A     | 118 | THR  | CA-CB-CG2  | -5.10 | 101.84      | 110.50   |
| 1   | B     | 10  | ALA  | O-C-N      | 5.09  | 127.95      | 122.15   |
| 1   | A     | 20  | TYR  | CA-C-O     | 5.08  | 126.66      | 120.81   |
| 1   | A     | 33  | LYS  | CD-CE-NZ   | -5.08 | 95.63       | 111.90   |
| 1   | B     | 122 | ALA  | N-CA-C     | 5.08  | 117.56      | 111.71   |
| 1   | A     | 121 | GLN  | O-C-N      | -5.07 | 115.81      | 122.39   |
| 1   | A     | 64  | CYS  | N-CA-C     | -5.06 | 101.59      | 109.24   |
| 1   | B     | 118 | THR  | N-CA-C     | 5.06  | 117.55      | 109.81   |
| 1   | A     | 101 | ASP  | CB-CG-OD2  | -5.05 | 106.79      | 118.40   |
| 1   | A     | 109 | VAL  | CA-CB-CG1  | -5.04 | 101.83      | 110.40   |
| 1   | B     | 122 | ALA  | N-CA-CB    | -5.04 | 102.46      | 110.22   |
| 1   | A     | 69  | THR  | OG1-CB-CG2 | -5.04 | 99.23       | 109.30   |
| 1   | B     | 15  | HIS  | N-CA-CB    | -5.03 | 102.71      | 110.46   |
| 1   | B     | 44  | ASN  | CA-CB-CG   | -5.03 | 107.57      | 112.60   |
| 1   | B     | 37  | ASN  | CA-C-N     | -5.03 | 115.91      | 124.31   |
| 1   | B     | 37  | ASN  | C-N-CA     | -5.03 | 115.91      | 124.31   |
| 1   | A     | 65  | ASN  | CB-CA-C    | 5.03  | 118.05      | 109.75   |
| 1   | B     | 38  | PHE  | CA-CB-CG   | 5.02  | 118.82      | 113.80   |
| 1   | A     | 42  | ALA  | CB-CA-C    | -5.02 | 102.07      | 109.90   |
| 1   | A     | 59  | ASN  | CB-CG-OD1  | 5.01  | 130.82      | 120.80   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 14  | ARG  | Sidechain |
| 1   | B     | 21  | ARG  | Sidechain |
| 1   | B     | 61  | ARG  | Sidechain |

## 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     | 1001  | 0        | 957      | 144     | 0            |
| 1   | B     | 1001  | 0        | 952      | 92      | 0            |
| 2   | A     | 11    | 0        | 0        | 2       | 0            |
| 2   | B     | 6     | 0        | 0        | 2       | 0            |
| 3   | A     | 143   | 0        | 0        | 6       | 0            |
| 3   | B     | 168   | 0        | 0        | 8       | 0            |
| All | All   | 2330  | 0        | 1909     | 237     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 60.

All (237) 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:14:ARG:CD   | 1:A:14:ARG:CG   | 1.78                     | 1.61              |
| 1:B:21:ARG:CB   | 1:B:21:ARG:CA   | 1.77                     | 1.60              |
| 1:B:15:HIS:CG   | 1:B:15:HIS:CB   | 1.80                     | 1.60              |
| 1:A:45:ARG:CB   | 1:A:45:ARG:CA   | 1.74                     | 1.59              |
| 1:B:76:CYS:CA   | 1:B:76:CYS:CB   | 1.74                     | 1.59              |
| 1:A:44:ASN:CB   | 1:A:44:ASN:CG   | 1.75                     | 1.59              |
| 1:A:76:CYS:CB   | 1:A:76:CYS:CA   | 1.74                     | 1.59              |
| 1:A:68:ARG:CD   | 1:A:68:ARG:CG   | 1.81                     | 1.58              |
| 1:B:21:ARG:CB   | 1:B:21:ARG:CG   | 1.82                     | 1.58              |
| 1:B:72:SER:CB   | 1:B:72:SER:CA   | 1.76                     | 1.58              |
| 1:B:46:ASN:CG   | 1:B:46:ASN:CB   | 1.74                     | 1.57              |
| 1:B:124:ILE:CD1 | 1:B:124:ILE:CG1 | 1.75                     | 1.57              |
| 1:B:58:ILE:CB   | 1:B:58:ILE:CG2  | 1.74                     | 1.57              |
| 1:B:1:LYS:CE    | 1:B:1:LYS:CD    | 1.81                     | 1.56              |
| 1:A:93:ASN:CG   | 1:A:93:ASN:CB   | 1.76                     | 1.56              |
| 1:B:37:ASN:CA   | 1:B:37:ASN:C    | 1.75                     | 1.55              |
| 1:A:112:ARG:CD  | 1:A:112:ARG:CG  | 1.81                     | 1.55              |
| 1:B:85:SER:C    | 1:B:85:SER:CA   | 1.76                     | 1.55              |
| 1:B:121:GLN:CD  | 1:B:121:GLN:CG  | 1.79                     | 1.55              |
| 1:A:127:CYS:C   | 1:A:127:CYS:CA  | 1.80                     | 1.54              |
| 1:B:61:ARG:CD   | 1:B:61:ARG:CG   | 1.83                     | 1.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:112:ARG:NH2  | 1:A:112:ARG:CZ   | 1.71                     | 1.54              |
| 1:A:21:ARG:N     | 1:A:21:ARG:CA    | 1.69                     | 1.53              |
| 1:A:101:ASP:CG   | 1:A:101:ASP:CB   | 1.80                     | 1.53              |
| 1:A:128:ARG:C    | 1:A:128:ARG:CA   | 1.79                     | 1.53              |
| 1:A:33:LYS:CE    | 1:A:33:LYS:CD    | 1.85                     | 1.53              |
| 1:A:72:SER:CB    | 1:A:72:SER:CA    | 1.82                     | 1.52              |
| 1:A:61:ARG:CD    | 1:A:61:ARG:CG    | 1.87                     | 1.51              |
| 1:A:62:TRP:CA    | 1:A:62:TRP:CB    | 1.87                     | 1.51              |
| 1:A:68:ARG:CD    | 1:A:68:ARG:NE    | 1.73                     | 1.50              |
| 1:B:61:ARG:NH2   | 1:B:61:ARG:CZ    | 1.67                     | 1.50              |
| 1:A:2:VAL:C      | 1:A:2:VAL:CA     | 1.82                     | 1.50              |
| 1:A:78:ILE:CB    | 1:A:78:ILE:CA    | 1.89                     | 1.49              |
| 1:A:48:ASP:CB    | 1:A:48:ASP:CA    | 1.85                     | 1.49              |
| 1:B:121:GLN:CD   | 1:B:121:GLN:NE2  | 1.69                     | 1.49              |
| 1:B:128:ARG:CD   | 1:B:128:ARG:CG   | 1.87                     | 1.49              |
| 1:B:73:ARG:CZ    | 1:B:73:ARG:NH1   | 1.74                     | 1.48              |
| 1:A:47:THR:CG2   | 1:A:47:THR:CB    | 1.87                     | 1.47              |
| 1:A:128:ARG:CA   | 1:A:128:ARG:N    | 1.75                     | 1.46              |
| 1:B:43:THR:CB    | 1:B:43:THR:CG2   | 1.91                     | 1.45              |
| 1:A:122:ALA:C    | 1:A:122:ALA:CA   | 1.87                     | 1.44              |
| 1:B:128:ARG:NH2  | 1:B:128:ARG:CZ   | 1.79                     | 1.43              |
| 1:B:114:ARG:NE   | 1:B:114:ARG:CZ   | 1.81                     | 1.42              |
| 1:B:128:ARG:CZ   | 1:B:128:ARG:NE   | 1.83                     | 1.41              |
| 1:A:129:LEU:CB   | 1:A:129:LEU:CA   | 1.99                     | 1.40              |
| 1:A:30:CYS:CB    | 1:A:30:CYS:SG    | 2.09                     | 1.40              |
| 1:A:87:ASP:CB    | 1:A:87:ASP:CA    | 1.95                     | 1.40              |
| 1:A:14:ARG:CD    | 1:A:14:ARG:NE    | 1.84                     | 1.39              |
| 1:B:69:THR:OG1   | 1:B:69:THR:CB    | 1.73                     | 1.37              |
| 1:A:48:ASP:C     | 1:A:49:GLY:N     | 1.86                     | 1.34              |
| 1:B:128:ARG:CD   | 1:B:128:ARG:HH11 | 1.38                     | 1.34              |
| 1:A:121:GLN:CG   | 1:A:121:GLN:CB   | 2.15                     | 1.24              |
| 1:B:47:THR:OG1   | 1:B:47:THR:CB    | 1.86                     | 1.23              |
| 1:A:87:ASP:CB    | 1:A:87:ASP:CG    | 2.14                     | 1.20              |
| 1:B:128:ARG:CD   | 1:B:128:ARG:NH1  | 2.05                     | 1.19              |
| 1:B:128:ARG:HH11 | 1:B:128:ARG:HD3  | 1.07                     | 1.19              |
| 1:A:87:ASP:CB    | 1:A:87:ASP:OD2   | 1.95                     | 1.15              |
| 1:A:45:ARG:CB    | 1:A:45:ARG:CG    | 2.31                     | 1.08              |
| 1:A:121:GLN:CB   | 1:A:121:GLN:CD   | 2.27                     | 1.07              |
| 1:A:14:ARG:CD    | 1:A:14:ARG:CZ    | 2.33                     | 1.07              |
| 1:B:61:ARG:CZ    | 1:B:61:ARG:NH1   | 2.18                     | 1.06              |
| 1:B:61:ARG:CG    | 1:B:61:ARG:NE    | 2.20                     | 1.05              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:127:CYS:C    | 1:A:128:ARG:CA  | 2.29                     | 1.04              |
| 1:A:112:ARG:CG   | 1:A:112:ARG:NE  | 2.20                     | 1.04              |
| 1:A:112:ARG:HD3  | 3:A:350:HOH:O   | 1.58                     | 1.02              |
| 1:A:129:LEU:CB   | 1:A:129:LEU:N   | 2.21                     | 1.02              |
| 1:A:68:ARG:CD    | 1:A:68:ARG:CZ   | 2.37                     | 1.00              |
| 1:A:14:ARG:CD    | 1:A:14:ARG:CB   | 2.41                     | 0.99              |
| 1:A:78:ILE:CA    | 1:A:78:ILE:CG1  | 2.41                     | 0.98              |
| 1:A:73:ARG:HD3   | 3:A:302:HOH:O   | 1.64                     | 0.97              |
| 1:A:48:ASP:C     | 1:A:49:GLY:CA   | 2.38                     | 0.96              |
| 1:B:43:THR:CG2   | 1:B:43:THR:CA   | 2.44                     | 0.96              |
| 1:B:128:ARG:NH1  | 1:B:128:ARG:HD3 | 1.75                     | 0.95              |
| 1:B:18:ASP:OD1   | 3:B:334:HOH:O   | 1.85                     | 0.95              |
| 1:B:114:ARG:CZ   | 1:B:114:ARG:CD  | 2.44                     | 0.94              |
| 1:A:44:ASN:CB    | 1:A:44:ASN:OD1  | 2.14                     | 0.94              |
| 1:A:33:LYS:CE    | 1:A:33:LYS:CG   | 2.44                     | 0.94              |
| 1:A:78:ILE:CB    | 1:A:78:ILE:C    | 2.40                     | 0.93              |
| 1:A:47:THR:CG2   | 1:A:47:THR:OG1  | 2.15                     | 0.93              |
| 1:B:124:ILE:CD1  | 1:B:124:ILE:CB  | 2.47                     | 0.93              |
| 1:B:128:ARG:CD   | 1:B:128:ARG:CZ  | 2.46                     | 0.92              |
| 1:B:21:ARG:CA    | 1:B:21:ARG:CG   | 2.49                     | 0.90              |
| 1:B:43:THR:CG2   | 1:B:43:THR:OG1  | 2.19                     | 0.90              |
| 1:A:128:ARG:CA   | 1:A:128:ARG:O   | 2.19                     | 0.89              |
| 1:B:128:ARG:HH11 | 1:B:128:ARG:HD2 | 1.38                     | 0.87              |
| 1:B:72:SER:CB    | 1:B:72:SER:N    | 2.39                     | 0.85              |
| 1:B:47:THR:OG1   | 1:B:47:THR:CA   | 2.24                     | 0.85              |
| 1:B:76:CYS:CB    | 1:B:76:CYS:C    | 2.49                     | 0.85              |
| 1:B:15:HIS:CG    | 1:B:15:HIS:CA   | 2.60                     | 0.85              |
| 1:B:58:ILE:CG2   | 1:B:58:ILE:CA   | 2.54                     | 0.85              |
| 1:B:21:ARG:CB    | 1:B:21:ARG:C    | 2.51                     | 0.84              |
| 1:A:87:ASP:CB    | 1:A:87:ASP:C    | 2.51                     | 0.84              |
| 1:A:14:ARG:HD3   | 1:A:14:ARG:HH11 | 1.41                     | 0.83              |
| 1:B:72:SER:CB    | 1:B:72:SER:C    | 2.53                     | 0.81              |
| 1:A:93:ASN:CG    | 1:A:93:ASN:CA   | 2.52                     | 0.81              |
| 1:A:78:ILE:CB    | 1:A:78:ILE:N    | 2.45                     | 0.79              |
| 1:A:48:ASP:C     | 1:A:49:GLY:HA3  | 2.06                     | 0.79              |
| 1:A:122:ALA:C    | 1:A:122:ALA:CB  | 2.56                     | 0.79              |
| 1:A:127:CYS:CA   | 1:A:128:ARG:N   | 2.46                     | 0.79              |
| 1:B:73:ARG:NH1   | 1:B:73:ARG:NE   | 2.29                     | 0.78              |
| 1:A:68:ARG:CD    | 1:A:68:ARG:CB   | 2.56                     | 0.78              |
| 1:B:128:ARG:NH2  | 1:B:128:ARG:NE  | 2.31                     | 0.78              |
| 1:B:69:THR:OG1   | 1:B:69:THR:CG2  | 2.32                     | 0.78              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:37:ASN:C    | 1:B:37:ASN:CB   | 2.56                     | 0.77              |
| 1:A:2:VAL:C     | 1:A:2:VAL:CB    | 2.54                     | 0.77              |
| 1:B:128:ARG:CG  | 1:B:128:ARG:NE  | 2.46                     | 0.77              |
| 1:A:127:CYS:CA  | 1:A:127:CYS:O   | 2.33                     | 0.77              |
| 1:B:61:ARG:CD   | 1:B:61:ARG:CB   | 2.62                     | 0.77              |
| 1:B:37:ASN:C    | 1:B:37:ASN:N    | 2.43                     | 0.76              |
| 1:A:62:TRP:CB   | 1:A:62:TRP:N    | 2.48                     | 0.76              |
| 1:B:46:ASN:CG   | 1:B:46:ASN:CA   | 2.59                     | 0.76              |
| 1:A:20:TYR:C    | 1:A:21:ARG:CA   | 2.56                     | 0.76              |
| 1:A:112:ARG:NH2 | 1:A:112:ARG:NH1 | 2.21                     | 0.76              |
| 1:A:112:ARG:NE  | 1:A:112:ARG:HG2 | 1.99                     | 0.76              |
| 1:B:85:SER:C    | 1:B:85:SER:CB   | 2.60                     | 0.75              |
| 1:A:76:CYS:CB   | 1:A:76:CYS:C    | 2.60                     | 0.75              |
| 1:A:112:ARG:CD  | 1:A:112:ARG:CZ  | 2.63                     | 0.75              |
| 1:A:48:ASP:CA   | 1:A:48:ASP:CG   | 2.60                     | 0.75              |
| 1:A:45:ARG:NE   | 1:A:45:ARG:NH2  | 2.31                     | 0.74              |
| 1:A:48:ASP:O    | 1:A:49:GLY:HA3  | 1.86                     | 0.74              |
| 1:B:58:ILE:CG2  | 1:B:58:ILE:CG1  | 2.65                     | 0.74              |
| 1:A:48:ASP:CB   | 1:A:48:ASP:C    | 2.60                     | 0.73              |
| 1:B:121:GLN:CG  | 1:B:121:GLN:NE2 | 2.52                     | 0.72              |
| 1:A:62:TRP:CB   | 1:A:62:TRP:C    | 2.62                     | 0.72              |
| 1:B:72:SER:CA   | 1:B:72:SER:OG   | 2.34                     | 0.72              |
| 1:A:14:ARG:CD   | 1:A:14:ARG:NH1  | 2.53                     | 0.72              |
| 1:A:21:ARG:N    | 1:A:21:ARG:C    | 2.48                     | 0.71              |
| 1:A:61:ARG:CD   | 1:A:61:ARG:CB   | 2.68                     | 0.71              |
| 1:A:72:SER:CA   | 1:A:72:SER:OG   | 2.38                     | 0.71              |
| 1:A:76:CYS:CA   | 1:A:76:CYS:SG   | 2.79                     | 0.71              |
| 1:B:114:ARG:NE  | 1:B:114:ARG:NH2 | 2.39                     | 0.70              |
| 1:A:72:SER:CB   | 1:A:72:SER:N    | 2.54                     | 0.70              |
| 1:B:114:ARG:CZ  | 1:B:114:ARG:HD3 | 2.22                     | 0.69              |
| 1:A:14:ARG:HD3  | 1:A:14:ARG:NH1  | 2.06                     | 0.69              |
| 1:A:76:CYS:CB   | 1:A:76:CYS:N    | 2.55                     | 0.69              |
| 1:A:72:SER:CB   | 1:A:72:SER:C    | 2.64                     | 0.69              |
| 1:A:129:LEU:CB  | 1:A:129:LEU:C   | 2.65                     | 0.68              |
| 1:A:121:GLN:CD  | 1:A:121:GLN:HB3 | 2.20                     | 0.67              |
| 1:B:46:ASN:CB   | 1:B:46:ASN:ND2  | 2.58                     | 0.67              |
| 1:A:93:ASN:CB   | 1:A:93:ASN:OD1  | 2.42                     | 0.67              |
| 1:B:21:ARG:CB   | 1:B:21:ARG:N    | 2.57                     | 0.66              |
| 1:A:122:ALA:CA  | 1:A:123:TRP:N   | 2.55                     | 0.66              |
| 1:A:101:ASP:CG  | 1:A:101:ASP:CA  | 2.69                     | 0.65              |
| 1:A:112:ARG:CD  | 1:A:112:ARG:CB  | 2.67                     | 0.65              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:30:CYS:SG   | 1:A:30:CYS:CA   | 2.84                     | 0.65              |
| 2:A:134:IOD:I   | 3:B:198:HOH:O   | 2.84                     | 0.64              |
| 1:A:44:ASN:CG   | 1:A:44:ASN:CA   | 2.69                     | 0.64              |
| 1:A:101:ASP:CB  | 1:A:101:ASP:OD2 | 2.39                     | 0.64              |
| 1:B:15:HIS:HB3  | 1:B:92:VAL:HG11 | 1.78                     | 0.64              |
| 1:A:78:ILE:CA   | 1:A:78:ILE:HG13 | 2.26                     | 0.64              |
| 1:A:33:LYS:CD   | 1:A:33:LYS:NZ   | 2.60                     | 0.64              |
| 1:A:47:THR:CB   | 1:A:47:THR:N    | 2.58                     | 0.64              |
| 1:A:125:ARG:NH1 | 1:A:125:ARG:HD3 | 2.12                     | 0.64              |
| 1:A:129:LEU:N   | 1:A:129:LEU:HG  | 2.13                     | 0.63              |
| 1:A:63:TRP:O    | 1:A:76:CYS:HB2  | 1.99                     | 0.63              |
| 1:B:76:CYS:CA   | 1:B:76:CYS:SG   | 2.87                     | 0.62              |
| 1:B:1:LYS:CD    | 1:B:1:LYS:NZ    | 2.56                     | 0.62              |
| 1:A:93:ASN:HA   | 1:A:93:ASN:HD22 | 1.65                     | 0.62              |
| 1:A:21:ARG:N    | 1:A:21:ARG:CB   | 2.63                     | 0.61              |
| 1:B:121:GLN:CG  | 1:B:121:GLN:OE1 | 2.41                     | 0.61              |
| 1:A:48:ASP:C    | 1:A:48:ASP:CG   | 2.70                     | 0.60              |
| 1:A:14:ARG:CD   | 1:A:14:ARG:HB2  | 2.31                     | 0.60              |
| 1:A:129:LEU:CB  | 1:A:129:LEU:H   | 2.09                     | 0.59              |
| 1:A:111:TRP:CD1 | 1:A:115:CYS:HB2 | 2.40                     | 0.56              |
| 1:A:75:LEU:HA   | 3:A:313:HOH:O   | 2.05                     | 0.55              |
| 1:A:88:ILE:HG12 | 2:A:133:IOD:I   | 2.77                     | 0.55              |
| 1:A:2:VAL:CA    | 1:A:2:VAL:O     | 2.50                     | 0.55              |
| 1:A:93:ASN:HA   | 1:A:93:ASN:ND2  | 2.22                     | 0.55              |
| 1:A:14:ARG:CZ   | 1:A:14:ARG:HD3  | 2.27                     | 0.55              |
| 1:B:73:ARG:NH1  | 1:B:73:ARG:CD   | 2.69                     | 0.55              |
| 1:A:68:ARG:CD   | 1:A:68:ARG:NH1  | 2.70                     | 0.55              |
| 1:A:45:ARG:CB   | 1:A:45:ARG:C    | 2.72                     | 0.55              |
| 1:A:127:CYS:C   | 1:A:127:CYS:CB  | 2.74                     | 0.54              |
| 1:A:129:LEU:H   | 1:A:129:LEU:HB2 | 1.73                     | 0.54              |
| 1:A:45:ARG:CA   | 1:A:45:ARG:CG   | 2.87                     | 0.53              |
| 1:A:62:TRP:CA   | 1:A:62:TRP:CG   | 2.88                     | 0.53              |
| 1:B:97:LYS:HE2  | 3:B:428:HOH:O   | 2.09                     | 0.53              |
| 1:A:45:ARG:CB   | 1:A:45:ARG:N    | 2.62                     | 0.52              |
| 1:A:15:HIS:HD2  | 3:A:444:HOH:O   | 1.93                     | 0.51              |
| 1:B:69:THR:O    | 1:B:72:SER:HB3  | 2.10                     | 0.51              |
| 1:B:76:CYS:CB   | 1:B:76:CYS:N    | 2.58                     | 0.51              |
| 1:A:14:ARG:CG   | 1:A:14:ARG:NE   | 2.74                     | 0.50              |
| 1:B:61:ARG:CG   | 1:B:61:ARG:CZ   | 2.86                     | 0.50              |
| 1:A:61:ARG:CG   | 1:A:61:ARG:NE   | 2.69                     | 0.50              |
| 1:A:128:ARG:N   | 1:A:128:ARG:CB  | 2.66                     | 0.49              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:93:ASN:CG   | 1:A:93:ASN:HA   | 2.34                     | 0.49              |
| 1:A:47:THR:N    | 1:A:48:ASP:N    | 2.59                     | 0.49              |
| 1:B:85:SER:CA   | 1:B:85:SER:O    | 2.46                     | 0.49              |
| 1:A:128:ARG:C   | 1:A:128:ARG:N   | 2.71                     | 0.48              |
| 1:A:87:ASP:CB   | 1:A:87:ASP:N    | 2.73                     | 0.48              |
| 1:A:68:ARG:CG   | 1:A:68:ARG:NE   | 2.74                     | 0.48              |
| 1:A:47:THR:N    | 1:A:47:THR:C    | 2.71                     | 0.48              |
| 1:A:78:ILE:CA   | 1:A:78:ILE:CD1  | 2.92                     | 0.48              |
| 1:B:21:ARG:HA   | 1:B:21:ARG:HD3  | 1.96                     | 0.47              |
| 1:A:63:TRP:CE2  | 1:A:98:ILE:HG12 | 2.49                     | 0.47              |
| 1:B:128:ARG:NH1 | 1:B:128:ARG:HD2 | 2.07                     | 0.47              |
| 1:B:96:LYS:NZ   | 3:B:384:HOH:O   | 2.47                     | 0.47              |
| 1:A:78:ILE:HG13 | 1:A:79:PRO:HD2  | 1.96                     | 0.47              |
| 1:B:1:LYS:HE3   | 3:B:342:HOH:O   | 2.15                     | 0.47              |
| 1:B:43:THR:CG2  | 1:B:43:THR:N    | 2.78                     | 0.47              |
| 1:A:129:LEU:CA  | 1:A:129:LEU:CG  | 2.81                     | 0.46              |
| 1:A:45:ARG:CB   | 1:A:45:ARG:HA   | 2.19                     | 0.46              |
| 1:A:1:LYS:NZ    | 3:A:333:HOH:O   | 2.49                     | 0.45              |
| 1:B:68:ARG:HH11 | 1:B:68:ARG:HD2  | 1.60                     | 0.45              |
| 1:A:93:ASN:CA   | 1:A:93:ASN:ND2  | 2.77                     | 0.45              |
| 1:A:121:GLN:CG  | 1:A:121:GLN:CA  | 2.94                     | 0.45              |
| 1:B:48:ASP:OD1  | 1:B:48:ASP:C    | 2.58                     | 0.45              |
| 1:A:33:LYS:NZ   | 3:A:415:HOH:O   | 2.50                     | 0.44              |
| 1:B:68:ARG:NH2  | 3:B:267:HOH:O   | 2.48                     | 0.44              |
| 1:A:18:ASP:O    | 1:A:19:ASN:HB2  | 2.18                     | 0.44              |
| 1:B:121:GLN:CD  | 1:B:121:GLN:CB  | 2.78                     | 0.44              |
| 1:B:121:GLN:HG2 | 2:B:131:IOD:I   | 2.87                     | 0.44              |
| 1:A:14:ARG:HD3  | 1:A:14:ARG:HB2  | 1.98                     | 0.44              |
| 1:A:2:VAL:C     | 1:A:2:VAL:CG1   | 2.90                     | 0.44              |
| 1:A:78:ILE:C    | 1:A:78:ILE:HG13 | 2.42                     | 0.44              |
| 1:B:97:LYS:CE   | 3:B:428:HOH:O   | 2.66                     | 0.44              |
| 1:A:51:THR:HB   | 1:A:53:TYR:CE1  | 2.52                     | 0.44              |
| 1:B:58:ILE:CG2  | 1:B:58:ILE:C    | 2.91                     | 0.44              |
| 1:B:114:ARG:HD3 | 1:B:114:ARG:NH1 | 2.33                     | 0.44              |
| 1:B:128:ARG:CD  | 1:B:128:ARG:CB  | 2.84                     | 0.44              |
| 1:A:48:ASP:CB   | 1:A:48:ASP:N    | 2.73                     | 0.43              |
| 1:A:78:ILE:CA   | 1:A:78:ILE:HD12 | 2.49                     | 0.43              |
| 1:B:61:ARG:NH1  | 1:B:61:ARG:HB2  | 2.33                     | 0.43              |
| 1:A:2:VAL:C     | 1:A:2:VAL:N     | 2.72                     | 0.42              |
| 1:A:14:ARG:CD   | 1:A:14:ARG:HH11 | 2.13                     | 0.42              |
| 1:B:88:ILE:HG12 | 2:B:138:IOD:I   | 2.90                     | 0.41              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:121:GLN:NE2 | 1:B:121:GLN:HG3 | 2.34                     | 0.41              |
| 1:B:124:ILE:CD1 | 1:B:124:ILE:HB  | 2.42                     | 0.41              |
| 1:A:61:ARG:HH11 | 1:A:61:ARG:HD2  | 1.14                     | 0.41              |
| 1:B:46:ASN:HB3  | 3:B:356:HOH:O   | 2.20                     | 0.41              |
| 1:A:1:LYS:HB2   | 1:A:86:SER:OG   | 2.21                     | 0.41              |
| 1:A:47:THR:N    | 1:A:48:ASP:H    | 2.19                     | 0.41              |
| 1:A:73:ARG:O    | 1:A:74:ASN:C    | 2.62                     | 0.41              |
| 1:B:52:ASP:OD1  | 1:B:59:ASN:HB2  | 2.21                     | 0.40              |
| 1:A:8:LEU:HD12  | 1:A:8:LEU:HA    | 1.87                     | 0.40              |
| 1:B:73:ARG:NH1  | 1:B:73:ARG:NH2  | 2.54                     | 0.40              |
| 1:B:111:TRP:CD1 | 1:B:115:CYS:HB2 | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 127/129 (98%) | 126 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | B     | 127/129 (98%) | 124 (98%) | 3 (2%)  | 0        | 100         | 100 |
| All | All   | 254/258 (98%) | 250 (98%) | 4 (2%)  | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 105/105 (100%) | 102 (97%) | 3 (3%)   | 37          | 14 |
| 1   | B     | 105/105 (100%) | 101 (96%) | 4 (4%)   | 29          | 9  |
| All | All   | 210/210 (100%) | 203 (97%) | 7 (3%)   | 33          | 12 |

All (7) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 44  | ASN  |
| 1   | A     | 55  | ILE  |
| 1   | A     | 86  | SER  |
| 1   | B     | 61  | ARG  |
| 1   | B     | 68  | ARG  |
| 1   | B     | 112 | ARG  |
| 1   | B     | 129 | LEU  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 46  | ASN  |
| 1   | A     | 57  | GLN  |
| 1   | A     | 65  | ASN  |
| 1   | A     | 77  | ASN  |
| 1   | A     | 93  | ASN  |
| 1   | B     | 44  | ASN  |
| 1   | B     | 57  | GLN  |
| 1   | B     | 77  | ASN  |
| 1   | B     | 121 | 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](#)

Of 17 ligands modelled in this entry, 17 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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   | B     | 11               |
| 1   | A     | 10               |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 48:ASP    | C      | 49:GLY    | N      | 1.86         |
| 1     | A     | 71:GLY    | C      | 72:SER    | N      | 1.19         |
| 1     | A     | 73:ARG    | C      | 74:ASN    | N      | 1.19         |
| 1     | B     | 43:THR    | C      | 44:ASN    | N      | 1.19         |
| 1     | B     | 84:LEU    | C      | 85:SER    | N      | 1.19         |
| 1     | B     | 102:GLY   | C      | 103:ASN   | N      | 1.19         |
| 1     | B     | 22:GLY    | C      | 23:TYR    | N      | 1.18         |
| 1     | B     | 88:ILE    | C      | 89:THR    | N      | 1.18         |
| 1     | A     | 75:LEU    | C      | 76:CYS    | N      | 1.17         |
| 1     | A     | 128:ARG   | C      | 129:LEU   | N      | 1.17         |
| 1     | B     | 99:VAL    | C      | 100:SER   | N      | 1.17         |
| 1     | B     | 114:ARG   | C      | 115:CYS   | N      | 1.17         |
| 1     | A     | 2:VAL     | C      | 3:PHE     | N      | 1.16         |
| 1     | A     | 4:GLY     | C      | 5:ARG     | N      | 1.16         |
| 1     | A     | 5:ARG     | C      | 6:CYS     | N      | 1.16         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 15:HIS    | C      | 16:GLY    | N      | 1.16         |
| 1     | A     | 107:ALA   | C      | 108:TRP   | N      | 1.15         |
| 1     | B     | 68:ARG    | C      | 69:THR    | N      | 1.14         |
| 1     | B     | 45:ARG    | C      | 46:ASN    | N      | 1.11         |
| 1     | B     | 49:GLY    | C      | 50:SER    | N      | 1.10         |
| 1     | B     | 42:ALA    | C      | 43:THR    | N      | 1.06         |

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2                                                                                                                                                                         | OWAB(Å <sup>2</sup> ) | Q<0.9    |
|-----|-------|----------------|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------|----------|
| 1   | A     | 129/129 (100%) | 2.33   | 68 (52%)    | 1, 5, 7, 8            | 20 (15%) |
| 1   | B     | 129/129 (100%) | 2.34   | 73 (56%)    | 1, 5, 8, 9            | 17 (13%) |
| All | All   | 258/258 (100%) | 2.34   | 141 (54%)   | 1, 5, 8, 9            | 37 (14%) |

All (141) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 126 | GLY  | 6.2  |
| 1   | A     | 51  | THR  | 6.1  |
| 1   | B     | 88  | ILE  | 5.8  |
| 1   | A     | 69  | THR  | 5.7  |
| 1   | B     | 124 | ILE  | 5.6  |
| 1   | B     | 36  | SER  | 5.3  |
| 1   | B     | 8   | LEU  | 5.3  |
| 1   | B     | 71  | GLY  | 5.2  |
| 1   | B     | 110 | ALA  | 5.2  |
| 1   | B     | 72  | SER  | 5.1  |
| 1   | A     | 102 | GLY  | 5.1  |
| 1   | B     | 34  | PHE  | 5.0  |
| 1   | B     | 108 | TRP  | 5.0  |
| 1   | A     | 11  | ALA  | 4.9  |
| 1   | A     | 82  | ALA  | 4.9  |
| 1   | A     | 119 | ASP  | 4.8  |
| 1   | A     | 72  | SER  | 4.8  |
| 1   | A     | 104 | GLY  | 4.8  |
| 1   | A     | 44  | ASN  | 4.7  |
| 1   | B     | 107 | ALA  | 4.7  |
| 1   | B     | 75  | LEU  | 4.5  |
| 1   | B     | 128 | ARG  | 4.5  |
| 1   | B     | 58  | ILE  | 4.4  |
| 1   | B     | 85  | SER  | 4.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 10  | ALA  | 4.3  |
| 1   | A     | 112 | ARG  | 4.3  |
| 1   | B     | 90  | ALA  | 4.2  |
| 1   | A     | 108 | TRP  | 4.2  |
| 1   | B     | 64  | CYS  | 4.1  |
| 1   | A     | 113 | ASN  | 4.1  |
| 1   | A     | 56  | LEU  | 4.1  |
| 1   | A     | 59  | ASN  | 4.0  |
| 1   | A     | 127 | CYS  | 3.9  |
| 1   | B     | 23  | TYR  | 3.7  |
| 1   | A     | 129 | LEU  | 3.7  |
| 1   | A     | 90  | ALA  | 3.6  |
| 1   | A     | 109 | VAL  | 3.6  |
| 1   | A     | 77  | ASN  | 3.6  |
| 1   | A     | 30  | CYS  | 3.6  |
| 1   | B     | 81  | SER  | 3.5  |
| 1   | A     | 62  | TRP  | 3.5  |
| 1   | A     | 88  | ILE  | 3.5  |
| 1   | A     | 39  | ASN  | 3.5  |
| 1   | B     | 46  | ASN  | 3.5  |
| 1   | B     | 11  | ALA  | 3.4  |
| 1   | B     | 129 | LEU  | 3.4  |
| 1   | B     | 24  | SER  | 3.4  |
| 1   | B     | 119 | ASP  | 3.4  |
| 1   | B     | 104 | GLY  | 3.3  |
| 1   | B     | 40  | THR  | 3.3  |
| 1   | A     | 2   | VAL  | 3.3  |
| 1   | B     | 9   | ALA  | 3.3  |
| 1   | A     | 75  | LEU  | 3.3  |
| 1   | A     | 34  | PHE  | 3.3  |
| 1   | A     | 107 | ALA  | 3.3  |
| 1   | B     | 59  | ASN  | 3.3  |
| 1   | B     | 67  | GLY  | 3.2  |
| 1   | B     | 78  | ILE  | 3.2  |
| 1   | B     | 76  | CYS  | 3.2  |
| 1   | B     | 115 | CYS  | 3.2  |
| 1   | B     | 94  | CYS  | 3.2  |
| 1   | B     | 51  | THR  | 3.2  |
| 1   | A     | 54  | GLY  | 3.1  |
| 1   | A     | 55  | ILE  | 3.1  |
| 1   | A     | 58  | ILE  | 3.1  |
| 1   | A     | 9   | ALA  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 78  | ILE  | 3.1  |
| 1   | B     | 127 | CYS  | 3.1  |
| 1   | A     | 6   | CYS  | 3.0  |
| 1   | A     | 13  | LYS  | 3.0  |
| 1   | B     | 100 | SER  | 3.0  |
| 1   | A     | 57  | GLN  | 2.9  |
| 1   | B     | 47  | THR  | 2.9  |
| 1   | A     | 63  | TRP  | 2.9  |
| 1   | A     | 8   | LEU  | 2.9  |
| 1   | B     | 63  | TRP  | 2.9  |
| 1   | A     | 52  | ASP  | 2.9  |
| 1   | B     | 101 | ASP  | 2.9  |
| 1   | A     | 60  | SER  | 2.9  |
| 1   | A     | 111 | TRP  | 2.9  |
| 1   | B     | 7   | GLU  | 2.8  |
| 1   | B     | 77  | ASN  | 2.8  |
| 1   | B     | 82  | ALA  | 2.8  |
| 1   | A     | 29  | VAL  | 2.8  |
| 1   | B     | 112 | ARG  | 2.8  |
| 1   | A     | 19  | ASN  | 2.7  |
| 1   | B     | 103 | ASN  | 2.7  |
| 1   | B     | 96  | LYS  | 2.7  |
| 1   | A     | 67  | GLY  | 2.6  |
| 1   | B     | 56  | LEU  | 2.6  |
| 1   | B     | 98  | ILE  | 2.6  |
| 1   | B     | 4   | GLY  | 2.6  |
| 1   | A     | 106 | ASN  | 2.6  |
| 1   | B     | 32  | ALA  | 2.6  |
| 1   | A     | 4   | GLY  | 2.5  |
| 1   | A     | 18  | ASP  | 2.5  |
| 1   | B     | 79  | PRO  | 2.5  |
| 1   | B     | 38  | PHE  | 2.5  |
| 1   | B     | 122 | ALA  | 2.5  |
| 1   | A     | 45  | ARG  | 2.5  |
| 1   | B     | 111 | TRP  | 2.4  |
| 1   | A     | 100 | SER  | 2.4  |
| 1   | B     | 109 | VAL  | 2.4  |
| 1   | A     | 46  | ASN  | 2.4  |
| 1   | B     | 89  | THR  | 2.4  |
| 1   | A     | 14  | ARG  | 2.4  |
| 1   | B     | 22  | GLY  | 2.4  |
| 1   | B     | 43  | THR  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 16  | GLY  | 2.3  |
| 1   | A     | 71  | GLY  | 2.3  |
| 1   | B     | 45  | ARG  | 2.3  |
| 1   | B     | 54  | GLY  | 2.3  |
| 1   | A     | 125 | ARG  | 2.3  |
| 1   | B     | 12  | MET  | 2.3  |
| 1   | B     | 121 | GLN  | 2.3  |
| 1   | A     | 124 | ILE  | 2.3  |
| 1   | B     | 74  | ASN  | 2.3  |
| 1   | A     | 80  | CYS  | 2.3  |
| 1   | A     | 68  | ARG  | 2.3  |
| 1   | B     | 91  | SER  | 2.3  |
| 1   | B     | 15  | HIS  | 2.2  |
| 1   | B     | 21  | ARG  | 2.2  |
| 1   | A     | 24  | SER  | 2.2  |
| 1   | B     | 69  | THR  | 2.1  |
| 1   | A     | 21  | ARG  | 2.1  |
| 1   | A     | 26  | GLY  | 2.1  |
| 1   | A     | 96  | LYS  | 2.1  |
| 1   | B     | 68  | ARG  | 2.1  |
| 1   | A     | 23  | TYR  | 2.1  |
| 1   | B     | 117 | GLY  | 2.1  |
| 1   | B     | 57  | GLN  | 2.1  |
| 1   | A     | 17  | LEU  | 2.1  |
| 1   | A     | 73  | ARG  | 2.1  |
| 1   | B     | 28  | TRP  | 2.1  |
| 1   | A     | 20  | TYR  | 2.1  |
| 1   | A     | 122 | ALA  | 2.0  |
| 1   | A     | 47  | THR  | 2.0  |
| 1   | B     | 16  | GLY  | 2.0  |
| 1   | A     | 123 | TRP  | 2.0  |
| 1   | B     | 55  | ILE  | 2.0  |
| 1   | B     | 29  | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

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

| Mol | Type | Chain | Res | Atoms | RSCC  | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|-------|------|-----------------------------|-------|
| 2   | IOD  | A     | 143 | 1/1   | -0.15 | 0.18 | 6,6,6,6                     | 1     |
| 2   | IOD  | A     | 133 | 1/1   | 0.21  | 0.11 | 1,1,1,1                     | 1     |
| 2   | IOD  | A     | 142 | 1/1   | 0.24  | 0.11 | 4,4,4,4                     | 1     |
| 2   | IOD  | A     | 140 | 1/1   | 0.38  | 0.11 | 9,9,9,9                     | 1     |
| 2   | IOD  | B     | 131 | 1/1   | 0.38  | 0.21 | 0,0,0,0                     | 1     |
| 2   | IOD  | A     | 141 | 1/1   | 0.43  | 0.14 | 9,9,9,9                     | 1     |
| 2   | IOD  | A     | 132 | 1/1   | 0.58  | 0.14 | 6,6,6,6                     | 1     |
| 2   | IOD  | B     | 146 | 1/1   | 0.59  | 0.18 | 3,3,3,3                     | 1     |
| 2   | IOD  | A     | 135 | 1/1   | 0.60  | 0.07 | 0,0,0,0                     | 1     |
| 2   | IOD  | A     | 134 | 1/1   | 0.67  | 0.22 | 6,6,6,6                     | 1     |
| 2   | IOD  | B     | 139 | 1/1   | 0.72  | 0.09 | 8,8,8,8                     | 1     |
| 2   | IOD  | B     | 136 | 1/1   | 0.74  | 0.11 | 5,5,5,5                     | 1     |
| 2   | IOD  | B     | 138 | 1/1   | 0.74  | 0.13 | 5,5,5,5                     | 1     |
| 2   | IOD  | A     | 130 | 1/1   | 0.76  | 0.04 | 3,3,3,3                     | 1     |
| 2   | IOD  | A     | 145 | 1/1   | 0.77  | 0.06 | 5,5,5,5                     | 0     |
| 2   | IOD  | A     | 144 | 1/1   | 0.77  | 0.06 | 5,5,5,5                     | 1     |
| 2   | IOD  | B     | 137 | 1/1   | 0.86  | 0.08 | 8,8,8,8                     | 1     |

## 6.5 Other polymers

There are no such residues in this entry.