



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 12:48 AM EST

PDB ID : 4DFR  
Title : CRYSTAL STRUCTURES OF ESCHERICHIA COLI AND LACTO-  
BACILLUS CASEI DIHYDROFOLATE REDUCTASE REFINED AT 1.7  
ANGSTROMS RESOLUTION. I. GENERAL FEATURES AND BINDING  
OF METHOTREXATE  
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Deposited on : unknown  
Resolution : 1.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Mogul                          | : | 1.7.2 (RC1), CSD as538be (2017)                                    |
| Xtriage (Phenix)               | : | NOT EXECUTED   |
| EDS                            | : | NOT EXECUTED   |
| Percentile statistics          | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | rb-20030345  |

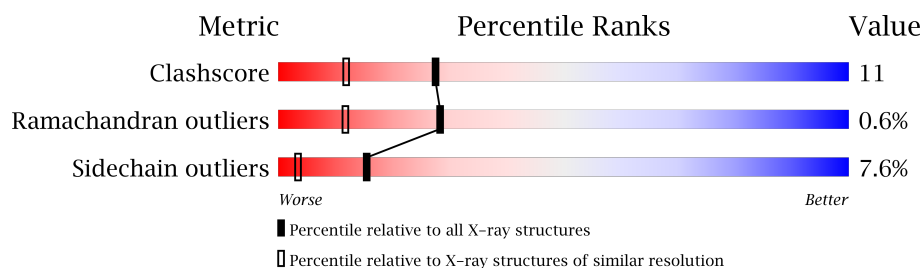
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 112137                      | 3876 (1.70-1.70)                                      |
| Ramachandran outliers | 110173                      | 3815 (1.70-1.70)                                      |
| Sidechain outliers    | 110143                      | 3815 (1.70-1.70)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|-------------------|
| 1   | A     | 159    | <br>13% 65% 18% . |
| 1   | B     | 159    | <br>8% 70% 16% 6% |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3035 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 DIHYDROFOLATE REDUCTASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 159      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1252  | 797 | 213 | 235 | 7 |         |         |       |
| 1   | B     | 159      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1286  | 817 | 222 | 240 | 7 |         |         |       |

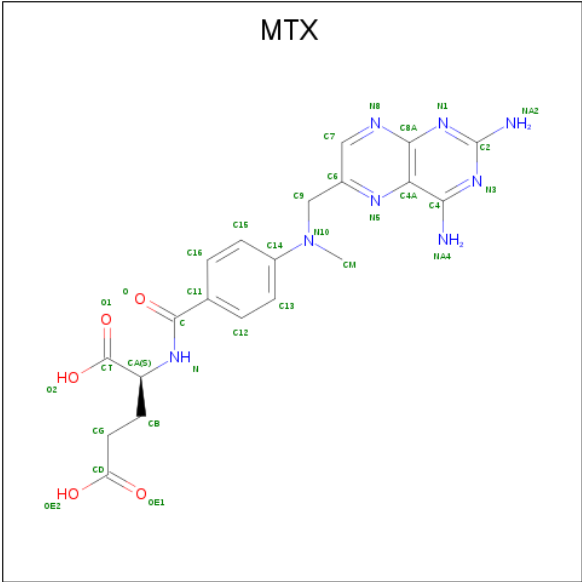
There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 37      | ASP      | ASN    | CONFLICT | UNP P0ABQ4 |
| A     | 154     | LYS      | GLU    | CONFLICT | UNP P0ABQ4 |
| B     | 37      | ASP      | ASN    | CONFLICT | UNP P0ABQ4 |
| B     | 154     | LYS      | GLU    | CONFLICT | UNP P0ABQ4 |

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | B     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | A     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is METHOTREXATE (three-letter code: MTX) (formula: C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 33    | 20 | 8 | 5 |         |         |
| 3   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 33    | 20 | 8 | 5 |         |         |

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 5   | A     | 239      | Total | O   | 0       | 0       |
|     |       |          | 239   | 239 |         |         |
| 5   | B     | 189      | Total | O   | 0       | 0       |
|     |       |          | 189   | 189 |         |         |

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

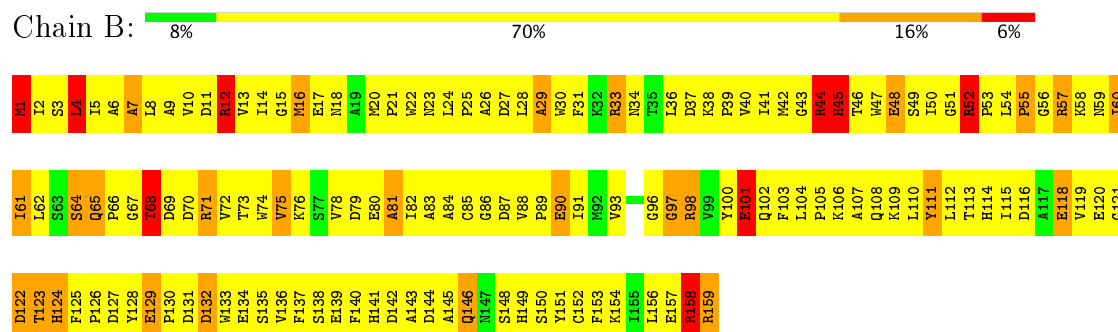
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

#### • Molecule 1: DIHYDROFOLATE REDUCTASE



#### • Molecule 1: DIHYDROFOLATE REDUCTASE



## 4 Data and refinement statistics

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

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | P 61  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 93.22Å 93.22Å 73.56Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å)   | (Not available) – 1.70                        | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) ((Not available)-1.70)        | Depositor |
| $R_{merge}$  | (Not available)                               | Depositor |
| $R_{sym}$  | (Not available)                               | Depositor |
| Refinement program                                       | unknown                                       | Depositor |
| R, $R_{free}$  | 0.155 , (Not available)                       | Depositor |
| Estimated twinning fraction                              | No twinning to report.                        | Xtriage   |
| Total number of atoms                                    | 3035  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 33.0  | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MTX, CA, CL

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

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$      | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 3.24         | 144/1285 (11.2%) | 4.42        | 311/1747 (17.8%) |
| 1   | B     | 3.44         | 163/1321 (12.3%) | 4.72        | 340/1795 (18.9%) |
| All | All   | 3.34         | 307/2606 (11.8%) | 4.58        | 651/3542 (18.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 7                   |
| 1   | B     | 0                   | 15                  |
| All | All   | 0                   | 22                  |

All (307) bond length outliers are listed below:

| Mol | Chain | Res   | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|---------|--------|-------------|----------|
| 1   | B     | 138   | SER  | CB-OG   | -20.55 | 1.15        | 1.42     |
| 1   | B     | 57    | ARG  | CZ-NH1  | 16.57  | 1.54        | 1.33     |
| 1   | B     | 100   | TYR  | CG-CD2  | 15.22  | 1.58        | 1.39     |
| 1   | A     | 48    | GLU  | CD-OE2  | 14.75  | 1.41        | 1.25     |
| 1   | B     | 118   | GLU  | CD-OE2  | 14.05  | 1.41        | 1.25     |
| 1   | B     | 33    | ARG  | NE-CZ   | 13.07  | 1.50        | 1.33     |
| 1   | A     | 33    | ARG  | CZ-NH2  | 13.06  | 1.50        | 1.33     |
| 1   | B     | 17    | GLU  | CD-OE2  | 12.58  | 1.39        | 1.25     |
| 1   | A     | 22    | TRP  | CD2-CE2 | -12.33 | 1.26        | 1.41     |
| 1   | A     | 64[A] | SER  | CB-OG   | 12.03  | 1.57        | 1.42     |
| 1   | A     | 64[B] | SER  | CB-OG   | 12.03  | 1.57        | 1.42     |
| 1   | B     | 159   | ARG  | N-CA    | 11.91  | 1.70        | 1.46     |
| 1   | B     | 55    | PRO  | C-O     | 11.84  | 1.47        | 1.23     |
| 1   | B     | 111   | TYR  | CG-CD1  | -11.16 | 1.24        | 1.39     |

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| Mol | Chain | Res   | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|---------|--------|-------------|----------|
| 1   | B     | 48    | GLU  | CD-OE2  | 10.64  | 1.37        | 1.25     |
| 1   | A     | 111   | TYR  | C-O     | 10.56  | 1.43        | 1.23     |
| 1   | A     | 43    | GLY  | C-O     | 10.54  | 1.40        | 1.23     |
| 1   | A     | 120   | GLU  | CD-OE2  | 10.47  | 1.37        | 1.25     |
| 1   | B     | 74    | TRP  | CD1-NE1 | -10.34 | 1.20        | 1.38     |
| 1   | B     | 22    | TRP  | CZ3-CH2 | -10.14 | 1.23        | 1.40     |
| 1   | B     | 101   | GLU  | CG-CD   | 10.10  | 1.67        | 1.51     |
| 1   | B     | 139   | GLU  | CD-OE2  | 9.98   | 1.36        | 1.25     |
| 1   | B     | 93    | VAL  | C-O     | 9.80   | 1.42        | 1.23     |
| 1   | A     | 48    | GLU  | CB-CG   | -9.76  | 1.33        | 1.52     |
| 1   | A     | 109   | LYS  | C-N     | -9.75  | 1.11        | 1.34     |
| 1   | A     | 58    | LYS  | CD-CE   | 9.71   | 1.75        | 1.51     |
| 1   | B     | 45[A] | HIS  | CB-CG   | 9.67   | 1.67        | 1.50     |
| 1   | B     | 45[B] | HIS  | CB-CG   | 9.67   | 1.67        | 1.50     |
| 1   | B     | 55    | PRO  | CA-C    | -9.64  | 1.33        | 1.52     |
| 1   | B     | 57    | ARG  | CA-CB   | 9.46   | 1.74        | 1.53     |
| 1   | A     | 22    | TRP  | CZ3-CH2 | -9.38  | 1.25        | 1.40     |
| 1   | B     | 38    | LYS  | CD-CE   | 9.27   | 1.74        | 1.51     |
| 1   | A     | 30    | TRP  | CD2-CE2 | -9.26  | 1.30        | 1.41     |
| 1   | B     | 12    | ARG  | CZ-NH1  | 9.26   | 1.45        | 1.33     |
| 1   | B     | 110   | LEU  | C-N     | -9.22  | 1.12        | 1.34     |
| 1   | B     | 118   | GLU  | CD-OE1  | 9.20   | 1.35        | 1.25     |
| 1   | B     | 139   | GLU  | CG-CD   | -9.19  | 1.38        | 1.51     |
| 1   | A     | 159   | ARG  | C-O     | 9.15   | 1.40        | 1.23     |
| 1   | A     | 111   | TYR  | C-N     | -8.95  | 1.13        | 1.34     |
| 1   | A     | 52    | ARG  | CZ-NH1  | 8.94   | 1.44        | 1.33     |
| 1   | A     | 57    | ARG  | CZ-NH2  | 8.90   | 1.44        | 1.33     |
| 1   | B     | 60    | ILE  | C-O     | 8.82   | 1.40        | 1.23     |
| 1   | B     | 101   | GLU  | CA-CB   | -8.77  | 1.34        | 1.53     |
| 1   | B     | 44    | ARG  | CA-CB   | 8.72   | 1.73        | 1.53     |
| 1   | B     | 17    | GLU  | CB-CG   | -8.64  | 1.35        | 1.52     |
| 1   | A     | 109   | LYS  | CE-NZ   | 8.59   | 1.70        | 1.49     |
| 1   | B     | 97    | GLY  | N-CA    | 8.59   | 1.58        | 1.46     |
| 1   | B     | 159   | ARG  | NE-CZ   | 8.59   | 1.44        | 1.33     |
| 1   | B     | 123   | THR  | CB-OG1  | 8.55   | 1.60        | 1.43     |
| 1   | B     | 149   | HIS  | CB-CG   | 8.53   | 1.65        | 1.50     |
| 1   | A     | 51    | GLY  | N-CA    | -8.52  | 1.33        | 1.46     |
| 1   | A     | 71    | ARG  | NE-CZ   | -8.45  | 1.22        | 1.33     |
| 1   | B     | 18    | ASN  | CB-CG   | 8.39   | 1.70        | 1.51     |
| 1   | A     | 33    | ARG  | CZ-NH1  | 8.36   | 1.44        | 1.33     |
| 1   | A     | 78    | VAL  | C-O     | 8.31   | 1.39        | 1.23     |
| 1   | A     | 47    | TRP  | CD2-CE3 | -8.25  | 1.27        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 78  | VAL  | CB-CG2  | 8.17  | 1.70        | 1.52     |
| 1   | B     | 44  | ARG  | NE-CZ   | 8.17  | 1.43        | 1.33     |
| 1   | B     | 74  | TRP  | CD2-CE2 | -8.16 | 1.31        | 1.41     |
| 1   | B     | 114 | HIS  | C-N     | -8.12 | 1.15        | 1.34     |
| 1   | B     | 80  | GLU  | CD-OE1  | 8.07  | 1.34        | 1.25     |
| 1   | A     | 77  | SER  | CA-CB   | 8.00  | 1.65        | 1.52     |
| 1   | A     | 109 | LYS  | CB-CG   | -8.00 | 1.30        | 1.52     |
| 1   | A     | 133 | TRP  | NE1-CE2 | 7.97  | 1.48        | 1.37     |
| 1   | B     | 80  | GLU  | CD-OE2  | 7.95  | 1.34        | 1.25     |
| 1   | A     | 143 | ALA  | C-O     | 7.93  | 1.38        | 1.23     |
| 1   | A     | 115 | ILE  | CA-CB   | 7.93  | 1.73        | 1.54     |
| 1   | A     | 100 | TYR  | C-O     | -7.92 | 1.08        | 1.23     |
| 1   | B     | 100 | TYR  | CE1-CZ  | -7.89 | 1.28        | 1.38     |
| 1   | A     | 113 | THR  | CB-OG1  | -7.86 | 1.27        | 1.43     |
| 1   | B     | 134 | GLU  | CB-CG   | 7.83  | 1.67        | 1.52     |
| 1   | B     | 114 | HIS  | CG-CD2  | -7.79 | 1.22        | 1.35     |
| 1   | A     | 103 | PHE  | CA-C    | -7.75 | 1.32        | 1.52     |
| 1   | B     | 151 | TYR  | CZ-OH   | -7.74 | 1.24        | 1.37     |
| 1   | B     | 22  | TRP  | CE3-CZ3 | 7.74  | 1.51        | 1.38     |
| 1   | A     | 133 | TRP  | CA-CB   | 7.71  | 1.71        | 1.53     |
| 1   | B     | 49  | SER  | CB-OG   | 7.71  | 1.52        | 1.42     |
| 1   | A     | 151 | TYR  | CD1-CE1 | 7.70  | 1.50        | 1.39     |
| 1   | B     | 72  | VAL  | C-O     | 7.67  | 1.38        | 1.23     |
| 1   | A     | 3   | SER  | CB-OG   | 7.67  | 1.52        | 1.42     |
| 1   | A     | 44  | ARG  | CD-NE   | 7.63  | 1.59        | 1.46     |
| 1   | B     | 1   | MET  | CA-C    | 7.58  | 1.72        | 1.52     |
| 1   | B     | 6   | ALA  | CA-CB   | 7.57  | 1.68        | 1.52     |
| 1   | B     | 111 | TYR  | CA-C    | -7.54 | 1.33        | 1.52     |
| 1   | A     | 157 | GLU  | CD-OE2  | 7.53  | 1.33        | 1.25     |
| 1   | A     | 65  | GLN  | C-O     | 7.52  | 1.37        | 1.23     |
| 1   | A     | 6   | ALA  | CA-CB   | 7.51  | 1.68        | 1.52     |
| 1   | A     | 90  | GLU  | CA-CB   | -7.50 | 1.37        | 1.53     |
| 1   | B     | 43  | GLY  | CA-C    | -7.49 | 1.39        | 1.51     |
| 1   | A     | 146 | GLN  | CD-OE1  | 7.47  | 1.40        | 1.24     |
| 1   | B     | 116 | ASP  | C-O     | 7.44  | 1.37        | 1.23     |
| 1   | B     | 111 | TYR  | CD2-CE2 | 7.43  | 1.50        | 1.39     |
| 1   | B     | 124 | HIS  | C-O     | 7.42  | 1.37        | 1.23     |
| 1   | B     | 31  | PHE  | CE2-CZ  | 7.40  | 1.51        | 1.37     |
| 1   | A     | 131 | ASP  | C-O     | 7.37  | 1.37        | 1.23     |
| 1   | A     | 9   | ALA  | C-O     | 7.37  | 1.37        | 1.23     |
| 1   | A     | 1   | MET  | CA-CB   | -7.36 | 1.37        | 1.53     |
| 1   | A     | 93  | VAL  | C-O     | 7.30  | 1.37        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 139 | GLU  | CD-OE2  | -7.26 | 1.17        | 1.25     |
| 1   | A     | 56  | GLY  | N-CA    | -7.25 | 1.35        | 1.46     |
| 1   | A     | 105 | PRO  | N-CD    | 7.21  | 1.57        | 1.47     |
| 1   | A     | 123 | THR  | C-O     | -7.17 | 1.09        | 1.23     |
| 1   | A     | 49  | SER  | CB-OG   | 7.17  | 1.51        | 1.42     |
| 1   | B     | 2   | ILE  | CB-CG1  | 7.16  | 1.74        | 1.54     |
| 1   | B     | 111 | TYR  | C-O     | 7.11  | 1.36        | 1.23     |
| 1   | A     | 126 | PRO  | N-CA    | 7.08  | 1.59        | 1.47     |
| 1   | B     | 159 | ARG  | CA-CB   | -7.07 | 1.38        | 1.53     |
| 1   | A     | 98  | ARG  | CD-NE   | 7.06  | 1.58        | 1.46     |
| 1   | A     | 90  | GLU  | CG-CD   | -7.05 | 1.41        | 1.51     |
| 1   | A     | 134 | GLU  | CD-OE1  | 7.04  | 1.33        | 1.25     |
| 1   | A     | 44  | ARG  | C-N     | -7.04 | 1.17        | 1.34     |
| 1   | B     | 47  | TRP  | CE2-CZ2 | 7.02  | 1.51        | 1.39     |
| 1   | B     | 90  | GLU  | CD-OE1  | -7.02 | 1.18        | 1.25     |
| 1   | B     | 12  | ARG  | NE-CZ   | -7.00 | 1.24        | 1.33     |
| 1   | B     | 154 | LYS  | CD-CE   | 6.99  | 1.68        | 1.51     |
| 1   | A     | 55  | PRO  | C-N     | -6.99 | 1.20        | 1.33     |
| 1   | A     | 53  | PRO  | C-O     | -6.95 | 1.09        | 1.23     |
| 1   | A     | 152 | CYS  | CA-C    | -6.95 | 1.34        | 1.52     |
| 1   | B     | 21  | PRO  | N-CD    | 6.93  | 1.57        | 1.47     |
| 1   | B     | 59  | ASN  | C-O     | 6.87  | 1.36        | 1.23     |
| 1   | A     | 120 | GLU  | CD-OE1  | 6.86  | 1.33        | 1.25     |
| 1   | B     | 68  | THR  | CB-OG1  | 6.86  | 1.56        | 1.43     |
| 1   | B     | 33  | ARG  | CG-CD   | 6.86  | 1.69        | 1.51     |
| 1   | B     | 97  | GLY  | CA-C    | -6.82 | 1.41        | 1.51     |
| 1   | B     | 116 | ASP  | CB-CG   | 6.82  | 1.66        | 1.51     |
| 1   | B     | 56  | GLY  | N-CA    | -6.81 | 1.35        | 1.46     |
| 1   | B     | 153 | PHE  | C-N     | -6.81 | 1.18        | 1.34     |
| 1   | B     | 114 | HIS  | CG-ND1  | 6.81  | 1.53        | 1.38     |
| 1   | B     | 54  | LEU  | CA-CB   | 6.80  | 1.69        | 1.53     |
| 1   | B     | 59  | ASN  | C-N     | -6.69 | 1.18        | 1.34     |
| 1   | B     | 141 | HIS  | CD2-NE2 | 6.68  | 1.55        | 1.42     |
| 1   | B     | 52  | ARG  | NE-CZ   | 6.68  | 1.41        | 1.33     |
| 1   | A     | 6   | ALA  | C-O     | 6.68  | 1.36        | 1.23     |
| 1   | A     | 44  | ARG  | CG-CD   | -6.66 | 1.35        | 1.51     |
| 1   | A     | 128 | TYR  | CG-CD1  | -6.66 | 1.30        | 1.39     |
| 1   | B     | 55  | PRO  | C-N     | -6.63 | 1.21        | 1.33     |
| 1   | B     | 39  | PRO  | N-CD    | -6.63 | 1.38        | 1.47     |
| 1   | B     | 154 | LYS  | C-O     | 6.62  | 1.35        | 1.23     |
| 1   | B     | 3   | SER  | CB-OG   | -6.60 | 1.33        | 1.42     |
| 1   | A     | 127 | ASP  | CG-OD2  | 6.58  | 1.40        | 1.25     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 1   | A     | 146    | GLN  | N-CA    | 6.58  | 1.59        | 1.46     |
| 1   | B     | 151    | TYR  | C-N     | -6.54 | 1.19        | 1.34     |
| 1   | A     | 12     | ARG  | CZ-NH2  | 6.53  | 1.41        | 1.33     |
| 1   | A     | 125    | PHE  | CG-CD1  | 6.53  | 1.48        | 1.38     |
| 1   | A     | 143    | ALA  | C-N     | -6.52 | 1.19        | 1.34     |
| 1   | B     | 10     | VAL  | CB-CG2  | 6.49  | 1.66        | 1.52     |
| 1   | A     | 155    | ILE  | N-CA    | -6.48 | 1.33        | 1.46     |
| 1   | B     | 42     | MET  | C-O     | -6.46 | 1.11        | 1.23     |
| 1   | B     | 139    | GLU  | CD-OE1  | -6.45 | 1.18        | 1.25     |
| 1   | A     | 12     | ARG  | CZ-NH1  | 6.45  | 1.41        | 1.33     |
| 1   | A     | 74     | TRP  | CB-CG   | -6.44 | 1.38        | 1.50     |
| 1   | A     | 116    | ASP  | CA-C    | -6.44 | 1.36        | 1.52     |
| 1   | B     | 57     | ARG  | NE-CZ   | -6.40 | 1.24        | 1.33     |
| 1   | B     | 102    | GLN  | CA-C    | -6.40 | 1.36        | 1.52     |
| 1   | A     | 135    | SER  | CB-OG   | -6.36 | 1.33        | 1.42     |
| 1   | B     | 135    | SER  | CA-CB   | 6.33  | 1.62        | 1.52     |
| 1   | A     | 57     | ARG  | CD-NE   | -6.31 | 1.35        | 1.46     |
| 1   | B     | 93     | VAL  | CA-C    | -6.31 | 1.36        | 1.52     |
| 1   | B     | 6      | ALA  | C-O     | 6.25  | 1.35        | 1.23     |
| 1   | B     | 131    | ASP  | CA-CB   | 6.24  | 1.67        | 1.53     |
| 1   | A     | 151    | TYR  | CD2-CE2 | -6.22 | 1.30        | 1.39     |
| 1   | A     | 151    | TYR  | C-N     | -6.20 | 1.19        | 1.34     |
| 1   | B     | 158    | ARG  | CA-CB   | 6.20  | 1.67        | 1.53     |
| 1   | A     | 127    | ASP  | C-N     | -6.18 | 1.19        | 1.34     |
| 1   | B     | 111    | TYR  | N-CA    | 6.18  | 1.58        | 1.46     |
| 1   | B     | 33     | ARG  | C-N     | 6.14  | 1.48        | 1.34     |
| 1   | B     | 18     | ASN  | C-O     | -6.14 | 1.11        | 1.23     |
| 1   | A     | 132    | ASP  | C-O     | -6.12 | 1.11        | 1.23     |
| 1   | A     | 158    | ARG  | CD-NE   | 6.08  | 1.56        | 1.46     |
| 1   | A     | 90     | GLU  | CD-OE1  | -6.04 | 1.19        | 1.25     |
| 1   | B     | 34     | ASN  | C-N     | -6.04 | 1.20        | 1.34     |
| 1   | A     | 142    | ASP  | CB-CG   | 6.02  | 1.64        | 1.51     |
| 1   | B     | 72     | VAL  | CA-CB   | 6.02  | 1.67        | 1.54     |
| 1   | A     | 30     | TRP  | C-N     | -6.02 | 1.20        | 1.34     |
| 1   | B     | 154    | LYS  | C-N     | -6.01 | 1.20        | 1.34     |
| 1   | B     | 17     | GLU  | CD-OE1  | 6.01  | 1.32        | 1.25     |
| 1   | B     | 12     | ARG  | CZ-NH2  | 6.01  | 1.40        | 1.33     |
| 1   | A     | 47     | TRP  | CG-CD1  | -5.98 | 1.28        | 1.36     |
| 1   | A     | 25     | PRO  | CA-CB   | -5.97 | 1.41        | 1.53     |
| 1   | B     | 122[A] | ASP  | CG-OD1  | 5.97  | 1.39        | 1.25     |
| 1   | B     | 122[B] | ASP  | CG-OD1  | 5.97  | 1.39        | 1.25     |
| 1   | A     | 98     | ARG  | C-O     | -5.96 | 1.12        | 1.23     |

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| Mol | Chain | Res   | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|---------|-------|-------------|----------|
| 1   | A     | 30    | TRP  | CD2-CE3 | 5.94  | 1.49        | 1.40     |
| 1   | A     | 43    | GLY  | N-CA    | -5.94 | 1.37        | 1.46     |
| 1   | A     | 158   | ARG  | CZ-NH2  | 5.93  | 1.40        | 1.33     |
| 1   | B     | 17    | GLU  | CG-CD   | 5.90  | 1.60        | 1.51     |
| 1   | B     | 159   | ARG  | C-OXT   | 5.90  | 1.34        | 1.23     |
| 1   | B     | 150   | SER  | CB-OG   | -5.90 | 1.34        | 1.42     |
| 1   | A     | 33    | ARG  | N-CA    | 5.89  | 1.58        | 1.46     |
| 1   | B     | 45[A] | HIS  | CA-CB   | 5.89  | 1.67        | 1.53     |
| 1   | B     | 45[B] | HIS  | CA-CB   | 5.89  | 1.67        | 1.53     |
| 1   | A     | 80    | GLU  | CD-OE2  | 5.87  | 1.32        | 1.25     |
| 1   | B     | 45[A] | HIS  | CG-CD2  | 5.83  | 1.45        | 1.35     |
| 1   | B     | 45[B] | HIS  | CG-CD2  | 5.83  | 1.45        | 1.35     |
| 1   | A     | 73    | THR  | C-O     | -5.83 | 1.12        | 1.23     |
| 1   | A     | 72    | VAL  | C-N     | -5.80 | 1.20        | 1.34     |
| 1   | A     | 103   | PHE  | CE1-CZ  | -5.80 | 1.26        | 1.37     |
| 1   | A     | 101   | GLU  | CD-OE1  | 5.79  | 1.32        | 1.25     |
| 1   | B     | 20    | MET  | CA-CB   | -5.79 | 1.41        | 1.53     |
| 1   | A     | 18    | ASN  | C-O     | 5.79  | 1.34        | 1.23     |
| 1   | A     | 44    | ARG  | N-CA    | -5.78 | 1.34        | 1.46     |
| 1   | B     | 51    | GLY  | CA-C    | -5.78 | 1.42        | 1.51     |
| 1   | A     | 103   | PHE  | CG-CD1  | 5.77  | 1.47        | 1.38     |
| 1   | A     | 22    | TRP  | CD1-NE1 | 5.77  | 1.47        | 1.38     |
| 1   | A     | 17    | GLU  | CA-C    | 5.77  | 1.68        | 1.52     |
| 1   | A     | 102   | GLN  | CD-OE1  | 5.76  | 1.36        | 1.24     |
| 1   | B     | 93    | VAL  | C-N     | -5.75 | 1.20        | 1.34     |
| 1   | A     | 154   | LYS  | CE-NZ   | 5.75  | 1.63        | 1.49     |
| 1   | A     | 139   | GLU  | C-O     | 5.74  | 1.34        | 1.23     |
| 1   | B     | 133   | TRP  | C-N     | -5.73 | 1.20        | 1.34     |
| 1   | B     | 158   | ARG  | CG-CD   | 5.71  | 1.66        | 1.51     |
| 1   | B     | 7     | ALA  | C-O     | 5.71  | 1.34        | 1.23     |
| 1   | B     | 104   | LEU  | N-CA    | 5.71  | 1.57        | 1.46     |
| 1   | B     | 128   | TYR  | CZ-OH   | 5.70  | 1.47        | 1.37     |
| 1   | A     | 26    | ALA  | CA-CB   | 5.69  | 1.64        | 1.52     |
| 1   | A     | 156   | LEU  | CA-C    | -5.67 | 1.38        | 1.52     |
| 1   | B     | 75    | VAL  | CB-CG2  | 5.67  | 1.64        | 1.52     |
| 1   | A     | 85    | CYS  | N-CA    | -5.66 | 1.35        | 1.46     |
| 1   | B     | 96    | GLY  | C-N     | 5.66  | 1.43        | 1.33     |
| 1   | A     | 98    | ARG  | CZ-NH1  | 5.65  | 1.40        | 1.33     |
| 1   | B     | 43    | GLY  | C-O     | 5.65  | 1.32        | 1.23     |
| 1   | B     | 120   | GLU  | CD-OE1  | 5.64  | 1.31        | 1.25     |
| 1   | B     | 159   | ARG  | CZ-NH1  | -5.61 | 1.25        | 1.33     |
| 1   | B     | 33    | ARG  | CD-NE   | 5.61  | 1.55        | 1.46     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 1   | B     | 143    | ALA  | C-O     | 5.60  | 1.33        | 1.23     |
| 1   | A     | 138    | SER  | CB-OG   | -5.59 | 1.34        | 1.42     |
| 1   | B     | 116    | ASP  | N-CA    | 5.59  | 1.57        | 1.46     |
| 1   | A     | 98     | ARG  | CZ-NH2  | 5.58  | 1.40        | 1.33     |
| 1   | A     | 98     | ARG  | NE-CZ   | 5.57  | 1.40        | 1.33     |
| 1   | B     | 59     | ASN  | CB-CG   | -5.55 | 1.38        | 1.51     |
| 1   | B     | 93     | VAL  | CB-CG2  | -5.54 | 1.41        | 1.52     |
| 1   | A     | 22     | TRP  | CB-CG   | -5.52 | 1.40        | 1.50     |
| 1   | B     | 5      | ILE  | CB-CG1  | 5.52  | 1.69        | 1.54     |
| 1   | A     | 88     | VAL  | CA-CB   | 5.51  | 1.66        | 1.54     |
| 1   | A     | 118    | GLU  | CD-OE2  | 5.50  | 1.31        | 1.25     |
| 1   | A     | 106    | LYS  | CG-CD   | 5.49  | 1.71        | 1.52     |
| 1   | A     | 124    | HIS  | CE1-NE2 | 5.48  | 1.45        | 1.32     |
| 1   | A     | 151    | TYR  | CA-C    | -5.47 | 1.38        | 1.52     |
| 1   | B     | 153    | PHE  | CD2-CE2 | 5.47  | 1.50        | 1.39     |
| 1   | A     | 107    | ALA  | N-CA    | -5.47 | 1.35        | 1.46     |
| 1   | A     | 38     | LYS  | CD-CE   | -5.47 | 1.37        | 1.51     |
| 1   | A     | 149    | HIS  | CG-CD2  | -5.44 | 1.26        | 1.35     |
| 1   | B     | 102    | GLN  | CD-OE1  | 5.44  | 1.35        | 1.24     |
| 1   | B     | 96     | GLY  | C-O     | -5.44 | 1.15        | 1.23     |
| 1   | B     | 10     | VAL  | CB-CG1  | 5.43  | 1.64        | 1.52     |
| 1   | B     | 85     | CYS  | C-O     | 5.41  | 1.33        | 1.23     |
| 1   | A     | 11     | ASP  | CA-C    | -5.41 | 1.38        | 1.52     |
| 1   | A     | 30     | TRP  | CE3-CZ3 | 5.40  | 1.47        | 1.38     |
| 1   | B     | 152    | CYS  | C-N     | -5.39 | 1.21        | 1.34     |
| 1   | B     | 129    | GLU  | CB-CG   | 5.39  | 1.62        | 1.52     |
| 1   | B     | 100    | TYR  | CB-CG   | 5.38  | 1.59        | 1.51     |
| 1   | A     | 90     | GLU  | CD-OE2  | 5.37  | 1.31        | 1.25     |
| 1   | B     | 140    | PHE  | C-O     | -5.36 | 1.13        | 1.23     |
| 1   | A     | 14     | ILE  | N-CA    | -5.36 | 1.35        | 1.46     |
| 1   | B     | 91     | ILE  | CB-CG1  | 5.35  | 1.69        | 1.54     |
| 1   | B     | 71     | ARG  | NE-CZ   | 5.35  | 1.40        | 1.33     |
| 1   | B     | 120    | GLU  | CD-OE2  | 5.35  | 1.31        | 1.25     |
| 1   | B     | 153    | PHE  | CG-CD1  | 5.34  | 1.46        | 1.38     |
| 1   | A     | 159    | ARG  | C-OXT   | 5.33  | 1.33        | 1.23     |
| 1   | B     | 136    | VAL  | N-CA    | -5.33 | 1.35        | 1.46     |
| 1   | B     | 40     | VAL  | C-O     | 5.32  | 1.33        | 1.23     |
| 1   | B     | 90     | GLU  | CD-OE2  | -5.32 | 1.19        | 1.25     |
| 1   | B     | 120    | GLU  | CB-CG   | -5.32 | 1.42        | 1.52     |
| 1   | B     | 20     | MET  | C-N     | 5.31  | 1.44        | 1.34     |
| 1   | B     | 122[A] | ASP  | CA-C    | -5.31 | 1.39        | 1.52     |
| 1   | B     | 122[B] | ASP  | CA-C    | -5.31 | 1.39        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 20  | MET  | N-CA    | 5.30  | 1.56        | 1.46     |
| 1   | A     | 143 | ALA  | CA-CB   | 5.30  | 1.63        | 1.52     |
| 1   | B     | 136 | VAL  | CB-CG1  | 5.30  | 1.64        | 1.52     |
| 1   | B     | 157 | GLU  | CD-OE1  | -5.30 | 1.19        | 1.25     |
| 1   | A     | 13  | VAL  | CB-CG2  | 5.29  | 1.64        | 1.52     |
| 1   | A     | 95  | GLY  | C-N     | -5.28 | 1.23        | 1.33     |
| 1   | B     | 101 | GLU  | CB-CG   | -5.27 | 1.42        | 1.52     |
| 1   | A     | 31  | PHE  | CE1-CZ  | 5.24  | 1.47        | 1.37     |
| 1   | A     | 48  | GLU  | CA-C    | -5.24 | 1.39        | 1.52     |
| 1   | A     | 30  | TRP  | CZ2-CH2 | -5.24 | 1.27        | 1.37     |
| 1   | A     | 42  | MET  | C-N     | 5.23  | 1.42        | 1.33     |
| 1   | A     | 71  | ARG  | CZ-NH2  | 5.21  | 1.39        | 1.33     |
| 1   | A     | 5   | ILE  | C-N     | -5.20 | 1.22        | 1.34     |
| 1   | B     | 76  | LYS  | CA-CB   | 5.20  | 1.65        | 1.53     |
| 1   | B     | 111 | TYR  | CG-CD2  | -5.19 | 1.32        | 1.39     |
| 1   | A     | 110 | LEU  | CG-CD1  | 5.19  | 1.71        | 1.51     |
| 1   | A     | 146 | GLN  | CA-C    | -5.18 | 1.39        | 1.52     |
| 1   | B     | 30  | TRP  | CD1-NE1 | -5.17 | 1.29        | 1.38     |
| 1   | B     | 44  | ARG  | CB-CG   | 5.17  | 1.66        | 1.52     |
| 1   | A     | 1   | MET  | C-O     | -5.16 | 1.13        | 1.23     |
| 1   | A     | 86  | GLY  | N-CA    | 5.13  | 1.53        | 1.46     |
| 1   | B     | 57  | ARG  | CZ-NH2  | -5.13 | 1.26        | 1.33     |
| 1   | B     | 53  | PRO  | CG-CD   | 5.12  | 1.67        | 1.50     |
| 1   | B     | 121 | GLY  | C-N     | -5.11 | 1.22        | 1.34     |
| 1   | A     | 10  | VAL  | N-CA    | 5.11  | 1.56        | 1.46     |
| 1   | B     | 52  | ARG  | CZ-NH2  | 5.10  | 1.39        | 1.33     |
| 1   | A     | 152 | CYS  | C-O     | 5.10  | 1.33        | 1.23     |
| 1   | B     | 15  | GLY  | C-N     | -5.10 | 1.22        | 1.34     |
| 1   | A     | 19  | ALA  | N-CA    | 5.09  | 1.56        | 1.46     |
| 1   | A     | 112 | LEU  | CA-C    | -5.08 | 1.39        | 1.52     |
| 1   | B     | 121 | GLY  | C-O     | -5.07 | 1.15        | 1.23     |
| 1   | B     | 20  | MET  | CA-C    | -5.07 | 1.39        | 1.52     |
| 1   | B     | 154 | LYS  | CE-NZ   | 5.06  | 1.61        | 1.49     |
| 1   | A     | 51  | GLY  | C-N     | -5.06 | 1.22        | 1.34     |
| 1   | B     | 153 | PHE  | CB-CG   | -5.05 | 1.42        | 1.51     |
| 1   | A     | 107 | ALA  | CA-CB   | 5.04  | 1.63        | 1.52     |
| 1   | B     | 48  | GLU  | CA-C    | -5.04 | 1.39        | 1.52     |
| 1   | A     | 10  | VAL  | C-O     | 5.04  | 1.32        | 1.23     |
| 1   | B     | 157 | GLU  | CG-CD   | 5.03  | 1.59        | 1.51     |
| 1   | B     | 103 | PHE  | CG-CD1  | 5.02  | 1.46        | 1.38     |
| 1   | A     | 47  | TRP  | NE1-CE2 | -5.01 | 1.31        | 1.37     |

All (651) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | B     | 87  | ASP  | CB-CG-OD2   | -39.34 | 82.89       | 118.30   |
| 1   | B     | 37  | ASP  | CB-CG-OD2   | -35.23 | 86.59       | 118.30   |
| 1   | A     | 57  | ARG  | NE-CZ-NH1   | 33.75  | 137.17      | 120.30   |
| 1   | A     | 98  | ARG  | NE-CZ-NH1   | 31.98  | 136.29      | 120.30   |
| 1   | B     | 71  | ARG  | NE-CZ-NH2   | -30.39 | 105.11      | 120.30   |
| 1   | B     | 100 | TYR  | CB-CG-CD2   | -29.24 | 103.46      | 121.00   |
| 1   | A     | 98  | ARG  | NE-CZ-NH2   | -28.79 | 105.91      | 120.30   |
| 1   | B     | 159 | ARG  | NE-CZ-NH2   | -26.19 | 107.20      | 120.30   |
| 1   | B     | 37  | ASP  | CB-CG-OD1   | 25.62  | 141.36      | 118.30   |
| 1   | B     | 52  | ARG  | NE-CZ-NH1   | 25.52  | 133.06      | 120.30   |
| 1   | A     | 116 | ASP  | CB-CG-OD1   | 25.25  | 141.02      | 118.30   |
| 1   | B     | 158 | ARG  | CD-NE-CZ    | 24.45  | 157.83      | 123.60   |
| 1   | A     | 57  | ARG  | NE-CZ-NH2   | -24.44 | 108.08      | 120.30   |
| 1   | A     | 127 | ASP  | CB-CG-OD1   | 23.54  | 139.49      | 118.30   |
| 1   | B     | 69  | ASP  | CB-CG-OD1   | 23.53  | 139.47      | 118.30   |
| 1   | A     | 44  | ARG  | NE-CZ-NH1   | 23.11  | 131.85      | 120.30   |
| 1   | A     | 158 | ARG  | NE-CZ-NH1   | 22.45  | 131.52      | 120.30   |
| 1   | A     | 71  | ARG  | NE-CZ-NH2   | 22.11  | 131.35      | 120.30   |
| 1   | B     | 52  | ARG  | CD-NE-CZ    | 21.95  | 154.32      | 123.60   |
| 1   | B     | 17  | GLU  | OE1-CD-OE2  | 20.68  | 148.12      | 123.30   |
| 1   | A     | 69  | ASP  | CB-CG-OD2   | -19.42 | 100.82      | 118.30   |
| 1   | A     | 16  | MET  | CG-SD-CE    | 19.05  | 130.68      | 100.20   |
| 1   | B     | 69  | ASP  | CB-CG-OD2   | -18.49 | 101.66      | 118.30   |
| 1   | A     | 108 | GLN  | CA-CB-CG    | 18.25  | 153.56      | 113.40   |
| 1   | B     | 44  | ARG  | NE-CZ-NH2   | -18.00 | 111.30      | 120.30   |
| 1   | A     | 79  | ASP  | CB-CG-OD1   | 17.98  | 134.49      | 118.30   |
| 1   | A     | 11  | ASP  | CB-CG-OD1   | 17.67  | 134.20      | 118.30   |
| 1   | B     | 55  | PRO  | CA-C-N      | 17.64  | 151.49      | 116.20   |
| 1   | B     | 111 | TYR  | CB-CG-CD2   | -17.46 | 110.52      | 121.00   |
| 1   | B     | 33  | ARG  | NE-CZ-NH1   | 17.44  | 129.02      | 120.30   |
| 1   | B     | 12  | ARG  | CD-NE-CZ    | 17.09  | 147.53      | 123.60   |
| 1   | B     | 118 | GLU  | OE1-CD-OE2  | -16.98 | 102.93      | 123.30   |
| 1   | B     | 27  | ASP  | CB-CG-OD1   | 16.85  | 133.46      | 118.30   |
| 1   | A     | 12  | ARG  | NE-CZ-NH2   | 16.80  | 128.70      | 120.30   |
| 1   | A     | 111 | TYR  | CB-CG-CD2   | -16.66 | 111.01      | 121.00   |
| 1   | A     | 22  | TRP  | CH2-CZ2-CE2 | -16.54 | 100.86      | 117.40   |
| 1   | A     | 52  | ARG  | CB-CG-CD    | 16.43  | 154.31      | 111.60   |
| 1   | B     | 87  | ASP  | CB-CG-OD1   | 16.21  | 132.89      | 118.30   |
| 1   | B     | 71  | ARG  | NE-CZ-NH1   | 15.90  | 128.25      | 120.30   |
| 1   | B     | 156 | LEU  | CB-CG-CD2   | 15.82  | 137.89      | 111.00   |
| 1   | B     | 73  | THR  | CA-CB-CG2   | 15.48  | 134.07      | 112.40   |
| 1   | B     | 52  | ARG  | CG-CD-NE    | 15.44  | 144.22      | 111.80   |
| 1   | A     | 142 | ASP  | CB-CG-OD2   | -15.33 | 104.50      | 118.30   |

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| Mol | Chain | Res    | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|--------|-------------|----------|
| 1   | B     | 1      | MET  | O-C-N       | 15.03  | 146.75      | 122.70   |
| 1   | A     | 22     | TRP  | NE1-CE2-CZ2 | -14.98 | 113.92      | 130.40   |
| 1   | B     | 52     | ARG  | CB-CG-CD    | 14.62  | 149.61      | 111.60   |
| 1   | A     | 100    | TYR  | CG-CD1-CE1  | -14.62 | 109.61      | 121.30   |
| 1   | B     | 74     | TRP  | CE3-CZ3-CH2 | -14.56 | 105.19      | 121.20   |
| 1   | B     | 116    | ASP  | CB-CG-OD2   | -14.56 | 105.20      | 118.30   |
| 1   | A     | 111    | TYR  | CG-CD1-CE1  | -14.23 | 109.92      | 121.30   |
| 1   | B     | 27     | ASP  | CB-CG-OD2   | -14.07 | 105.64      | 118.30   |
| 1   | B     | 100    | TYR  | CB-CG-CD1   | 14.06  | 129.44      | 121.00   |
| 1   | B     | 100    | TYR  | CG-CD1-CE1  | -13.82 | 110.25      | 121.30   |
| 1   | B     | 128    | TYR  | CB-CG-CD1   | -13.70 | 112.78      | 121.00   |
| 1   | A     | 31     | PHE  | CB-CG-CD2   | -13.65 | 111.25      | 120.80   |
| 1   | B     | 98     | ARG  | NE-CZ-NH2   | 13.51  | 127.05      | 120.30   |
| 1   | B     | 158    | ARG  | NE-CZ-NH2   | 13.40  | 127.00      | 120.30   |
| 1   | B     | 78     | VAL  | CA-CB-CG1   | 13.33  | 130.90      | 110.90   |
| 1   | B     | 44     | ARG  | NE-CZ-NH1   | 13.31  | 126.96      | 120.30   |
| 1   | A     | 135    | SER  | N-CA-CB     | 13.29  | 130.43      | 110.50   |
| 1   | A     | 100    | TYR  | CB-CG-CD2   | -13.26 | 113.04      | 121.00   |
| 1   | A     | 109    | LYS  | CA-CB-CG    | 12.92  | 141.83      | 113.40   |
| 1   | B     | 120    | GLU  | CB-CG-CD    | 12.89  | 149.00      | 114.20   |
| 1   | A     | 8      | LEU  | CB-CG-CD2   | 12.63  | 132.47      | 111.00   |
| 1   | A     | 128    | TYR  | CB-CG-CD1   | 12.62  | 128.57      | 121.00   |
| 1   | B     | 79     | ASP  | CB-CG-OD1   | 12.56  | 129.60      | 118.30   |
| 1   | A     | 132    | ASP  | CB-CG-OD2   | -12.47 | 107.08      | 118.30   |
| 1   | B     | 55     | PRO  | O-C-N       | -12.46 | 102.01      | 123.20   |
| 1   | B     | 111    | TYR  | O-C-N       | -12.28 | 103.05      | 122.70   |
| 1   | B     | 80     | GLU  | OE1-CD-OE2  | 12.09  | 137.81      | 123.30   |
| 1   | B     | 122[A] | ASP  | CB-CG-OD2   | -12.05 | 107.45      | 118.30   |
| 1   | B     | 122[B] | ASP  | CB-CG-OD2   | -12.05 | 107.45      | 118.30   |
| 1   | A     | 22     | TRP  | CD1-NE1-CE2 | -11.69 | 98.48       | 109.00   |
| 1   | A     | 78     | VAL  | CA-CB-CG1   | 11.69  | 128.44      | 110.90   |
| 1   | A     | 48     | GLU  | OE1-CD-OE2  | 11.63  | 137.26      | 123.30   |
| 1   | A     | 73     | THR  | CA-CB-CG2   | 11.62  | 128.68      | 112.40   |
| 1   | B     | 101    | GLU  | CA-CB-CG    | 11.57  | 138.85      | 113.40   |
| 1   | B     | 135    | SER  | O-C-N       | -11.51 | 104.29      | 122.70   |
| 1   | B     | 118    | GLU  | CG-CD-OE2   | 11.49  | 141.28      | 118.30   |
| 1   | B     | 18     | ASN  | OD1-CG-ND2  | 11.44  | 148.20      | 121.90   |
| 1   | A     | 71     | ARG  | CG-CD-NE    | 11.43  | 135.81      | 111.80   |
| 1   | A     | 109    | LYS  | CB-CG-CD    | 11.37  | 141.16      | 111.60   |
| 1   | B     | 10     | VAL  | CG1-CB-CG2  | -11.35 | 92.74       | 110.90   |
| 1   | A     | 87     | ASP  | CB-CG-OD1   | -11.27 | 108.16      | 118.30   |
| 1   | B     | 140    | PHE  | CB-CG-CD1   | 11.24  | 128.67      | 120.80   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | A     | 95  | GLY  | C-N-CA      | 11.21  | 145.85      | 122.30   |
| 1   | A     | 22  | TRP  | CD1-CG-CD2  | -11.15 | 97.38       | 106.30   |
| 1   | B     | 23  | ASN  | OD1-CG-ND2  | -11.09 | 96.39       | 121.90   |
| 1   | B     | 11  | ASP  | CB-CG-OD1   | 10.97  | 128.17      | 118.30   |
| 1   | B     | 87  | ASP  | OD1-CG-OD2  | 10.97  | 144.14      | 123.30   |
| 1   | B     | 101 | GLU  | O-C-N       | -10.95 | 105.18      | 122.70   |
| 1   | A     | 65  | GLN  | CB-CA-C     | 10.95  | 132.30      | 110.40   |
| 1   | B     | 74  | TRP  | CZ3-CH2-CZ2 | 10.91  | 134.70      | 121.60   |
| 1   | A     | 55  | PRO  | CA-C-N      | 10.88  | 137.96      | 116.20   |
| 1   | B     | 142 | ASP  | CB-CG-OD2   | -10.83 | 108.56      | 118.30   |
| 1   | B     | 158 | ARG  | O-C-N       | 10.78  | 139.95      | 122.70   |
| 1   | B     | 11  | ASP  | CB-CG-OD2   | -10.75 | 108.62      | 118.30   |
| 1   | A     | 44  | ARG  | CB-CG-CD    | 10.75  | 139.54      | 111.60   |
| 1   | B     | 154 | LYS  | CG-CD-CE    | -10.74 | 79.69       | 111.90   |
| 1   | B     | 119 | VAL  | CA-CB-CG1   | -10.66 | 94.91       | 110.90   |
| 1   | B     | 4   | LEU  | CB-CG-CD1   | 10.57  | 128.98      | 111.00   |
| 1   | B     | 111 | TYR  | CB-CG-CD1   | 10.54  | 127.33      | 121.00   |
| 1   | A     | 116 | ASP  | CB-CG-OD2   | -10.50 | 108.85      | 118.30   |
| 1   | A     | 22  | TRP  | CE2-CD2-CG  | 10.49  | 115.69      | 107.30   |
| 1   | B     | 50  | ILE  | O-C-N       | 10.42  | 140.92      | 123.20   |
| 1   | A     | 48  | GLU  | CG-CD-OE2   | -10.38 | 97.53       | 118.30   |
| 1   | A     | 10  | VAL  | CG1-CB-CG2  | -10.37 | 94.31       | 110.90   |
| 1   | A     | 134 | GLU  | OE1-CD-OE2  | 10.31  | 135.67      | 123.30   |
| 1   | B     | 103 | PHE  | CB-CG-CD1   | -10.30 | 113.59      | 120.80   |
| 1   | B     | 93  | VAL  | O-C-N       | -10.28 | 106.25      | 122.70   |
| 1   | A     | 71  | ARG  | CD-NE-CZ    | 10.25  | 137.96      | 123.60   |
| 1   | B     | 36  | LEU  | CB-CG-CD1   | 10.25  | 128.42      | 111.00   |
| 1   | A     | 71  | ARG  | NH1-CZ-NH2  | -10.23 | 108.15      | 119.40   |
| 1   | A     | 22  | TRP  | CD2-CE2-CZ2 | 10.22  | 134.56      | 122.30   |
| 1   | A     | 104 | LEU  | CA-CB-CG    | 10.21  | 138.79      | 115.30   |
| 1   | B     | 101 | GLU  | OE1-CD-OE2  | 10.16  | 135.49      | 123.30   |
| 1   | A     | 120 | GLU  | CA-CB-CG    | 10.15  | 135.74      | 113.40   |
| 1   | A     | 144 | ASP  | CB-CG-OD2   | -10.15 | 109.17      | 118.30   |
| 1   | A     | 151 | TYR  | CD1-CE1-CZ  | -10.09 | 110.72      | 119.80   |
| 1   | A     | 128 | TYR  | CG-CD1-CE1  | 9.98   | 129.29      | 121.30   |
| 1   | B     | 132 | ASP  | CB-CG-OD2   | -9.95  | 109.34      | 118.30   |
| 1   | B     | 127 | ASP  | CB-CG-OD1   | 9.94   | 127.25      | 118.30   |
| 1   | B     | 93  | VAL  | CA-C-N      | 9.94   | 139.06      | 117.20   |
| 1   | B     | 12  | ARG  | NE-CZ-NH1   | 9.94   | 125.27      | 120.30   |
| 1   | B     | 59  | ASN  | CA-C-N      | 9.92   | 139.02      | 117.20   |
| 1   | B     | 23  | ASN  | O-C-N       | 9.91   | 138.56      | 122.70   |
| 1   | A     | 79  | ASP  | O-C-N       | 9.85   | 138.47      | 122.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 143 | ALA  | C-N-CA      | 9.85  | 146.34      | 121.70   |
| 1   | A     | 158 | ARG  | O-C-N       | 9.80  | 138.39      | 122.70   |
| 1   | A     | 4   | LEU  | CB-CG-CD1   | 9.79  | 127.65      | 111.00   |
| 1   | A     | 111 | TYR  | CA-C-N      | 9.79  | 138.73      | 117.20   |
| 1   | A     | 31  | PHE  | CG-CD2-CE2  | -9.75 | 110.08      | 120.80   |
| 1   | A     | 127 | ASP  | CB-CG-OD2   | -9.73 | 109.55      | 118.30   |
| 1   | B     | 1   | MET  | CA-CB-CG    | 9.72  | 129.83      | 113.30   |
| 1   | A     | 139 | GLU  | CG-CD-OE1   | 9.71  | 137.72      | 118.30   |
| 1   | A     | 136 | VAL  | CA-CB-CG1   | 9.67  | 125.41      | 110.90   |
| 1   | B     | 23  | ASN  | CB-CG-OD1   | 9.62  | 140.84      | 121.60   |
| 1   | B     | 6   | ALA  | O-C-N       | -9.60 | 107.34      | 122.70   |
| 1   | B     | 104 | LEU  | C-N-CD      | 9.59  | 148.54      | 128.40   |
| 1   | B     | 158 | ARG  | NH1-CZ-NH2  | -9.59 | 108.85      | 119.40   |
| 1   | A     | 22  | TRP  | CG-CD2-CE3  | -9.58 | 125.28      | 133.90   |
| 1   | A     | 1   | MET  | CG-SD-CE    | 9.53  | 115.45      | 100.20   |
| 1   | B     | 98  | ARG  | NH1-CZ-NH2  | -9.52 | 108.93      | 119.40   |
| 1   | B     | 52  | ARG  | NH1-CZ-NH2  | -9.51 | 108.94      | 119.40   |
| 1   | B     | 100 | TYR  | CZ-CE2-CD2  | -9.51 | 111.24      | 119.80   |
| 1   | A     | 6   | ALA  | O-C-N       | -9.45 | 107.58      | 122.70   |
| 1   | A     | 70  | ASP  | CB-CG-OD2   | 9.44  | 126.80      | 118.30   |
| 1   | B     | 81  | ALA  | CA-C-O      | -9.31 | 100.54      | 120.10   |
| 1   | B     | 140 | PHE  | CG-CD2-CE2  | 9.28  | 131.01      | 120.80   |
| 1   | B     | 30  | TRP  | CD1-NE1-CE2 | 9.25  | 117.32      | 109.00   |
| 1   | B     | 38  | LYS  | O-C-N       | 9.23  | 138.65      | 121.10   |
| 1   | B     | 111 | TYR  | CA-C-O      | 9.16  | 139.33      | 120.10   |
| 1   | B     | 153 | PHE  | CB-CG-CD1   | 9.10  | 127.17      | 120.80   |
| 1   | A     | 44  | ARG  | CD-NE-CZ    | -9.10 | 110.86      | 123.60   |
| 1   | B     | 103 | PHE  | CB-CG-CD2   | 9.08  | 127.16      | 120.80   |
| 1   | A     | 143 | ALA  | CA-C-N      | 9.08  | 137.17      | 117.20   |
| 1   | B     | 22  | TRP  | CZ3-CH2-CZ2 | 9.07  | 132.49      | 121.60   |
| 1   | B     | 9   | ALA  | O-C-N       | -9.05 | 108.22      | 122.70   |
| 1   | A     | 78  | VAL  | CG1-CB-CG2  | -9.04 | 96.43       | 110.90   |
| 1   | B     | 38  | LYS  | C-N-CD      | 9.03  | 147.37      | 128.40   |
| 1   | A     | 145 | ALA  | O-C-N       | 9.02  | 137.13      | 122.70   |
| 1   | A     | 103 | PHE  | CB-CG-CD2   | 9.00  | 127.10      | 120.80   |
| 1   | B     | 159 | ARG  | CD-NE-CZ    | -8.99 | 111.01      | 123.60   |
| 1   | B     | 16  | MET  | CA-CB-CG    | -8.98 | 98.03       | 113.30   |
| 1   | A     | 105 | PRO  | CA-CB-CG    | 8.96  | 121.83      | 104.80   |
| 1   | B     | 98  | ARG  | CG-CD-NE    | 8.94  | 130.58      | 111.80   |
| 1   | B     | 74  | TRP  | CD2-CE3-CZ3 | 8.87  | 130.33      | 118.80   |
| 1   | A     | 150 | SER  | O-C-N       | -8.86 | 108.53      | 122.70   |
| 1   | B     | 50  | ILE  | C-N-CA      | -8.86 | 103.70      | 122.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 128 | TYR  | CB-CG-CD2   | 8.85  | 126.31      | 121.00   |
| 1   | A     | 72  | VAL  | CG1-CB-CG2  | -8.85 | 96.74       | 110.90   |
| 1   | B     | 33  | ARG  | NE-CZ-NH2   | -8.84 | 115.88      | 120.30   |
| 1   | B     | 88  | VAL  | CG1-CB-CG2  | 8.83  | 125.02      | 110.90   |
| 1   | B     | 159 | ARG  | NE-CZ-NH1   | 8.82  | 124.71      | 120.30   |
| 1   | B     | 79  | ASP  | CA-C-N      | 8.76  | 136.47      | 117.20   |
| 1   | B     | 61  | ILE  | CG1-CB-CG2  | -8.75 | 92.15       | 111.40   |
| 1   | A     | 69  | ASP  | OD1-CG-OD2  | 8.74  | 139.91      | 123.30   |
| 1   | A     | 85  | CYS  | C-N-CA      | -8.71 | 104.01      | 122.30   |
| 1   | A     | 33  | ARG  | NE-CZ-NH2   | 8.70  | 124.65      | 120.30   |
| 1   | A     | 143 | ALA  | O-C-N       | -8.69 | 108.80      | 122.70   |
| 1   | B     | 157 | GLU  | CG-CD-OE2   | -8.65 | 100.99      | 118.30   |
| 1   | B     | 101 | GLU  | CG-CD-OE2   | -8.65 | 101.00      | 118.30   |
| 1   | B     | 18  | ASN  | CB-CG-ND2   | -8.64 | 95.96       | 116.70   |
| 1   | A     | 79  | ASP  | CA-C-O      | -8.63 | 101.98      | 120.10   |
| 1   | B     | 100 | TYR  | CG-CD2-CE2  | -8.61 | 114.41      | 121.30   |
| 1   | B     | 54  | LEU  | CB-CG-CD1   | -8.60 | 96.38       | 111.00   |
| 1   | A     | 158 | ARG  | NE-CZ-NH2   | -8.59 | 116.00      | 120.30   |
| 1   | B     | 81  | ALA  | CA-C-N      | 8.57  | 136.06      | 117.20   |
| 1   | B     | 31  | PHE  | CB-CG-CD2   | -8.57 | 114.80      | 120.80   |
| 1   | A     | 23  | ASN  | CB-CG-OD1   | 8.56  | 138.72      | 121.60   |
| 1   | B     | 61  | ILE  | CA-CB-CG1   | 8.56  | 127.27      | 111.00   |
| 1   | A     | 82  | ILE  | CA-CB-CG2   | 8.55  | 128.00      | 110.90   |
| 1   | B     | 96  | GLY  | CA-C-O      | 8.55  | 135.98      | 120.60   |
| 1   | A     | 103 | PHE  | CZ-CE2-CD2  | -8.54 | 109.85      | 120.10   |
| 1   | A     | 145 | ALA  | CB-CA-C     | 8.54  | 122.90      | 110.10   |
| 1   | A     | 22  | TRP  | CD2-CE3-CZ3 | -8.48 | 107.78      | 118.80   |
| 1   | A     | 21  | PRO  | N-CD-CG     | 8.48  | 115.92      | 103.20   |
| 1   | A     | 22  | TRP  | CE3-CZ3-CH2 | 8.48  | 130.53      | 121.20   |
| 1   | A     | 110 | LEU  | CB-CG-CD1   | -8.47 | 96.60       | 111.00   |
| 1   | A     | 92  | MET  | CG-SD-CE    | 8.46  | 113.74      | 100.20   |
| 1   | B     | 100 | TYR  | CD1-CE1-CZ  | 8.46  | 127.42      | 119.80   |
| 1   | A     | 128 | TYR  | CB-CG-CD2   | -8.43 | 115.94      | 121.00   |
| 1   | A     | 159 | ARG  | CA-CB-CG    | 8.42  | 131.91      | 113.40   |
| 1   | A     | 80  | GLU  | OE1-CD-OE2  | 8.39  | 133.37      | 123.30   |
| 1   | B     | 100 | TYR  | CD1-CG-CD2  | 8.35  | 127.09      | 117.90   |
| 1   | B     | 9   | ALA  | CA-C-O      | 8.35  | 137.64      | 120.10   |
| 1   | A     | 37  | ASP  | CB-CG-OD2   | 8.33  | 125.80      | 118.30   |
| 1   | B     | 88  | VAL  | CA-CB-CG1   | -8.30 | 98.44       | 110.90   |
| 1   | A     | 10  | VAL  | CA-CB-CG1   | 8.29  | 123.33      | 110.90   |
| 1   | B     | 17  | GLU  | CA-CB-CG    | 8.28  | 131.62      | 113.40   |
| 1   | B     | 84  | ALA  | N-CA-CB     | -8.28 | 98.50       | 110.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 90  | GLU  | OE1-CD-OE2  | -8.27 | 113.37      | 123.30   |
| 1   | B     | 22  | TRP  | CH2-CZ2-CE2 | -8.23 | 109.17      | 117.40   |
| 1   | A     | 103 | PHE  | CB-CG-CD1   | -8.23 | 115.04      | 120.80   |
| 1   | A     | 76  | LYS  | CA-C-N      | 8.21  | 135.26      | 117.20   |
| 1   | B     | 133 | TRP  | NE1-CE2-CZ2 | 8.21  | 139.43      | 130.40   |
| 1   | B     | 50  | ILE  | CA-C-O      | -8.21 | 102.86      | 120.10   |
| 1   | B     | 30  | TRP  | CB-CG-CD1   | 8.18  | 137.63      | 127.00   |
| 1   | B     | 118 | GLU  | O-C-N       | -8.12 | 109.71      | 122.70   |
| 1   | B     | 103 | PHE  | CZ-CE2-CD2  | 8.11  | 129.84      | 120.10   |
| 1   | A     | 30  | TRP  | CA-C-O      | -8.11 | 103.07      | 120.10   |
| 1   | B     | 42  | MET  | O-C-N       | 8.11  | 136.98      | 123.20   |
| 1   | B     | 138 | SER  | N-CA-CB     | -8.06 | 98.40       | 110.50   |
| 1   | A     | 126 | PRO  | CA-C-N      | 8.06  | 134.93      | 117.20   |
| 1   | B     | 33  | ARG  | CA-C-O      | 8.06  | 137.02      | 120.10   |
| 1   | A     | 111 | TYR  | CD1-CG-CD2  | 8.06  | 126.76      | 117.90   |
| 1   | A     | 43  | GLY  | O-C-N       | -8.05 | 109.83      | 122.70   |
| 1   | A     | 12  | ARG  | CD-NE-CZ    | 7.99  | 134.79      | 123.60   |
| 1   | B     | 65  | GLN  | CB-CA-C     | 7.98  | 126.36      | 110.40   |
| 1   | A     | 90  | GLU  | CG-CD-OE1   | 7.98  | 134.25      | 118.30   |
| 1   | B     | 72  | VAL  | CA-C-O      | -7.95 | 103.40      | 120.10   |
| 1   | A     | 30  | TRP  | CA-C-N      | 7.93  | 134.65      | 117.20   |
| 1   | B     | 17  | GLU  | CG-CD-OE2   | -7.92 | 102.46      | 118.30   |
| 1   | B     | 118 | GLU  | CB-CG-CD    | 7.92  | 135.58      | 114.20   |
| 1   | A     | 69  | ASP  | N-CA-CB     | -7.90 | 96.38       | 110.60   |
| 1   | A     | 44  | ARG  | NH1-CZ-NH2  | -7.88 | 110.73      | 119.40   |
| 1   | B     | 5   | ILE  | CA-CB-CG1   | -7.87 | 96.05       | 111.00   |
| 1   | B     | 119 | VAL  | CG1-CB-CG2  | 7.85  | 123.45      | 110.90   |
| 1   | B     | 121 | GLY  | O-C-N       | 7.85  | 135.26      | 122.70   |
| 1   | B     | 72  | VAL  | CA-C-N      | 7.84  | 134.44      | 117.20   |
| 1   | A     | 156 | LEU  | CB-CG-CD1   | 7.82  | 124.30      | 111.00   |
| 1   | A     | 88  | VAL  | CG1-CB-CG2  | -7.78 | 98.45       | 110.90   |
| 1   | B     | 93  | VAL  | C-N-CA      | 7.78  | 141.15      | 121.70   |
| 1   | B     | 140 | PHE  | CB-CG-CD2   | -7.77 | 115.36      | 120.80   |
| 1   | A     | 131 | ASP  | CB-CA-C     | -7.76 | 94.87       | 110.40   |
| 1   | B     | 48  | GLU  | CA-CB-CG    | 7.75  | 130.44      | 113.40   |
| 1   | A     | 12  | ARG  | CG-CD-NE    | 7.74  | 128.05      | 111.80   |
| 1   | B     | 1   | MET  | CB-CG-SD    | 7.73  | 135.58      | 112.40   |
| 1   | A     | 87  | ASP  | CA-C-N      | -7.73 | 100.20      | 117.20   |
| 1   | A     | 47  | TRP  | CE2-CD2-CG  | -7.72 | 101.12      | 107.30   |
| 1   | A     | 111 | TYR  | CD1-CE1-CZ  | 7.72  | 126.75      | 119.80   |
| 1   | B     | 159 | ARG  | NH1-CZ-NH2  | 7.72  | 127.89      | 119.40   |
| 1   | B     | 55  | PRO  | N-CA-C      | 7.71  | 132.16      | 112.10   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1   | A     | 79     | ASP  | OD1-CG-OD2  | -7.70 | 108.67      | 123.30   |
| 1   | A     | 111    | TYR  | O-C-N       | -7.69 | 110.39      | 122.70   |
| 1   | B     | 122[A] | ASP  | N-CA-CB     | -7.69 | 96.77       | 110.60   |
| 1   | B     | 122[B] | ASP  | N-CA-CB     | -7.69 | 96.77       | 110.60   |
| 1   | B     | 57     | ARG  | NE-CZ-NH1   | -7.68 | 116.46      | 120.30   |
| 1   | A     | 55     | PRO  | O-C-N       | -7.68 | 110.14      | 123.20   |
| 1   | B     | 52     | ARG  | CA-CB-CG    | 7.67  | 130.27      | 113.40   |
| 1   | A     | 69     | ASP  | CA-C-O      | 7.66  | 136.19      | 120.10   |
| 1   | A     | 140    | PHE  | CG-CD2-CE2  | -7.66 | 112.38      | 120.80   |
| 1   | A     | 21     | PRO  | CA-N-CD     | -7.66 | 100.78      | 111.50   |
| 1   | B     | 140    | PHE  | CZ-CE2-CD2  | -7.65 | 110.92      | 120.10   |
| 1   | A     | 144    | ASP  | O-C-N       | -7.64 | 110.48      | 122.70   |
| 1   | A     | 146    | GLN  | N-CA-CB     | -7.62 | 96.88       | 110.60   |
| 1   | A     | 152    | CYS  | CA-C-N      | 7.62  | 133.96      | 117.20   |
| 1   | B     | 142    | ASP  | OD1-CG-OD2  | 7.62  | 137.77      | 123.30   |
| 1   | B     | 7      | ALA  | CB-CA-C     | 7.59  | 121.49      | 110.10   |
| 1   | B     | 139    | GLU  | CG-CD-OE1   | 7.59  | 133.49      | 118.30   |
| 1   | B     | 29     | ALA  | CA-C-N      | 7.59  | 133.90      | 117.20   |
| 1   | B     | 55     | PRO  | C-N-CA      | 7.59  | 138.24      | 122.30   |
| 1   | A     | 158    | ARG  | CG-CD-NE    | -7.58 | 95.88       | 111.80   |
| 1   | A     | 88     | VAL  | CA-CB-CG2   | 7.57  | 122.26      | 110.90   |
| 1   | B     | 122[A] | ASP  | OD1-CG-OD2  | 7.57  | 137.69      | 123.30   |
| 1   | B     | 122[B] | ASP  | OD1-CG-OD2  | 7.57  | 137.69      | 123.30   |
| 1   | A     | 47     | TRP  | CA-C-O      | 7.57  | 135.99      | 120.10   |
| 1   | B     | 30     | TRP  | NE1-CE2-CD2 | -7.56 | 99.74       | 107.30   |
| 1   | B     | 44     | ARG  | O-C-N       | -7.55 | 110.62      | 122.70   |
| 1   | B     | 30     | TRP  | NE1-CE2-CZ2 | 7.55  | 138.70      | 130.40   |
| 1   | B     | 79     | ASP  | OD1-CG-OD2  | -7.52 | 109.01      | 123.30   |
| 1   | A     | 158    | ARG  | CA-C-N      | -7.50 | 100.69      | 117.20   |
| 1   | B     | 60     | ILE  | CB-CA-C     | 7.50  | 126.61      | 111.60   |
| 1   | A     | 142    | ASP  | O-C-N       | 7.50  | 134.70      | 122.70   |
| 1   | B     | 72     | VAL  | CG1-CB-CG2  | 7.49  | 122.88      | 110.90   |
| 1   | B     | 114    | HIS  | CA-C-N      | 7.49  | 133.67      | 117.20   |
| 1   | B     | 65     | GLN  | CG-CD-OE1   | 7.45  | 136.50      | 121.60   |
| 1   | A     | 38     | LYS  | CA-CB-CG    | 7.45  | 129.78      | 113.40   |
| 1   | B     | 105    | PRO  | CA-N-CD     | -7.45 | 101.07      | 111.50   |
| 1   | B     | 98     | ARG  | NE-CZ-NH1   | 7.37  | 123.99      | 120.30   |
| 1   | B     | 146    | GLN  | CG-CD-NE2   | 7.37  | 134.40      | 116.70   |
| 1   | B     | 44     | ARG  | CA-C-O      | 7.35  | 135.54      | 120.10   |
| 1   | A     | 55     | PRO  | C-N-CA      | 7.34  | 137.72      | 122.30   |
| 1   | A     | 74     | TRP  | CA-C-N      | 7.33  | 133.33      | 117.20   |
| 1   | A     | 128    | TYR  | CD1-CE1-CZ  | -7.29 | 113.24      | 119.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 158 | ARG  | NE-CZ-NH1   | 7.29  | 123.94      | 120.30   |
| 1   | A     | 47  | TRP  | CG-CD2-CE3  | 7.28  | 140.45      | 133.90   |
| 1   | B     | 104 | LEU  | CB-CG-CD2   | -7.28 | 98.63       | 111.00   |
| 1   | A     | 159 | ARG  | CA-C-O      | -7.28 | 104.82      | 120.10   |
| 1   | A     | 30  | TRP  | CZ3-CH2-CZ2 | 7.25  | 130.30      | 121.60   |
| 1   | B     | 53  | PRO  | O-C-N       | -7.23 | 111.13      | 122.70   |
| 1   | B     | 1   | MET  | CA-C-O      | -7.23 | 104.93      | 120.10   |
| 1   | B     | 6   | ALA  | C-N-CA      | 7.22  | 139.75      | 121.70   |
| 1   | A     | 61  | ILE  | CA-CB-CG1   | 7.20  | 124.68      | 111.00   |
| 1   | B     | 38  | LYS  | CD-CE-NZ    | -7.19 | 95.16       | 111.70   |
| 1   | A     | 141 | HIS  | CG-CD2-NE2  | -7.18 | 95.55       | 109.20   |
| 1   | A     | 128 | TYR  | CA-C-N      | -7.18 | 101.41      | 117.20   |
| 1   | B     | 68  | THR  | CA-CB-CG2   | 7.18  | 122.45      | 112.40   |
| 1   | A     | 30  | TRP  | CG-CD2-CE3  | -7.16 | 127.45      | 133.90   |
| 1   | A     | 48  | GLU  | CB-CA-C     | -7.14 | 96.12       | 110.40   |
| 1   | A     | 116 | ASP  | OD1-CG-OD2  | -7.14 | 109.73      | 123.30   |
| 1   | A     | 147 | ASN  | CB-CG-OD1   | 7.13  | 135.86      | 121.60   |
| 1   | A     | 114 | HIS  | N-CA-CB     | 7.12  | 123.42      | 110.60   |
| 1   | B     | 70  | ASP  | CB-CG-OD2   | 7.11  | 124.70      | 118.30   |
| 1   | B     | 31  | PHE  | O-C-N       | 7.11  | 134.07      | 122.70   |
| 1   | B     | 28  | LEU  | CB-CG-CD2   | 7.10  | 123.08      | 111.00   |
| 1   | A     | 139 | GLU  | CG-CD-OE2   | -7.09 | 104.11      | 118.30   |
| 1   | A     | 82  | ILE  | CG1-CB-CG2  | -7.06 | 95.87       | 111.40   |
| 1   | A     | 43  | GLY  | CA-C-N      | 7.04  | 132.70      | 117.20   |
| 1   | B     | 89  | PRO  | CA-N-CD     | 7.04  | 121.55      | 111.70   |
| 1   | B     | 5   | ILE  | CB-CA-C     | 7.03  | 125.67      | 111.60   |
| 1   | A     | 105 | PRO  | O-C-N       | -7.03 | 111.45      | 122.70   |
| 1   | B     | 68  | THR  | O-C-N       | -7.01 | 111.49      | 122.70   |
| 1   | A     | 30  | TRP  | CE3-CZ3-CH2 | -7.00 | 113.50      | 121.20   |
| 1   | B     | 51  | GLY  | O-C-N       | -6.99 | 111.52      | 122.70   |
| 1   | A     | 10  | VAL  | O-C-N       | -6.96 | 111.56      | 122.70   |
| 1   | B     | 137 | PHE  | CD1-CE1-CZ  | -6.94 | 111.78      | 120.10   |
| 1   | B     | 40  | VAL  | CA-CB-CG1   | 6.90  | 121.25      | 110.90   |
| 1   | A     | 121 | GLY  | C-N-CA      | -6.90 | 104.45      | 121.70   |
| 1   | A     | 36  | LEU  | CB-CG-CD1   | 6.89  | 122.72      | 111.00   |
| 1   | A     | 18  | ASN  | OD1-CG-ND2  | 6.87  | 137.70      | 121.90   |
| 1   | A     | 48  | GLU  | O-C-N       | -6.86 | 111.73      | 122.70   |
| 1   | B     | 52  | ARG  | N-CA-CB     | -6.85 | 98.27       | 110.60   |
| 1   | B     | 133 | TRP  | CD2-CE2-CZ2 | -6.84 | 114.09      | 122.30   |
| 1   | B     | 59  | ASN  | OD1-CG-ND2  | -6.84 | 106.16      | 121.90   |
| 1   | A     | 22  | TRP  | CG-CD1-NE1  | 6.82  | 116.92      | 110.10   |
| 1   | B     | 13  | VAL  | CA-CB-CG2   | -6.80 | 100.70      | 110.90   |

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| Mol | Chain | Res   | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-------------|-------|-------------|----------|
| 1   | B     | 39    | PRO  | N-CD-CG     | 6.80  | 113.40      | 103.20   |
| 1   | B     | 133   | TRP  | CE3-CZ3-CH2 | -6.79 | 113.72      | 121.20   |
| 1   | A     | 93    | VAL  | CG1-CB-CG2  | 6.77  | 121.73      | 110.90   |
| 1   | B     | 67    | GLY  | N-CA-C      | 6.77  | 130.02      | 113.10   |
| 1   | A     | 151   | TYR  | C-N-CA      | 6.77  | 138.62      | 121.70   |
| 1   | B     | 123   | THR  | CA-CB-CG2   | 6.76  | 121.86      | 112.40   |
| 1   | A     | 100   | TYR  | O-C-N       | 6.75  | 133.50      | 122.70   |
| 1   | A     | 140   | PHE  | CB-CG-CD1   | -6.74 | 116.08      | 120.80   |
| 1   | A     | 155   | ILE  | CA-CB-CG1   | -6.74 | 98.19       | 111.00   |
| 1   | B     | 141   | HIS  | CG-CD2-NE2  | -6.74 | 96.39       | 109.20   |
| 1   | B     | 30    | TRP  | O-C-N       | -6.74 | 111.92      | 122.70   |
| 1   | B     | 57    | ARG  | N-CA-CB     | -6.72 | 98.50       | 110.60   |
| 1   | A     | 34    | ASN  | CA-C-N      | 6.72  | 131.98      | 117.20   |
| 1   | B     | 57    | ARG  | CA-CB-CG    | -6.71 | 98.65       | 113.40   |
| 1   | A     | 120   | GLU  | CB-CG-CD    | 6.70  | 132.28      | 114.20   |
| 1   | B     | 61    | ILE  | N-CA-CB     | 6.67  | 126.14      | 110.80   |
| 1   | B     | 59    | ASN  | C-N-CA      | 6.67  | 138.37      | 121.70   |
| 1   | A     | 125   | PHE  | CB-CG-CD1   | 6.66  | 125.46      | 120.80   |
| 1   | A     | 127   | ASP  | CB-CA-C     | -6.65 | 97.11       | 110.40   |
| 1   | B     | 118   | GLU  | CA-C-O      | 6.63  | 134.03      | 120.10   |
| 1   | A     | 74    | TRP  | O-C-N       | -6.62 | 112.10      | 122.70   |
| 1   | A     | 29    | ALA  | O-C-N       | -6.62 | 112.11      | 122.70   |
| 1   | B     | 53    | PRO  | N-CA-CB     | 6.62  | 111.24      | 103.30   |
| 1   | B     | 80    | GLU  | N-CA-CB     | -6.58 | 98.75       | 110.60   |
| 1   | B     | 89    | PRO  | N-CA-CB     | -6.58 | 95.36       | 102.60   |
| 1   | A     | 130   | PRO  | N-CA-CB     | 6.58  | 111.19      | 103.30   |
| 1   | B     | 30    | TRP  | CB-CG-CD2   | -6.56 | 118.07      | 126.60   |
| 1   | A     | 64[A] | SER  | CA-CB-OG    | -6.56 | 93.50       | 111.20   |
| 1   | A     | 64[B] | SER  | CA-CB-OG    | -6.56 | 93.50       | 111.20   |
| 1   | A     | 87    | ASP  | CA-CB-CG    | -6.55 | 98.98       | 113.40   |
| 1   | A     | 155   | ILE  | N-CA-CB     | 6.54  | 125.85      | 110.80   |
| 1   | A     | 150   | SER  | CB-CA-C     | 6.54  | 122.52      | 110.10   |
| 1   | A     | 127   | ASP  | OD1-CG-OD2  | -6.53 | 110.89      | 123.30   |
| 1   | B     | 1     | MET  | C-N-CA      | -6.52 | 105.39      | 121.70   |
| 1   | A     | 105   | PRO  | CA-C-O      | 6.52  | 135.84      | 120.20   |
| 1   | B     | 6     | ALA  | CA-C-N      | 6.52  | 131.54      | 117.20   |
| 1   | A     | 78    | VAL  | CA-C-O      | 6.52  | 133.79      | 120.10   |
| 1   | A     | 129   | GLU  | CB-CA-C     | 6.51  | 123.42      | 110.40   |
| 1   | B     | 23    | ASN  | CA-C-N      | -6.51 | 102.88      | 117.20   |
| 1   | A     | 144   | ASP  | CB-CG-OD1   | 6.50  | 124.15      | 118.30   |
| 1   | B     | 54    | LEU  | O-C-N       | 6.49  | 133.43      | 121.10   |
| 1   | B     | 116   | ASP  | OD1-CG-OD2  | 6.49  | 135.62      | 123.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 31  | PHE  | CD1-CG-CD2  | 6.48  | 126.72      | 118.30   |
| 1   | A     | 30  | TRP  | CG-CD1-NE1  | -6.47 | 103.63      | 110.10   |
| 1   | A     | 120 | GLU  | CA-C-N      | 6.45  | 129.10      | 116.20   |
| 1   | B     | 58  | LYS  | CD-CE-NZ    | 6.44  | 126.50      | 111.70   |
| 1   | A     | 87  | ASP  | CA-C-O      | 6.43  | 133.60      | 120.10   |
| 1   | A     | 52  | ARG  | NE-CZ-NH2   | 6.42  | 123.51      | 120.30   |
| 1   | A     | 111 | TYR  | C-N-CA      | 6.42  | 137.74      | 121.70   |
| 1   | A     | 151 | TYR  | CB-CG-CD2   | 6.41  | 124.85      | 121.00   |
| 1   | A     | 107 | ALA  | CA-C-O      | 6.40  | 133.55      | 120.10   |
| 1   | B     | 59  | ASN  | CA-C-O      | -6.40 | 106.66      | 120.10   |
| 1   | B     | 106 | LYS  | CB-CG-CD    | 6.40  | 128.24      | 111.60   |
| 1   | A     | 65  | GLN  | O-C-N       | -6.39 | 108.95      | 121.10   |
| 1   | A     | 132 | ASP  | CB-CG-OD1   | 6.39  | 124.06      | 118.30   |
| 1   | B     | 46  | THR  | CA-CB-CG2   | 6.39  | 121.35      | 112.40   |
| 1   | B     | 157 | GLU  | OE1-CD-OE2  | 6.37  | 130.94      | 123.30   |
| 1   | B     | 111 | TYR  | CZ-CE2-CD2  | -6.36 | 114.07      | 119.80   |
| 1   | A     | 153 | PHE  | CB-CG-CD2   | -6.35 | 116.36      | 120.80   |
| 1   | B     | 137 | PHE  | O-C-N       | 6.34  | 132.85      | 122.70   |
| 1   | A     | 48  | GLU  | CA-CB-CG    | 6.33  | 127.33      | 113.40   |
| 1   | A     | 133 | TRP  | NE1-CE2-CZ2 | -6.33 | 123.44      | 130.40   |
| 1   | A     | 158 | ARG  | CB-CG-CD    | -6.33 | 95.16       | 111.60   |
| 1   | B     | 78  | VAL  | CA-CB-CG2   | -6.32 | 101.42      | 110.90   |
| 1   | B     | 120 | GLU  | OE1-CD-OE2  | 6.32  | 130.89      | 123.30   |
| 1   | B     | 16  | MET  | O-C-N       | -6.32 | 112.59      | 122.70   |
| 1   | B     | 149 | HIS  | CA-CB-CG    | 6.31  | 124.33      | 113.60   |
| 1   | B     | 47  | TRP  | N-CA-CB     | -6.31 | 99.25       | 110.60   |
| 1   | A     | 158 | ARG  | NH1-CZ-NH2  | -6.30 | 112.47      | 119.40   |
| 1   | B     | 54  | LEU  | C-N-CD      | 6.30  | 141.62      | 128.40   |
| 1   | B     | 134 | GLU  | CG-CD-OE2   | -6.29 | 105.73      | 118.30   |
| 1   | A     | 80  | GLU  | CB-CA-C     | -6.29 | 97.83       | 110.40   |
| 1   | B     | 24  | LEU  | CB-CG-CD2   | -6.28 | 100.33      | 111.00   |
| 1   | B     | 7   | ALA  | CA-C-N      | 6.28  | 131.01      | 117.20   |
| 1   | B     | 137 | PHE  | CA-C-N      | -6.26 | 103.42      | 117.20   |
| 1   | A     | 47  | TRP  | CD2-CE3-CZ3 | 6.24  | 126.91      | 118.80   |
| 1   | B     | 86  | GLY  | CA-C-N      | -6.22 | 103.51      | 117.20   |
| 1   | B     | 71  | ARG  | NH1-CZ-NH2  | 6.22  | 126.24      | 119.40   |
| 1   | A     | 25  | PRO  | O-C-N       | -6.21 | 112.76      | 122.70   |
| 1   | A     | 109 | LYS  | C-N-CA      | 6.20  | 137.20      | 121.70   |
| 1   | A     | 11  | ASP  | OD1-CG-OD2  | -6.19 | 111.54      | 123.30   |
| 1   | B     | 101 | GLU  | CA-C-O      | 6.18  | 133.09      | 120.10   |
| 1   | A     | 37  | ASP  | CB-CG-OD1   | -6.18 | 112.74      | 118.30   |
| 1   | B     | 44  | ARG  | N-CA-C      | 6.17  | 127.66      | 111.00   |

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| Mol | Chain | Res   | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-------------|-------|-------------|----------|
| 1   | A     | 112   | LEU  | CA-C-O      | 6.17  | 133.06      | 120.10   |
| 1   | B     | 59    | ASN  | CB-CG-OD1   | 6.16  | 133.93      | 121.60   |
| 1   | A     | 126   | PRO  | O-C-N       | -6.16 | 112.84      | 122.70   |
| 1   | A     | 80    | GLU  | N-CA-CB     | -6.16 | 99.51       | 110.60   |
| 1   | B     | 125   | PHE  | CB-CG-CD1   | 6.16  | 125.11      | 120.80   |
| 1   | B     | 16    | MET  | CA-C-O      | 6.16  | 133.03      | 120.10   |
| 1   | A     | 150   | SER  | C-N-CA      | 6.15  | 137.08      | 121.70   |
| 1   | A     | 132   | ASP  | N-CA-CB     | -6.15 | 99.53       | 110.60   |
| 1   | B     | 55    | PRO  | CA-C-O      | -6.14 | 105.47      | 120.20   |
| 1   | A     | 125   | PHE  | C-N-CD      | 6.12  | 141.26      | 128.40   |
| 1   | A     | 32    | LYS  | O-C-N       | 6.12  | 132.49      | 122.70   |
| 1   | B     | 79    | ASP  | O-C-N       | -6.12 | 112.91      | 122.70   |
| 1   | B     | 141   | HIS  | ND1-CG-CD2  | 6.11  | 117.35      | 108.80   |
| 1   | A     | 47    | TRP  | CA-C-N      | -6.10 | 103.79      | 117.20   |
| 1   | B     | 74    | TRP  | CD1-CG-CD2  | -6.10 | 101.42      | 106.30   |
| 1   | A     | 93    | VAL  | CA-CB-CG2   | -6.07 | 101.79      | 110.90   |
| 1   | A     | 17    | GLU  | O-C-N       | 6.07  | 132.41      | 122.70   |
| 1   | B     | 154   | LYS  | CB-CG-CD    | -6.07 | 95.83       | 111.60   |
| 1   | B     | 25    | PRO  | O-C-N       | -6.06 | 113.00      | 122.70   |
| 1   | A     | 152   | CYS  | O-C-N       | -6.05 | 113.02      | 122.70   |
| 1   | A     | 103   | PHE  | O-C-N       | -6.04 | 113.03      | 122.70   |
| 1   | B     | 103   | PHE  | CG-CD2-CE2  | -6.02 | 114.17      | 120.80   |
| 1   | B     | 14    | ILE  | O-C-N       | -6.02 | 112.97      | 123.20   |
| 1   | A     | 135   | SER  | CB-CA-C     | -6.01 | 98.69       | 110.10   |
| 1   | B     | 153   | PHE  | CZ-CE2-CD2  | -6.01 | 112.89      | 120.10   |
| 1   | A     | 141   | HIS  | ND1-CG-CD2  | 6.00  | 117.21      | 108.80   |
| 1   | A     | 37    | ASP  | N-CA-CB     | 5.99  | 121.39      | 110.60   |
| 1   | A     | 46    | THR  | N-CA-CB     | 5.99  | 121.69      | 110.30   |
| 1   | A     | 125   | PHE  | CA-C-O      | -5.98 | 107.55      | 120.10   |
| 1   | B     | 45[A] | HIS  | CA-CB-CG    | -5.96 | 103.46      | 113.60   |
| 1   | B     | 45[B] | HIS  | CA-CB-CG    | -5.96 | 103.46      | 113.60   |
| 1   | A     | 69    | ASP  | N-CA-C      | 5.95  | 127.07      | 111.00   |
| 1   | A     | 141   | HIS  | CE1-NE2-CD2 | 5.95  | 121.47      | 106.60   |
| 1   | A     | 157   | GLU  | CB-CG-CD    | 5.95  | 130.26      | 114.20   |
| 1   | A     | 141   | HIS  | O-C-N       | -5.94 | 113.20      | 122.70   |
| 1   | B     | 74    | TRP  | CH2-CZ2-CE2 | -5.92 | 111.48      | 117.40   |
| 1   | A     | 87    | ASP  | OD1-CG-OD2  | 5.92  | 134.55      | 123.30   |
| 1   | A     | 152   | CYS  | C-N-CA      | 5.92  | 136.50      | 121.70   |
| 1   | B     | 157   | GLU  | CA-CB-CG    | 5.92  | 126.41      | 113.40   |
| 1   | A     | 27    | ASP  | CB-CG-OD1   | -5.89 | 113.00      | 118.30   |
| 1   | B     | 26    | ALA  | CA-C-O      | 5.88  | 132.45      | 120.10   |
| 1   | B     | 141   | HIS  | CA-C-O      | 5.88  | 132.44      | 120.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 90  | GLU  | CA-C-O      | 5.88  | 132.44      | 120.10   |
| 1   | B     | 36  | LEU  | CB-CG-CD2   | -5.86 | 101.03      | 111.00   |
| 1   | B     | 31  | PHE  | CA-C-O      | -5.86 | 107.80      | 120.10   |
| 1   | B     | 53  | PRO  | CA-CB-CG    | -5.86 | 92.87       | 104.00   |
| 1   | B     | 154 | LYS  | CD-CE-NZ    | -5.85 | 98.25       | 111.70   |
| 1   | B     | 53  | PRO  | CA-C-O      | 5.84  | 134.22      | 120.20   |
| 1   | B     | 31  | PHE  | CB-CG-CD1   | 5.84  | 124.89      | 120.80   |
| 1   | B     | 96  | GLY  | CA-C-N      | -5.83 | 104.54      | 116.20   |
| 1   | A     | 79  | ASP  | N-CA-CB     | -5.83 | 100.11      | 110.60   |
| 1   | A     | 125 | PHE  | O-C-N       | 5.83  | 132.17      | 121.10   |
| 1   | A     | 40  | VAL  | O-C-N       | 5.82  | 132.01      | 122.70   |
| 1   | A     | 133 | TRP  | CH2-CZ2-CE2 | -5.82 | 111.58      | 117.40   |
| 1   | A     | 44  | ARG  | CA-C-N      | 5.81  | 129.98      | 117.20   |
| 1   | A     | 34  | ASN  | O-C-N       | -5.80 | 113.43      | 122.70   |
| 1   | A     | 100 | TYR  | CD1-CG-CD2  | 5.79  | 124.27      | 117.90   |
| 1   | B     | 119 | VAL  | CA-CB-CG2   | 5.79  | 119.59      | 110.90   |
| 1   | A     | 74  | TRP  | CD1-NE1-CE2 | 5.79  | 114.21      | 109.00   |
| 1   | B     | 2   | ILE  | CA-CB-CG2   | 5.79  | 122.47      | 110.90   |
| 1   | A     | 3   | SER  | N-CA-CB     | 5.78  | 119.17      | 110.50   |
| 1   | B     | 62  | LEU  | N-CA-CB     | 5.78  | 121.97      | 110.40   |
| 1   | A     | 133 | TRP  | CD1-NE1-CE2 | -5.78 | 103.80      | 109.00   |
| 1   | B     | 109 | LYS  | CD-CE-NZ    | 5.78  | 124.98      | 111.70   |
| 1   | B     | 139 | GLU  | OE1-CD-OE2  | -5.77 | 116.37      | 123.30   |
| 1   | A     | 44  | ARG  | NE-CZ-NH2   | -5.77 | 117.42      | 120.30   |
| 1   | A     | 74  | TRP  | C-N-CA      | 5.75  | 136.08      | 121.70   |
| 1   | B     | 83  | ALA  | N-CA-CB     | -5.75 | 102.05      | 110.10   |
| 1   | B     | 65  | GLN  | OE1-CD-NE2  | -5.75 | 108.67      | 121.90   |
| 1   | B     | 34  | ASN  | CB-CG-OD1   | 5.74  | 133.07      | 121.60   |
| 1   | A     | 158 | ARG  | N-CA-CB     | 5.73  | 120.91      | 110.60   |
| 1   | B     | 20  | MET  | N-CA-CB     | 5.72  | 120.91      | 110.60   |
| 1   | B     | 115 | ILE  | O-C-N       | 5.71  | 131.84      | 122.70   |
| 1   | A     | 47  | TRP  | CB-CG-CD1   | -5.70 | 119.59      | 127.00   |
| 1   | B     | 135 | SER  | CA-C-N      | 5.70  | 129.74      | 117.20   |
| 1   | B     | 112 | LEU  | O-C-N       | 5.69  | 131.81      | 122.70   |
| 1   | A     | 53  | PRO  | N-CA-CB     | 5.69  | 110.12      | 103.30   |
| 1   | A     | 54  | LEU  | CB-CG-CD1   | -5.69 | 101.33      | 111.00   |
| 1   | B     | 81  | ALA  | CB-CA-C     | 5.68  | 118.62      | 110.10   |
| 1   | B     | 145 | ALA  | CB-CA-C     | -5.68 | 101.58      | 110.10   |
| 1   | A     | 140 | PHE  | O-C-N       | 5.68  | 131.78      | 122.70   |
| 1   | A     | 156 | LEU  | O-C-N       | -5.67 | 113.62      | 122.70   |
| 1   | B     | 24  | LEU  | CB-CG-CD1   | -5.67 | 101.36      | 111.00   |
| 1   | B     | 151 | TYR  | CA-C-O      | -5.67 | 108.20      | 120.10   |

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| Mol | Chain | Res   | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-------------|-------|-------------|----------|
| 1   | B     | 45[A] | HIS  | O-C-N       | -5.66 | 113.64      | 122.70   |
| 1   | B     | 45[B] | HIS  | O-C-N       | -5.66 | 113.64      | 122.70   |
| 1   | A     | 104   | LEU  | CB-CG-CD1   | 5.66  | 120.62      | 111.00   |
| 1   | B     | 45[A] | HIS  | CG-CD2-NE2  | -5.66 | 98.45       | 109.20   |
| 1   | B     | 45[B] | HIS  | CG-CD2-NE2  | -5.66 | 98.45       | 109.20   |
| 1   | A     | 158   | ARG  | CB-CA-C     | -5.65 | 99.11       | 110.40   |
| 1   | A     | 81    | ALA  | CA-C-O      | -5.64 | 108.25      | 120.10   |
| 1   | A     | 78    | VAL  | CA-C-N      | -5.64 | 104.79      | 117.20   |
| 1   | B     | 113   | THR  | CA-CB-CG2   | 5.63  | 120.29      | 112.40   |
| 1   | B     | 120   | GLU  | C-N-CA      | -5.63 | 110.47      | 122.30   |
| 1   | A     | 103   | PHE  | CE1-CZ-CE2  | 5.63  | 130.13      | 120.00   |
| 1   | A     | 74    | TRP  | CB-CG-CD1   | -5.63 | 119.69      | 127.00   |
| 1   | A     | 29    | ALA  | N-CA-CB     | -5.62 | 102.22      | 110.10   |
| 1   | B     | 133   | TRP  | CH2-CZ2-CE2 | 5.62  | 123.02      | 117.40   |
| 1   | A     | 24    | LEU  | CB-CG-CD1   | -5.61 | 101.46      | 111.00   |
| 1   | B     | 17    | GLU  | CB-CG-CD    | 5.60  | 129.32      | 114.20   |
| 1   | B     | 100   | TYR  | CE1-CZ-CE2  | 5.60  | 128.76      | 119.80   |
| 1   | B     | 97    | GLY  | N-CA-C      | 5.59  | 127.09      | 113.10   |
| 1   | B     | 8     | LEU  | CB-CG-CD2   | 5.59  | 120.51      | 111.00   |
| 1   | A     | 18    | ASN  | CB-CG-ND2   | -5.59 | 103.28      | 116.70   |
| 1   | A     | 112   | LEU  | CB-CG-CD2   | 5.57  | 120.47      | 111.00   |
| 1   | B     | 23    | ASN  | N-CA-CB     | -5.57 | 100.58      | 110.60   |
| 1   | B     | 140   | PHE  | CA-C-O      | 5.56  | 131.78      | 120.10   |
| 1   | A     | 32    | LYS  | N-CA-CB     | -5.55 | 100.61      | 110.60   |
| 1   | A     | 140   | PHE  | CD1-CG-CD2  | 5.54  | 125.50      | 118.30   |
| 1   | B     | 44    | ARG  | CD-NE-CZ    | -5.53 | 115.86      | 123.60   |
| 1   | A     | 151   | TYR  | CG-CD1-CE1  | 5.53  | 125.72      | 121.30   |
| 1   | A     | 154   | LYS  | CB-CG-CD    | 5.53  | 125.97      | 111.60   |
| 1   | A     | 11    | ASP  | CB-CG-OD2   | -5.52 | 113.33      | 118.30   |
| 1   | A     | 30    | TRP  | CE2-CD2-CG  | 5.52  | 111.72      | 107.30   |
| 1   | A     | 100   | TYR  | CD1-CE1-CZ  | 5.49  | 124.74      | 119.80   |
| 1   | B     | 134   | GLU  | CG-CD-OE1   | 5.48  | 129.26      | 118.30   |
| 1   | B     | 98    | ARG  | CB-CA-C     | -5.48 | 99.44       | 110.40   |
| 1   | B     | 45[A] | HIS  | CE1-NE2-CD2 | 5.48  | 120.30      | 106.60   |
| 1   | B     | 45[B] | HIS  | CE1-NE2-CD2 | 5.48  | 120.30      | 106.60   |
| 1   | A     | 31    | PHE  | CD1-CE1-CZ  | -5.47 | 113.53      | 120.10   |
| 1   | A     | 82    | ILE  | N-CA-CB     | 5.47  | 123.39      | 110.80   |
| 1   | A     | 100   | TYR  | CA-C-N      | -5.46 | 105.18      | 117.20   |
| 1   | A     | 6     | ALA  | CA-C-O      | 5.46  | 131.56      | 120.10   |
| 1   | A     | 76    | LYS  | CA-C-O      | -5.45 | 108.65      | 120.10   |
| 1   | B     | 18    | ASN  | N-CA-CB     | -5.45 | 100.78      | 110.60   |
| 1   | A     | 144   | ASP  | CA-C-N      | 5.45  | 129.19      | 117.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 58  | LYS  | CA-CB-CG    | -5.45 | 101.42      | 113.40   |
| 1   | B     | 97  | GLY  | CA-C-O      | 5.44  | 130.39      | 120.60   |
| 1   | B     | 133 | TRP  | CD1-NE1-CE2 | 5.43  | 113.89      | 109.00   |
| 1   | B     | 144 | ASP  | CB-CG-OD2   | -5.43 | 113.41      | 118.30   |
| 1   | B     | 62  | LEU  | CD1-CG-CD2  | -5.43 | 94.21       | 110.50   |
| 1   | A     | 23  | ASN  | CB-CG-ND2   | -5.42 | 103.70      | 116.70   |
| 1   | B     | 86  | GLY  | O-C-N       | 5.41  | 131.35      | 122.70   |
| 1   | B     | 126 | PRO  | CA-C-O      | 5.41  | 133.18      | 120.20   |
| 1   | B     | 22  | TRP  | NE1-CE2-CZ2 | -5.40 | 124.46      | 130.40   |
| 1   | B     | 89  | PRO  | N-CA-C      | 5.39  | 126.12      | 112.10   |
| 1   | B     | 42  | MET  | C-N-CA      | -5.39 | 110.98      | 122.30   |
| 1   | B     | 48  | GLU  | CB-CG-CD    | 5.38  | 128.73      | 114.20   |
| 1   | A     | 122 | ASP  | CB-CG-OD2   | -5.38 | 113.46      | 118.30   |
| 1   | B     | 142 | ASP  | CB-CG-OD1   | -5.37 | 113.47      | 118.30   |
| 1   | A     | 12  | ARG  | NE-CZ-NH1   | -5.36 | 117.62      | 120.30   |
| 1   | A     | 128 | TYR  | O-C-N       | 5.35  | 131.27      | 122.70   |
| 1   | B     | 158 | ARG  | C-N-CA      | -5.35 | 108.33      | 121.70   |
| 1   | A     | 45  | HIS  | CE1-NE2-CD2 | 5.35  | 119.97      | 106.60   |
| 1   | A     | 150 | SER  | CA-C-O      | 5.35  | 131.33      | 120.10   |
| 1   | B     | 105 | PRO  | CB-CG-CD    | -5.34 | 85.66       | 106.50   |
| 1   | B     | 130 | PRO  | O-C-N       | 5.34  | 131.25      | 122.70   |
| 1   | A     | 74  | TRP  | CG-CD1-NE1  | -5.34 | 104.76      | 110.10   |
| 1   | A     | 89  | PRO  | CB-CA-C     | -5.33 | 98.66       | 112.00   |
| 1   | B     | 127 | ASP  | CB-CG-OD2   | -5.33 | 113.50      | 118.30   |
| 1   | A     | 103 | PHE  | CG-CD2-CE2  | 5.33  | 126.67      | 120.80   |
| 1   | B     | 8   | LEU  | O-C-N       | -5.33 | 114.17      | 122.70   |
| 1   | A     | 68  | THR  | O-C-N       | -5.33 | 114.17      | 122.70   |
| 1   | B     | 158 | ARG  | CG-CD-NE    | -5.32 | 100.62      | 111.80   |
| 1   | A     | 62  | LEU  | O-C-N       | -5.32 | 114.20      | 122.70   |
| 1   | B     | 61  | ILE  | CA-CB-CG2   | 5.31  | 121.52      | 110.90   |
| 1   | A     | 71  | ARG  | N-CA-CB     | -5.31 | 101.04      | 110.60   |
| 1   | B     | 43  | GLY  | CA-C-O      | 5.31  | 130.16      | 120.60   |
| 1   | B     | 74  | TRP  | CB-CG-CD2   | 5.30  | 133.49      | 126.60   |
| 1   | B     | 31  | PHE  | CG-CD2-CE2  | -5.30 | 114.97      | 120.80   |
| 1   | B     | 156 | LEU  | CA-C-N      | -5.30 | 105.54      | 117.20   |
| 1   | B     | 2   | ILE  | CA-CB-CG1   | -5.29 | 100.94      | 111.00   |
| 1   | A     | 14  | ILE  | C-N-CA      | -5.29 | 111.19      | 122.30   |
| 1   | A     | 47  | TRP  | C-N-CA      | -5.29 | 108.48      | 121.70   |
| 1   | B     | 130 | PRO  | N-CA-CB     | 5.28  | 109.64      | 103.30   |
| 1   | A     | 14  | ILE  | O-C-N       | 5.27  | 132.16      | 123.20   |
| 1   | A     | 154 | LYS  | CG-CD-CE    | 5.26  | 127.70      | 111.90   |
| 1   | B     | 40  | VAL  | O-C-N       | 5.26  | 131.11      | 122.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 32  | LYS  | CD-CE-NZ    | -5.26 | 99.61       | 111.70   |
| 1   | A     | 12  | ARG  | NH1-CZ-NH2  | -5.25 | 113.62      | 119.40   |
| 1   | A     | 17  | GLU  | CA-CB-CG    | 5.25  | 124.96      | 113.40   |
| 1   | B     | 15  | GLY  | O-C-N       | 5.25  | 131.10      | 122.70   |
| 1   | B     | 59  | ASN  | O-C-N       | -5.25 | 114.30      | 122.70   |
| 1   | A     | 45  | HIS  | ND1-CE1-NE2 | -5.24 | 98.37       | 109.90   |
| 1   | B     | 135 | SER  | C-N-CA      | 5.24  | 134.80      | 121.70   |
| 1   | B     | 102 | GLN  | N-CA-CB     | -5.23 | 101.19      | 110.60   |
| 1   | A     | 153 | PHE  | CA-C-O      | -5.22 | 109.13      | 120.10   |
| 1   | B     | 153 | PHE  | CA-C-O      | -5.22 | 109.14      | 120.10   |
| 1   | B     | 141 | HIS  | O-C-N       | -5.21 | 114.36      | 122.70   |
| 1   | B     | 57  | ARG  | CB-CA-C     | -5.19 | 100.02      | 110.40   |
| 1   | A     | 44  | ARG  | CG-CD-NE    | -5.18 | 100.92      | 111.80   |
| 1   | A     | 74  | TRP  | NE1-CE2-CD2 | -5.18 | 102.12      | 107.30   |
| 1   | A     | 84  | ALA  | N-CA-CB     | 5.18  | 117.36      | 110.10   |
| 1   | A     | 98  | ARG  | CA-CB-CG    | -5.18 | 102.00      | 113.40   |
| 1   | A     | 114 | HIS  | CG-ND1-CE1  | 5.18  | 115.45      | 108.20   |
| 1   | B     | 82  | ILE  | CB-CG1-CD1  | 5.17  | 128.39      | 113.90   |
| 1   | A     | 134 | GLU  | O-C-N       | -5.17 | 114.43      | 122.70   |
| 1   | B     | 28  | LEU  | CA-C-O      | -5.17 | 109.24      | 120.10   |
| 1   | A     | 4   | LEU  | N-CA-CB     | 5.16  | 120.73      | 110.40   |
| 1   | A     | 103 | PHE  | CA-C-N      | 5.16  | 128.56      | 117.20   |
| 1   | A     | 88  | VAL  | CA-C-N      | -5.16 | 102.65      | 117.10   |
| 1   | B     | 17  | GLU  | N-CA-CB     | -5.16 | 101.31      | 110.60   |
| 1   | A     | 21  | PRO  | N-CA-CB     | 5.16  | 109.49      | 103.30   |
| 1   | A     | 58  | LYS  | CD-CE-NZ    | -5.15 | 99.86       | 111.70   |
| 1   | A     | 142 | ASP  | CB-CG-OD1   | 5.15  | 122.93      | 118.30   |
| 1   | B     | 9   | ALA  | N-CA-C      | -5.15 | 97.10       | 111.00   |
| 1   | B     | 33  | ARG  | CA-C-N      | -5.15 | 105.88      | 117.20   |
| 1   | B     | 148 | SER  | N-CA-CB     | -5.14 | 102.79      | 110.50   |
| 1   | A     | 82  | ILE  | CA-C-O      | 5.14  | 130.89      | 120.10   |
| 1   | A     | 1   | MET  | N-CA-C      | -5.13 | 97.15       | 111.00   |
| 1   | B     | 65  | GLN  | CA-C-O      | 5.13  | 130.87      | 120.10   |
| 1   | A     | 61  | ILE  | CB-CG1-CD1  | 5.12  | 128.25      | 113.90   |
| 1   | A     | 36  | LEU  | CB-CG-CD2   | -5.12 | 102.30      | 111.00   |
| 1   | B     | 104 | LEU  | N-CA-CB     | 5.12  | 120.64      | 110.40   |
| 1   | A     | 52  | ARG  | C-N-CD      | 5.10  | 139.11      | 128.40   |
| 1   | A     | 74  | TRP  | CH2-CZ2-CE2 | -5.10 | 112.30      | 117.40   |
| 1   | B     | 103 | PHE  | O-C-N       | 5.10  | 130.86      | 122.70   |
| 1   | B     | 146 | GLN  | CA-CB-CG    | -5.10 | 102.17      | 113.40   |
| 1   | B     | 76  | LYS  | N-CA-CB     | -5.10 | 101.42      | 110.60   |
| 1   | B     | 22  | TRP  | CD1-NE1-CE2 | -5.10 | 104.41      | 109.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 22  | TRP  | CA-CB-CG   | 5.10  | 123.39      | 113.70   |
| 1   | B     | 26  | ALA  | O-C-N      | -5.10 | 114.55      | 122.70   |
| 1   | B     | 38  | LYS  | CA-C-N     | -5.09 | 102.84      | 117.10   |
| 1   | B     | 145 | ALA  | O-C-N      | 5.09  | 130.85      | 122.70   |
| 1   | A     | 77  | SER  | C-N-CA     | 5.09  | 134.42      | 121.70   |
| 1   | A     | 103 | PHE  | CG-CD1-CE1 | -5.09 | 115.20      | 120.80   |
| 1   | A     | 124 | HIS  | C-N-CA     | 5.09  | 134.43      | 121.70   |
| 1   | B     | 14  | ILE  | N-CA-CB    | 5.08  | 122.49      | 110.80   |
| 1   | A     | 44  | ARG  | CA-C-O     | -5.08 | 109.43      | 120.10   |
| 1   | B     | 23  | ASN  | CA-CB-CG   | -5.08 | 102.23      | 113.40   |
| 1   | A     | 54  | LEU  | O-C-N      | 5.08  | 130.75      | 121.10   |
| 1   | B     | 7   | ALA  | CA-C-O     | -5.08 | 109.44      | 120.10   |
| 1   | B     | 132 | ASP  | O-C-N      | 5.07  | 130.81      | 122.70   |
| 1   | B     | 140 | PHE  | CA-C-N     | -5.06 | 106.07      | 117.20   |
| 1   | A     | 109 | LYS  | CG-CD-CE   | 5.05  | 127.05      | 111.90   |
| 1   | A     | 46  | THR  | CA-CB-OG1  | -5.04 | 98.41       | 109.00   |
| 1   | A     | 133 | TRP  | C-N-CA     | 5.03  | 134.28      | 121.70   |
| 1   | B     | 18  | ASN  | CA-C-O     | 5.00  | 130.61      | 120.10   |
| 1   | B     | 44  | ARG  | N-CA-CB    | -5.00 | 101.59      | 110.60   |
| 1   | A     | 144 | ASP  | C-N-CA     | 5.00  | 134.20      | 121.70   |

There are no chirality outliers.

All (22) planarity outliers are listed below:

| Mol | Chain | Res   | Type | Group               |
|-----|-------|-------|------|---------------------|
| 1   | A     | 117   | ALA  | Mainchain           |
| 1   | A     | 33    | ARG  | Sidechain           |
| 1   | A     | 44    | ARG  | Sidechain           |
| 1   | A     | 52    | ARG  | Sidechain           |
| 1   | A     | 65    | GLN  | Mainchain,Peptide   |
| 1   | A     | 98    | ARG  | Sidechain           |
| 1   | B     | 101   | GLU  | Mainchain           |
| 1   | B     | 12    | ARG  | Sidechain,Mainchain |
| 1   | B     | 29    | ALA  | Mainchain           |
| 1   | B     | 33    | ARG  | Sidechain           |
| 1   | B     | 41    | ILE  | Mainchain           |
| 1   | B     | 44    | ARG  | Sidechain           |
| 1   | B     | 45[B] | HIS  | Mainchain           |
| 1   | B     | 52    | ARG  | Sidechain           |
| 1   | B     | 55    | PRO  | Mainchain           |
| 1   | B     | 60    | ILE  | Mainchain           |
| 1   | B     | 64[B] | SER  | Mainchain           |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 7   | ALA  | Mainchain |
| 1   | B     | 71  | ARG  | Sidechain |
| 1   | B     | 98  | 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     | 1252  | 0        | 1175     | 24      | 0            |
| 1   | B     | 1286  | 0        | 1217     | 32      | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 33    | 0        | 19       | 2       | 0            |
| 3   | B     | 33    | 0        | 20       | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 239   | 0        | 0        | 11      | 0            |
| 5   | B     | 189   | 0        | 0        | 9       | 0            |
| All | All   | 3035  | 0        | 2431     | 57      | 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 11.

All (57) 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:B:57:ARG:CB     | 1:B:57:ARG:CA  | 1.74                     | 1.61              |
| 1:A:58:LYS:CD     | 1:A:58:LYS:CE  | 1.75                     | 1.57              |
| 1:A:109:LYS:NZ    | 1:A:109:LYS:CE | 1.70                     | 1.52              |
| 1:B:159:ARG:N     | 1:B:159:ARG:CA | 1.70                     | 1.49              |
| 1:B:122[B]:ASP:C  | 1:B:123:THR:N  | 1.82                     | 1.32              |
| 1:B:64[B]:SER:OG  | 1:B:65:GLN:NE2 | 1.86                     | 1.06              |
| 1:A:64[B]:SER:HB3 | 5:A:229:HOH:O  | 1.60                     | 1.01              |
| 1:B:124:HIS:HB3   | 5:B:342:HOH:O  | 1.59                     | 0.99              |
| 1:A:51:GLY:HA3    | 5:B:167:HOH:O  | 1.70                     | 0.89              |
| 1:B:57:ARG:CG     | 1:B:57:ARG:CA  | 2.50                     | 0.89              |
| 1:A:58:LYS:CG     | 1:A:58:LYS:CE  | 2.52                     | 0.88              |

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| Atom-1            | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-----------------|--------------------------|-------------------|
| 1:B:159:ARG:N     | 1:B:159:ARG:CB  | 2.40                     | 0.84              |
| 1:B:57:ARG:N      | 1:B:57:ARG:CB   | 2.42                     | 0.81              |
| 1:B:158:ARG:C     | 1:B:159:ARG:CA  | 2.49                     | 0.80              |
| 1:A:46:THR:OG1    | 5:A:376:HOH:O   | 2.05                     | 0.75              |
| 1:B:57:ARG:CB     | 1:B:57:ARG:C    | 2.56                     | 0.73              |
| 1:A:58:LYS:CD     | 1:A:58:LYS:NZ   | 2.54                     | 0.71              |
| 1:B:108:GLN:HG2   | 5:B:181:HOH:O   | 1.93                     | 0.68              |
| 1:B:129:GLU:HB3   | 1:B:132:ASP:OD2 | 1.99                     | 0.61              |
| 1:A:33:ARG:HG3    | 5:A:239:HOH:O   | 2.01                     | 0.60              |
| 1:A:109:LYS:NZ    | 1:A:109:LYS:CD  | 2.58                     | 0.59              |
| 1:B:159:ARG:C     | 1:B:159:ARG:N   | 2.54                     | 0.58              |
| 1:A:67:GLY:HA2    | 1:A:74:TRP:CE2  | 2.38                     | 0.58              |
| 1:B:45[B]:HIS:HD2 | 5:B:329:HOH:O   | 1.86                     | 0.57              |
| 1:A:78:VAL:O      | 1:A:82:ILE:HD12 | 2.04                     | 0.57              |
| 1:B:12:ARG:NH1    | 5:B:342:HOH:O   | 2.38                     | 0.56              |
| 1:B:75:VAL:HG21   | 1:B:81:ALA:HB2  | 1.87                     | 0.55              |
| 1:A:128:TYR:O     | 1:A:130:PRO:HD3 | 2.07                     | 0.55              |
| 1:A:67:GLY:HA2    | 1:A:74:TRP:CD2  | 2.43                     | 0.54              |
| 1:B:64[A]:SER:HB2 | 1:B:65:GLN:NE2  | 2.21                     | 0.54              |
| 1:A:95:GLY:C      | 5:A:376:HOH:O   | 2.46                     | 0.53              |
| 3:A:161:MTX:HG1   | 5:A:328:HOH:O   | 2.11                     | 0.51              |
| 1:B:97:GLY:O      | 1:B:101:GLU:HG3 | 2.11                     | 0.50              |
| 1:B:12:ARG:HB2    | 5:B:342:HOH:O   | 2.12                     | 0.49              |
| 1:A:134:GLU:HG3   | 5:A:373:HOH:O   | 2.11                     | 0.49              |
| 1:B:146:GLN:OE1   | 5:B:167:HOH:O   | 2.20                     | 0.49              |
| 1:B:57:ARG:HG3    | 1:B:57:ARG:CA   | 2.42                     | 0.48              |
| 1:A:44:ARG:HG3    | 1:A:44:ARG:O    | 2.15                     | 0.47              |
| 1:A:27:ASP:OD2    | 3:A:161:MTX:N1  | 2.48                     | 0.46              |
| 1:B:64[A]:SER:CB  | 1:B:65:GLN:HE21 | 2.28                     | 0.46              |
| 1:B:44:ARG:O      | 1:B:48:GLU:HG3  | 2.16                     | 0.46              |
| 1:B:16:MET:HE1    | 5:B:211:HOH:O   | 2.16                     | 0.46              |
| 1:B:64[A]:SER:HB2 | 1:B:65:GLN:HE21 | 1.80                     | 0.46              |
| 1:B:1:MET:O       | 1:B:90:GLU:HA   | 2.17                     | 0.45              |
| 1:A:10:VAL:HG22   | 1:A:117:ALA:O   | 2.17                     | 0.45              |
| 1:A:114:HIS:CD2   | 5:A:381:HOH:O   | 2.70                     | 0.44              |
| 1:A:46:THR:CB     | 5:A:376:HOH:O   | 2.62                     | 0.43              |
| 1:B:12:ARG:CZ     | 5:B:342:HOH:O   | 2.67                     | 0.43              |
| 1:B:65:GLN:HA     | 1:B:66:PRO:HD3  | 1.79                     | 0.43              |
| 1:A:95:GLY:CA     | 5:A:376:HOH:O   | 2.67                     | 0.42              |
| 1:B:44:ARG:HH12   | 1:B:68:THR:HG23 | 1.84                     | 0.42              |
| 1:B:75:VAL:HG21   | 1:B:81:ALA:CB   | 2.49                     | 0.41              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:46:THR:CG2  | 5:A:376:HOH:O   | 2.69                     | 0.41              |
| 1:A:158:ARG:NH2 | 5:A:199:HOH:O   | 2.54                     | 0.40              |
| 1:B:4:LEU:HD13  | 1:B:107:ALA:HB2 | 2.03                     | 0.40              |
| 1:A:54:LEU:HA   | 1:A:55:PRO:HD3  | 1.96                     | 0.40              |
| 1:B:44:ARG:HH12 | 1:B:68:THR:CG2  | 2.34                     | 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     | 158/159 (99%)  | 146 (92%) | 10 (6%) | 2 (1%)   | 14          | 2   |
| 1   | B     | 160/159 (101%) | 156 (98%) | 4 (2%)  | 0        | 100         | 100 |
| All | All   | 318/318 (100%) | 302 (95%) | 14 (4%) | 2 (1%)   | 28          | 12  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 67  | GLY  |
| 1   | A     | 66  | PRO  |

### 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     | 130/136 (96%)  | 117 (90%) | 13 (10%) | 9           | 2 |
| 1   | B     | 137/136 (101%) | 129 (94%) | 8 (6%)   | 23          | 7 |
| All | All   | 267/272 (98%)  | 246 (92%) | 21 (8%)  | 15          | 3 |

All (21) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | A     | 4     | LEU  |
| 1   | A     | 21    | PRO  |
| 1   | A     | 61    | ILE  |
| 1   | A     | 62    | LEU  |
| 1   | A     | 64[A] | SER  |
| 1   | A     | 64[B] | SER  |
| 1   | A     | 80    | GLU  |
| 1   | A     | 87    | ASP  |
| 1   | A     | 98    | ARG  |
| 1   | A     | 104   | LEU  |
| 1   | A     | 109   | LYS  |
| 1   | A     | 120   | GLU  |
| 1   | A     | 136   | VAL  |
| 1   | B     | 1     | MET  |
| 1   | B     | 4     | LEU  |
| 1   | B     | 52    | ARG  |
| 1   | B     | 61    | ILE  |
| 1   | B     | 68    | THR  |
| 1   | B     | 111   | TYR  |
| 1   | B     | 118   | GLU  |
| 1   | B     | 158   | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 102 | GLN  |
| 1   | A     | 114 | HIS  |
| 1   | B     | 65  | GLN  |
| 1   | B     | 124 | HIS  |

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | MTX  | A     | 161 | -    | 28,35,35     | 2.91 | 12 (42%)    | 36,49,49    | 3.55 | 18 (50%)    |
| 3   | MTX  | B     | 162 | -    | 28,35,35     | 2.67 | 12 (42%)    | 36,49,49    | 3.14 | 14 (38%)    |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | MTX  | A     | 161 | -    | -       | 0/19/25/25 | 0/3/3/3 |
| 3   | MTX  | B     | 162 | -    | -       | 0/19/25/25 | 0/3/3/3 |

All (24) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | B     | 162 | MTX  | C7-C6   | -5.98 | 1.28        | 1.39     |
| 3   | A     | 161 | MTX  | C16-C11 | -3.62 | 1.33        | 1.39     |
| 3   | B     | 162 | MTX  | CA-N    | -3.19 | 1.42        | 1.46     |
| 3   | B     | 162 | MTX  | CB-CA   | -2.75 | 1.49        | 1.53     |
| 3   | A     | 161 | MTX  | C4-NA4  | -2.48 | 1.23        | 1.34     |
| 3   | B     | 162 | MTX  | C16-C15 | -2.47 | 1.34        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | A     | 161 | MTX  | C13-C14 | -2.34 | 1.34        | 1.39     |
| 3   | A     | 161 | MTX  | C2-N3   | -2.06 | 1.31        | 1.35     |
| 3   | B     | 162 | MTX  | C7-N8   | 2.13  | 1.35        | 1.31     |
| 3   | B     | 162 | MTX  | C16-C11 | 2.14  | 1.42        | 1.39     |
| 3   | B     | 162 | MTX  | C8A-N8  | 2.27  | 1.40        | 1.37     |
| 3   | B     | 162 | MTX  | CB-CG   | 2.73  | 1.65        | 1.53     |
| 3   | A     | 161 | MTX  | C15-C14 | 3.09  | 1.45        | 1.39     |
| 3   | A     | 161 | MTX  | C8A-N8  | 3.72  | 1.43        | 1.37     |
| 3   | B     | 162 | MTX  | C2-NA2  | 3.76  | 1.41        | 1.34     |
| 3   | B     | 162 | MTX  | C8A-N1  | 4.05  | 1.44        | 1.36     |
| 3   | A     | 161 | MTX  | C9-N10  | 4.33  | 1.53        | 1.46     |
| 3   | A     | 161 | MTX  | C7-C6   | 4.67  | 1.47        | 1.39     |
| 3   | A     | 161 | MTX  | C14-N10 | 4.93  | 1.54        | 1.39     |
| 3   | B     | 162 | MTX  | CM-N10  | 4.97  | 1.54        | 1.46     |
| 3   | A     | 161 | MTX  | CM-N10  | 5.13  | 1.54        | 1.46     |
| 3   | A     | 161 | MTX  | O-C     | 5.15  | 1.34        | 1.23     |
| 3   | B     | 162 | MTX  | C9-N10  | 6.86  | 1.57        | 1.46     |
| 3   | A     | 161 | MTX  | CA-N    | 7.13  | 1.56        | 1.46     |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 161 | MTX  | C2-N1-C8A   | -8.95 | 104.71      | 115.16   |
| 3   | A     | 161 | MTX  | N8-C8A-N1   | -8.52 | 105.02      | 116.04   |
| 3   | A     | 161 | MTX  | CB-CA-CT    | -7.30 | 101.68      | 112.28   |
| 3   | B     | 162 | MTX  | C15-C16-C11 | -6.16 | 113.90      | 120.79   |
| 3   | A     | 161 | MTX  | C11-C-N     | -5.64 | 106.55      | 116.97   |
| 3   | A     | 161 | MTX  | CG-CB-CA    | -5.45 | 102.30      | 113.19   |
| 3   | B     | 162 | MTX  | CB-CA-CT    | -5.05 | 104.95      | 112.28   |
| 3   | B     | 162 | MTX  | CM-N10-C9   | -4.56 | 101.83      | 114.18   |
| 3   | B     | 162 | MTX  | C13-C14-N10 | -4.43 | 115.08      | 121.65   |
| 3   | A     | 161 | MTX  | C6-C7-N8    | -4.01 | 119.03      | 123.09   |
| 3   | A     | 161 | MTX  | C15-C16-C11 | -3.48 | 116.90      | 120.79   |
| 3   | B     | 162 | MTX  | C13-C12-C11 | -3.46 | 116.92      | 120.79   |
| 3   | A     | 161 | MTX  | C12-C13-C14 | -3.29 | 115.86      | 120.34   |
| 3   | B     | 162 | MTX  | C6-N5-C4A   | -3.27 | 112.16      | 117.72   |
| 3   | B     | 162 | MTX  | CG-CB-CA    | -3.17 | 106.86      | 113.19   |
| 3   | B     | 162 | MTX  | N8-C8A-N1   | -2.64 | 112.62      | 116.04   |
| 3   | A     | 161 | MTX  | NA2-C2-N1   | -2.31 | 113.49      | 117.75   |
| 3   | B     | 162 | MTX  | C12-C11-C   | -2.12 | 113.80      | 120.61   |
| 3   | B     | 162 | MTX  | N1-C2-N3    | -2.03 | 124.49      | 127.46   |
| 3   | A     | 161 | MTX  | C16-C15-C14 | 2.19  | 123.33      | 120.34   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3   | B     | 162 | MTX  | C7-C6-N5    | 2.64 | 122.54      | 120.80   |
| 3   | A     | 161 | MTX  | CB-CA-N     | 3.16 | 115.03      | 110.22   |
| 3   | A     | 161 | MTX  | C4A-C4-NA4  | 3.18 | 126.95      | 120.47   |
| 3   | A     | 161 | MTX  | C9-N10-C14  | 3.42 | 126.52      | 119.49   |
| 3   | A     | 161 | MTX  | C2-N3-C4    | 3.55 | 127.73      | 116.73   |
| 3   | A     | 161 | MTX  | NA4-C4-N3   | 3.64 | 127.83      | 116.59   |
| 3   | A     | 161 | MTX  | C13-C12-C11 | 3.93 | 125.18      | 120.79   |
| 3   | A     | 161 | MTX  | O-C-N       | 4.43 | 130.56      | 122.46   |
| 3   | A     | 161 | MTX  | C4A-C8A-N1  | 5.01 | 130.03      | 122.07   |
| 3   | B     | 162 | MTX  | C16-C11-C12 | 5.33 | 125.95      | 118.58   |
| 3   | B     | 162 | MTX  | C6-C7-N8    | 7.99 | 131.18      | 123.09   |
| 3   | B     | 162 | MTX  | CM-N10-C14  | 8.40 | 134.54      | 119.60   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 161 | MTX  | 2       | 0            |

## 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     | 12               |
| 1   | A     | 7                |

All chain breaks are listed below:

| Model | Chain | Residue-1  | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|------------|--------|-----------|--------|--------------|
| 1     | B     | 122[B]:ASP | C      | 123:THR   | N      | 1.82         |
| 1     | B     | 44:ARG     | C      | 45[B]:HIS | N      | 1.65         |
| 1     | A     | 30:TRP     | C      | 31:PHE    | N      | 1.20         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2  | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|------------|--------|--------------|
| 1     | B     | 34:ASN    | C      | 35:THR     | N      | 1.20         |
| 1     | B     | 154:LYS   | C      | 155:ILE    | N      | 1.20         |
| 1     | A     | 127:ASP   | C      | 128:TYR    | N      | 1.19         |
| 1     | A     | 143:ALA   | C      | 144:ASP    | N      | 1.19         |
| 1     | A     | 151:TYR   | C      | 152:CYS    | N      | 1.19         |
| 1     | B     | 151:TYR   | C      | 152:CYS    | N      | 1.19         |
| 1     | B     | 59:ASN    | C      | 60:ILE     | N      | 1.18         |
| 1     | B     | 153:PHE   | C      | 154:LYS    | N      | 1.18         |
| 1     | A     | 44:ARG    | C      | 45:HIS     | N      | 1.17         |
| 1     | B     | 64[B]:SER | C      | 65:GLN     | N      | 1.15         |
| 1     | B     | 114:HIS   | C      | 115:ILE    | N      | 1.15         |
| 1     | A     | 111:TYR   | C      | 112:LEU    | N      | 1.13         |
| 1     | B     | 110:LEU   | C      | 111:TYR    | N      | 1.12         |
| 1     | A     | 109:LYS   | C      | 110:LEU    | N      | 1.11         |
| 1     | B     | 63:SER    | C      | 64[B]:SER  | N      | 1.02         |
| 1     | B     | 121:GLY   | C      | 122[B]:ASP | N      | 0.97         |

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.