



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:13 PM UTC

PDB ID : 8TIM / pdb\_00008tim  
Title : TRIOSE PHOSPHATE ISOMERASE  
Authors : Artymiuk, P.J.; Taylor, W.R.; Phillips, D.C.  
Deposited on : 1998-08-25  
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

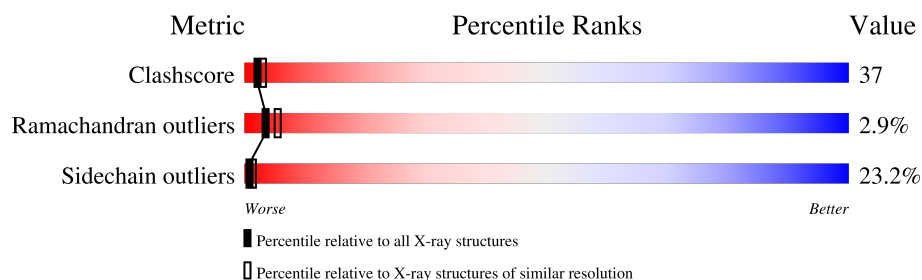
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



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

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 247    |                  |
| 1   | B     | 247    |                  |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3778 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 TRIOSE PHOSPHATE ISOMERASE.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 247      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1867  | 1184 | 327 | 350 | 6 |         |         |       |
| 1   | B     | 247      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1867  | 1184 | 327 | 350 | 6 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 194     | THR      | SER    | conflict | UNP P00940 |
| B     | 194     | THR      | SER    | conflict | UNP P00940 |

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 3 is water.

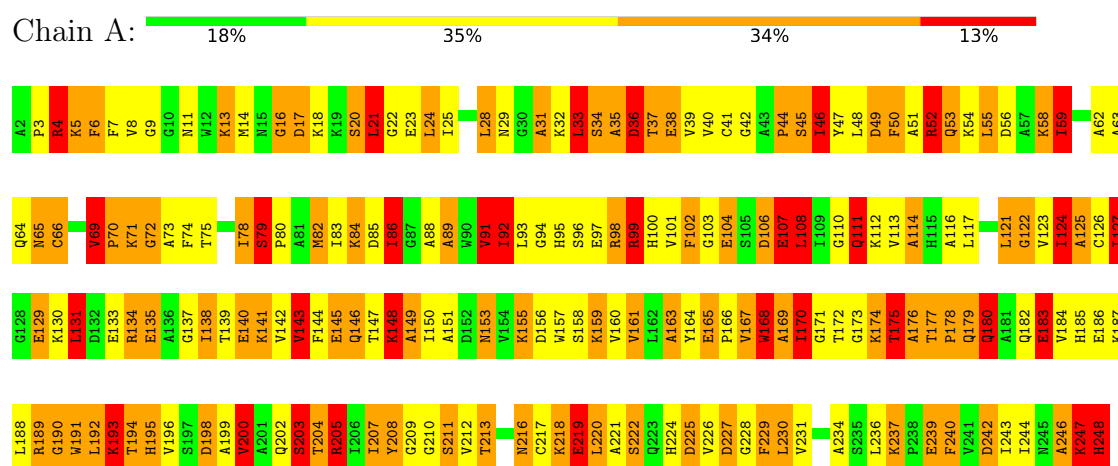
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 3   | B     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |

### 3 Residue-property plots

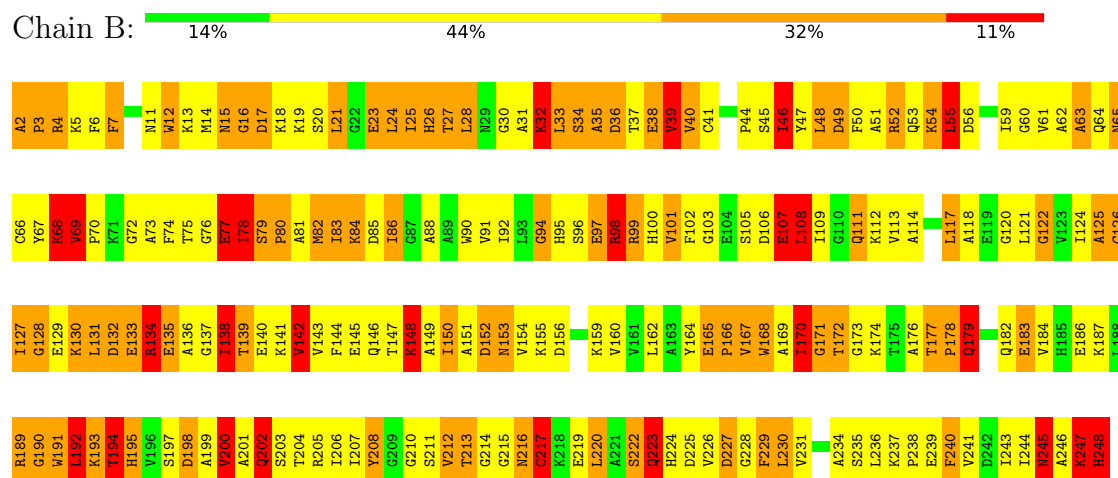
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

#### • Molecule 1: TRIOSE PHOSPHATE ISOMERASE



#### • Molecule 1: TRIOSE PHOSPHATE ISOMERASE



## 4 Data and refinement statistics

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

| Property                                                 | Value                                         | Source    |
|----------------------------------------------------------|-----------------------------------------------|-----------|
| Space group                                              | P 21 21 21                                    | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 106.01Å 74.76Å 61.74Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 10.00 – 2.50                                  | Depositor |
| % Data completeness<br>(in resolution range)             | 100.0 (10.00-2.50)                            | Depositor |
| $R_{merge}$                                              | (Not available)                               | Depositor |
| $R_{sym}$                                                | (Not available)                               | Depositor |
| Refinement program                                       | PROLSQ                                        | Depositor |
| R, $R_{free}$                                            | 0.177 , (Not available)                       | Depositor |
| Estimated twinning fraction                              | No twinning to report.                        | Xtriage   |
| Total number of atoms                                    | 3778                                          | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 19.0                                          | 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: SO4

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     | 1.83         | 35/1903 (1.8%) | 3.63        | 395/2571 (15.4%) |
| 1   | B     | 1.77         | 22/1903 (1.2%) | 3.42        | 322/2571 (12.5%) |
| All | All   | 1.80         | 57/3806 (1.5%) | 3.53        | 717/5142 (13.9%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 4                   |
| 1   | B     | 0                   | 3                   |
| All | All   | 0                   | 7                   |

All (57) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 122 | GLY  | CA-C  | 13.50 | 1.62        | 1.52     |
| 1   | A     | 170 | ILE  | C-O   | 8.96  | 1.34        | 1.24     |
| 1   | A     | 100 | HIS  | CA-CB | 8.21  | 1.66        | 1.53     |
| 1   | B     | 190 | GLY  | N-CA  | 7.81  | 1.55        | 1.45     |
| 1   | B     | 69  | VAL  | N-CA  | 7.76  | 1.53        | 1.46     |
| 1   | A     | 216 | ASN  | CA-CB | 7.36  | 1.65        | 1.53     |
| 1   | A     | 121 | LEU  | N-CA  | 7.19  | 1.54        | 1.45     |
| 1   | A     | 237 | LYS  | N-CA  | 7.18  | 1.50        | 1.46     |
| 1   | A     | 175 | THR  | CA-CB | 7.04  | 1.65        | 1.53     |
| 1   | A     | 35  | ALA  | CA-C  | 6.92  | 1.62        | 1.53     |
| 1   | A     | 174 | LYS  | CA-CB | 6.91  | 1.66        | 1.52     |
| 1   | B     | 31  | ALA  | N-CA  | 6.79  | 1.53        | 1.45     |
| 1   | A     | 8   | VAL  | N-CA  | 6.77  | 1.54        | 1.46     |
| 1   | B     | 167 | VAL  | N-CA  | 6.70  | 1.54        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 148 | LYS  | N-CA    | 6.65  | 1.54        | 1.46     |
| 1   | A     | 82  | MET  | N-CA    | 6.64  | 1.54        | 1.46     |
| 1   | A     | 91  | VAL  | CA-C    | 6.56  | 1.60        | 1.52     |
| 1   | B     | 194 | THR  | CA-CB   | 6.42  | 1.63        | 1.53     |
| 1   | A     | 95  | HIS  | CD2-NE2 | -6.19 | 1.31        | 1.37     |
| 1   | A     | 86  | ILE  | CA-CB   | 6.10  | 1.61        | 1.54     |
| 1   | B     | 201 | ALA  | C-O     | 6.07  | 1.31        | 1.24     |
| 1   | A     | 114 | ALA  | C-O     | 6.06  | 1.31        | 1.24     |
| 1   | B     | 208 | TYR  | N-CA    | 5.99  | 1.53        | 1.46     |
| 1   | A     | 111 | GLN  | N-CA    | 5.95  | 1.53        | 1.46     |
| 1   | B     | 186 | GLU  | CA-CB   | -5.90 | 1.43        | 1.53     |
| 1   | A     | 177 | THR  | CB-OG1  | 5.90  | 1.53        | 1.43     |
| 1   | B     | 38  | GLU  | C-O     | 5.75  | 1.30        | 1.24     |
| 1   | B     | 194 | THR  | N-CA    | -5.72 | 1.39        | 1.46     |
| 1   | A     | 170 | ILE  | CA-CB   | 5.71  | 1.62        | 1.54     |
| 1   | A     | 107 | GLU  | CA-CB   | -5.69 | 1.44        | 1.53     |
| 1   | B     | 204 | THR  | CA-CB   | 5.66  | 1.62        | 1.53     |
| 1   | A     | 226 | VAL  | N-CA    | 5.66  | 1.53        | 1.46     |
| 1   | A     | 72  | GLY  | N-CA    | -5.61 | 1.38        | 1.44     |
| 1   | A     | 66  | CYS  | C-O     | 5.61  | 1.30        | 1.23     |
| 1   | A     | 185 | HIS  | N-CA    | 5.60  | 1.53        | 1.46     |
| 1   | A     | 166 | PRO  | CA-CB   | -5.57 | 1.45        | 1.53     |
| 1   | B     | 21  | LEU  | N-CA    | 5.56  | 1.53        | 1.46     |
| 1   | B     | 75  | THR  | N-CA    | 5.55  | 1.53        | 1.46     |
| 1   | B     | 120 | GLY  | N-CA    | 5.54  | 1.52        | 1.45     |
| 1   | B     | 102 | PHE  | N-CA    | 5.51  | 1.53        | 1.46     |
| 1   | B     | 98  | ARG  | CD-NE   | -5.50 | 1.38        | 1.46     |
| 1   | B     | 174 | LYS  | N-CA    | 5.49  | 1.52        | 1.45     |
| 1   | A     | 114 | ALA  | N-CA    | 5.47  | 1.53        | 1.46     |
| 1   | B     | 19  | LYS  | C-N     | -5.44 | 1.26        | 1.34     |
| 1   | A     | 33  | LEU  | N-CA    | 5.38  | 1.52        | 1.45     |
| 1   | A     | 112 | LYS  | N-CA    | 5.34  | 1.52        | 1.46     |
| 1   | A     | 220 | LEU  | C-N     | -5.25 | 1.27        | 1.33     |
| 1   | B     | 91  | VAL  | C-N     | -5.15 | 1.26        | 1.33     |
| 1   | A     | 35  | ALA  | C-N     | -5.14 | 1.26        | 1.33     |
| 1   | A     | 100 | HIS  | C-N     | -5.12 | 1.26        | 1.33     |
| 1   | B     | 41  | CYS  | CA-C    | 5.09  | 1.58        | 1.52     |
| 1   | A     | 185 | HIS  | ND1-CE1 | 5.08  | 1.37        | 1.32     |
| 1   | A     | 175 | THR  | CB-OG1  | 5.05  | 1.51        | 1.43     |
| 1   | A     | 69  | VAL  | N-CA    | 5.04  | 1.52        | 1.46     |
| 1   | A     | 49  | ASP  | N-CA    | 5.03  | 1.52        | 1.46     |
| 1   | B     | 31  | ALA  | CA-CB   | -5.03 | 1.46        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 204 | THR  | CA-CB | 5.01 | 1.60        | 1.53     |

All (717) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | A     | 107 | GLU  | CA-CB-CG  | 24.32  | 162.75      | 114.10   |
| 1   | B     | 245 | ASN  | CA-CB-CG  | 22.17  | 134.77      | 112.60   |
| 1   | A     | 216 | ASN  | N-CA-C    | 19.07  | 131.76      | 110.97   |
| 1   | A     | 205 | ARG  | CD-NE-CZ  | 19.01  | 151.01      | 124.40   |
| 1   | A     | 35  | ALA  | N-CA-C    | -18.73 | 86.38       | 110.53   |
| 1   | A     | 35  | ALA  | N-CA-CB   | 17.62  | 135.63      | 110.44   |
| 1   | B     | 69  | VAL  | CB-CA-C   | 17.55  | 128.84      | 109.89   |
| 1   | B     | 98  | ARG  | NE-CZ-NH2 | -17.00 | 103.90      | 119.20   |
| 1   | B     | 33  | LEU  | CA-C-O    | -16.29 | 103.11      | 120.70   |
| 1   | A     | 174 | LYS  | N-CA-C    | 16.29  | 135.61      | 108.08   |
| 1   | A     | 72  | GLY  | N-CA-C    | 16.19  | 134.23      | 110.60   |
| 1   | A     | 216 | ASN  | CA-C-O    | 15.84  | 137.63      | 121.00   |
| 1   | A     | 100 | HIS  | CA-CB-CG  | -15.30 | 98.50       | 113.80   |
| 1   | A     | 34  | SER  | CA-C-O    | -14.28 | 105.05      | 121.47   |
| 1   | B     | 16  | GLY  | CA-C-O    | -14.25 | 112.40      | 122.23   |
| 1   | A     | 174 | LYS  | CB-CA-C   | -13.85 | 100.57      | 116.63   |
| 1   | B     | 45  | SER  | CA-C-O    | -13.74 | 105.53      | 120.92   |
| 1   | B     | 100 | HIS  | CA-CB-CG  | -13.52 | 100.28      | 113.80   |
| 1   | A     | 92  | ILE  | N-CA-CB   | 13.49  | 125.42      | 110.72   |
| 1   | A     | 143 | VAL  | CA-C-O    | -13.08 | 107.35      | 120.95   |
| 1   | B     | 184 | VAL  | O-C-N     | 12.99  | 135.41      | 121.90   |
| 1   | B     | 225 | ASP  | O-C-N     | 12.77  | 137.69      | 122.24   |
| 1   | B     | 219 | GLU  | CA-C-O    | 12.65  | 133.96      | 120.55   |
| 1   | A     | 107 | GLU  | CB-CG-CD  | 12.62  | 134.05      | 112.60   |
| 1   | B     | 49  | ASP  | CA-CB-CG  | 12.50  | 125.10      | 112.60   |
| 1   | B     | 69  | VAL  | N-CA-CB   | -12.42 | 98.20       | 111.87   |
| 1   | A     | 74  | PHE  | CA-CB-CG  | -12.36 | 101.44      | 113.80   |
| 1   | A     | 143 | VAL  | O-C-N     | 11.90  | 133.42      | 121.87   |
| 1   | A     | 98  | ARG  | NE-CZ-NH1 | 11.87  | 133.37      | 121.50   |
| 1   | A     | 121 | LEU  | CB-CA-C   | 11.68  | 130.74      | 109.37   |
| 1   | A     | 176 | ALA  | N-CA-C    | -11.46 | 95.81       | 111.28   |
| 1   | B     | 94  | GLY  | CA-C-N    | 11.31  | 136.77      | 120.82   |
| 1   | B     | 94  | GLY  | C-N-CA    | 11.31  | 136.77      | 120.82   |
| 1   | B     | 248 | HIS  | CA-CB-CG  | 11.20  | 125.00      | 113.80   |
| 1   | B     | 52  | ARG  | NE-CZ-NH2 | 11.18  | 129.26      | 119.20   |
| 1   | B     | 98  | ARG  | CD-NE-CZ  | 11.10  | 139.94      | 124.40   |
| 1   | A     | 96  | SER  | CA-CB-OG  | 11.10  | 133.29      | 111.10   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 69  | VAL  | CB-CA-C    | 11.02  | 120.13      | 109.33   |
| 1   | B     | 21  | LEU  | CB-CA-C    | 11.00  | 128.28      | 110.90   |
| 1   | A     | 55  | LEU  | O-C-N      | 10.99  | 135.38      | 122.96   |
| 1   | B     | 184 | VAL  | CA-C-O     | -10.98 | 108.86      | 121.05   |
| 1   | B     | 6   | PHE  | O-C-N      | 10.94  | 136.19      | 123.06   |
| 1   | B     | 98  | ARG  | NH1-CZ-NH2 | 10.91  | 133.49      | 119.30   |
| 1   | B     | 239 | GLU  | CG-CD-OE2  | 10.91  | 143.48      | 118.40   |
| 1   | A     | 160 | VAL  | N-CA-C     | 10.90  | 123.38      | 108.11   |
| 1   | B     | 194 | THR  | CB-CA-C    | -10.90 | 92.32       | 110.85   |
| 1   | B     | 224 | HIS  | N-CA-C     | 10.85  | 125.78      | 112.54   |
| 1   | B     | 96  | SER  | CA-C-O     | -10.84 | 108.06      | 120.20   |
| 1   | A     | 129 | GLU  | CG-CD-OE2  | 10.64  | 142.88      | 118.40   |
| 1   | B     | 201 | ALA  | CA-C-O     | 10.60  | 132.24      | 120.90   |
| 1   | A     | 71  | LYS  | CA-CB-CG   | 10.58  | 135.26      | 114.10   |
| 1   | B     | 200 | VAL  | O-C-N      | 10.56  | 132.88      | 121.90   |
| 1   | B     | 74  | PHE  | CA-CB-CG   | -10.54 | 103.26      | 113.80   |
| 1   | B     | 122 | GLY  | N-CA-C     | -10.54 | 91.96       | 110.71   |
| 1   | B     | 125 | ALA  | CA-C-N     | 10.46  | 137.44      | 123.00   |
| 1   | B     | 125 | ALA  | C-N-CA     | 10.46  | 137.44      | 123.00   |
| 1   | A     | 36  | ASP  | N-CA-C     | -10.44 | 88.56       | 110.80   |
| 1   | A     | 100 | HIS  | CA-C-O     | -10.40 | 107.43      | 119.60   |
| 1   | B     | 153 | ASN  | CA-CB-CG   | 10.35  | 122.95      | 112.60   |
| 1   | B     | 38  | GLU  | CB-CG-CD   | 10.34  | 130.18      | 112.60   |
| 1   | A     | 36  | ASP  | O-C-N      | 10.26  | 136.24      | 122.59   |
| 1   | A     | 142 | VAL  | N-CA-CB    | -10.25 | 99.45       | 110.62   |
| 1   | B     | 26  | HIS  | CA-CB-CG   | -10.22 | 103.58      | 113.80   |
| 1   | B     | 165 | GLU  | O-C-N      | 10.20  | 132.76      | 121.23   |
| 1   | A     | 138 | ILE  | CA-CB-CG2  | 10.19  | 127.82      | 110.50   |
| 1   | A     | 193 | LYS  | CA-C-O     | 10.17  | 131.50      | 120.82   |
| 1   | A     | 138 | ILE  | N-CA-C     | 10.17  | 121.85      | 112.29   |
| 1   | A     | 204 | THR  | CA-C-O     | 10.16  | 132.27      | 120.69   |
| 1   | B     | 167 | VAL  | CB-CA-C    | 9.99   | 125.63      | 112.14   |
| 1   | A     | 192 | LEU  | N-CA-CB    | -9.98  | 95.44       | 110.12   |
| 1   | A     | 121 | LEU  | N-CA-CB    | -9.96  | 94.92       | 110.85   |
| 1   | A     | 216 | ASN  | CB-CA-C    | -9.92  | 95.68       | 110.96   |
| 1   | A     | 79  | SER  | CB-CA-C    | -9.89  | 93.47       | 108.61   |
| 1   | B     | 183 | GLU  | CA-C-O     | 9.89   | 131.20      | 120.82   |
| 1   | B     | 16  | GLY  | N-CA-C     | 9.88   | 123.36      | 112.29   |
| 1   | A     | 151 | ALA  | O-C-N      | 9.87   | 132.59      | 122.12   |
| 1   | B     | 224 | HIS  | CA-CB-CG   | 9.85   | 123.65      | 113.80   |
| 1   | A     | 126 | CYS  | CA-C-O     | 9.82   | 131.08      | 120.38   |
| 1   | A     | 56  | ASP  | O-C-N      | 9.76   | 133.99      | 122.96   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 153 | ASN  | CA-CB-CG   | -9.69 | 102.91      | 112.60   |
| 1   | A     | 112 | LYS  | CA-C-N     | -9.65 | 108.64      | 120.70   |
| 1   | A     | 112 | LYS  | C-N-CA     | -9.65 | 108.64      | 120.70   |
| 1   | A     | 3   | PRO  | CA-C-N     | 9.64  | 139.95      | 121.54   |
| 1   | A     | 3   | PRO  | C-N-CA     | 9.64  | 139.95      | 121.54   |
| 1   | A     | 56  | ASP  | CA-CB-CG   | 9.62  | 122.22      | 112.60   |
| 1   | B     | 46  | ILE  | CA-CB-CG2  | 9.59  | 126.80      | 110.50   |
| 1   | B     | 113 | VAL  | O-C-N      | 9.54  | 131.25      | 121.91   |
| 1   | A     | 150 | ILE  | O-C-N      | 9.49  | 131.77      | 121.90   |
| 1   | B     | 52  | ARG  | O-C-N      | 9.48  | 131.83      | 122.07   |
| 1   | B     | 207 | ILE  | CA-C-O     | -9.47 | 109.46      | 121.48   |
| 1   | A     | 58  | LYS  | CA-CB-CG   | 9.44  | 132.99      | 114.10   |
| 1   | A     | 138 | ILE  | N-CA-CB    | -9.41 | 98.32       | 112.15   |
| 1   | B     | 173 | GLY  | N-CA-C     | -9.38 | 102.21      | 115.43   |
| 1   | B     | 169 | ALA  | CA-C-O     | -9.36 | 108.64      | 119.78   |
| 1   | A     | 71  | LYS  | O-C-N      | 9.34  | 134.47      | 123.17   |
| 1   | A     | 52  | ARG  | O-C-N      | 9.32  | 132.00      | 122.12   |
| 1   | A     | 112 | LYS  | O-C-N      | 9.29  | 132.75      | 122.15   |
| 1   | A     | 170 | ILE  | CA-C-O     | -9.26 | 109.21      | 120.78   |
| 1   | A     | 55  | LEU  | CA-C-O     | -9.25 | 110.84      | 121.47   |
| 1   | A     | 29  | ASN  | OD1-CG-ND2 | 9.24  | 131.84      | 122.60   |
| 1   | B     | 85  | ASP  | CA-CB-CG   | 9.23  | 121.83      | 112.60   |
| 1   | B     | 80  | PRO  | CA-C-O     | 9.20  | 134.18      | 119.64   |
| 1   | B     | 132 | ASP  | CB-CA-C    | 9.20  | 125.53      | 110.81   |
| 1   | B     | 169 | ALA  | N-CA-CB    | 9.09  | 124.24      | 110.70   |
| 1   | A     | 69  | VAL  | N-CA-C     | -9.08 | 101.75      | 109.19   |
| 1   | A     | 96  | SER  | O-C-N      | 9.03  | 131.48      | 122.09   |
| 1   | B     | 21  | LEU  | N-CA-CB    | -9.02 | 96.98       | 110.07   |
| 1   | A     | 71  | LYS  | CA-C-O     | -9.02 | 111.21      | 121.40   |
| 1   | A     | 100 | HIS  | N-CA-C     | 8.98  | 124.66      | 112.90   |
| 1   | B     | 197 | SER  | O-C-N      | 8.96  | 133.06      | 123.56   |
| 1   | B     | 203 | SER  | CA-C-N     | 8.95  | 133.48      | 120.95   |
| 1   | B     | 203 | SER  | C-N-CA     | 8.95  | 133.48      | 120.95   |
| 1   | A     | 198 | ASP  | N-CA-C     | -8.93 | 101.81      | 112.89   |
| 1   | A     | 199 | ALA  | CB-CA-C    | 8.91  | 124.67      | 110.96   |
| 1   | A     | 173 | GLY  | CA-C-N     | 8.90  | 138.06      | 122.66   |
| 1   | A     | 173 | GLY  | C-N-CA     | 8.90  | 138.06      | 122.66   |
| 1   | B     | 68  | LYS  | CA-C-N     | -8.88 | 108.41      | 122.17   |
| 1   | B     | 68  | LYS  | C-N-CA     | -8.88 | 108.41      | 122.17   |
| 1   | B     | 182 | GLN  | CB-CG-CD   | 8.87  | 127.68      | 112.60   |
| 1   | A     | 248 | HIS  | CA-CB-CG   | 8.86  | 122.66      | 113.80   |
| 1   | A     | 142 | VAL  | CA-C-O     | 8.82  | 130.73      | 121.29   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 34  | SER  | O-C-N     | 8.76  | 132.86      | 122.96   |
| 1   | B     | 35  | ALA  | CA-C-N    | 8.75  | 133.60      | 120.31   |
| 1   | B     | 35  | ALA  | C-N-CA    | 8.75  | 133.60      | 120.31   |
| 1   | B     | 186 | GLU  | CB-CG-CD  | -8.74 | 97.74       | 112.60   |
| 1   | B     | 152 | ASP  | CA-C-O    | -8.73 | 108.02      | 120.51   |
| 1   | A     | 143 | VAL  | CB-CA-C   | 8.72  | 123.91      | 112.14   |
| 1   | B     | 45  | SER  | O-C-N     | 8.72  | 132.14      | 122.11   |
| 1   | A     | 216 | ASN  | CA-CB-CG  | -8.70 | 103.90      | 112.60   |
| 1   | B     | 3   | PRO  | CB-CA-C   | 8.69  | 124.34      | 111.22   |
| 1   | B     | 127 | ILE  | CA-C-O    | -8.67 | 113.05      | 121.63   |
| 1   | A     | 168 | TRP  | O-C-N     | 8.67  | 134.12      | 122.59   |
| 1   | A     | 174 | LYS  | CA-C-O    | 8.64  | 133.39      | 119.13   |
| 1   | A     | 103 | GLY  | O-C-N     | 8.62  | 130.85      | 122.41   |
| 1   | B     | 101 | VAL  | N-CA-C    | -8.59 | 101.64      | 111.00   |
| 1   | A     | 208 | TYR  | O-C-N     | 8.58  | 133.00      | 123.22   |
| 1   | A     | 79  | SER  | CA-C-O    | -8.56 | 111.81      | 120.63   |
| 1   | B     | 142 | VAL  | N-CA-CB   | -8.54 | 101.31      | 110.62   |
| 1   | B     | 33  | LEU  | O-C-N     | 8.54  | 134.33      | 123.23   |
| 1   | B     | 3   | PRO  | N-CA-C    | -8.50 | 99.32       | 111.22   |
| 1   | A     | 195 | HIS  | CA-CB-CG  | -8.49 | 105.31      | 113.80   |
| 1   | A     | 160 | VAL  | CA-CB-CG2 | 8.48  | 124.81      | 110.40   |
| 1   | B     | 25  | ILE  | N-CA-C    | -8.46 | 100.98      | 110.62   |
| 1   | B     | 207 | ILE  | O-C-N     | 8.46  | 132.33      | 122.69   |
| 1   | A     | 56  | ASP  | CA-C-O    | -8.45 | 111.75      | 121.47   |
| 1   | B     | 40  | VAL  | O-C-N     | -8.45 | 114.06      | 123.10   |
| 1   | B     | 216 | ASN  | CA-C-N    | 8.44  | 133.49      | 120.82   |
| 1   | B     | 216 | ASN  | C-N-CA    | 8.44  | 133.49      | 120.82   |
| 1   | B     | 40  | VAL  | CA-C-N    | 8.44  | 134.90      | 122.99   |
| 1   | B     | 40  | VAL  | C-N-CA    | 8.44  | 134.90      | 122.99   |
| 1   | A     | 216 | ASN  | N-CA-CB   | -8.44 | 97.59       | 109.91   |
| 1   | B     | 113 | VAL  | CA-C-O    | -8.42 | 112.24      | 121.17   |
| 1   | B     | 17  | ASP  | CA-CB-CG  | 8.40  | 121.00      | 112.60   |
| 1   | B     | 184 | VAL  | N-CA-C    | -8.34 | 102.69      | 110.53   |
| 1   | A     | 102 | PHE  | N-CA-CB   | -8.32 | 98.04       | 110.61   |
| 1   | A     | 183 | GLU  | CA-CB-CG  | 8.32  | 130.74      | 114.10   |
| 1   | A     | 122 | GLY  | N-CA-C    | -8.32 | 101.34      | 112.82   |
| 1   | A     | 237 | LYS  | O-C-N     | 8.31  | 128.39      | 121.32   |
| 1   | A     | 157 | TRP  | CA-C-O    | -8.30 | 108.64      | 119.10   |
| 1   | B     | 200 | VAL  | CA-C-O    | -8.29 | 111.84      | 121.05   |
| 1   | B     | 2   | ALA  | CB-CA-C   | 8.26  | 122.89      | 110.50   |
| 1   | B     | 191 | TRP  | O-C-N     | 8.26  | 130.87      | 122.12   |
| 1   | B     | 105 | SER  | O-C-N     | 8.21  | 132.31      | 123.03   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 153 | ASN  | OD1-CG-ND2 | -8.20 | 114.41      | 122.60   |
| 1   | B     | 229 | PHE  | CA-CB-CG   | 8.17  | 121.97      | 113.80   |
| 1   | B     | 206 | ILE  | CB-CA-C    | 8.17  | 120.45      | 110.73   |
| 1   | A     | 45  | SER  | CA-C-O     | -8.16 | 110.88      | 120.10   |
| 1   | A     | 225 | ASP  | CA-C-N     | -8.15 | 112.46      | 122.90   |
| 1   | A     | 225 | ASP  | C-N-CA     | -8.15 | 112.46      | 122.90   |
| 1   | B     | 96  | SER  | O-C-N      | 8.12  | 131.45      | 122.20   |
| 1   | B     | 154 | VAL  | CA-C-O     | -8.11 | 111.88      | 120.48   |
| 1   | A     | 4   | ARG  | CD-NE-CZ   | -8.10 | 113.06      | 124.40   |
| 1   | A     | 138 | ILE  | CA-CB-CG1  | -8.09 | 96.64       | 110.40   |
| 1   | B     | 170 | ILE  | CB-CG1-CD1 | 8.08  | 130.77      | 113.80   |
| 1   | A     | 199 | ALA  | N-CA-C     | -8.05 | 102.20      | 110.97   |
| 1   | A     | 88  | ALA  | N-CA-C     | -8.04 | 99.70       | 110.55   |
| 1   | A     | 143 | VAL  | N-CA-C     | -8.02 | 102.44      | 110.62   |
| 1   | A     | 160 | VAL  | CB-CA-C    | -8.02 | 98.77       | 110.63   |
| 1   | A     | 99  | ARG  | N-CA-CB    | 8.01  | 121.62      | 110.01   |
| 1   | A     | 174 | LYS  | CA-CB-CG   | -7.99 | 98.11       | 114.10   |
| 1   | B     | 6   | PHE  | CA-C-N     | -7.99 | 111.97      | 123.00   |
| 1   | B     | 6   | PHE  | C-N-CA     | -7.99 | 111.97      | 123.00   |
| 1   | B     | 195 | HIS  | CA-CB-CG   | -7.97 | 105.83      | 113.80   |
| 1   | B     | 182 | GLN  | CA-C-O     | 7.96  | 129.42      | 120.90   |
| 1   | A     | 210 | GLY  | CA-C-O     | -7.95 | 112.89      | 122.03   |
| 1   | B     | 17  | ASP  | CA-C-O     | -7.94 | 112.59      | 121.40   |
| 1   | A     | 230 | LEU  | CA-C-O     | -7.94 | 112.28      | 120.54   |
| 1   | A     | 99  | ARG  | N-CA-C     | -7.94 | 102.58      | 111.07   |
| 1   | A     | 36  | ASP  | CA-C-N     | -7.93 | 112.06      | 123.00   |
| 1   | A     | 36  | ASP  | C-N-CA     | -7.93 | 112.06      | 123.00   |
| 1   | B     | 142 | VAL  | N-CA-C     | 7.93  | 117.99      | 110.30   |
| 1   | A     | 17  | ASP  | N-CA-CB    | 7.91  | 124.87      | 111.66   |
| 1   | B     | 32  | LYS  | O-C-N      | 7.90  | 132.59      | 123.27   |
| 1   | A     | 82  | MET  | CA-C-O     | 7.88  | 128.82      | 120.70   |
| 1   | A     | 176 | ALA  | CA-C-N     | 7.87  | 131.66      | 120.49   |
| 1   | A     | 176 | ALA  | C-N-CA     | 7.87  | 131.66      | 120.49   |
| 1   | A     | 53  | GLN  | OE1-CD-NE2 | -7.86 | 114.74      | 122.60   |
| 1   | A     | 94  | GLY  | O-C-N      | 7.85  | 132.06      | 122.32   |
| 1   | A     | 100 | HIS  | O-C-N      | 7.84  | 133.50      | 122.36   |
| 1   | A     | 169 | ALA  | CA-C-O     | -7.82 | 109.32      | 120.51   |
| 1   | A     | 177 | THR  | N-CA-CB    | 7.82  | 122.37      | 110.02   |
| 1   | A     | 194 | THR  | CA-C-O     | -7.81 | 110.57      | 119.79   |
| 1   | B     | 138 | ILE  | CA-CB-CG2  | 7.80  | 123.77      | 110.50   |
| 1   | A     | 38  | GLU  | CG-CD-OE1  | 7.80  | 136.35      | 118.40   |
| 1   | B     | 216 | ASN  | CA-C-O     | 7.79  | 127.42      | 118.77   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 165 | GLU  | CB-CA-C   | -7.77 | 100.23      | 110.34   |
| 1   | A     | 102 | PHE  | CA-CB-CG  | -7.77 | 106.03      | 113.80   |
| 1   | B     | 214 | GLY  | N-CA-C    | -7.76 | 103.42      | 112.73   |
| 1   | A     | 229 | PHE  | O-C-N     | 7.75  | 132.09      | 123.33   |
| 1   | B     | 63  | ALA  | CB-CA-C   | 7.75  | 122.76      | 109.51   |
| 1   | B     | 75  | THR  | CA-C-O    | 7.75  | 129.75      | 120.92   |
| 1   | B     | 48  | LEU  | CA-C-N    | 7.70  | 130.45      | 120.44   |
| 1   | B     | 48  | LEU  | C-N-CA    | 7.70  | 130.45      | 120.44   |
| 1   | A     | 247 | LYS  | O-C-N     | 7.68  | 132.80      | 122.59   |
| 1   | A     | 205 | ARG  | N-CA-CB   | 7.66  | 122.35      | 109.87   |
| 1   | A     | 165 | GLU  | CA-CB-CG  | 7.63  | 129.37      | 114.10   |
| 1   | A     | 23  | GLU  | CB-CG-CD  | 7.62  | 125.56      | 112.60   |
| 1   | B     | 46  | ILE  | CB-CA-C   | -7.60 | 100.95      | 112.05   |
| 1   | B     | 44  | PRO  | CB-CA-C   | 7.59  | 121.26      | 111.46   |
| 1   | A     | 85  | ASP  | O-C-N     | 7.59  | 129.98      | 122.09   |
| 1   | B     | 48  | LEU  | CB-CA-C   | 7.54  | 122.82      | 110.90   |
| 1   | A     | 52  | ARG  | N-CA-C    | -7.54 | 103.06      | 111.28   |
| 1   | A     | 239 | GLU  | CA-C-O    | 7.53  | 128.49      | 119.61   |
| 1   | A     | 13  | LYS  | CA-CB-CG  | -7.51 | 99.08       | 114.10   |
| 1   | A     | 209 | GLY  | CA-C-N    | 7.51  | 132.85      | 122.04   |
| 1   | A     | 209 | GLY  | C-N-CA    | 7.51  | 132.85      | 122.04   |
| 1   | A     | 231 | VAL  | CA-C-O    | 7.50  | 128.43      | 120.48   |
| 1   | A     | 147 | THR  | CA-C-N    | -7.49 | 109.65      | 120.29   |
| 1   | A     | 147 | THR  | C-N-CA    | -7.49 | 109.65      | 120.29   |
| 1   | B     | 88  | ALA  | CA-C-O    | -7.48 | 112.87      | 121.47   |
| 1   | B     | 193 | LYS  | CA-C-N    | 7.48  | 130.91      | 120.29   |
| 1   | B     | 193 | LYS  | C-N-CA    | 7.48  | 130.91      | 120.29   |
| 1   | A     | 180 | GLN  | CG-CD-NE2 | 7.47  | 127.60      | 116.40   |
| 1   | A     | 155 | LYS  | CA-C-N    | 7.46  | 134.72      | 123.23   |
| 1   | A     | 155 | LYS  | C-N-CA    | 7.46  | 134.72      | 123.23   |
| 1   | B     | 26  | HIS  | CA-C-N    | 7.45  | 130.26      | 120.28   |
| 1   | B     | 26  | HIS  | C-N-CA    | 7.45  | 130.26      | 120.28   |
| 1   | A     | 224 | HIS  | N-CA-C    | 7.45  | 119.04      | 111.07   |
| 1   | A     | 49  | ASP  | CA-CB-CG  | 7.44  | 120.04      | 112.60   |
| 1   | A     | 178 | PRO  | CA-C-O    | 7.43  | 134.13      | 120.60   |
| 1   | A     | 8   | VAL  | CA-C-O    | 7.43  | 127.61      | 120.25   |
| 1   | B     | 92  | ILE  | CA-C-O    | -7.42 | 112.50      | 120.59   |
| 1   | B     | 189 | ARG  | NE-CZ-NH1 | -7.42 | 114.08      | 121.50   |
| 1   | B     | 48  | LEU  | N-CA-CB   | -7.42 | 99.32       | 110.07   |
| 1   | A     | 46  | ILE  | CA-CB-CG2 | 7.42  | 123.11      | 110.50   |
| 1   | A     | 23  | GLU  | N-CA-CB   | 7.41  | 120.98      | 109.94   |
| 1   | A     | 36  | ASP  | CA-CB-CG  | -7.41 | 105.19      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 38  | GLU  | CA-C-O     | -7.38 | 112.16      | 120.43   |
| 1   | A     | 192 | LEU  | CA-C-O     | 7.38  | 128.37      | 120.55   |
| 1   | A     | 230 | LEU  | N-CA-C     | -7.37 | 95.59       | 108.20   |
| 1   | B     | 247 | LYS  | CA-C-O     | -7.37 | 109.97      | 120.51   |
| 1   | A     | 157 | TRP  | CA-CB-CG   | -7.37 | 99.60       | 113.60   |
| 1   | B     | 154 | VAL  | O-C-N      | 7.36  | 130.91      | 123.18   |
| 1   | A     | 79  | SER  | N-CA-C     | 7.35  | 119.94      | 110.39   |
| 1   | A     | 167 | VAL  | O-C-N      | 7.34  | 129.39      | 121.83   |
| 1   | A     | 91  | VAL  | N-CA-C     | -7.34 | 97.59       | 108.45   |
| 1   | A     | 224 | HIS  | CA-C-O     | -7.33 | 113.12      | 120.82   |
| 1   | B     | 132 | ASP  | N-CA-C     | -7.33 | 102.31      | 111.11   |
| 1   | A     | 84  | LYS  | O-C-N      | 7.32  | 130.49      | 122.15   |
| 1   | B     | 52  | ARG  | N-CA-CB    | 7.31  | 120.61      | 110.01   |
| 1   | B     | 107 | GLU  | CA-CB-CG   | 7.31  | 128.72      | 114.10   |
| 1   | A     | 222 | SER  | O-C-N      | 7.28  | 129.84      | 122.12   |
| 1   | A     | 33  | LEU  | CA-C-O     | -7.28 | 112.59      | 121.11   |
| 1   | B     | 231 | VAL  | O-C-N      | 7.26  | 131.22      | 122.95   |
| 1   | B     | 69  | VAL  | CA-CB-CG1  | 7.24  | 122.71      | 110.40   |
| 1   | A     | 216 | ASN  | O-C-N      | -7.22 | 114.52      | 122.03   |
| 1   | A     | 175 | THR  | CA-CB-CG2  | 7.22  | 122.77      | 110.50   |
| 1   | B     | 101 | VAL  | CA-C-N     | -7.20 | 110.65      | 122.54   |
| 1   | B     | 101 | VAL  | C-N-CA     | -7.20 | 110.65      | 122.54   |
| 1   | B     | 63  | ALA  | N-CA-C     | -7.19 | 98.88       | 110.32   |
| 1   | B     | 106 | ASP  | CA-C-O     | -7.19 | 112.61      | 121.02   |
| 1   | B     | 48  | LEU  | CA-C-O     | -7.19 | 113.30      | 120.70   |
| 1   | A     | 59  | ILE  | CA-C-O     | 7.18  | 128.26      | 120.57   |
| 1   | A     | 14  | MET  | CA-C-O     | -7.18 | 113.37      | 122.63   |
| 1   | A     | 170 | ILE  | CB-CG1-CD1 | -7.18 | 98.72       | 113.80   |
| 1   | A     | 180 | GLN  | CA-C-O     | -7.18 | 112.81      | 120.42   |
| 1   | A     | 237 | LYS  | CA-C-O     | -7.17 | 113.70      | 120.94   |
| 1   | B     | 239 | GLU  | CA-C-O     | 7.16  | 128.15      | 119.49   |
| 1   | A     | 102 | PHE  | CA-C-N     | 7.15  | 133.22      | 120.77   |
| 1   | A     | 102 | PHE  | C-N-CA     | 7.15  | 133.22      | 120.77   |
| 1   | A     | 180 | GLN  | N-CA-C     | -7.15 | 103.57      | 111.36   |
| 1   | B     | 33  | LEU  | CA-C-N     | -7.15 | 110.82      | 120.90   |
| 1   | B     | 33  | LEU  | C-N-CA     | -7.15 | 110.82      | 120.90   |
| 1   | B     | 68  | LYS  | CB-CA-C    | -7.14 | 96.21       | 110.42   |
| 1   | B     | 65  | ASN  | CA-C-O     | -7.13 | 113.27      | 121.26   |
| 1   | A     | 142 | VAL  | N-CA-C     | 7.13  | 117.21      | 110.30   |
| 1   | A     | 112 | LYS  | N-CA-C     | -7.10 | 103.62      | 111.36   |
| 1   | A     | 36  | ASP  | CB-CA-C    | 7.09  | 124.53      | 110.42   |
| 1   | B     | 199 | ALA  | O-C-N      | 7.08  | 129.74      | 122.09   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 92  | ILE  | N-CA-C     | -7.07 | 98.39       | 108.58   |
| 1   | A     | 230 | LEU  | CB-CA-C    | 7.07  | 122.09      | 110.78   |
| 1   | A     | 135 | GLU  | CA-C-O     | -7.07 | 111.84      | 119.97   |
| 1   | B     | 192 | LEU  | CA-C-O     | -7.06 | 112.93      | 120.42   |
| 1   | A     | 91  | VAL  | N-CA-CB    | 7.06  | 123.02      | 111.45   |
| 1   | B     | 102 | PHE  | N-CA-CB    | -7.05 | 100.05      | 110.49   |
| 1   | A     | 239 | GLU  | CA-CB-CG   | 7.05  | 128.20      | 114.10   |
| 1   | B     | 138 | ILE  | N-CA-CB    | -7.05 | 99.60       | 111.23   |
| 1   | B     | 217 | CYS  | CA-CB-SG   | 7.03  | 130.56      | 114.40   |
| 1   | A     | 176 | ALA  | CB-CA-C    | 7.02  | 122.36      | 112.11   |
| 1   | B     | 177 | THR  | CA-C-O     | 7.00  | 128.55      | 121.27   |
| 1   | A     | 193 | LYS  | CB-CG-CD   | 7.00  | 127.39      | 111.30   |
| 1   | B     | 83  | ILE  | CB-CA-C    | 6.99  | 120.65      | 111.70   |
| 1   | A     | 38  | GLU  | CB-CG-CD   | 6.97  | 124.45      | 112.60   |
| 1   | A     | 160 | VAL  | O-C-N      | 6.97  | 130.79      | 123.26   |
| 1   | A     | 158 | SER  | CA-C-O     | -6.95 | 110.83      | 119.38   |
| 1   | B     | 192 | LEU  | O-C-N      | 6.95  | 130.07      | 122.15   |
| 1   | B     | 169 | ALA  | CB-CA-C    | -6.95 | 99.47       | 110.94   |
| 1   | A     | 13  | LYS  | CB-CA-C    | -6.94 | 106.73      | 115.89   |
| 1   | A     | 155 | LYS  | N-CA-CB    | 6.94  | 122.31      | 110.51   |
| 1   | A     | 175 | THR  | N-CA-C     | 6.94  | 125.58      | 110.80   |
| 1   | A     | 157 | TRP  | O-C-N      | 6.92  | 131.64      | 122.43   |
| 1   | A     | 168 | TRP  | CA-CB-CG   | 6.92  | 126.76      | 113.60   |
| 1   | A     | 135 | GLU  | O-C-N      | 6.92  | 130.78      | 122.27   |
| 1   | A     | 164 | TYR  | O-C-N      | 6.89  | 131.06      | 123.13   |
| 1   | B     | 6   | PHE  | N-CA-CB    | 6.88  | 120.15      | 109.48   |
| 1   | A     | 59  | ILE  | CA-CB-CG1  | 6.88  | 122.10      | 110.40   |
| 1   | B     | 244 | ILE  | O-C-N      | 6.84  | 129.53      | 121.80   |
| 1   | B     | 127 | ILE  | CB-CG1-CD1 | 6.83  | 128.13      | 113.80   |
| 1   | B     | 239 | GLU  | CA-CB-CG   | 6.82  | 127.73      | 114.10   |
| 1   | A     | 110 | GLY  | O-C-N      | 6.81  | 129.46      | 122.24   |
| 1   | A     | 191 | TRP  | CA-C-N     | 6.80  | 129.40      | 120.28   |
| 1   | A     | 191 | TRP  | C-N-CA     | 6.80  | 129.40      | 120.28   |
| 1   | B     | 132 | ASP  | CA-CB-CG   | 6.80  | 119.40      | 112.60   |
| 1   | B     | 195 | HIS  | CA-C-O     | -6.80 | 111.70      | 118.97   |
| 1   | B     | 207 | ILE  | CA-C-N     | -6.76 | 112.66      | 122.19   |
| 1   | B     | 207 | ILE  | C-N-CA     | -6.76 | 112.66      | 122.19   |
| 1   | B     | 30  | GLY  | CA-C-N     | -6.75 | 110.69      | 122.64   |
| 1   | B     | 30  | GLY  | C-N-CA     | -6.75 | 110.69      | 122.64   |
| 1   | A     | 198 | ASP  | CA-C-N     | -6.75 | 111.74      | 120.65   |
| 1   | A     | 198 | ASP  | C-N-CA     | -6.75 | 111.74      | 120.65   |
| 1   | A     | 192 | LEU  | CA-C-N     | 6.74  | 129.20      | 120.44   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 192 | LEU  | C-N-CA     | 6.74  | 129.20      | 120.44   |
| 1   | B     | 167 | VAL  | O-C-N      | 6.74  | 128.41      | 121.87   |
| 1   | A     | 240 | PHE  | CA-CB-CG   | 6.74  | 120.53      | 113.80   |
| 1   | B     | 179 | GLN  | CB-CG-CD   | 6.73  | 124.05      | 112.60   |
| 1   | A     | 225 | ASP  | CA-CB-CG   | -6.70 | 105.90      | 112.60   |
| 1   | B     | 102 | PHE  | CA-CB-CG   | -6.69 | 107.11      | 113.80   |
| 1   | B     | 183 | GLU  | N-CA-CB    | -6.69 | 100.31      | 110.01   |
| 1   | A     | 6   | PHE  | CA-C-O     | 6.68  | 128.24      | 120.96   |
| 1   | A     | 124 | ILE  | CA-CB-CG2  | 6.68  | 121.86      | 110.50   |
| 1   | B     | 78  | ILE  | CA-CB-CG2  | 6.68  | 121.85      | 110.50   |
| 1   | B     | 170 | ILE  | CA-C-N     | 6.68  | 134.50      | 121.41   |
| 1   | B     | 170 | ILE  | C-N-CA     | 6.68  | 134.50      | 121.41   |
| 1   | A     | 96  | SER  | CA-C-O     | -6.67 | 113.76      | 120.90   |
| 1   | B     | 7   | PHE  | CA-C-N     | -6.66 | 113.91      | 123.11   |
| 1   | B     | 7   | PHE  | C-N-CA     | -6.66 | 113.91      | 123.11   |
| 1   | A     | 33  | LEU  | O-C-N      | 6.65  | 131.42      | 123.24   |
| 1   | A     | 102 | PHE  | CB-CA-C    | 6.65  | 121.41      | 110.17   |
| 1   | B     | 82  | MET  | O-C-N      | 6.65  | 129.73      | 122.15   |
| 1   | B     | 20  | SER  | CA-C-N     | -6.65 | 111.40      | 120.44   |
| 1   | B     | 20  | SER  | C-N-CA     | -6.65 | 111.40      | 120.44   |
| 1   | A     | 99  | ARG  | NE-CZ-NH2  | 6.62  | 125.16      | 119.20   |
| 1   | B     | 4   | ARG  | NE-CZ-NH1  | -6.62 | 114.88      | 121.50   |
| 1   | A     | 114 | ALA  | N-CA-CB    | -6.62 | 100.14      | 110.06   |
| 1   | B     | 245 | ASN  | OD1-CG-ND2 | -6.61 | 115.99      | 122.60   |
| 1   | A     | 225 | ASP  | CA-C-O     | -6.60 | 111.93      | 119.78   |
| 1   | B     | 224 | HIS  | N-CA-CB    | -6.58 | 99.47       | 110.39   |
| 1   | A     | 184 | VAL  | N-CA-C     | -6.57 | 104.12      | 110.42   |
| 1   | A     | 32  | LYS  | CA-C-O     | -6.56 | 113.71      | 120.54   |
| 1   | B     | 165 | GLU  | CA-C-O     | -6.56 | 114.47      | 119.59   |
| 1   | A     | 127 | ILE  | CA-CB-CG1  | 6.55  | 121.54      | 110.40   |
| 1   | B     | 78  | ILE  | CA-CB-CG1  | -6.54 | 99.28       | 110.40   |
| 1   | B     | 103 | GLY  | O-C-N      | 6.53  | 130.57      | 122.41   |
| 1   | A     | 24  | LEU  | CB-CA-C    | -6.53 | 100.54      | 110.92   |
| 1   | B     | 40  | VAL  | CB-CA-C    | 6.52  | 120.54      | 110.50   |
| 1   | B     | 176 | ALA  | CA-C-O     | -6.51 | 113.86      | 121.16   |
| 1   | B     | 222 | SER  | N-CA-CB    | -6.51 | 99.47       | 110.41   |
| 1   | A     | 182 | GLN  | CB-CG-CD   | 6.50  | 123.64      | 112.60   |
| 1   | B     | 95  | HIS  | CA-CB-CG   | -6.48 | 107.32      | 113.80   |
| 1   | A     | 121 | LEU  | O-C-N      | -6.47 | 115.01      | 123.16   |
| 1   | B     | 7   | PHE  | CA-CB-CG   | 6.44  | 120.24      | 113.80   |
| 1   | B     | 138 | ILE  | CA-CB-CG1  | -6.44 | 99.44       | 110.40   |
| 1   | A     | 177 | THR  | CA-CB-CG2  | 6.44  | 121.45      | 110.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 170 | ILE  | N-CA-CB    | 6.44  | 118.72      | 110.99   |
| 1   | A     | 242 | ASP  | O-C-N      | 6.42  | 128.92      | 122.12   |
| 1   | A     | 125 | ALA  | CA-C-O     | 6.42  | 127.37      | 120.38   |
| 1   | A     | 114 | ALA  | CB-CA-C    | 6.41  | 121.57      | 110.68   |
| 1   | B     | 215 | GLY  | CA-C-O     | -6.41 | 113.25      | 120.30   |
| 1   | A     | 177 | THR  | N-CA-C     | -6.40 | 101.70      | 109.83   |
| 1   | B     | 124 | ILE  | N-CA-CB    | 6.40  | 119.70      | 111.83   |
| 1   | B     | 170 | ILE  | CA-C-O     | -6.39 | 113.73      | 120.57   |
| 1   | B     | 133 | GLU  | N-CA-C     | 6.38  | 118.03      | 111.14   |
| 1   | B     | 202 | GLN  | OE1-CD-NE2 | 6.38  | 128.98      | 122.60   |
| 1   | A     | 31  | ALA  | N-CA-CB    | -6.36 | 101.64      | 110.29   |
| 1   | A     | 22  | GLY  | N-CA-C     | -6.36 | 105.10      | 112.73   |
| 1   | B     | 96  | SER  | CA-C-N     | -6.36 | 111.80      | 120.44   |
| 1   | B     | 96  | SER  | C-N-CA     | -6.36 | 111.80      | 120.44   |
| 1   | A     | 133 | GLU  | N-CA-C     | -6.35 | 103.66      | 111.40   |
| 1   | A     | 121 | LEU  | CA-C-N     | 6.34  | 128.63      | 120.64   |
| 1   | A     | 121 | LEU  | C-N-CA     | 6.34  | 128.63      | 120.64   |
| 1   | B     | 62  | ALA  | N-CA-CB    | -6.34 | 99.80       | 110.83   |
| 1   | A     | 156 | ASP  | CB-CA-C    | -6.34 | 102.14      | 111.77   |
| 1   | A     | 58  | LYS  | CB-CG-CD   | 6.33  | 125.86      | 111.30   |
| 1   | A     | 5   | LYS  | N-CA-C     | 6.32  | 119.80      | 109.76   |
| 1   | B     | 106 | ASP  | O-C-N      | 6.31  | 129.84      | 122.20   |
| 1   | A     | 190 | GLY  | N-CA-C     | -6.26 | 104.98      | 113.37   |
| 1   | A     | 70  | PRO  | O-C-N      | -6.25 | 114.42      | 122.23   |
| 1   | A     | 221 | ALA  | CA-C-N     | 6.25  | 128.94      | 120.38   |
| 1   | A     | 221 | ALA  | C-N-CA     | 6.25  | 128.94      | 120.38   |
| 1   | B     | 148 | LYS  | CA-C-O     | 6.24  | 127.58      | 120.90   |
| 1   | B     | 227 | ASP  | N-CA-CB    | -6.24 | 100.93      | 110.92   |
| 1   | A     | 21  | LEU  | N-CA-CB    | -6.24 | 101.03      | 110.07   |
| 1   | A     | 124 | ILE  | CA-C-N     | 6.24  | 131.61      | 123.00   |
| 1   | A     | 124 | ILE  | C-N-CA     | 6.24  | 131.61      | 123.00   |
| 1   | B     | 172 | THR  | O-C-N      | 6.22  | 130.98      | 122.46   |
| 1   | A     | 124 | ILE  | CB-CA-C    | 6.21  | 119.07      | 110.99   |
| 1   | A     | 203 | SER  | O-C-N      | 6.21  | 131.18      | 122.36   |
| 1   | B     | 213 | THR  | CA-CB-OG1  | -6.21 | 100.28      | 109.60   |
| 1   | A     | 168 | TRP  | CA-C-N     | -6.20 | 109.70      | 121.54   |
| 1   | A     | 168 | TRP  | C-N-CA     | -6.20 | 109.70      | 121.54   |
| 1   | A     | 161 | VAL  | CB-CA-C    | 6.20  | 120.04      | 110.50   |
| 1   | A     | 63  | ALA  | N-CA-C     | -6.19 | 101.32      | 110.48   |
| 1   | B     | 176 | ALA  | O-C-N      | 6.19  | 130.44      | 122.89   |
| 1   | A     | 32  | LYS  | CA-C-N     | -6.18 | 112.97      | 122.62   |
| 1   | A     | 32  | LYS  | C-N-CA     | -6.18 | 112.97      | 122.62   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 179 | GLN  | O-C-N     | 6.18  | 129.20      | 122.15   |
| 1   | B     | 186 | GLU  | CA-CB-CG  | 6.18  | 126.47      | 114.10   |
| 1   | B     | 227 | ASP  | CA-CB-CG  | 6.18  | 118.78      | 112.60   |
| 1   | A     | 173 | GLY  | CA-C-O    | 6.16  | 131.29      | 120.57   |
| 1   | B     | 91  | VAL  | CA-C-N    | 6.16  | 130.78      | 122.90   |
| 1   | B     | 91  | VAL  | C-N-CA    | 6.16  | 130.78      | 122.90   |
| 1   | B     | 189 | ARG  | CA-C-N    | -6.16 | 113.23      | 120.00   |
| 1   | B     | 189 | ARG  | C-N-CA    | -6.16 | 113.23      | 120.00   |
| 1   | B     | 31  | ALA  | N-CA-C    | -6.15 | 100.89      | 110.17   |
| 1   | B     | 239 | GLU  | CG-CD-OE1 | -6.15 | 104.26      | 118.40   |
| 1   | B     | 130 | LYS  | CA-C-O    | -6.14 | 114.87      | 121.94   |
| 1   | B     | 134 | ARG  | NE-CZ-NH1 | -6.14 | 115.36      | 121.50   |
| 1   | A     | 44  | PRO  | CB-CA-C   | 6.13  | 119.23      | 111.39   |
| 1   | A     | 46  | ILE  | N-CA-CB   | 6.12  | 118.87      | 110.54   |
| 1   | B     | 220 | LEU  | N-CA-CB   | -6.12 | 101.13      | 110.01   |
| 1   | B     | 46  | ILE  | CA-CB-CG1 | -6.12 | 100.00      | 110.40   |
| 1   | A     | 98  | ARG  | NE-CZ-NH2 | -6.11 | 113.70      | 119.20   |
| 1   | A     | 155 | LYS  | N-CA-C    | -6.11 | 105.73      | 113.43   |
| 1   | B     | 61  | VAL  | CA-C-O    | 6.10  | 126.80      | 120.39   |
| 1   | A     | 224 | HIS  | CB-CA-C   | -6.10 | 101.31      | 110.88   |
| 1   | A     | 239 | GLU  | CG-CD-OE1 | -6.10 | 104.38      | 118.40   |
| 1   | B     | 193 | LYS  | CA-C-O    | -6.09 | 112.61      | 119.79   |
| 1   | A     | 175 | THR  | CA-C-N    | -6.08 | 113.87      | 122.63   |
| 1   | A     | 175 | THR  | C-N-CA    | -6.08 | 113.87      | 122.63   |
| 1   | B     | 227 | ASP  | N-CA-C    | 6.08  | 120.01      | 112.59   |
| 1   | A     | 37  | THR  | CA-C-O    | 6.07  | 127.00      | 120.38   |
| 1   | B     | 194 | THR  | N-CA-CB   | 6.06  | 119.13      | 110.16   |
| 1   | A     | 71  | LYS  | CB-CA-C   | -6.06 | 96.74       | 110.07   |
| 1   | A     | 140 | GLU  | CG-CD-OE1 | -6.04 | 104.50      | 118.40   |
| 1   | B     | 150 | ILE  | O-C-N     | 6.02  | 128.39      | 121.94   |
| 1   | A     | 41  | CYS  | O-C-N     | 6.01  | 130.84      | 123.21   |
| 1   | A     | 40  | VAL  | O-C-N     | 6.00  | 130.05      | 123.09   |
| 1   | B     | 230 | LEU  | CA-C-N    | 6.00  | 130.11      | 122.37   |
| 1   | B     | 230 | LEU  | C-N-CA    | 6.00  | 130.11      | 122.37   |
| 1   | B     | 229 | PHE  | O-C-N     | 6.00  | 129.99      | 123.10   |
| 1   | A     | 41  | CYS  | N-CA-CB   | 5.99  | 120.34      | 110.69   |
| 1   | B     | 72  | GLY  | O-C-N     | 5.99  | 129.82      | 123.23   |
| 1   | B     | 160 | VAL  | CA-CB-CG1 | 5.98  | 120.56      | 110.40   |
| 1   | B     | 52  | ARG  | CB-CA-C   | -5.97 | 101.50      | 110.88   |
| 1   | A     | 226 | VAL  | CB-CA-C   | 5.97  | 119.16      | 110.98   |
| 1   | A     | 191 | TRP  | CA-C-O    | 5.95  | 127.07      | 120.82   |
| 1   | B     | 217 | CYS  | N-CA-CB   | -5.95 | 100.07      | 109.78   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 21  | LEU  | CB-CA-C    | 5.95  | 120.30      | 110.90   |
| 1   | A     | 39  | VAL  | N-CA-C     | 5.95  | 117.05      | 108.48   |
| 1   | B     | 103 | GLY  | CA-C-O     | -5.95 | 111.87      | 119.13   |
| 1   | B     | 114 | ALA  | O-C-N      | 5.95  | 128.43      | 122.12   |
| 1   | A     | 211 | SER  | O-C-N      | 5.95  | 130.23      | 122.68   |
| 1   | A     | 45  | SER  | N-CA-C     | 5.94  | 118.54      | 111.71   |
| 1   | A     | 146 | GLN  | CA-CB-CG   | -5.94 | 102.22      | 114.10   |
| 1   | A     | 145 | GLU  | CA-C-O     | 5.94  | 127.06      | 120.82   |
| 1   | A     | 179 | GLN  | CA-C-N     | -5.94 | 111.85      | 120.29   |
| 1   | A     | 179 | GLN  | C-N-CA     | -5.94 | 111.85      | 120.29   |
| 1   | A     | 239 | GLU  | N-CA-C     | 5.94  | 120.06      | 112.34   |
| 1   | B     | 84  | LYS  | O-C-N      | 5.93  | 128.41      | 122.12   |
| 1   | B     | 205 | ARG  | NH1-CZ-NH2 | -5.93 | 111.59      | 119.30   |
| 1   | A     | 16  | GLY  | CA-C-N     | 5.92  | 131.99      | 121.75   |
| 1   | A     | 16  | GLY  | C-N-CA     | 5.92  | 131.99      | 121.75   |
| 1   | B     | 99  | ARG  | CA-C-O     | -5.91 | 114.80      | 121.00   |
| 1   | B     | 134 | ARG  | N-CA-C     | -5.91 | 103.81      | 111.02   |
| 1   | B     | 34  | SER  | N-CA-C     | 5.91  | 118.57      | 110.24   |
| 1   | A     | 4   | ARG  | CA-C-O     | 5.90  | 128.95      | 120.51   |
| 1   | A     | 108 | LEU  | CA-C-N     | -5.89 | 110.63      | 120.30   |
| 1   | A     | 108 | LEU  | C-N-CA     | -5.89 | 110.63      | 120.30   |
| 1   | A     | 124 | ILE  | CA-C-O     | 5.89  | 126.97      | 120.48   |
| 1   | B     | 167 | VAL  | N-CA-CB    | -5.89 | 102.53      | 110.54   |
| 1   | A     | 138 | ILE  | CA-C-N     | 5.89  | 128.49      | 120.54   |
| 1   | A     | 138 | ILE  | C-N-CA     | 5.89  | 128.49      | 120.54   |
| 1   | B     | 178 | PRO  | CB-CA-C    | 5.89  | 122.42      | 113.06   |
| 1   | A     | 163 | ALA  | CA-C-N     | -5.88 | 114.36      | 122.30   |
| 1   | A     | 163 | ALA  | C-N-CA     | -5.88 | 114.36      | 122.30   |
| 1   | A     | 69  | VAL  | CA-CB-CG1  | 5.87  | 120.38      | 110.40   |
| 1   | A     | 103 | GLY  | CA-C-O     | -5.87 | 112.70      | 119.80   |
| 1   | A     | 160 | VAL  | CA-C-N     | -5.86 | 114.80      | 122.94   |
| 1   | A     | 160 | VAL  | C-N-CA     | -5.86 | 114.80      | 122.94   |
| 1   | B     | 100 | HIS  | CA-C-O     | -5.85 | 112.75      | 119.60   |
| 1   | B     | 200 | VAL  | N-CA-C     | -5.85 | 105.03      | 110.53   |
| 1   | B     | 240 | PHE  | N-CA-C     | -5.85 | 104.90      | 111.28   |
| 1   | A     | 186 | GLU  | CA-CB-CG   | 5.84  | 125.78      | 114.10   |
| 1   | A     | 134 | ARG  | CA-CB-CG   | -5.83 | 102.43      | 114.10   |
| 1   | A     | 100 | HIS  | CB-CG-CD2  | -5.83 | 123.62      | 131.20   |
| 1   | B     | 137 | GLY  | CA-C-N     | 5.83  | 132.47      | 121.97   |
| 1   | B     | 137 | GLY  | C-N-CA     | 5.83  | 132.47      | 121.97   |
| 1   | A     | 48  | LEU  | N-CA-C     | 5.83  | 118.10      | 111.11   |
| 1   | B     | 139 | THR  | O-C-N      | 5.81  | 128.07      | 122.03   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 186 | GLU  | CB-CA-C   | -5.80 | 101.77      | 110.88   |
| 1   | A     | 239 | GLU  | CG-CD-OE2 | 5.80  | 131.74      | 118.40   |
| 1   | A     | 234 | ALA  | N-CA-CB   | -5.80 | 100.25      | 110.39   |
| 1   | B     | 245 | ASN  | CA-C-O    | -5.79 | 113.12      | 122.20   |
| 1   | B     | 4   | ARG  | NE-CZ-NH2 | 5.78  | 124.40      | 119.20   |
| 1   | B     | 32  | LYS  | N-CA-C    | -5.77 | 99.11       | 108.52   |
| 1   | A     | 173 | GLY  | O-C-N     | -5.77 | 115.20      | 122.70   |
| 1   | A     | 179 | GLN  | CA-C-O    | -5.76 | 114.31      | 120.42   |
| 1   | A     | 208 | TYR  | CA-C-O    | -5.76 | 114.03      | 120.54   |
| 1   | A     | 46  | ILE  | N-CA-C    | -5.75 | 104.75      | 110.62   |
| 1   | B     | 122 | GLY  | O-C-N     | 5.75  | 129.81      | 123.49   |
| 1   | A     | 17  | ASP  | O-C-N     | 5.74  | 129.79      | 123.25   |
| 1   | A     | 170 | ILE  | N-CA-C    | 5.74  | 121.27      | 109.34   |
| 1   | A     | 209 | GLY  | N-CA-C    | 5.74  | 126.77      | 113.18   |
| 1   | B     | 136 | ALA  | CA-C-N    | 5.73  | 133.74      | 121.18   |
| 1   | B     | 136 | ALA  | C-N-CA    | 5.73  | 133.74      | 121.18   |
| 1   | A     | 49  | ASP  | N-CA-CB   | -5.73 | 101.68      | 110.16   |
| 1   | A     | 111 | GLN  | CB-CG-CD  | -5.73 | 102.86      | 112.60   |
| 1   | B     | 40  | VAL  | N-CA-CB   | -5.73 | 102.04      | 111.44   |
| 1   | B     | 98  | ARG  | CA-C-O    | 5.72  | 126.61      | 120.55   |
| 1   | A     | 106 | ASP  | N-CA-C    | -5.71 | 105.14      | 111.36   |
| 1   | A     | 123 | VAL  | CA-CB-CG2 | 5.69  | 120.08      | 110.40   |
| 1   | A     | 146 | GLN  | CA-C-N    | 5.69  | 128.22      | 120.54   |
| 1   | A     | 146 | GLN  | C-N-CA    | 5.69  | 128.22      | 120.54   |
| 1   | A     | 35  | ALA  | O-C-N     | 5.68  | 129.64      | 122.65   |
| 1   | B     | 23  | GLU  | CA-C-N    | 5.68  | 128.36      | 120.29   |
| 1   | B     | 23  | GLU  | C-N-CA    | 5.68  | 128.36      | 120.29   |
| 1   | A     | 9   | GLY  | O-C-N     | 5.68  | 129.03      | 123.80   |
| 1   | B     | 39  | VAL  | CA-C-O    | 5.68  | 127.31      | 120.67   |
| 1   | A     | 163 | ALA  | O-C-N     | 5.67  | 130.28      | 123.13   |
| 1   | B     | 109 | ILE  | CA-CB-CG2 | 5.67  | 120.15      | 110.50   |
| 1   | A     | 127 | ILE  | CA-CB-CG2 | -5.66 | 100.88      | 110.50   |
| 1   | A     | 156 | ASP  | N-CA-C    | 5.66  | 120.44      | 107.48   |
| 1   | A     | 179 | GLN  | CA-CB-CG  | -5.66 | 102.78      | 114.10   |
| 1   | B     | 81  | ALA  | O-C-N     | 5.65  | 128.11      | 122.12   |
| 1   | A     | 35  | ALA  | CB-CA-C   | -5.65 | 98.71       | 110.40   |
| 1   | A     | 158 | SER  | CA-CB-OG  | 5.64  | 122.39      | 111.10   |
| 1   | A     | 184 | VAL  | O-C-N     | 5.64  | 127.44      | 121.91   |
| 1   | B     | 202 | GLN  | O-C-N     | 5.63  | 128.57      | 122.15   |
| 1   | A     | 95  | HIS  | O-C-N     | 5.63  | 129.73      | 122.81   |
| 1   | A     | 149 | ALA  | CA-C-N    | 5.63  | 127.77      | 120.56   |
| 1   | A     | 149 | ALA  | C-N-CA    | 5.63  | 127.77      | 120.56   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 17  | ASP  | N-CA-C     | -5.62 | 100.53      | 109.07   |
| 1   | A     | 213 | THR  | O-C-N      | 5.62  | 129.49      | 122.92   |
| 1   | A     | 126 | CYS  | N-CA-CB    | -5.60 | 101.77      | 110.57   |
| 1   | B     | 155 | LYS  | CB-CA-C    | -5.60 | 99.66       | 109.07   |
| 1   | A     | 34  | SER  | CA-C-N     | -5.60 | 109.47      | 121.45   |
| 1   | A     | 34  | SER  | C-N-CA     | -5.60 | 109.47      | 121.45   |
| 1   | A     | 221 | ALA  | CA-C-O     | 5.59  | 126.67      | 120.63   |
| 1   | A     | 112 | LYS  | CA-C-O     | -5.59 | 114.49      | 120.42   |
| 1   | B     | 55  | LEU  | N-CA-CB    | 5.58  | 118.21      | 110.17   |
| 1   | B     | 225 | ASP  | CA-C-O     | -5.57 | 112.69      | 119.32   |
| 1   | A     | 247 | LYS  | CA-C-O     | -5.56 | 112.56      | 120.51   |
| 1   | B     | 79  | SER  | CA-CB-OG   | -5.56 | 99.99       | 111.10   |
| 1   | A     | 130 | LYS  | CA-C-N     | 5.55  | 127.99      | 120.38   |
| 1   | A     | 130 | LYS  | C-N-CA     | 5.55  | 127.99      | 120.38   |
| 1   | A     | 72  | GLY  | CA-C-O     | 5.54  | 126.73      | 121.30   |
| 1   | A     | 211 | SER  | CA-C-O     | -5.54 | 115.16      | 120.92   |
| 1   | B     | 4   | ARG  | CD-NE-CZ   | -5.54 | 116.65      | 124.40   |
| 1   | B     | 134 | ARG  | O-C-N      | 5.54  | 128.00      | 122.08   |
| 1   | A     | 182 | GLN  | OE1-CD-NE2 | -5.53 | 117.07      | 122.60   |
| 1   | B     | 12  | TRP  | O-C-N      | 5.53  | 129.84      | 122.43   |
| 1   | B     | 162 | LEU  | CA-C-N     | 5.53  | 130.80      | 123.00   |
| 1   | B     | 162 | LEU  | C-N-CA     | 5.53  | 130.80      | 123.00   |
| 1   | A     | 121 | LEU  | N-CA-C     | -5.53 | 101.16      | 109.95   |
| 1   | B     | 121 | LEU  | O-C-N      | 5.52  | 129.14      | 122.68   |
| 1   | B     | 101 | VAL  | O-C-N      | 5.51  | 129.12      | 121.84   |
| 1   | B     | 76  | GLY  | CA-C-N     | 5.51  | 132.77      | 122.74   |
| 1   | B     | 76  | GLY  | C-N-CA     | 5.51  | 132.77      | 122.74   |
| 1   | A     | 137 | GLY  | CA-C-N     | 5.51  | 130.10      | 122.28   |
| 1   | A     | 137 | GLY  | C-N-CA     | 5.51  | 130.10      | 122.28   |
| 1   | B     | 17  | ASP  | CA-C-N     | -5.50 | 112.91      | 120.28   |
| 1   | B     | 17  | ASP  | C-N-CA     | -5.50 | 112.91      | 120.28   |
| 1   | A     | 86  | ILE  | CA-CB-CG2  | 5.50  | 119.85      | 110.50   |
| 1   | B     | 77  | GLU  | CA-C-O     | 5.49  | 128.35      | 121.66   |
| 1   | B     | 168 | TRP  | CA-C-O     | -5.49 | 113.14      | 119.61   |
| 1   | A     | 126 | CYS  | N-CA-C     | 5.48  | 117.90      | 109.07   |
| 1   | A     | 34  | SER  | N-CA-C     | 5.48  | 118.59      | 110.48   |
| 1   | A     | 82  | MET  | N-CA-C     | -5.48 | 105.22      | 111.14   |
| 1   | B     | 195 | HIS  | CA-C-N     | -5.48 | 112.10      | 121.97   |
| 1   | B     | 195 | HIS  | C-N-CA     | -5.48 | 112.10      | 121.97   |
| 1   | A     | 89  | ALA  | O-C-N      | 5.47  | 128.19      | 122.23   |
| 1   | A     | 186 | GLU  | CB-CG-CD   | 5.47  | 121.90      | 112.60   |
| 1   | B     | 77  | GLU  | CA-C-N     | 5.47  | 130.58      | 122.71   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 77  | GLU  | C-N-CA     | 5.47  | 130.58      | 122.71   |
| 1   | B     | 230 | LEU  | N-CA-C     | -5.46 | 96.28       | 107.70   |
| 1   | B     | 74  | PHE  | O-C-N      | 5.46  | 131.02      | 122.61   |
| 1   | B     | 133 | GLU  | CA-C-O     | 5.46  | 126.33      | 120.70   |
| 1   | A     | 100 | HIS  | CB-CA-C    | -5.46 | 98.69       | 109.67   |
| 1   | B     | 147 | THR  | CA-C-O     | 5.46  | 126.32      | 120.70   |
| 1   | B     | 240 | PHE  | O-C-N      | 5.46  | 127.90      | 122.12   |
| 1   | A     | 195 | HIS  | CA-C-O     | -5.45 | 112.97      | 119.35   |
| 1   | A     | 52  | ARG  | CA-C-O     | -5.45 | 114.78      | 120.55   |
| 1   | B     | 75  | THR  | CA-CB-OG1  | -5.44 | 101.44      | 109.60   |
| 1   | A     | 52  | ARG  | NH1-CZ-NH2 | 5.44  | 126.37      | 119.30   |
| 1   | B     | 69  | VAL  | CA-C-O     | 5.44  | 127.82      | 121.13   |
| 1   | A     | 193 | LYS  | CA-CB-CG   | 5.42  | 124.95      | 114.10   |
| 1   | B     | 79  | SER  | CA-C-O     | 5.42  | 127.21      | 120.54   |
| 1   | A     | 99  | ARG  | O-C-N      | 5.42  | 127.65      | 122.07   |
| 1   | A     | 150 | ILE  | CB-CG1-CD1 | 5.42  | 125.18      | 113.80   |
| 1   | A     | 178 | PRO  | O-C-N      | -5.41 | 115.34      | 122.64   |
| 1   | A     | 174 | LYS  | CA-C-N     | 5.41  | 131.87      | 121.54   |
| 1   | A     | 174 | LYS  | C-N-CA     | 5.41  | 131.87      | 121.54   |
| 1   | B     | 128 | GLY  | CA-C-O     | -5.41 | 111.16      | 120.57   |
| 1   | A     | 224 | HIS  | O-C-N      | 5.39  | 127.62      | 122.07   |
| 1   | A     | 82  | MET  | CB-CA-C    | 5.39  | 119.41      | 110.90   |
| 1   | B     | 241 | VAL  | N-CA-C     | -5.39 | 105.13      | 110.62   |
| 1   | A     | 127 | ILE  | CB-CA-C    | 5.38  | 118.73      | 110.55   |
| 1   | A     | 198 | ASP  | O-C-N      | 5.38  | 129.88      | 122.46   |
| 1   | B     | 137 | GLY  | O-C-N      | -5.38 | 115.20      | 122.35   |
| 1   | A     | 143 | VAL  | N-CA-CB    | -5.37 | 103.24      | 110.54   |
| 1   | A     | 180 | GLN  | O-C-N      | 5.37  | 128.27      | 122.15   |
| 1   | A     | 236 | LEU  | N-CA-CB    | -5.36 | 102.24      | 110.44   |
| 1   | A     | 131 | LEU  | CA-CB-CG   | 5.34  | 135.00      | 116.30   |
| 1   | B     | 225 | ASP  | CA-CB-CG   | -5.34 | 107.26      | 112.60   |
| 1   | A     | 41  | CYS  | CA-CB-SG   | -5.34 | 102.12      | 114.40   |
| 1   | B     | 197 | SER  | CA-C-O     | -5.34 | 114.77      | 120.75   |
| 1   | B     | 83  | ILE  | N-CA-CB    | -5.32 | 105.03      | 110.62   |
| 1   | A     | 219 | GLU  | N-CA-CB    | -5.32 | 102.01      | 109.94   |
| 1   | A     | 129 | GLU  | CG-CD-OE1  | -5.32 | 106.16      | 118.40   |
| 1   | B     | 45  | SER  | CA-CB-OG   | 5.32  | 121.74      | 111.10   |
| 1   | A     | 59  | ILE  | CA-C-N     | 5.31  | 127.33      | 120.64   |
| 1   | A     | 59  | ILE  | C-N-CA     | 5.31  | 127.33      | 120.64   |
| 1   | A     | 153 | ASN  | OD1-CG-ND2 | 5.30  | 127.91      | 122.60   |
| 1   | B     | 19  | LYS  | CA-C-O     | -5.30 | 115.43      | 121.00   |
| 1   | B     | 19  | LYS  | CB-CA-C    | 5.30  | 119.12      | 110.96   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 191 | TRP  | CA-C-O    | -5.29 | 114.92      | 120.63   |
| 1   | B     | 220 | LEU  | CB-CA-C   | 5.29  | 119.18      | 110.88   |
| 1   | A     | 149 | ALA  | CB-CA-C   | 5.28  | 119.66      | 110.68   |
| 1   | A     | 194 | THR  | CA-C-N    | -5.28 | 113.83      | 122.54   |
| 1   | A     | 194 | THR  | C-N-CA    | -5.28 | 113.83      | 122.54   |
| 1   | A     | 207 | ILE  | CA-C-O    | 5.28  | 128.10      | 121.40   |
| 1   | B     | 97  | GLU  | CG-CD-OE2 | -5.28 | 106.26      | 118.40   |
| 1   | B     | 240 | PHE  | CA-CB-CG  | 5.28  | 119.08      | 113.80   |
| 1   | B     | 75  | THR  | CB-CA-C   | 5.27  | 118.12      | 109.90   |
| 1   | B     | 212 | VAL  | O-C-N     | 5.27  | 128.74      | 123.10   |
| 1   | B     | 82  | MET  | N-CA-C    | -5.27 | 105.62      | 111.36   |
| 1   | A     | 200 | VAL  | CA-C-N    | 5.26  | 127.33      | 120.28   |
| 1   | A     | 200 | VAL  | C-N-CA    | 5.26  | 127.33      | 120.28   |
| 1   | A     | 104 | GLU  | CB-CG-CD  | 5.26  | 121.53      | 112.60   |
| 1   | A     | 151 | ALA  | CA-C-O    | -5.26 | 114.98      | 120.55   |
| 1   | A     | 204 | THR  | CA-C-N    | 5.25  | 129.34      | 121.72   |
| 1   | A     | 204 | THR  | C-N-CA    | 5.25  | 129.34      | 121.72   |
| 1   | B     | 28  | LEU  | CA-C-O    | 5.25  | 126.31      | 120.90   |
| 1   | A     | 8   | VAL  | CB-CA-C   | 5.25  | 117.25      | 110.12   |
| 1   | A     | 91  | VAL  | CA-C-O    | 5.24  | 126.53      | 120.76   |
| 1   | A     | 50  | PHE  | CA-CB-CG  | -5.24 | 108.56      | 113.80   |
| 1   | B     | 235 | SER  | N-CA-C    | -5.24 | 106.39      | 112.89   |
| 1   | B     | 66  | CYS  | CA-C-O    | -5.23 | 115.69      | 121.28   |
| 1   | B     | 106 | ASP  | CA-CB-CG  | -5.22 | 107.38      | 112.60   |
| 1   | A     | 198 | ASP  | N-CA-CB   | 5.22  | 118.91      | 110.40   |
| 1   | A     | 116 | ALA  | CB-CA-C   | 5.22  | 119.45      | 110.79   |
| 1   | B     | 156 | ASP  | N-CA-CB   | 5.22  | 119.97      | 110.95   |
| 1   | B     | 204 | THR  | CA-C-O    | 5.21  | 126.80      | 120.81   |
| 1   | B     | 240 | PHE  | CA-C-O    | -5.21 | 115.03      | 120.55   |
| 1   | A     | 159 | LYS  | N-CA-C    | -5.20 | 106.79      | 112.72   |
| 1   | A     | 167 | VAL  | CA-C-O    | 5.20  | 126.36      | 120.85   |
| 1   | B     | 126 | CYS  | CA-CB-SG  | -5.20 | 102.44      | 114.40   |
| 1   | B     | 223 | GLN  | CB-CG-CD  | 5.20  | 121.44      | 112.60   |
| 1   | B     | 41  | CYS  | O-C-N     | 5.19  | 129.48      | 123.30   |
| 1   | B     | 231 | VAL  | CB-CA-C   | -5.19 | 104.47      | 110.91   |
| 1   | B     | 223 | GLN  | N-CA-CB   | -5.19 | 102.00      | 109.83   |
| 1   | A     | 59  | ILE  | N-CA-C    | 5.18  | 115.76      | 108.36   |
| 1   | B     | 230 | LEU  | N-CA-CB   | 5.17  | 119.30      | 110.87   |
| 1   | A     | 103 | GLY  | CA-C-N    | -5.17 | 113.53      | 120.82   |
| 1   | A     | 103 | GLY  | C-N-CA    | -5.17 | 113.53      | 120.82   |
| 1   | A     | 174 | LYS  | N-CA-CB   | -5.17 | 96.69       | 111.16   |
| 1   | B     | 6   | PHE  | CA-C-O    | -5.16 | 115.34      | 120.96   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 46  | ILE  | N-CA-CB    | 5.16  | 118.64      | 110.54   |
| 1   | B     | 53  | GLN  | OE1-CD-NE2 | -5.15 | 117.45      | 122.60   |
| 1   | A     | 240 | PHE  | CB-CA-C    | 5.15  | 119.33      | 110.79   |
| 1   | A     | 52  | ARG  | N-CA-CB    | 5.15  | 117.68      | 110.12   |
| 1   | B     | 150 | ILE  | N-CA-C     | -5.14 | 105.59      | 110.42   |
| 1   | A     | 192 | LEU  | CB-CA-C    | 5.13  | 119.31      | 110.79   |
| 1   | B     | 15  | ASN  | CB-CG-ND2  | 5.13  | 124.09      | 116.40   |
| 1   | A     | 117 | LEU  | O-C-N      | 5.13  | 127.35      | 122.07   |
| 1   | A     | 98  | ARG  | CA-C-O     | 5.11  | 125.82      | 119.79   |
| 1   | A     | 3   | PRO  | N-CA-C     | 5.11  | 122.99      | 112.47   |
| 1   | A     | 20  | SER  | CA-C-N     | 5.11  | 127.38      | 120.44   |
| 1   | A     | 20  | SER  | C-N-CA     | 5.11  | 127.38      | 120.44   |
| 1   | A     | 31  | ALA  | N-CA-C     | 5.10  | 116.91      | 110.33   |
| 1   | B     | 27  | THR  | CA-CB-OG1  | -5.10 | 101.95      | 109.60   |
| 1   | A     | 71  | LYS  | N-CA-C     | 5.09  | 116.93      | 109.24   |
| 1   | A     | 58  | LYS  | CA-C-N     | 5.09  | 129.34      | 122.93   |
| 1   | A     | 58  | LYS  | C-N-CA     | 5.09  | 129.34      | 122.93   |
| 1   | A     | 4   | ARG  | NH1-CZ-NH2 | 5.07  | 125.89      | 119.30   |
| 1   | B     | 85  | ASP  | OD1-CG-OD2 | -5.07 | 110.74      | 122.90   |
| 1   | A     | 216 | ASN  | CA-C-N     | 5.07  | 129.24      | 121.19   |
| 1   | A     | 216 | ASN  | C-N-CA     | 5.07  | 129.24      | 121.19   |
| 1   | A     | 227 | ASP  | CB-CG-OD2  | 5.06  | 130.04      | 118.40   |
| 1   | A     | 31  | ALA  | O-C-N      | -5.06 | 116.71      | 122.68   |
| 1   | A     | 147 | THR  | O-C-N      | 5.06  | 127.35      | 122.09   |
| 1   | B     | 103 | GLY  | CA-C-N     | -5.06 | 113.87      | 120.95   |
| 1   | B     | 103 | GLY  | C-N-CA     | -5.06 | 113.87      | 120.95   |
| 1   | A     | 44  | PRO  | CA-C-O     | -5.05 | 115.77      | 121.43   |
| 1   | A     | 231 | VAL  | CA-CB-CG2  | 5.05  | 118.98      | 110.40   |
| 1   | A     | 14  | MET  | O-C-N      | 5.04  | 129.01      | 122.71   |
| 1   | B     | 118 | ALA  | CA-C-N     | 5.04  | 130.31      | 122.49   |
| 1   | B     | 118 | ALA  | C-N-CA     | 5.04  | 130.31      | 122.49   |
| 1   | B     | 234 | ALA  | O-C-N      | 5.04  | 129.42      | 122.46   |
| 1   | B     | 187 | LYS  | CA-C-N     | 5.04  | 127.30      | 120.44   |
| 1   | B     | 187 | LYS  | C-N-CA     | 5.04  | 127.30      | 120.44   |
| 1   | B     | 100 | HIS  | CA-C-N     | -5.04 | 112.49      | 120.55   |
| 1   | B     | 100 | HIS  | C-N-CA     | -5.04 | 112.49      | 120.55   |
| 1   | B     | 108 | LEU  | CB-CA-C    | 5.04  | 118.71      | 110.96   |
| 1   | A     | 131 | LEU  | O-C-N      | 5.03  | 127.45      | 122.12   |
| 1   | B     | 236 | LEU  | CA-C-O     | -5.03 | 112.67      | 119.11   |
| 1   | A     | 219 | GLU  | OE1-CD-OE2 | 5.03  | 134.97      | 122.90   |
| 1   | A     | 113 | VAL  | CA-C-N     | -5.03 | 113.49      | 120.38   |
| 1   | A     | 113 | VAL  | C-N-CA     | -5.03 | 113.49      | 120.38   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 48  | LEU  | O-C-N      | 5.02  | 127.31      | 122.09   |
| 1   | B     | 190 | GLY  | N-CA-C     | -5.02 | 106.35      | 112.77   |
| 1   | B     | 145 | GLU  | CG-CD-OE1  | -5.01 | 106.87      | 118.40   |
| 1   | B     | 247 | LYS  | O-C-N      | 5.01  | 129.25      | 122.59   |
| 1   | A     | 247 | LYS  | N-CA-C     | -5.00 | 100.15      | 110.80   |
| 1   | B     | 145 | GLU  | OE1-CD-OE2 | 5.00  | 134.90      | 122.90   |
| 1   | B     | 183 | GLU  | CA-C-N     | -5.00 | 114.16      | 120.56   |
| 1   | B     | 183 | GLU  | C-N-CA     | -5.00 | 114.16      | 120.56   |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 134 | ARG  | Sidechain |
| 1   | A     | 205 | ARG  | Sidechain |
| 1   | A     | 52  | ARG  | Sidechain |
| 1   | A     | 99  | ARG  | Sidechain |
| 1   | B     | 134 | ARG  | Sidechain |
| 1   | B     | 52  | ARG  | Sidechain |
| 1   | B     | 99  | 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     | 1867  | 0        | 1875     | 150     | 0            |
| 1   | B     | 1867  | 0        | 1875     | 139     | 0            |
| 2   | A     | 5     | 0        | 0        | 0       | 0            |
| 2   | B     | 5     | 0        | 0        | 1       | 0            |
| 3   | A     | 18    | 0        | 0        | 0       | 0            |
| 3   | B     | 16    | 0        | 0        | 4       | 0            |
| All | All   | 3778  | 0        | 3750     | 277     | 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 37.

All (277) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:82:MET:HB3   | 1:B:46:ILE:HD13  | 1.33                     | 1.08              |
| 1:A:129:GLU:OE2  | 1:A:168:TRP:CD1  | 2.17                     | 0.97              |
| 1:A:84:LYS:HG3   | 1:A:121:LEU:HD13 | 1.47                     | 0.97              |
| 1:B:178:PRO:HD2  | 1:B:179:GLN:NE2  | 1.80                     | 0.97              |
| 1:A:49:ASP:O     | 1:A:53:GLN:HG3   | 1.68                     | 0.94              |
| 1:A:141:LYS:O    | 1:A:145:GLU:HG3  | 1.68                     | 0.94              |
| 1:A:175:THR:HG22 | 1:A:177:THR:HG23 | 1.47                     | 0.92              |
| 1:A:124:ILE:CD1  | 1:A:163:ALA:HB2  | 2.00                     | 0.92              |
| 1:B:69:VAL:HG22  | 1:B:70:PRO:CD    | 2.02                     | 0.90              |
| 1:A:35:ALA:O     | 1:A:36:ASP:HB2   | 1.69                     | 0.89              |
| 1:B:25:ILE:HG21  | 1:B:54:LYS:HB3   | 1.54                     | 0.89              |
| 1:A:170:ILE:HD12 | 1:A:171:GLY:N    | 1.85                     | 0.89              |
| 1:B:178:PRO:HD2  | 1:B:179:GLN:HE22 | 1.32                     | 0.88              |
| 1:A:212:VAL:HA   | 1:A:216:ASN:HD22 | 1.39                     | 0.87              |
| 1:B:23:GLU:O     | 1:B:26:HIS:HB3   | 1.75                     | 0.87              |
| 1:A:177:THR:OG1  | 1:A:180:GLN:HG2  | 1.74                     | 0.86              |
| 1:A:46:ILE:HD12  | 1:A:47:TYR:H     | 1.39                     | 0.85              |
| 1:B:67:TYR:HB2   | 1:B:77:GLU:HG3   | 1.58                     | 0.85              |
| 1:B:2:ALA:HB3    | 1:B:3:PRO:HD3    | 1.60                     | 0.83              |
| 1:B:129:GLU:OE2  | 1:B:134:ARG:NH1  | 2.11                     | 0.83              |
| 1:A:17:ASP:O     | 1:A:21:LEU:HB2   | 1.78                     | 0.81              |
| 1:B:177:THR:HB   | 1:B:179:GLN:NE2  | 1.96                     | 0.81              |
| 1:B:213:THR:O    | 1:B:217:CYS:HB3  | 1.79                     | 0.81              |
| 1:A:82:MET:SD    | 1:B:46:ILE:HD11  | 2.21                     | 0.80              |
| 1:B:5:LYS:HE2    | 1:B:38:GLU:HB2   | 1.63                     | 0.80              |
| 1:A:175:THR:HB   | 1:A:180:GLN:OE1  | 1.81                     | 0.79              |
| 1:A:178:PRO:HG3  | 1:A:219:GLU:HG3  | 1.64                     | 0.79              |
| 1:A:247:LYS:O    | 1:A:248:HIS:CD2  | 2.36                     | 0.79              |
| 1:A:42:GLY:HA2   | 1:A:62:ALA:O     | 1.82                     | 0.78              |
| 1:A:82:MET:HB3   | 1:B:46:ILE:CD1   | 2.13                     | 0.78              |
| 1:A:64:GLN:HA    | 1:A:92:ILE:HG13  | 1.66                     | 0.77              |
| 1:B:17:ASP:O     | 1:B:21:LEU:HB2   | 1.83                     | 0.77              |
| 1:A:219:GLU:O    | 1:A:222:SER:OG   | 2.03                     | 0.76              |
| 1:B:69:VAL:HG22  | 1:B:70:PRO:HD2   | 1.66                     | 0.76              |
| 1:B:107:GLU:HG3  | 1:B:111:GLN:HE22 | 1.51                     | 0.76              |
| 1:A:246:ALA:O    | 1:A:248:HIS:N    | 2.19                     | 0.75              |
| 1:B:69:VAL:HG22  | 1:B:70:PRO:HD3   | 1.68                     | 0.75              |
| 1:B:25:ILE:HG23  | 1:B:55:LEU:HD13  | 1.68                     | 0.74              |
| 1:A:247:LYS:O    | 1:A:248:HIS:HD2  | 1.71                     | 0.74              |
| 1:B:189:ARG:NH2  | 1:B:227:ASP:OD2  | 2.20                     | 0.74              |
| 1:A:46:ILE:HD12  | 1:A:47:TYR:N     | 2.03                     | 0.73              |
| 1:A:176:ALA:HB1  | 1:A:208:TYR:OH   | 1.88                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:75:THR:O     | 1:B:98:ARG:HD2   | 1.90                     | 0.72              |
| 1:A:35:ALA:O     | 1:A:36:ASP:CB    | 2.38                     | 0.72              |
| 1:A:104:GLU:HG2  | 1:A:108:LEU:CD1  | 2.20                     | 0.72              |
| 1:B:192:LEU:HD22 | 1:B:200:VAL:CG1  | 2.19                     | 0.72              |
| 1:B:7:PHE:O      | 1:B:228:GLY:HA3  | 1.90                     | 0.71              |
| 1:A:141:LYS:HD2  | 1:A:145:GLU:OE2  | 1.91                     | 0.71              |
| 1:B:177:THR:HB   | 1:B:179:GLN:HE22 | 1.54                     | 0.70              |
| 1:B:192:LEU:HD22 | 1:B:200:VAL:HG12 | 1.72                     | 0.70              |
| 1:A:175:THR:HG22 | 1:A:177:THR:CG2  | 2.21                     | 0.70              |
| 1:A:218:LYS:HD2  | 1:A:219:GLU:N    | 2.07                     | 0.70              |
| 1:A:46:ILE:HD12  | 1:A:46:ILE:N     | 2.06                     | 0.69              |
| 1:A:52:ARG:NH1   | 1:A:59:ILE:O     | 2.24                     | 0.69              |
| 1:B:194:THR:HB   | 1:B:195:HIS:CE1  | 2.28                     | 0.69              |
| 1:A:190:GLY:O    | 1:A:194:THR:HG23 | 1.92                     | 0.69              |
| 1:B:2:ALA:HB3    | 1:B:3:PRO:CD     | 2.24                     | 0.68              |
| 1:B:5:LYS:HE3    | 1:B:36:ASP:O     | 1.94                     | 0.68              |
| 2:B:560:SO4:O2   | 3:B:621:HOH:O    | 2.12                     | 0.68              |
| 1:B:223:GLN:HB3  | 1:B:226:VAL:CG2  | 2.23                     | 0.68              |
| 1:B:125:ALA:HB1  | 1:B:150:ILE:HD13 | 1.76                     | 0.68              |
| 1:B:220:LEU:O    | 1:B:223:GLN:HB2  | 1.92                     | 0.68              |
| 1:B:69:VAL:CG2   | 1:B:70:PRO:HD3   | 2.24                     | 0.67              |
| 1:A:49:ASP:HB2   | 1:A:86:ILE:HG12  | 1.76                     | 0.67              |
| 1:A:168:TRP:CE3  | 1:A:169:ALA:HB2  | 2.30                     | 0.67              |
| 1:B:213:THR:O    | 1:B:217:CYS:CB   | 2.43                     | 0.67              |
| 1:A:70:PRO:HA    | 1:A:79:SER:OG    | 1.94                     | 0.67              |
| 1:A:175:THR:CG2  | 1:A:177:THR:HG23 | 2.25                     | 0.66              |
| 1:B:194:THR:HB   | 1:B:195:HIS:ND1  | 2.09                     | 0.66              |
| 1:A:44:PRO:HA    | 3:B:623:HOH:O    | 1.96                     | 0.66              |
| 1:A:129:GLU:OE2  | 1:A:168:TRP:HD1  | 1.79                     | 0.66              |
| 1:A:34:SER:O     | 1:A:37:THR:HG22  | 1.95                     | 0.65              |
| 1:A:122:GLY:HA2  | 1:A:159:LYS:HB3  | 1.78                     | 0.65              |
| 1:B:179:GLN:CD   | 1:B:179:GLN:H    | 2.03                     | 0.65              |
| 1:A:124:ILE:HD13 | 1:A:163:ALA:HB2  | 1.79                     | 0.65              |
| 1:A:131:LEU:HA   | 1:A:168:TRP:HB2  | 1.79                     | 0.65              |
| 1:B:237:LYS:HB3  | 1:B:238:PRO:HD2  | 1.78                     | 0.65              |
| 1:A:64:GLN:O     | 1:A:65:ASN:HB2   | 1.96                     | 0.64              |
| 1:A:170:ILE:HD12 | 1:A:170:ILE:C    | 2.21                     | 0.64              |
| 1:B:55:LEU:HG    | 1:B:59:ILE:HG21  | 1.79                     | 0.64              |
| 1:B:223:GLN:HB3  | 1:B:226:VAL:HG23 | 1.79                     | 0.64              |
| 1:A:124:ILE:HD11 | 1:A:163:ALA:HB2  | 1.77                     | 0.64              |
| 1:B:131:LEU:O    | 1:B:132:ASP:C    | 2.41                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:84:LYS:CG    | 1:A:121:LEU:HD13 | 2.28                     | 0.62              |
| 1:B:178:PRO:CD   | 1:B:179:GLN:NE2  | 2.61                     | 0.62              |
| 1:A:82:MET:CB    | 1:B:46:ILE:HD13  | 2.21                     | 0.62              |
| 1:B:216:ASN:O    | 1:B:220:LEU:HD12 | 2.00                     | 0.61              |
| 1:B:211:SER:O    | 1:B:216:ASN:ND2  | 2.32                     | 0.61              |
| 1:B:55:LEU:HD12  | 1:B:59:ILE:HD13  | 1.82                     | 0.61              |
| 1:B:168:TRP:O    | 1:B:172:THR:HG21 | 1.99                     | 0.61              |
| 1:A:175:THR:CB   | 1:A:180:GLN:OE1  | 2.49                     | 0.61              |
| 1:B:212:VAL:HG12 | 1:B:243:ILE:HD13 | 1.82                     | 0.61              |
| 1:B:142:VAL:O    | 1:B:146:GLN:HG3  | 2.00                     | 0.61              |
| 1:B:212:VAL:HA   | 1:B:216:ASN:HD21 | 1.66                     | 0.61              |
| 1:A:13:LYS:O     | 1:A:44:PRO:HG3   | 2.01                     | 0.60              |
| 1:B:2:ALA:CB     | 1:B:3:PRO:HD3    | 2.30                     | 0.60              |
| 1:A:127:ILE:CG2  | 1:A:146:GLN:HB3  | 2.31                     | 0.60              |
| 1:B:216:ASN:C    | 1:B:220:LEU:HD12 | 2.27                     | 0.59              |
| 1:A:208:TYR:O    | 1:A:229:PHE:HA   | 2.03                     | 0.59              |
| 1:A:167:VAL:C    | 1:A:169:ALA:N    | 2.58                     | 0.59              |
| 1:B:131:LEU:O    | 1:B:135:GLU:HB2  | 2.03                     | 0.58              |
| 1:B:108:LEU:O    | 1:B:112:LYS:HG3  | 2.04                     | 0.58              |
| 1:B:178:PRO:CD   | 1:B:179:GLN:HE22 | 2.10                     | 0.58              |
| 1:B:83:ILE:O     | 1:B:86:ILE:HG13  | 2.03                     | 0.57              |
| 1:A:73:ALA:HA    | 1:B:13:LYS:HD2   | 1.85                     | 0.57              |
| 1:B:193:LYS:HB2  | 1:B:198:ASP:HA   | 1.85                     | 0.57              |
| 1:A:91:VAL:HG22  | 1:A:93:LEU:HG    | 1.87                     | 0.57              |
| 1:A:124:ILE:CD1  | 1:A:163:ALA:CB   | 2.78                     | 0.56              |
| 1:B:48:LEU:HD21  | 1:B:63:ALA:HB2   | 1.87                     | 0.56              |
| 1:A:78:ILE:HG21  | 1:B:46:ILE:HG12  | 1.87                     | 0.56              |
| 1:A:124:ILE:HD11 | 1:A:163:ALA:CB   | 2.35                     | 0.56              |
| 1:B:144:PHE:O    | 1:B:148:LYS:HB2  | 2.06                     | 0.56              |
| 1:B:177:THR:CB   | 1:B:179:GLN:NE2  | 2.66                     | 0.56              |
| 1:B:208:TYR:CZ   | 1:B:210:GLY:HA3  | 2.41                     | 0.56              |
| 1:A:129:GLU:CD   | 1:A:139:THR:HG23 | 2.31                     | 0.56              |
| 1:A:191:TRP:O    | 1:A:195:HIS:N    | 2.38                     | 0.55              |
| 1:B:18:LYS:HE2   | 1:B:50:PHE:CD1   | 2.41                     | 0.55              |
| 1:A:82:MET:SD    | 1:B:46:ILE:CD1   | 2.94                     | 0.55              |
| 1:A:175:THR:O    | 1:A:176:ALA:C    | 2.47                     | 0.55              |
| 1:A:239:GLU:O    | 1:A:242:ASP:HB2  | 2.05                     | 0.55              |
| 1:B:159:LYS:HE2  | 3:B:633:HOH:O    | 2.07                     | 0.55              |
| 1:A:213:THR:OG1  | 1:A:216:ASN:HB2  | 2.06                     | 0.55              |
| 1:A:49:ASP:HB2   | 1:A:86:ILE:CG1   | 2.37                     | 0.54              |
| 1:B:191:TRP:CD1  | 1:B:195:HIS:CE1  | 2.95                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:46:ILE:CD1   | 1:A:47:TYR:N     | 2.70                     | 0.54              |
| 1:A:98:ARG:HA    | 1:A:102:PHE:HB2  | 1.89                     | 0.54              |
| 1:A:240:PHE:CE2  | 1:A:244:ILE:HD11 | 2.42                     | 0.54              |
| 1:B:5:LYS:HE3    | 1:B:36:ASP:C     | 2.33                     | 0.54              |
| 1:B:142:VAL:HG12 | 1:B:143:VAL:N    | 2.22                     | 0.54              |
| 1:A:131:LEU:O    | 1:A:135:GLU:HB2  | 2.08                     | 0.54              |
| 1:A:218:LYS:HD2  | 1:A:218:LYS:C    | 2.33                     | 0.54              |
| 1:A:139:THR:O    | 1:A:143:VAL:HB   | 2.08                     | 0.53              |
| 1:B:16:GLY:HA3   | 1:B:21:LEU:HD13  | 1.90                     | 0.53              |
| 1:B:4:ARG:HD3    | 1:B:202:GLN:O    | 2.08                     | 0.53              |
| 1:B:69:VAL:CG2   | 1:B:70:PRO:CD    | 2.80                     | 0.53              |
| 1:A:89:ALA:HA    | 1:A:121:LEU:HD12 | 1.91                     | 0.53              |
| 1:A:129:GLU:OE2  | 1:A:168:TRP:NE1  | 2.40                     | 0.53              |
| 1:A:219:GLU:HG2  | 1:A:220:LEU:N    | 2.22                     | 0.53              |
| 1:B:14:MET:O     | 1:B:14:MET:HG2   | 2.09                     | 0.53              |
| 1:B:149:ALA:O    | 1:B:153:ASN:ND2  | 2.41                     | 0.53              |
| 1:A:31:ALA:HB3   | 1:A:33:LEU:HD21  | 1.91                     | 0.53              |
| 1:A:187:LYS:O    | 1:A:191:TRP:N    | 2.42                     | 0.52              |
| 1:B:171:GLY:N    | 3:B:624:HOH:O    | 2.42                     | 0.52              |
| 1:A:140:GLU:HG2  | 1:A:144:PHE:CE2  | 2.44                     | 0.52              |
| 1:A:240:PHE:HA   | 1:A:243:ILE:HD12 | 1.90                     | 0.52              |
| 1:A:169:ALA:O    | 1:A:170:ILE:C    | 2.53                     | 0.52              |
| 1:A:4:ARG:HD3    | 1:A:202:GLN:O    | 2.10                     | 0.52              |
| 1:B:128:GLY:HA3  | 1:B:165:GLU:O    | 2.09                     | 0.52              |
| 1:A:246:ALA:O    | 1:A:247:LYS:C    | 2.51                     | 0.52              |
| 1:B:50:PHE:HE1   | 1:B:54:LYS:HZ2   | 1.58                     | 0.51              |
| 1:B:33:LEU:HA    | 1:B:245:ASN:HD22 | 1.75                     | 0.51              |
| 1:B:2:ALA:CB     | 1:B:3:PRO:CD     | 2.86                     | 0.51              |
| 1:A:108:LEU:HD22 | 1:A:108:LEU:O    | 2.12                     | 0.50              |
| 1:A:167:VAL:C    | 1:A:169:ALA:H    | 2.19                     | 0.50              |
| 1:B:94:GLY:C     | 1:B:126:CYS:HB2  | 2.37                     | 0.50              |
| 1:A:170:ILE:CD1  | 1:A:171:GLY:N    | 2.69                     | 0.50              |
| 1:B:129:GLU:OE1  | 1:B:129:GLU:N    | 2.44                     | 0.50              |
| 1:B:165:GLU:O    | 1:B:167:VAL:HG23 | 2.11                     | 0.50              |
| 1:B:12:TRP:O     | 1:B:15:ASN:HB2   | 2.12                     | 0.50              |
| 1:A:70:PRO:HA    | 1:A:79:SER:HG    | 1.76                     | 0.49              |
| 1:B:178:PRO:HD2  | 1:B:179:GLN:CD   | 2.35                     | 0.49              |
| 1:A:18:LYS:NZ    | 1:B:49:ASP:OD1   | 2.45                     | 0.49              |
| 1:A:127:ILE:HG22 | 1:A:146:GLN:HB3  | 1.93                     | 0.49              |
| 1:A:50:PHE:O     | 1:A:54:LYS:HG2   | 2.13                     | 0.49              |
| 1:B:24:LEU:O     | 1:B:25:ILE:C     | 2.54                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:79:SER:HB3   | 1:A:82:MET:HG3   | 1.94                     | 0.49              |
| 1:A:124:ILE:O    | 1:A:124:ILE:HG13 | 2.12                     | 0.49              |
| 1:B:11:ASN:OD1   | 1:B:11:ASN:C     | 2.54                     | 0.49              |
| 1:B:46:ILE:HD12  | 1:B:47:TYR:CE2   | 2.47                     | 0.49              |
| 1:A:189:ARG:NE   | 1:A:225:ASP:OD1  | 2.45                     | 0.48              |
| 1:B:79:SER:HB2   | 1:B:80:PRO:HD2   | 1.96                     | 0.48              |
| 1:A:97:GLU:O     | 1:A:101:VAL:HB   | 2.13                     | 0.48              |
| 1:B:5:LYS:NZ     | 1:B:35:ALA:O     | 2.43                     | 0.48              |
| 1:A:104:GLU:HG2  | 1:A:108:LEU:HD12 | 1.95                     | 0.48              |
| 1:A:212:VAL:HG21 | 1:A:229:PHE:CD2  | 2.49                     | 0.48              |
| 1:B:80:PRO:HA    | 1:B:83:ILE:HD12  | 1.96                     | 0.48              |
| 1:B:237:LYS:HB3  | 1:B:238:PRO:CD   | 2.43                     | 0.48              |
| 1:B:246:ALA:O    | 1:B:248:HIS:N    | 2.46                     | 0.48              |
| 1:A:168:TRP:CZ3  | 1:A:169:ALA:HB2  | 2.49                     | 0.48              |
| 1:B:192:LEU:HD22 | 1:B:200:VAL:HG11 | 1.94                     | 0.48              |
| 1:B:37:THR:HG22  | 1:B:38:GLU:N     | 2.29                     | 0.48              |
| 1:B:69:VAL:O     | 1:B:79:SER:HB2   | 2.13                     | 0.48              |
| 1:A:148:LYS:HB2  | 1:A:191:TRP:CZ2  | 2.49                     | 0.47              |
| 1:A:230:LEU:HD12 | 1:A:230:LEU:HA   | 1.54                     | 0.47              |
| 1:B:7:PHE:O      | 1:B:228:GLY:CA   | 2.62                     | 0.47              |
| 1:A:45:SER:OG    | 1:B:78:ILE:CD1   | 2.62                     | 0.47              |
| 1:A:66:CYS:HB3   | 1:A:83:ILE:HD11  | 1.95                     | 0.47              |
| 1:B:179:GLN:O    | 1:B:183:GLU:HB2  | 2.13                     | 0.47              |
| 1:A:7:PHE:O      | 1:A:228:GLY:HA3  | 2.15                     | 0.47              |
| 1:A:46:ILE:CD1   | 1:A:47:TYR:H     | 2.19                     | 0.47              |
| 1:B:50:PHE:HE1   | 1:B:54:LYS:NZ    | 2.13                     | 0.47              |
| 1:B:64:GLN:O     | 1:B:65:ASN:HB2   | 2.15                     | 0.47              |
| 1:A:6:PHE:CE1    | 1:A:228:GLY:HA2  | 2.50                     | 0.47              |
| 1:A:174:LYS:N    | 1:A:174:LYS:CD   | 2.78                     | 0.47              |
| 1:B:130:LYS:HE3  | 1:B:133:GLU:OE2  | 2.15                     | 0.47              |
| 1:A:93:LEU:O     | 1:A:125:ALA:HA   | 2.14                     | 0.46              |
| 1:A:35:ALA:C     | 1:A:37:THR:H     | 2.21                     | 0.46              |
| 1:B:50:PHE:CE1   | 1:B:54:LYS:HD3   | 2.50                     | 0.46              |
| 1:B:56:ASP:HB3   | 1:B:59:ILE:HD12  | 1.96                     | 0.46              |
| 1:B:198:ASP:O    | 1:B:202:GLN:HB2  | 2.15                     | 0.46              |
| 1:B:55:LEU:HG    | 1:B:59:ILE:CG2   | 2.44                     | 0.46              |
| 1:A:16:GLY:HA3   | 1:A:21:LEU:HD13  | 1.97                     | 0.46              |
| 1:A:127:ILE:HD13 | 1:A:127:ILE:H    | 1.81                     | 0.46              |
| 1:B:177:THR:CB   | 1:B:179:GLN:HE21 | 2.27                     | 0.46              |
| 1:B:39:VAL:C     | 1:B:40:VAL:HG23  | 2.40                     | 0.46              |
| 1:A:28:LEU:HA    | 1:A:28:LEU:HD13  | 1.53                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:79:SER:CB    | 1:A:82:MET:HG3   | 2.46                     | 0.46              |
| 1:A:188:LEU:HD23 | 1:A:188:LEU:HA   | 1.76                     | 0.46              |
| 1:A:4:ARG:NH2    | 1:A:227:ASP:OD1  | 2.43                     | 0.45              |
| 1:A:4:ARG:HD3    | 1:A:4:ARG:HH11   | 1.40                     | 0.45              |
| 1:B:167:VAL:HA   | 1:B:170:ILE:HG12 | 1.98                     | 0.45              |
| 1:A:31:ALA:CB    | 1:A:33:LEU:HD21  | 2.47                     | 0.45              |
| 1:A:11:ASN:C     | 1:A:11:ASN:OD1   | 2.59                     | 0.45              |
| 1:B:238:PRO:C    | 1:B:240:PHE:N    | 2.74                     | 0.45              |
| 1:A:174:LYS:HB3  | 1:A:175:THR:H    | 1.06                     | 0.45              |
| 1:A:25:ILE:HG23  | 1:A:55:LEU:HD23  | 1.98                     | 0.45              |
| 1:A:45:SER:OG    | 1:B:78:ILE:HD13  | 2.17                     | 0.45              |
| 1:A:114:ALA:HB2  | 1:A:153:ASN:HB3  | 1.99                     | 0.44              |
| 1:A:38:GLU:OE1   | 1:A:205:ARG:NH1  | 2.41                     | 0.44              |
| 1:B:50:PHE:CE1   | 1:B:54:LYS:NZ    | 2.85                     | 0.44              |
| 1:B:69:VAL:O     | 1:B:79:SER:CB    | 2.65                     | 0.44              |
| 1:B:129:GLU:CD   | 1:B:139:THR:HG23 | 2.42                     | 0.44              |
| 1:A:216:ASN:O    | 1:A:219:GLU:HG2  | 2.18                     | 0.44              |
| 1:B:97:GLU:O     | 1:B:101:VAL:N    | 2.44                     | 0.44              |
| 1:B:48:LEU:HG    | 1:B:86:ILE:HD11  | 1.98                     | 0.44              |
| 1:B:90:TRP:HA    | 1:B:122:GLY:O    | 2.18                     | 0.44              |
| 1:B:237:LYS:CB   | 1:B:238:PRO:HD2  | 2.47                     | 0.44              |
| 1:A:4:ARG:HG2    | 1:A:203:SER:O    | 2.18                     | 0.44              |
| 1:A:51:ALA:O     | 1:A:55:LEU:HB2   | 2.18                     | 0.44              |
| 1:B:39:VAL:C     | 1:B:40:VAL:CG2   | 2.91                     | 0.44              |
| 1:A:5:LYS:HG3    | 1:A:36:ASP:O     | 2.17                     | 0.44              |
| 1:A:193:LYS:HZ2  | 1:A:193:LYS:HG3  | 1.58                     | 0.44              |
| 1:A:79:SER:O     | 1:A:82:MET:N     | 2.50                     | 0.43              |
| 1:A:192:LEU:O    | 1:A:196:VAL:N    | 2.51                     | 0.43              |
| 1:B:32:LYS:O     | 1:B:32:LYS:CG    | 2.63                     | 0.43              |
| 1:A:91:VAL:HG22  | 1:A:92:ILE:O     | 2.19                     | 0.43              |
| 1:A:212:VAL:HG21 | 1:A:229:PHE:HD2  | 1.82                     | 0.43              |
| 1:B:117:LEU:HD12 | 1:B:117:LEU:HA   | 1.80                     | 0.43              |
| 1:A:99:ARG:NH1   | 1:A:106:ASP:OD1  | 2.48                     | 0.43              |
| 1:A:131:LEU:HD21 | 1:A:174:LYS:NZ   | 2.34                     | 0.43              |
| 1:A:196:VAL:HG11 | 1:A:200:VAL:HG21 | 2.01                     | 0.43              |
| 1:A:124:ILE:HA   | 1:A:161:VAL:O    | 2.19                     | 0.43              |
| 1:B:128:GLY:HA2  | 1:B:164:TYR:CE1  | 2.54                     | 0.43              |
| 1:B:247:LYS:HA   | 1:B:247:LYS:HD2  | 1.39                     | 0.43              |
| 1:A:211:SER:O    | 1:A:216:ASN:ND2  | 2.52                     | 0.43              |
| 1:B:69:VAL:HA    | 1:B:70:PRO:HD3   | 1.66                     | 0.43              |
| 1:B:177:THR:HB   | 1:B:178:PRO:CD   | 2.48                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:192:LEU:O    | 1:A:196:VAL:HB   | 2.19                     | 0.42              |
| 1:B:146:GLN:O    | 1:B:150:ILE:HG13 | 2.19                     | 0.42              |
| 1:B:190:GLY:O    | 1:B:191:TRP:C    | 2.62                     | 0.42              |
| 1:A:148:LYS:O    | 1:A:149:ALA:C    | 2.62                     | 0.42              |
| 1:B:55:LEU:HD13  | 1:B:55:LEU:HA    | 1.59                     | 0.42              |
| 1:B:213:THR:HA   | 1:B:243:ILE:HD11 | 2.01                     | 0.42              |
| 1:A:46:ILE:HD13  | 1:A:47:TYR:CG    | 2.55                     | 0.42              |
| 1:B:179:GLN:NE2  | 1:B:179:GLN:H    | 2.18                     | 0.42              |
| 1:B:79:SER:O     | 1:B:82:MET:N     | 2.52                     | 0.41              |
| 1:B:107:GLU:HG3  | 1:B:111:GLN:NE2  | 2.28                     | 0.41              |
| 1:A:183:GLU:O    | 1:A:187:LYS:HG3  | 2.20                     | 0.41              |
| 1:B:151:ALA:C    | 1:B:153:ASN:H    | 2.29                     | 0.41              |
| 1:A:107:GLU:O    | 1:A:111:GLN:NE2  | 2.52                     | 0.41              |
| 1:A:193:LYS:HD2  | 1:A:193:LYS:C    | 2.46                     | 0.41              |
| 1:A:217:CYS:O    | 1:A:218:LYS:C    | 2.64                     | 0.41              |
| 1:A:218:LYS:HD2  | 1:A:219:GLU:CA   | 2.50                     | 0.41              |
| 1:B:166:PRO:O    | 1:B:170:ILE:HD13 | 2.21                     | 0.41              |
| 1:A:239:GLU:O    | 1:A:243:ILE:HD12 | 2.20                     | 0.41              |
| 1:B:40:VAL:HA    | 1:B:60:GLY:O     | 2.21                     | 0.41              |
| 1:A:82:MET:O     | 1:A:83:ILE:C     | 2.61                     | 0.41              |
| 1:B:14:MET:O     | 1:B:14:MET:CG    | 2.67                     | 0.40              |
| 1:A:46:ILE:CD1   | 1:A:46:ILE:H     | 2.34                     | 0.40              |
| 1:B:230:LEU:HD12 | 1:B:230:LEU:HA   | 1.93                     | 0.40              |
| 1:A:64:GLN:O     | 1:A:65:ASN:CB    | 2.66                     | 0.40              |
| 1:A:69:VAL:O     | 1:B:14:MET:HE3   | 2.21                     | 0.40              |
| 1:A:72:GLY:N     | 1:B:14:MET:O     | 2.51                     | 0.40              |
| 1:B:48:LEU:O     | 1:B:51:ALA:HB3   | 2.21                     | 0.40              |
| 1:A:66:CYS:HB3   | 1:A:83:ILE:CD1   | 2.51                     | 0.40              |
| 1:A:243:ILE:O    | 1:A:244:ILE:C    | 2.64                     | 0.40              |
| 1:B:195:HIS:ND1  | 1:B:195:HIS:N    | 2.69                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|---------|----------|-------------|---|
| 1   | A     | 245/247 (99%) | 219 (89%) | 18 (7%) | 8 (3%)   | 3           | 4 |
| 1   | B     | 245/247 (99%) | 221 (90%) | 18 (7%) | 6 (2%)   | 4           | 8 |
| All | All   | 490/494 (99%) | 440 (90%) | 36 (7%) | 14 (3%)  | 3           | 5 |

All (14) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 170 | ILE  |
| 1   | B     | 247 | LYS  |
| 1   | A     | 36  | ASP  |
| 1   | A     | 247 | LYS  |
| 1   | B     | 152 | ASP  |
| 1   | A     | 168 | TRP  |
| 1   | A     | 172 | THR  |
| 1   | A     | 246 | ALA  |
| 1   | B     | 171 | GLY  |
| 1   | A     | 4   | ARG  |
| 1   | A     | 65  | ASN  |
| 1   | B     | 68  | LYS  |
| 1   | B     | 73  | ALA  |
| 1   | B     | 138 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |   |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1   | A     | 192/192 (100%) | 147 (77%) | 45 (23%) | 1           | 1 |
| 1   | B     | 192/192 (100%) | 148 (77%) | 44 (23%) | 1           | 1 |
| All | All   | 384/384 (100%) | 295 (77%) | 89 (23%) | 1           | 1 |

All (89) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | SER  |
| 1   | A     | 21  | LEU  |
| 1   | A     | 24  | LEU  |
| 1   | A     | 28  | LEU  |
| 1   | A     | 33  | LEU  |
| 1   | A     | 46  | ILE  |
| 1   | A     | 58  | LYS  |
| 1   | A     | 59  | ILE  |
| 1   | A     | 69  | VAL  |
| 1   | A     | 71  | LYS  |
| 1   | A     | 78  | ILE  |
| 1   | A     | 79  | SER  |
| 1   | A     | 80  | PRO  |
| 1   | A     | 86  | ILE  |
| 1   | A     | 91  | VAL  |
| 1   | A     | 92  | ILE  |
| 1   | A     | 107 | GLU  |
| 1   | A     | 108 | LEU  |
| 1   | A     | 111 | GLN  |
| 1   | A     | 124 | ILE  |
| 1   | A     | 127 | ILE  |
| 1   | A     | 131 | LEU  |
| 1   | A     | 138 | ILE  |
| 1   | A     | 141 | LYS  |
| 1   | A     | 143 | VAL  |
| 1   | A     | 148 | LYS  |
| 1   | A     | 155 | LYS  |
| 1   | A     | 165 | GLU  |
| 1   | A     | 170 | ILE  |
| 1   | A     | 175 | THR  |
| 1   | A     | 179 | GLN  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 183 | GLU  |
| 1   | A     | 189 | ARG  |
| 1   | A     | 193 | LYS  |
| 1   | A     | 198 | ASP  |
| 1   | A     | 200 | VAL  |
| 1   | A     | 203 | SER  |
| 1   | A     | 204 | THR  |
| 1   | A     | 207 | ILE  |
| 1   | A     | 218 | LYS  |
| 1   | A     | 219 | GLU  |
| 1   | A     | 237 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 247 | LYS  |
| 1   | A     | 248 | HIS  |
| 1   | B     | 24  | LEU  |
| 1   | B     | 27  | THR  |
| 1   | B     | 28  | LEU  |
| 1   | B     | 32  | LYS  |
| 1   | B     | 34  | SER  |
| 1   | B     | 36  | ASP  |
| 1   | B     | 39  | VAL  |
| 1   | B     | 46  | ILE  |
| 1   | B     | 54  | LYS  |
| 1   | B     | 55  | LEU  |
| 1   | B     | 68  | LYS  |
| 1   | B     | 69  | VAL  |
| 1   | B     | 77  | GLU  |
| 1   | B     | 78  | ILE  |
| 1   | B     | 84  | LYS  |
| 1   | B     | 86  | ILE  |
| 1   | B     | 98  | ARG  |
| 1   | B     | 107 | GLU  |
| 1   | B     | 108 | LEU  |
| 1   | B     | 111 | GLN  |
| 1   | B     | 117 | LEU  |
| 1   | B     | 127 | ILE  |
| 1   | B     | 131 | LEU  |
| 1   | B     | 135 | GLU  |
| 1   | B     | 138 | ILE  |
| 1   | B     | 140 | GLU  |
| 1   | B     | 141 | LYS  |
| 1   | B     | 142 | VAL  |
| 1   | B     | 148 | LYS  |
| 1   | B     | 166 | PRO  |
| 1   | B     | 170 | ILE  |
| 1   | B     | 179 | GLN  |
| 1   | B     | 192 | LEU  |
| 1   | B     | 194 | THR  |
| 1   | B     | 198 | ASP  |
| 1   | B     | 200 | VAL  |
| 1   | B     | 202 | GLN  |
| 1   | B     | 217 | CYS  |
| 1   | B     | 222 | SER  |
| 1   | B     | 223 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 229 | PHE  |
| 1   | B     | 245 | ASN  |
| 1   | B     | 247 | LYS  |
| 1   | B     | 248 | HIS  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 53  | GLN  |
| 1   | A     | 179 | GLN  |
| 1   | A     | 202 | GLN  |
| 1   | A     | 248 | HIS  |
| 1   | B     | 111 | GLN  |
| 1   | B     | 153 | ASN  |
| 1   | B     | 179 | GLN  |
| 1   | B     | 245 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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 | $\# Z  > 2$ |
| 2   | SO4  | A     | 561 | -    | 4,4,4        | 0.98 | 0           | 6,6,6       | 0.47 | 0           |
| 2   | SO4  | B     | 560 | -    | 4,4,4        | 0.92 | 0           | 6,6,6       | 0.37 | 0           |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 560 | SO4  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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.