



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:20 AM UTC

PDB ID : 1XLB / pdb\_00001xlb  
Title : MECHANISM FOR ALDOSE-KETOSE INTERCONVERSION BY D-XYLOSE ISOMERASE INVOLVING RING OPENING FOLLOWED BY A 1,2-HYDRIDE SHIFT  
Authors : Collyer, C.A.; Henrick, K.; Blow, D.M.  
Deposited on : 1991-10-09  
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

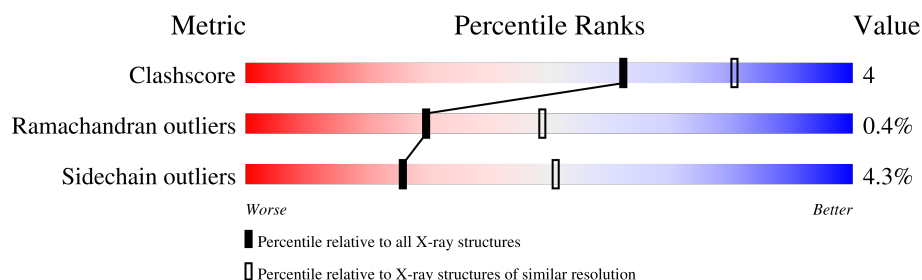
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



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

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 394    | <br>54% 38% 6% • |
| 1   | B     | 394    | <br>50% 42% 7%   |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6640 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 D-XYLOSE ISOMERASE.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 393      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3026  | 1919 | 521 | 577 | 9 |         |         |       |
| 1   | B     | 393      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3026  | 1919 | 521 | 577 | 9 |         |         |       |

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 298      | Total | O   | 0       | 0       |
|     |       |          | 298   | 298 |         |         |
| 3   | B     | 288      | Total | O   | 0       | 0       |
|     |       |          | 288   | 288 |         |         |

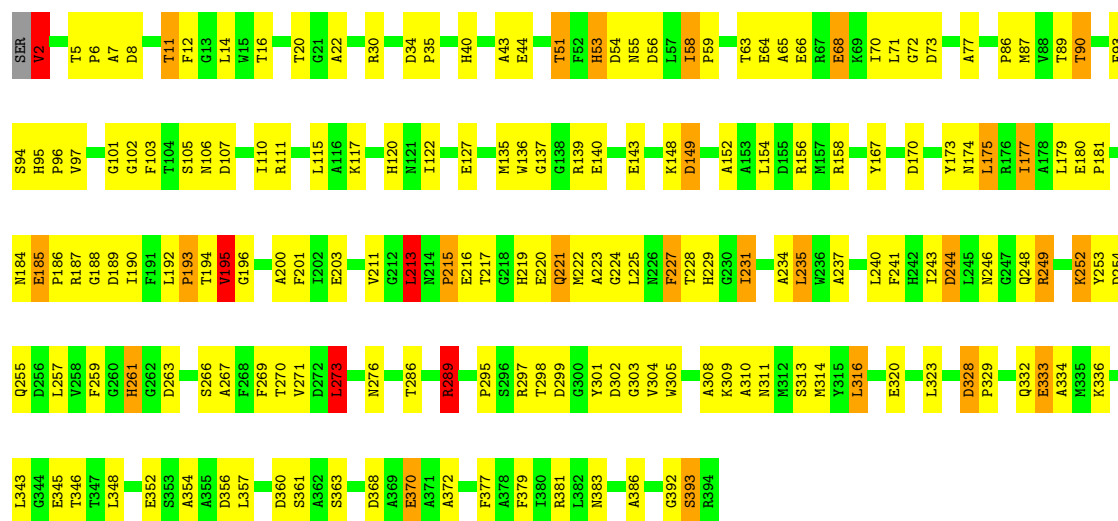
### 3 Residue-property plots

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.

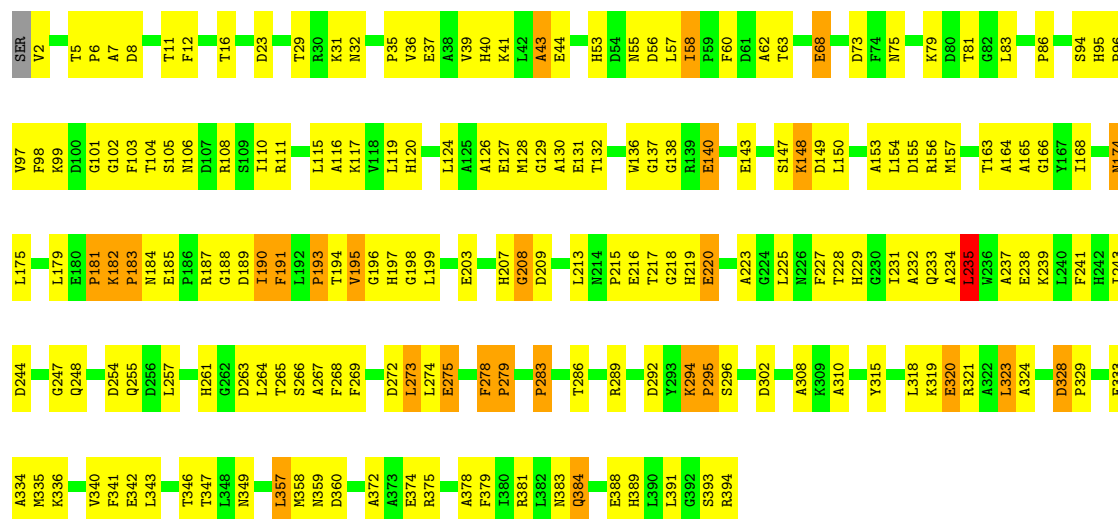
#### • Molecule 1: D-XYLOSE ISOMERASE

Chain A: 



#### • Molecule 1: D-XYLOSE ISOMERASE

Chain B: 



## 4 Data and refinement statistics

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

| Property                                                 | Value                                            | Source    |
|----------------------------------------------------------|--------------------------------------------------|-----------|
| Space group                                              | P 31 2 1                                         | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 105.30Å 105.30Å 153.50Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å)                                           | 10.00 – 2.50                                     | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (10.00-2.50)                     | Depositor |
| $R_{merge}$                                              | (Not available)                                  | Depositor |
| $R_{sym}$                                                | (Not available)                                  | Depositor |
| Refinement program                                       | PROLSQ                                           | Depositor |
| R, $R_{free}$                                            | 0.157 , (Not available)                          | Depositor |
| Estimated twinning fraction                              | No twinning to report.                           | Xtriage   |
| Total number of atoms                                    | 6640                                             | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 25.0                                             | wwPDB-VP  |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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     | 1.32         | 4/3100 (0.1%)  | 2.63        | 272/4201 (6.5%) |
| 1   | B     | 1.32         | 9/3100 (0.3%)  | 2.78        | 304/4201 (7.2%) |
| All | All   | 1.32         | 13/6200 (0.2%) | 2.71        | 576/8402 (6.9%) |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 252 | LYS  | C-O     | 7.30  | 1.31        | 1.24     |
| 1   | A     | 102 | GLY  | CA-C    | 6.59  | 1.55        | 1.51     |
| 1   | B     | 148 | LYS  | N-CA    | -6.50 | 1.37        | 1.45     |
| 1   | B     | 102 | GLY  | CA-C    | 6.33  | 1.55        | 1.51     |
| 1   | B     | 324 | ALA  | N-CA    | 6.12  | 1.53        | 1.46     |
| 1   | A     | 254 | ASP  | CA-CB   | -5.96 | 1.45        | 1.53     |
| 1   | B     | 105 | SER  | N-CA    | -5.96 | 1.38        | 1.46     |
| 1   | B     | 194 | THR  | CA-CB   | 5.63  | 1.62        | 1.53     |
| 1   | B     | 81  | THR  | CA-CB   | 5.44  | 1.62        | 1.53     |
| 1   | B     | 101 | GLY  | C-N     | -5.35 | 1.28        | 1.33     |
| 1   | B     | 324 | ALA  | CA-CB   | -5.32 | 1.45        | 1.53     |
| 1   | B     | 104 | THR  | C-N     | -5.13 | 1.26        | 1.33     |
| 1   | A     | 261 | HIS  | CD2-NE2 | -5.04 | 1.32        | 1.37     |

All (576) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | B     | 187 | ARG  | CD-NE-CZ | 17.86 | 149.41      | 124.40   |
| 1   | B     | 68  | GLU  | CB-CG-CD | 17.83 | 142.91      | 112.60   |
| 1   | B     | 68  | GLU  | CA-CB-CG | 16.39 | 146.88      | 114.10   |
| 1   | A     | 103 | PHE  | CA-CB-CG | 16.33 | 130.13      | 113.80   |
| 1   | A     | 254 | ASP  | CA-CB-CG | 14.27 | 126.87      | 112.60   |
| 1   | B     | 217 | THR  | CA-C-N   | 14.19 | 135.92      | 120.03   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | B     | 217 | THR  | C-N-CA     | 14.19  | 135.92      | 120.03   |
| 1   | A     | 6   | PRO  | CA-C-N     | 13.95  | 140.36      | 120.28   |
| 1   | A     | 6   | PRO  | C-N-CA     | 13.95  | 140.36      | 120.28   |
| 1   | A     | 379 | PHE  | CA-CB-CG   | 12.65  | 126.45      | 113.80   |
| 1   | B     | 384 | GLN  | OE1-CD-NE2 | -12.20 | 110.41      | 122.60   |
| 1   | A     | 196 | GLY  | CA-C-N     | 11.96  | 136.31      | 120.28   |
| 1   | A     | 196 | GLY  | C-N-CA     | 11.96  | 136.31      | 120.28   |
| 1   | A     | 68  | GLU  | CB-CG-CD   | 11.51  | 132.17      | 112.60   |
| 1   | B     | 220 | GLU  | CA-C-N     | 11.47  | 137.74      | 120.31   |
| 1   | B     | 220 | GLU  | C-N-CA     | 11.47  | 137.74      | 120.31   |
| 1   | B     | 195 | VAL  | CA-C-O     | -11.43 | 109.06      | 121.17   |
| 1   | B     | 208 | GLY  | CA-C-N     | 11.28  | 135.83      | 120.38   |
| 1   | B     | 208 | GLY  | C-N-CA     | 11.28  | 135.83      | 120.38   |
| 1   | A     | 249 | ARG  | CD-NE-CZ   | 11.24  | 140.13      | 124.40   |
| 1   | B     | 104 | THR  | CA-C-N     | 11.20  | 137.06      | 121.05   |
| 1   | B     | 104 | THR  | C-N-CA     | 11.20  | 137.06      | 121.05   |
| 1   | B     | 343 | LEU  | CA-C-N     | 10.42  | 133.45      | 120.22   |
| 1   | B     | 343 | LEU  | C-N-CA     | 10.42  | 133.45      | 120.22   |
| 1   | B     | 244 | ASP  | CA-CB-CG   | 10.36  | 122.96      | 112.60   |
| 1   | B     | 241 | PHE  | CA-CB-CG   | 10.27  | 124.07      | 113.80   |
| 1   | B     | 43  | ALA  | CA-C-N     | 10.21  | 134.98      | 120.28   |
| 1   | B     | 43  | ALA  | C-N-CA     | 10.21  | 134.98      | 120.28   |
| 1   | B     | 359 | ASN  | CA-CB-CG   | 9.97   | 122.57      | 112.60   |
| 1   | A     | 383 | ASN  | CA-CB-CG   | -9.79  | 102.81      | 112.60   |
| 1   | A     | 334 | ALA  | CA-C-N     | 9.61   | 133.16      | 120.28   |
| 1   | A     | 334 | ALA  | C-N-CA     | 9.61   | 133.16      | 120.28   |
| 1   | B     | 207 | HIS  | CA-C-N     | 9.56   | 130.74      | 120.03   |
| 1   | B     | 207 | HIS  | C-N-CA     | 9.56   | 130.74      | 120.03   |
| 1   | B     | 197 | HIS  | CB-CG-CD2  | 9.56   | 143.62      | 131.20   |
| 1   | B     | 102 | GLY  | N-CA-C     | -9.55  | 101.52      | 110.21   |
| 1   | B     | 229 | HIS  | CA-C-O     | -9.40  | 109.16      | 119.97   |
| 1   | A     | 190 | ILE  | O-C-N      | 9.40   | 132.72      | 123.14   |
| 1   | A     | 360 | ASP  | CA-CB-CG   | 9.29   | 121.89      | 112.60   |
| 1   | B     | 103 | PHE  | CA-CB-CG   | 9.24   | 123.04      | 113.80   |
| 1   | B     | 358 | MET  | CA-C-N     | 9.22   | 139.56      | 121.58   |
| 1   | B     | 358 | MET  | C-N-CA     | 9.22   | 139.56      | 121.58   |
| 1   | B     | 255 | GLN  | OE1-CD-NE2 | 9.16   | 131.76      | 122.60   |
| 1   | A     | 158 | ARG  | CD-NE-CZ   | 9.13   | 137.19      | 124.40   |
| 1   | B     | 374 | GLU  | CA-CB-CG   | 9.13   | 132.36      | 114.10   |
| 1   | B     | 238 | GLU  | CB-CG-CD   | 9.09   | 128.05      | 112.60   |
| 1   | B     | 198 | GLY  | CA-C-N     | 9.08   | 132.25      | 120.44   |
| 1   | B     | 198 | GLY  | C-N-CA     | 9.08   | 132.25      | 120.44   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 72  | GLY  | O-C-N      | -9.03 | 113.53      | 122.19   |
| 1   | A     | 102 | GLY  | N-CA-C     | -9.01 | 102.01      | 110.21   |
| 1   | A     | 14  | LEU  | CA-C-N     | 8.98  | 133.96      | 120.31   |
| 1   | A     | 14  | LEU  | C-N-CA     | 8.98  | 133.96      | 120.31   |
| 1   | B     | 279 | PRO  | CA-C-N     | 8.93  | 137.28      | 122.54   |
| 1   | B     | 279 | PRO  | C-N-CA     | 8.93  | 137.28      | 122.54   |
| 1   | B     | 286 | THR  | CA-CB-OG1  | -8.90 | 96.24       | 109.60   |
| 1   | B     | 324 | ALA  | CA-C-N     | 8.88  | 131.99      | 120.44   |
| 1   | B     | 324 | ALA  | C-N-CA     | 8.88  | 131.99      | 120.44   |
| 1   | A     | 298 | THR  | CA-C-N     | 8.87  | 134.70      | 122.19   |
| 1   | A     | 298 | THR  | C-N-CA     | 8.87  | 134.70      | 122.19   |
| 1   | A     | 360 | ASP  | CA-C-N     | 8.86  | 132.51      | 120.38   |
| 1   | A     | 360 | ASP  | C-N-CA     | 8.86  | 132.51      | 120.38   |
| 1   | A     | 117 | LYS  | CA-C-N     | 8.85  | 131.88      | 120.56   |
| 1   | A     | 117 | LYS  | C-N-CA     | 8.85  | 131.88      | 120.56   |
| 1   | A     | 228 | THR  | CA-C-O     | -8.82 | 111.10      | 120.63   |
| 1   | A     | 381 | ARG  | CD-NE-CZ   | 8.74  | 136.64      | 124.40   |
| 1   | A     | 96  | PRO  | CA-C-N     | 8.73  | 134.26      | 120.47   |
| 1   | A     | 96  | PRO  | C-N-CA     | 8.73  | 134.26      | 120.47   |
| 1   | A     | 44  | GLU  | CA-CB-CG   | 8.71  | 131.53      | 114.10   |
| 1   | B     | 197 | HIS  | CA-C-N     | 8.71  | 129.60      | 119.94   |
| 1   | B     | 197 | HIS  | C-N-CA     | 8.71  | 129.60      | 119.94   |
| 1   | B     | 36  | VAL  | CA-C-N     | 8.70  | 131.94      | 120.28   |
| 1   | B     | 36  | VAL  | C-N-CA     | 8.70  | 131.94      | 120.28   |
| 1   | A     | 295 | PRO  | CA-C-O     | -8.62 | 112.22      | 121.27   |
| 1   | B     | 372 | ALA  | O-C-N      | -8.57 | 113.03      | 122.12   |
| 1   | B     | 302 | ASP  | CA-C-N     | 8.56  | 129.48      | 119.98   |
| 1   | B     | 302 | ASP  | C-N-CA     | 8.56  | 129.48      | 119.98   |
| 1   | A     | 188 | GLY  | CA-C-O     | -8.53 | 111.62      | 120.66   |
| 1   | B     | 174 | ASN  | N-CA-CB    | 8.44  | 124.54      | 110.53   |
| 1   | B     | 2   | VAL  | CA-C-N     | 8.39  | 133.13      | 122.64   |
| 1   | B     | 2   | VAL  | C-N-CA     | 8.39  | 133.13      | 122.64   |
| 1   | B     | 383 | ASN  | CB-CG-ND2  | 8.37  | 128.96      | 116.40   |
| 1   | B     | 174 | ASN  | OD1-CG-ND2 | 8.33  | 130.93      | 122.60   |
| 1   | A     | 392 | GLY  | CA-C-N     | 8.30  | 136.94      | 122.09   |
| 1   | A     | 392 | GLY  | C-N-CA     | 8.30  | 136.94      | 122.09   |
| 1   | A     | 263 | ASP  | CA-C-N     | 8.28  | 131.58      | 120.65   |
| 1   | A     | 263 | ASP  | C-N-CA     | 8.28  | 131.58      | 120.65   |
| 1   | B     | 23  | ASP  | CB-CA-C    | 8.26  | 126.44      | 110.17   |
| 1   | B     | 181 | PRO  | CB-CA-C    | 8.24  | 121.77      | 110.98   |
| 1   | B     | 188 | GLY  | O-C-N      | -8.22 | 113.33      | 122.28   |
| 1   | A     | 289 | ARG  | CD-NE-CZ   | 8.21  | 135.90      | 124.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 375 | ARG  | NE-CZ-NH2  | -8.21 | 111.81      | 119.20   |
| 1   | B     | 143 | GLU  | N-CA-C     | -8.18 | 103.50      | 113.97   |
| 1   | A     | 305 | TRP  | CA-C-N     | 8.15  | 131.55      | 120.54   |
| 1   | A     | 305 | TRP  | C-N-CA     | 8.15  | 131.55      | 120.54   |
| 1   | B     | 247 | GLY  | CA-C-O     | 8.12  | 130.13      | 121.76   |
| 1   | B     | 53  | HIS  | N-CA-CB    | 8.12  | 123.91      | 110.52   |
| 1   | B     | 269 | PHE  | CA-C-N     | 8.08  | 131.43      | 120.44   |
| 1   | B     | 269 | PHE  | C-N-CA     | 8.08  | 131.43      | 120.44   |
| 1   | B     | 229 | HIS  | CA-CB-CG   | 8.06  | 121.86      | 113.80   |
| 1   | A     | 137 | GLY  | CA-C-N     | 7.93  | 130.06      | 120.14   |
| 1   | A     | 137 | GLY  | C-N-CA     | 7.93  | 130.06      | 120.14   |
| 1   | B     | 193 | PRO  | O-C-N      | -7.93 | 111.56      | 122.27   |
| 1   | A     | 255 | GLN  | OE1-CD-NE2 | 7.91  | 130.51      | 122.60   |
| 1   | A     | 143 | GLU  | CB-CG-CD   | 7.86  | 125.96      | 112.60   |
| 1   | B     | 143 | GLU  | N-CA-CB    | 7.84  | 121.57      | 110.67   |
| 1   | B     | 381 | ARG  | NE-CZ-NH2  | -7.78 | 112.20      | 119.20   |
| 1   | A     | 267 | ALA  | CA-C-N     | 7.72  | 130.96      | 120.54   |
| 1   | A     | 267 | ALA  | C-N-CA     | 7.72  | 130.96      | 120.54   |
| 1   | A     | 269 | PHE  | CA-C-N     | 7.69  | 130.90      | 120.44   |
| 1   | A     | 269 | PHE  | C-N-CA     | 7.69  | 130.90      | 120.44   |
| 1   | A     | 187 | ARG  | CA-CB-CG   | 7.66  | 129.42      | 114.10   |
| 1   | A     | 305 | TRP  | O-C-N      | -7.65 | 113.43      | 122.15   |
| 1   | A     | 332 | GLN  | CA-C-N     | 7.64  | 130.83      | 120.44   |
| 1   | A     | 332 | GLN  | C-N-CA     | 7.64  | 130.83      | 120.44   |
| 1   | A     | 249 | ARG  | CB-CA-C    | 7.63  | 122.20      | 111.74   |
| 1   | B     | 68  | GLU  | N-CA-CB    | 7.63  | 121.08      | 110.01   |
| 1   | B     | 264 | LEU  | N-CA-C     | 7.63  | 119.24      | 111.07   |
| 1   | A     | 105 | SER  | CA-C-N     | 7.63  | 131.91      | 120.31   |
| 1   | A     | 105 | SER  | C-N-CA     | 7.63  | 131.91      | 120.31   |
| 1   | B     | 231 | ILE  | CA-C-N     | 7.60  | 130.79      | 120.54   |
| 1   | B     | 231 | ILE  | C-N-CA     | 7.60  | 130.79      | 120.54   |
| 1   | B     | 12  | PHE  | CA-CB-CG   | 7.58  | 121.38      | 113.80   |
| 1   | A     | 235 | LEU  | CA-C-N     | 7.55  | 130.73      | 120.38   |
| 1   | A     | 235 | LEU  | C-N-CA     | 7.55  | 130.73      | 120.38   |
| 1   | A     | 381 | ARG  | NE-CZ-NH2  | -7.55 | 112.40      | 119.20   |
| 1   | B     | 111 | ARG  | CD-NE-CZ   | 7.53  | 134.94      | 124.40   |
| 1   | B     | 219 | HIS  | CB-CG-CD2  | 7.52  | 140.97      | 131.20   |
| 1   | B     | 56  | ASP  | CA-CB-CG   | 7.50  | 120.10      | 112.60   |
| 1   | B     | 105 | SER  | N-CA-CB    | 7.49  | 121.09      | 109.48   |
| 1   | B     | 320 | GLU  | N-CA-CB    | 7.48  | 120.92      | 110.07   |
| 1   | A     | 224 | GLY  | CA-C-O     | -7.47 | 109.73      | 119.44   |
| 1   | A     | 227 | PHE  | N-CA-CB    | 7.46  | 121.06      | 109.94   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 379 | PHE  | CB-CG-CD2 | 7.44  | 133.34      | 120.70   |
| 1   | A     | 215 | PRO  | O-C-N     | 7.42  | 132.00      | 123.10   |
| 1   | B     | 126 | ALA  | CA-C-N    | 7.42  | 130.54      | 120.38   |
| 1   | B     | 126 | ALA  | C-N-CA    | 7.42  | 130.54      | 120.38   |
| 1   | A     | 381 | ARG  | NE-CZ-NH1 | 7.41  | 128.91      | 121.50   |
| 1   | B     | 103 | PHE  | CA-C-O    | -7.41 | 111.73      | 120.10   |
| 1   | B     | 165 | ALA  | CA-C-N    | 7.40  | 128.20      | 119.98   |
| 1   | B     | 165 | ALA  | C-N-CA    | 7.40  | 128.20      | 119.98   |
| 1   | B     | 60  | PHE  | CA-C-N    | 7.37  | 131.51      | 120.31   |
| 1   | B     | 60  | PHE  | C-N-CA    | 7.37  | 131.51      | 120.31   |
| 1   | A     | 229 | HIS  | CA-C-N    | 7.36  | 128.11      | 119.94   |
| 1   | A     | 229 | HIS  | C-N-CA    | 7.36  | 128.11      | 119.94   |
| 1   | B     | 197 | HIS  | CB-CG-ND1 | -7.35 | 111.67      | 122.70   |
| 1   | B     | 232 | ALA  | CA-C-N    | 7.33  | 130.71      | 120.29   |
| 1   | B     | 232 | ALA  | C-N-CA    | 7.33  | 130.71      | 120.29   |
| 1   | A     | 309 | LYS  | CA-CB-CG  | 7.33  | 128.76      | 114.10   |
| 1   | A     | 72  | GLY  | N-CA-C    | -7.32 | 103.64      | 112.49   |
| 1   | B     | 8   | ASP  | CA-C-N    | 7.31  | 132.50      | 122.34   |
| 1   | B     | 8   | ASP  | C-N-CA    | 7.31  | 132.50      | 122.34   |
| 1   | A     | 297 | ARG  | CA-C-N    | 7.30  | 131.41      | 120.31   |
| 1   | A     | 297 | ARG  | C-N-CA    | 7.30  | 131.41      | 120.31   |
| 1   | A     | 173 | TYR  | CA-C-N    | -7.24 | 112.06      | 122.77   |
| 1   | A     | 173 | TYR  | C-N-CA    | -7.24 | 112.06      | 122.77   |
| 1   | B     | 294 | LYS  | CB-CA-C   | -7.23 | 100.54      | 110.16   |
| 1   | B     | 384 | GLN  | CG-CD-OE1 | 7.22  | 135.23      | 120.80   |
| 1   | B     | 73  | ASP  | CA-CB-CG  | 7.19  | 119.79      | 112.60   |
| 1   | A     | 180 | GLU  | CA-C-O    | 7.15  | 126.21      | 119.99   |
| 1   | A     | 357 | LEU  | CA-C-O    | -7.14 | 113.32      | 120.82   |
| 1   | B     | 182 | LYS  | CA-C-N    | 7.14  | 126.39      | 118.97   |
| 1   | B     | 182 | LYS  | C-N-CA    | 7.14  | 126.39      | 118.97   |
| 1   | B     | 215 | PRO  | CA-C-O    | -7.14 | 112.96      | 121.67   |
| 1   | B     | 340 | VAL  | CB-CA-C   | 7.14  | 121.11      | 111.97   |
| 1   | B     | 219 | HIS  | CB-CG-ND1 | -7.13 | 112.00      | 122.70   |
| 1   | B     | 267 | ALA  | CA-C-O    | 7.05  | 128.22      | 120.82   |
| 1   | A     | 320 | GLU  | CA-CB-CG  | 7.03  | 128.16      | 114.10   |
| 1   | A     | 152 | ALA  | CA-C-O    | -7.00 | 113.00      | 120.42   |
| 1   | A     | 259 | PHE  | CA-C-N    | 7.00  | 134.72      | 122.05   |
| 1   | A     | 259 | PHE  | C-N-CA    | 7.00  | 134.72      | 122.05   |
| 1   | A     | 7   | ALA  | CA-C-N    | 7.00  | 132.41      | 120.72   |
| 1   | A     | 7   | ALA  | C-N-CA    | 7.00  | 132.41      | 120.72   |
| 1   | B     | 308 | ALA  | CA-C-N    | 6.98  | 129.52      | 120.44   |
| 1   | B     | 308 | ALA  | C-N-CA    | 6.98  | 129.52      | 120.44   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 110 | ILE  | O-C-N     | -6.98 | 115.07      | 121.91   |
| 1   | B     | 265 | THR  | CA-C-N    | 6.97  | 129.62      | 120.28   |
| 1   | B     | 265 | THR  | C-N-CA    | 6.97  | 129.62      | 120.28   |
| 1   | A     | 149 | ASP  | N-CA-C    | -6.96 | 97.21       | 108.41   |
| 1   | B     | 383 | ASN  | CA-C-O    | 6.96  | 127.93      | 120.55   |
| 1   | A     | 180 | GLU  | CA-CB-CG  | 6.95  | 128.00      | 114.10   |
| 1   | A     | 73  | ASP  | N-CA-CB   | 6.92  | 120.05      | 110.01   |
| 1   | B     | 7   | ALA  | CA-C-N    | 6.92  | 130.83      | 120.31   |
| 1   | B     | 7   | ALA  | C-N-CA    | 6.92  | 130.83      | 120.31   |
| 1   | B     | 106 | ASN  | N-CA-CB   | 6.92  | 121.01      | 110.28   |
| 1   | B     | 94  | SER  | N-CA-C    | 6.92  | 122.06      | 112.45   |
| 1   | A     | 305 | TRP  | CB-CA-C   | 6.91  | 122.60      | 110.85   |
| 1   | B     | 130 | ALA  | CA-C-O    | -6.91 | 113.42      | 121.16   |
| 1   | B     | 223 | ALA  | O-C-N     | -6.91 | 114.03      | 122.25   |
| 1   | B     | 310 | ALA  | O-C-N     | -6.90 | 114.92      | 122.09   |
| 1   | A     | 143 | GLU  | CA-C-O    | 6.89  | 126.72      | 119.14   |
| 1   | A     | 219 | HIS  | CB-CG-CD2 | 6.89  | 140.16      | 131.20   |
| 1   | A     | 194 | THR  | CA-CB-CG2 | 6.89  | 122.21      | 110.50   |
| 1   | B     | 149 | ASP  | N-CA-C    | -6.89 | 96.43       | 108.20   |
| 1   | B     | 117 | LYS  | N-CA-C    | -6.88 | 103.71      | 111.07   |
| 1   | A     | 70  | ILE  | CA-C-O    | -6.87 | 114.13      | 121.27   |
| 1   | B     | 196 | GLY  | CA-C-O    | -6.87 | 113.68      | 120.75   |
| 1   | A     | 345 | GLU  | CB-CG-CD  | 6.86  | 124.27      | 112.60   |
| 1   | A     | 215 | PRO  | CA-C-O    | -6.85 | 113.09      | 121.31   |
| 1   | B     | 266 | SER  | CA-C-N    | 6.84  | 129.34      | 120.44   |
| 1   | B     | 266 | SER  | C-N-CA    | 6.84  | 129.34      | 120.44   |
| 1   | B     | 110 | ILE  | O-C-N     | -6.83 | 114.80      | 121.83   |
| 1   | A     | 40  | HIS  | CA-CB-CG  | -6.81 | 106.99      | 113.80   |
| 1   | B     | 175 | LEU  | O-C-N     | 6.80  | 131.37      | 123.41   |
| 1   | A     | 16  | THR  | CA-CB-OG1 | -6.79 | 99.41       | 109.60   |
| 1   | A     | 54  | ASP  | CA-C-O    | -6.79 | 113.31      | 120.92   |
| 1   | A     | 308 | ALA  | CA-C-N    | 6.79  | 129.93      | 120.29   |
| 1   | A     | 308 | ALA  | C-N-CA    | 6.79  | 129.93      | 120.29   |
| 1   | B     | 203 | GLU  | CA-C-N    | 6.79  | 133.05      | 122.26   |
| 1   | B     | 203 | GLU  | C-N-CA    | 6.79  | 133.05      | 122.26   |
| 1   | B     | 346 | THR  | CA-CB-OG1 | -6.79 | 99.42       | 109.60   |
| 1   | B     | 263 | ASP  | CB-CA-C   | 6.78  | 122.59      | 111.41   |
| 1   | A     | 30  | ARG  | NE-CZ-NH2 | -6.77 | 113.11      | 119.20   |
| 1   | A     | 93  | PHE  | CA-C-O    | -6.77 | 110.01      | 118.54   |
| 1   | A     | 223 | ALA  | N-CA-CB   | 6.76  | 120.50      | 110.49   |
| 1   | B     | 96  | PRO  | CA-C-N    | 6.76  | 131.14      | 120.47   |
| 1   | B     | 96  | PRO  | C-N-CA    | 6.76  | 131.14      | 120.47   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 336 | LYS  | CA-C-N    | 6.74  | 129.61      | 120.38   |
| 1   | A     | 336 | LYS  | C-N-CA    | 6.74  | 129.61      | 120.38   |
| 1   | B     | 56  | ASP  | N-CA-C    | -6.74 | 103.40      | 111.69   |
| 1   | B     | 257 | LEU  | O-C-N     | 6.73  | 131.18      | 122.23   |
| 1   | A     | 105 | SER  | N-CA-C    | -6.73 | 101.20      | 110.35   |
| 1   | A     | 107 | ASP  | CA-C-O    | 6.70  | 128.26      | 120.49   |
| 1   | B     | 37  | GLU  | CB-CG-CD  | 6.68  | 123.96      | 112.60   |
| 1   | A     | 101 | GLY  | O-C-N     | 6.67  | 130.15      | 123.48   |
| 1   | A     | 174 | ASN  | CA-CB-CG  | 6.67  | 119.27      | 112.60   |
| 1   | A     | 194 | THR  | CA-CB-OG1 | -6.67 | 99.60       | 109.60   |
| 1   | A     | 289 | ARG  | NE-CZ-NH1 | 6.67  | 128.17      | 121.50   |
| 1   | A     | 254 | ASP  | N-CA-CB   | 6.66  | 120.73      | 109.87   |
| 1   | B     | 233 | GLN  | CB-CG-CD  | 6.63  | 123.86      | 112.60   |
| 1   | A     | 96  | PRO  | O-C-N     | -6.62 | 113.37      | 122.24   |
| 1   | B     | 190 | ILE  | CA-C-O    | -6.61 | 113.09      | 121.48   |
| 1   | B     | 106 | ASN  | CB-CG-ND2 | 6.60  | 126.30      | 116.40   |
| 1   | B     | 115 | LEU  | CB-CA-C   | 6.59  | 122.06      | 110.85   |
| 1   | A     | 64  | GLU  | CA-C-N    | 6.56  | 128.97      | 120.44   |
| 1   | A     | 64  | GLU  | C-N-CA    | 6.56  | 128.97      | 120.44   |
| 1   | B     | 223 | ALA  | CA-C-O    | 6.55  | 127.32      | 119.59   |
| 1   | B     | 378 | ALA  | CA-C-N    | 6.55  | 130.26      | 120.31   |
| 1   | B     | 378 | ALA  | C-N-CA    | 6.55  | 130.26      | 120.31   |
| 1   | A     | 148 | LYS  | N-CA-C    | 6.54  | 119.83      | 109.50   |
| 1   | A     | 259 | PHE  | CA-CB-CG  | 6.54  | 120.34      | 113.80   |
| 1   | B     | 150 | LEU  | CA-C-N    | 6.51  | 129.29      | 120.44   |
| 1   | B     | 150 | LEU  | C-N-CA    | 6.51  | 129.29      | 120.44   |
| 1   | B     | 223 | ALA  | CA-C-N    | 6.51  | 133.69      | 120.80   |
| 1   | B     | 223 | ALA  | C-N-CA    | 6.51  | 133.69      | 120.80   |
| 1   | A     | 200 | ALA  | CA-C-N    | 6.50  | 128.99      | 120.28   |
| 1   | A     | 200 | ALA  | C-N-CA    | 6.50  | 128.99      | 120.28   |
| 1   | B     | 108 | ARG  | NE-CZ-NH2 | -6.49 | 113.36      | 119.20   |
| 1   | B     | 379 | PHE  | CA-CB-CG  | 6.48  | 120.28      | 113.80   |
| 1   | B     | 335 | MET  | CA-C-N    | 6.48  | 129.25      | 120.44   |
| 1   | B     | 335 | MET  | C-N-CA    | 6.48  | 129.25      | 120.44   |
| 1   | B     | 56  | ASP  | N-CA-CB   | 6.47  | 119.83      | 110.20   |
| 1   | A     | 8   | ASP  | CA-C-N    | 6.46  | 131.30      | 122.19   |
| 1   | A     | 8   | ASP  | C-N-CA    | 6.46  | 131.30      | 122.19   |
| 1   | A     | 237 | ALA  | CA-C-N    | 6.46  | 132.18      | 122.68   |
| 1   | A     | 237 | ALA  | C-N-CA    | 6.46  | 132.18      | 122.68   |
| 1   | A     | 149 | ASP  | N-CA-CB   | 6.46  | 120.48      | 110.21   |
| 1   | A     | 314 | MET  | N-CA-CB   | 6.45  | 119.62      | 109.82   |
| 1   | A     | 316 | LEU  | CB-CA-C   | 6.43  | 121.79      | 110.85   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 209 | ASP  | CA-CB-CG  | 6.42  | 119.02      | 112.60   |
| 1   | A     | 220 | GLU  | CA-C-N    | 6.42  | 131.44      | 120.72   |
| 1   | A     | 220 | GLU  | C-N-CA    | 6.42  | 131.44      | 120.72   |
| 1   | B     | 44  | GLU  | CA-CB-CG  | 6.41  | 126.91      | 114.10   |
| 1   | B     | 150 | LEU  | CB-CA-C   | 6.39  | 121.55      | 110.68   |
| 1   | A     | 328 | ASP  | CA-C-O    | 6.38  | 126.18      | 119.80   |
| 1   | B     | 147 | SER  | CA-C-N    | 6.38  | 132.61      | 122.59   |
| 1   | B     | 147 | SER  | C-N-CA    | 6.38  | 132.61      | 122.59   |
| 1   | A     | 111 | ARG  | CA-C-N    | 6.37  | 129.10      | 120.44   |
| 1   | A     | 111 | ARG  | C-N-CA    | 6.37  | 129.10      | 120.44   |
| 1   | A     | 149 | ASP  | CA-CB-CG  | 6.37  | 118.97      | 112.60   |
| 1   | A     | 213 | LEU  | N-CA-C    | 6.36  | 120.00      | 110.14   |
| 1   | A     | 56  | ASP  | N-CA-CB   | 6.36  | 119.56      | 110.16   |
| 1   | B     | 168 | ILE  | CA-C-O    | 6.36  | 128.10      | 121.05   |
| 1   | B     | 213 | LEU  | CA-CB-CG  | 6.32  | 138.41      | 116.30   |
| 1   | A     | 115 | LEU  | CA-C-N    | 6.29  | 128.61      | 120.44   |
| 1   | A     | 115 | LEU  | C-N-CA    | 6.29  | 128.61      | 120.44   |
| 1   | A     | 196 | GLY  | O-C-N     | -6.27 | 115.93      | 122.13   |
| 1   | B     | 106 | ASN  | CA-C-N    | 6.25  | 130.24      | 121.24   |
| 1   | B     | 106 | ASN  | C-N-CA    | 6.25  | 130.24      | 121.24   |
| 1   | B     | 102 | GLY  | O-C-N     | 6.25  | 125.35      | 121.85   |
| 1   | A     | 56  | ASP  | CA-CB-CG  | 6.24  | 118.84      | 112.60   |
| 1   | A     | 253 | TYR  | CA-C-N    | -6.23 | 112.68      | 121.72   |
| 1   | A     | 253 | TYR  | C-N-CA    | -6.23 | 112.68      | 121.72   |
| 1   | B     | 120 | HIS  | CA-C-N    | 6.23  | 129.77      | 120.31   |
| 1   | B     | 120 | HIS  | C-N-CA    | 6.23  | 129.77      | 120.31   |
| 1   | A     | 308 | ALA  | N-CA-C    | -6.21 | 104.51      | 111.28   |
| 1   | A     | 203 | GLU  | CA-C-N    | 6.21  | 132.11      | 122.49   |
| 1   | A     | 203 | GLU  | C-N-CA    | 6.21  | 132.11      | 122.49   |
| 1   | A     | 348 | LEU  | N-CA-CB   | -6.20 | 101.57      | 110.44   |
| 1   | B     | 127 | GLU  | CA-CB-CG  | 6.20  | 126.50      | 114.10   |
| 1   | A     | 228 | THR  | CA-C-N    | 6.20  | 129.09      | 120.29   |
| 1   | A     | 228 | THR  | C-N-CA    | 6.20  | 129.09      | 120.29   |
| 1   | A     | 43  | ALA  | CB-CA-C   | 6.20  | 121.38      | 110.85   |
| 1   | A     | 56  | ASP  | N-CA-C    | -6.20 | 104.61      | 111.36   |
| 1   | B     | 98  | PHE  | CA-C-N    | 6.19  | 129.20      | 120.28   |
| 1   | B     | 98  | PHE  | C-N-CA    | 6.19  | 129.20      | 120.28   |
| 1   | B     | 140 | GLU  | CB-CA-C   | -6.18 | 100.61      | 110.81   |
| 1   | B     | 199 | LEU  | CA-C-N    | 6.16  | 128.82      | 120.44   |
| 1   | B     | 199 | LEU  | C-N-CA    | 6.16  | 128.82      | 120.44   |
| 1   | A     | 136 | TRP  | N-CA-CB   | 6.15  | 120.36      | 110.65   |
| 1   | B     | 187 | ARG  | NE-CZ-NH2 | -6.14 | 113.67      | 119.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 102 | GLY  | CA-C-N     | 6.13  | 129.11      | 120.28   |
| 1   | B     | 102 | GLY  | C-N-CA     | 6.13  | 129.11      | 120.28   |
| 1   | A     | 179 | LEU  | CB-CA-C    | 6.12  | 119.62      | 109.53   |
| 1   | A     | 221 | GLN  | CA-C-N     | 6.11  | 130.93      | 120.72   |
| 1   | A     | 221 | GLN  | C-N-CA     | 6.11  | 130.93      | 120.72   |
| 1   | B     | 32  | ASN  | CA-CB-CG   | -6.11 | 106.49      | 112.60   |
| 1   | B     | 129 | GLY  | CA-C-N     | 6.08  | 129.50      | 120.87   |
| 1   | B     | 129 | GLY  | C-N-CA     | 6.08  | 129.50      | 120.87   |
| 1   | B     | 29  | THR  | CA-CB-OG1  | -6.06 | 100.50      | 109.60   |
| 1   | A     | 310 | ALA  | CA-C-O     | -6.06 | 114.13      | 120.55   |
| 1   | A     | 187 | ARG  | N-CA-C     | -6.05 | 101.56      | 110.52   |
| 1   | B     | 40  | HIS  | CA-CB-CG   | -6.05 | 107.75      | 113.80   |
| 1   | B     | 117 | LYS  | N-CA-CB    | 6.03  | 118.75      | 110.01   |
| 1   | B     | 117 | LYS  | CA-C-N     | 6.03  | 128.15      | 120.56   |
| 1   | B     | 117 | LYS  | C-N-CA     | 6.03  | 128.15      | 120.56   |
| 1   | A     | 53  | HIS  | N-CA-CB    | 6.02  | 120.45      | 110.63   |
| 1   | B     | 261 | HIS  | CA-CB-CG   | 6.01  | 119.81      | 113.80   |
| 1   | A     | 225 | LEU  | CB-CA-C    | 6.01  | 121.72      | 109.76   |
| 1   | A     | 139 | ARG  | NE-CZ-NH2  | 6.00  | 124.60      | 119.20   |
| 1   | B     | 388 | GLU  | O-C-N      | -6.00 | 115.76      | 122.12   |
| 1   | B     | 360 | ASP  | CA-CB-CG   | 6.00  | 118.60      | 112.60   |
| 1   | B     | 267 | ALA  | O-C-N      | -5.99 | 115.90      | 122.07   |
| 1   | B     | 286 | THR  | CA-CB-CG2  | 5.98  | 120.67      | 110.50   |
| 1   | A     | 195 | VAL  | CA-C-N     | 5.95  | 126.71      | 119.99   |
| 1   | A     | 195 | VAL  | C-N-CA     | 5.95  | 126.71      | 119.99   |
| 1   | B     | 203 | GLU  | CG-CD-OE2  | 5.94  | 132.06      | 118.40   |
| 1   | A     | 93  | PHE  | N-CA-C     | 5.94  | 121.39      | 114.62   |
| 1   | B     | 57  | LEU  | N-CA-CB    | -5.92 | 101.01      | 110.19   |
| 1   | B     | 389 | HIS  | CA-CB-CG   | -5.92 | 107.88      | 113.80   |
| 1   | A     | 219 | HIS  | CB-CG-ND1  | -5.92 | 113.82      | 122.70   |
| 1   | B     | 116 | ALA  | CA-C-N     | 5.92  | 128.13      | 120.44   |
| 1   | B     | 116 | ALA  | C-N-CA     | 5.92  | 128.13      | 120.44   |
| 1   | A     | 2   | VAL  | CB-CA-C    | 5.91  | 122.62      | 111.40   |
| 1   | B     | 233 | GLN  | OE1-CD-NE2 | -5.89 | 116.71      | 122.60   |
| 1   | A     | 271 | VAL  | CA-C-N     | 5.89  | 128.49      | 120.54   |
| 1   | A     | 271 | VAL  | C-N-CA     | 5.89  | 128.49      | 120.54   |
| 1   | A     | 234 | ALA  | CA-C-N     | 5.89  | 128.09      | 120.44   |
| 1   | A     | 234 | ALA  | C-N-CA     | 5.89  | 128.09      | 120.44   |
| 1   | B     | 349 | ASN  | CB-CG-ND2  | 5.88  | 125.23      | 116.40   |
| 1   | B     | 148 | LYS  | N-CA-C     | 5.88  | 118.63      | 109.52   |
| 1   | A     | 356 | ASP  | CA-CB-CG   | 5.87  | 118.47      | 112.60   |
| 1   | A     | 174 | ASN  | CB-CA-C    | 5.86  | 121.47      | 111.68   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 22  | ALA  | CB-CA-C    | 5.86  | 119.67      | 109.65   |
| 1   | A     | 189 | ASP  | CA-C-O     | -5.85 | 113.08      | 120.28   |
| 1   | B     | 216 | GLU  | CB-CG-CD   | 5.85  | 122.55      | 112.60   |
| 1   | B     | 391 | LEU  | CA-C-N     | 5.85  | 132.87      | 121.41   |
| 1   | B     | 391 | LEU  | C-N-CA     | 5.85  | 132.87      | 121.41   |
| 1   | A     | 370 | GLU  | CB-CG-CD   | 5.84  | 122.53      | 112.60   |
| 1   | B     | 247 | GLY  | O-C-N      | -5.83 | 118.12      | 123.42   |
| 1   | A     | 261 | HIS  | N-CA-CB    | 5.81  | 119.09      | 110.49   |
| 1   | B     | 119 | LEU  | CB-CA-C    | 5.81  | 120.01      | 110.88   |
| 1   | B     | 120 | HIS  | CA-CB-CG   | -5.80 | 108.00      | 113.80   |
| 1   | A     | 16  | THR  | OG1-CB-CG2 | 5.79  | 120.89      | 109.30   |
| 1   | A     | 252 | LYS  | CG-CD-CE   | 5.78  | 124.60      | 111.30   |
| 1   | A     | 257 | LEU  | N-CA-C     | -5.78 | 103.08      | 110.53   |
| 1   | A     | 12  | PHE  | CA-C-N     | -5.77 | 115.33      | 121.45   |
| 1   | A     | 12  | PHE  | C-N-CA     | -5.77 | 115.33      | 121.45   |
| 1   | A     | 301 | TYR  | N-CA-C     | 5.77  | 118.34      | 111.71   |
| 1   | A     | 377 | PHE  | CA-CB-CG   | 5.76  | 119.56      | 113.80   |
| 1   | A     | 261 | HIS  | CA-C-N     | 5.76  | 132.70      | 121.41   |
| 1   | A     | 261 | HIS  | C-N-CA     | 5.76  | 132.70      | 121.41   |
| 1   | B     | 342 | GLU  | CG-CD-OE2  | -5.76 | 105.15      | 118.40   |
| 1   | B     | 328 | ASP  | CA-C-N     | 5.76  | 125.29      | 119.19   |
| 1   | B     | 328 | ASP  | C-N-CA     | 5.76  | 125.29      | 119.19   |
| 1   | B     | 163 | THR  | CA-C-O     | -5.76 | 114.77      | 120.70   |
| 1   | A     | 243 | ILE  | CA-C-O     | -5.75 | 114.75      | 120.90   |
| 1   | B     | 243 | ILE  | CA-C-O     | -5.74 | 114.75      | 120.90   |
| 1   | A     | 174 | ASN  | OD1-CG-ND2 | 5.74  | 128.34      | 122.60   |
| 1   | A     | 72  | GLY  | CA-C-O     | 5.73  | 127.32      | 120.90   |
| 1   | A     | 127 | GLU  | CA-C-N     | 5.72  | 132.51      | 121.18   |
| 1   | A     | 127 | GLU  | C-N-CA     | 5.72  | 132.51      | 121.18   |
| 1   | B     | 383 | ASN  | CA-CB-CG   | -5.72 | 106.88      | 112.60   |
| 1   | B     | 318 | LEU  | CA-C-N     | 5.72  | 127.94      | 120.28   |
| 1   | B     | 318 | LEU  | C-N-CA     | 5.72  | 127.94      | 120.28   |
| 1   | A     | 343 | LEU  | CA-C-N     | 5.71  | 130.96      | 120.79   |
| 1   | A     | 343 | LEU  | C-N-CA     | 5.71  | 130.96      | 120.79   |
| 1   | A     | 181 | PRO  | O-C-N      | 5.71  | 130.08      | 123.06   |
| 1   | A     | 386 | ALA  | CA-C-O     | -5.70 | 114.83      | 120.82   |
| 1   | A     | 44  | GLU  | N-CA-CB    | 5.70  | 119.00      | 110.22   |
| 1   | B     | 154 | LEU  | CA-C-O     | -5.70 | 114.51      | 120.55   |
| 1   | A     | 90  | THR  | CA-C-O     | -5.70 | 114.21      | 120.36   |
| 1   | A     | 286 | THR  | CA-C-O     | -5.69 | 112.77      | 119.48   |
| 1   | B     | 227 | PHE  | CA-CB-CG   | 5.69  | 119.49      | 113.80   |
| 1   | A     | 167 | TYR  | CA-C-N     | 5.68  | 127.93      | 120.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 167 | TYR  | C-N-CA     | 5.68  | 127.93      | 120.60   |
| 1   | B     | 254 | ASP  | CA-CB-CG   | 5.68  | 118.28      | 112.60   |
| 1   | B     | 383 | ASN  | CB-CG-OD1  | -5.68 | 109.43      | 120.80   |
| 1   | B     | 63  | THR  | N-CA-C     | -5.68 | 102.89      | 110.55   |
| 1   | B     | 347 | THR  | CA-CB-OG1  | -5.66 | 101.10      | 109.60   |
| 1   | A     | 328 | ASP  | CA-CB-CG   | 5.66  | 118.26      | 112.60   |
| 1   | A     | 143 | GLU  | CA-C-N     | 5.65  | 131.42      | 122.94   |
| 1   | A     | 143 | GLU  | C-N-CA     | 5.65  | 131.42      | 122.94   |
| 1   | A     | 276 | ASN  | CA-C-O     | -5.65 | 112.46      | 119.18   |
| 1   | A     | 370 | GLU  | CA-C-O     | -5.65 | 113.47      | 119.97   |
| 1   | A     | 140 | GLU  | CB-CG-CD   | 5.65  | 122.20      | 112.60   |
| 1   | A     | 289 | ARG  | N-CA-CB    | 5.65  | 119.90      | 110.53   |
| 1   | A     | 273 | LEU  | CA-C-O     | -5.64 | 114.89      | 120.82   |
| 1   | A     | 11  | THR  | O-C-N      | -5.64 | 115.86      | 123.19   |
| 1   | A     | 170 | ASP  | CB-CA-C    | -5.64 | 101.43      | 110.79   |
| 1   | A     | 370 | GLU  | CA-CB-CG   | 5.64  | 125.37      | 114.10   |
| 1   | B     | 148 | LYS  | CB-CA-C    | -5.62 | 98.26       | 109.79   |
| 1   | B     | 295 | PRO  | CA-C-O     | -5.61 | 114.36      | 120.92   |
| 1   | B     | 248 | GLN  | OE1-CD-NE2 | -5.60 | 117.00      | 122.60   |
| 1   | B     | 105 | SER  | N-CA-C     | -5.59 | 102.02      | 110.24   |
| 1   | B     | 164 | ALA  | CA-C-N     | 5.59  | 128.04      | 120.44   |
| 1   | B     | 164 | ALA  | C-N-CA     | 5.59  | 128.04      | 120.44   |
| 1   | B     | 334 | ALA  | CA-C-N     | 5.59  | 127.77      | 120.28   |
| 1   | B     | 334 | ALA  | C-N-CA     | 5.59  | 127.77      | 120.28   |
| 1   | B     | 137 | GLY  | CA-C-N     | 5.58  | 127.12      | 120.14   |
| 1   | B     | 137 | GLY  | C-N-CA     | 5.58  | 127.12      | 120.14   |
| 1   | A     | 6   | PRO  | O-C-N      | -5.58 | 115.42      | 122.17   |
| 1   | A     | 90  | THR  | O-C-N      | 5.58  | 129.94      | 123.30   |
| 1   | A     | 174 | ASN  | CA-C-N     | 5.58  | 131.77      | 122.73   |
| 1   | A     | 174 | ASN  | C-N-CA     | 5.58  | 131.77      | 122.73   |
| 1   | B     | 75  | ASN  | CA-C-N     | 5.58  | 127.69      | 120.44   |
| 1   | B     | 75  | ASN  | C-N-CA     | 5.58  | 127.69      | 120.44   |
| 1   | A     | 352 | GLU  | N-CA-C     | -5.58 | 100.61      | 109.59   |
| 1   | B     | 278 | PHE  | CA-C-N     | 5.57  | 125.94      | 119.47   |
| 1   | B     | 278 | PHE  | C-N-CA     | 5.57  | 125.94      | 119.47   |
| 1   | B     | 189 | ASP  | CA-C-O     | -5.57 | 114.33      | 120.24   |
| 1   | B     | 261 | HIS  | CA-C-O     | -5.57 | 112.54      | 119.28   |
| 1   | A     | 193 | PRO  | N-CA-C     | 5.57  | 121.16      | 113.65   |
| 1   | B     | 191 | PHE  | CA-CB-CG   | 5.55  | 119.35      | 113.80   |
| 1   | B     | 275 | GLU  | CA-C-O     | -5.54 | 114.99      | 120.70   |
| 1   | B     | 31  | LYS  | CA-C-O     | -5.54 | 115.28      | 121.81   |
| 1   | A     | 58  | ILE  | CA-C-O     | 5.52  | 123.44      | 119.25   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 225 | LEU  | O-C-N     | 5.52  | 129.12      | 122.94   |
| 1   | B     | 279 | PRO  | O-C-N     | -5.52 | 115.49      | 122.17   |
| 1   | B     | 215 | PRO  | CA-C-N    | -5.51 | 113.07      | 122.33   |
| 1   | B     | 215 | PRO  | C-N-CA    | -5.51 | 113.07      | 122.33   |
| 1   | B     | 295 | PRO  | O-C-N     | 5.51  | 128.87      | 123.03   |
| 1   | B     | 342 | GLU  | CB-CG-CD  | 5.50  | 121.96      | 112.60   |
| 1   | B     | 155 | ASP  | CA-CB-CG  | 5.50  | 118.10      | 112.60   |
| 1   | B     | 143 | GLU  | O-C-N     | -5.50 | 115.83      | 122.48   |
| 1   | B     | 359 | ASN  | N-CA-CB   | -5.48 | 101.20      | 110.41   |
| 1   | A     | 156 | ARG  | NE-CZ-NH2 | -5.48 | 114.27      | 119.20   |
| 1   | A     | 51  | THR  | CA-CB-CG2 | 5.46  | 119.79      | 110.50   |
| 1   | B     | 254 | ASP  | CB-CA-C   | 5.46  | 121.30      | 110.42   |
| 1   | B     | 220 | GLU  | O-C-N     | -5.46 | 115.84      | 122.22   |
| 1   | B     | 73  | ASP  | CA-C-N    | 5.45  | 127.52      | 120.44   |
| 1   | B     | 73  | ASP  | C-N-CA    | 5.45  | 127.52      | 120.44   |
| 1   | A     | 302 | ASP  | N-CA-C    | -5.45 | 105.34      | 111.28   |
| 1   | B     | 166 | GLY  | CA-C-N    | 5.44  | 128.12      | 120.28   |
| 1   | B     | 166 | GLY  | C-N-CA    | 5.44  | 128.12      | 120.28   |
| 1   | B     | 289 | ARG  | CD-NE-CZ  | 5.44  | 132.02      | 124.40   |
| 1   | B     | 381 | ARG  | NE-CZ-NH1 | 5.44  | 126.94      | 121.50   |
| 1   | A     | 59  | PRO  | CB-CA-C   | 5.43  | 118.18      | 111.23   |
| 1   | A     | 106 | ASN  | N-CA-C    | -5.43 | 105.53      | 111.82   |
| 1   | B     | 181 | PRO  | O-C-N     | -5.43 | 116.39      | 123.06   |
| 1   | A     | 120 | HIS  | CA-CB-CG  | -5.42 | 108.38      | 113.80   |
| 1   | B     | 239 | LYS  | CA-C-O    | -5.41 | 113.44      | 119.34   |
| 1   | A     | 235 | LEU  | CA-C-O    | 5.41  | 126.50      | 120.82   |
| 1   | B     | 156 | ARG  | NE-CZ-NH2 | 5.40  | 124.06      | 119.20   |
| 1   | A     | 393 | SER  | CB-CA-C   | -5.39 | 99.81       | 109.24   |
| 1   | A     | 222 | MET  | CA-C-N    | 5.38  | 131.41      | 122.54   |
| 1   | A     | 222 | MET  | C-N-CA    | 5.38  | 131.41      | 122.54   |
| 1   | A     | 63  | THR  | CA-CB-OG1 | -5.38 | 101.53      | 109.60   |
| 1   | A     | 368 | ASP  | CA-C-N    | 5.37  | 127.48      | 120.28   |
| 1   | A     | 368 | ASP  | C-N-CA    | 5.37  | 127.48      | 120.28   |
| 1   | A     | 215 | PRO  | N-CA-CB   | 5.37  | 108.33      | 103.34   |
| 1   | B     | 111 | ARG  | CG-CD-NE  | 5.37  | 123.82      | 112.00   |
| 1   | A     | 35  | PRO  | CA-C-N    | 5.37  | 127.33      | 120.56   |
| 1   | A     | 35  | PRO  | C-N-CA    | 5.37  | 127.33      | 120.56   |
| 1   | A     | 270 | THR  | CA-CB-CG2 | 5.36  | 119.62      | 110.50   |
| 1   | A     | 43  | ALA  | O-C-N     | -5.36 | 116.05      | 122.15   |
| 1   | B     | 323 | LEU  | CA-C-N    | -5.35 | 113.11      | 120.28   |
| 1   | B     | 323 | LEU  | C-N-CA    | -5.35 | 113.11      | 120.28   |
| 1   | B     | 283 | PRO  | CB-CA-C   | 5.34  | 117.95      | 110.95   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 249 | ARG  | O-C-N     | -5.34 | 114.55      | 122.67   |
| 1   | B     | 190 | ILE  | CA-C-N    | 5.34  | 129.06      | 121.42   |
| 1   | B     | 190 | ILE  | C-N-CA    | 5.34  | 129.06      | 121.42   |
| 1   | A     | 65  | ALA  | N-CA-C    | -5.34 | 105.35      | 111.07   |
| 1   | B     | 101 | GLY  | O-C-N     | 5.34  | 128.42      | 123.35   |
| 1   | B     | 218 | GLY  | N-CA-C    | 5.33  | 119.34      | 112.83   |
| 1   | A     | 354 | ALA  | CA-C-N    | 5.32  | 127.72      | 120.54   |
| 1   | A     | 354 | ALA  | C-N-CA    | 5.32  | 127.72      | 120.54   |
| 1   | A     | 177 | ILE  | O-C-N     | 5.31  | 128.99      | 122.83   |
| 1   | B     | 58  | ILE  | O-C-N     | 5.31  | 125.81      | 120.92   |
| 1   | B     | 292 | ASP  | CA-C-N    | 5.31  | 131.08      | 122.53   |
| 1   | B     | 292 | ASP  | C-N-CA    | 5.31  | 131.08      | 122.53   |
| 1   | A     | 227 | PHE  | CA-C-N    | 5.30  | 127.65      | 120.38   |
| 1   | A     | 227 | PHE  | C-N-CA    | 5.30  | 127.65      | 120.38   |
| 1   | B     | 357 | LEU  | CA-C-O    | -5.30 | 114.93      | 120.55   |
| 1   | B     | 342 | GLU  | CA-C-N    | 5.30  | 127.91      | 120.28   |
| 1   | B     | 342 | GLU  | C-N-CA    | 5.30  | 127.91      | 120.28   |
| 1   | B     | 219 | HIS  | CA-CB-CG  | -5.29 | 108.51      | 113.80   |
| 1   | B     | 324 | ALA  | N-CA-CB   | -5.29 | 102.34      | 110.12   |
| 1   | A     | 107 | ASP  | CA-CB-CG  | 5.29  | 117.89      | 112.60   |
| 1   | A     | 304 | VAL  | CA-C-O    | -5.29 | 115.77      | 121.27   |
| 1   | A     | 372 | ALA  | O-C-N     | -5.29 | 116.51      | 122.12   |
| 1   | B     | 136 | TRP  | N-CA-CB   | 5.29  | 119.25      | 110.47   |
| 1   | B     | 189 | ASP  | N-CA-CB   | 5.29  | 119.07      | 110.77   |
| 1   | A     | 5   | THR  | CA-C-N    | 5.29  | 125.60      | 119.47   |
| 1   | A     | 5   | THR  | C-N-CA    | 5.29  | 125.60      | 119.47   |
| 1   | B     | 379 | PHE  | CA-C-N    | 5.28  | 127.32      | 120.56   |
| 1   | B     | 379 | PHE  | C-N-CA    | 5.28  | 127.32      | 120.56   |
| 1   | B     | 5   | THR  | CA-CB-CG2 | 5.28  | 119.47      | 110.50   |
| 1   | B     | 37  | GLU  | CA-C-N    | 5.27  | 127.29      | 120.44   |
| 1   | B     | 37  | GLU  | C-N-CA    | 5.27  | 127.29      | 120.44   |
| 1   | A     | 175 | LEU  | O-C-N     | 5.26  | 129.68      | 123.27   |
| 1   | B     | 315 | TYR  | N-CA-CB   | 5.25  | 117.84      | 110.12   |
| 1   | A     | 211 | VAL  | CA-CB-CG2 | 5.25  | 119.33      | 110.40   |
| 1   | A     | 231 | ILE  | CB-CA-C   | 5.25  | 120.76      | 112.26   |
| 1   | A     | 53  | HIS  | CB-CA-C   | -5.24 | 100.65      | 109.50   |
| 1   | A     | 241 | PHE  | CA-CB-CG  | 5.23  | 119.03      | 113.80   |
| 1   | A     | 244 | ASP  | CA-CB-CG  | 5.22  | 117.82      | 112.60   |
| 1   | A     | 30  | ARG  | CD-NE-CZ  | 5.22  | 131.70      | 124.40   |
| 1   | A     | 259 | PHE  | O-C-N     | -5.21 | 116.48      | 122.95   |
| 1   | A     | 53  | HIS  | N-CA-C    | -5.20 | 101.79      | 110.17   |
| 1   | B     | 106 | ASN  | CA-CB-CG  | 5.20  | 117.80      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 274 | LEU  | CA-C-N     | 5.20  | 127.51      | 120.44   |
| 1   | B     | 274 | LEU  | C-N-CA     | 5.20  | 127.51      | 120.44   |
| 1   | A     | 34  | ASP  | CA-CB-CG   | 5.20  | 117.80      | 112.60   |
| 1   | A     | 20  | THR  | N-CA-C     | 5.19  | 119.48      | 113.20   |
| 1   | A     | 311 | ASN  | OD1-CG-ND2 | 5.18  | 127.78      | 122.60   |
| 1   | B     | 296 | SER  | CA-C-N     | 5.18  | 128.89      | 120.60   |
| 1   | B     | 296 | SER  | C-N-CA     | 5.18  | 128.89      | 120.60   |
| 1   | B     | 341 | PHE  | CA-C-N     | 5.18  | 127.74      | 120.28   |
| 1   | B     | 341 | PHE  | C-N-CA     | 5.18  | 127.74      | 120.28   |
| 1   | A     | 68  | GLU  | N-CA-CB    | 5.17  | 117.82      | 110.16   |
| 1   | B     | 132 | THR  | O-C-N      | 5.17  | 129.58      | 123.27   |
| 1   | B     | 235 | LEU  | CA-C-N     | 5.17  | 127.52      | 120.54   |
| 1   | B     | 235 | LEU  | C-N-CA     | 5.17  | 127.52      | 120.54   |
| 1   | B     | 181 | PRO  | CA-C-O     | 5.17  | 127.98      | 121.67   |
| 1   | B     | 220 | GLU  | N-CA-C     | 5.17  | 117.65      | 111.71   |
| 1   | B     | 237 | ALA  | CA-C-N     | 5.17  | 129.95      | 122.36   |
| 1   | B     | 237 | ALA  | C-N-CA     | 5.17  | 129.95      | 122.36   |
| 1   | B     | 272 | ASP  | O-C-N      | -5.16 | 116.76      | 122.07   |
| 1   | B     | 62  | ALA  | CA-C-O     | 5.15  | 127.87      | 120.51   |
| 1   | A     | 259 | PHE  | CB-CA-C    | 5.14  | 117.92      | 109.90   |
| 1   | A     | 246 | ASN  | OD1-CG-ND2 | -5.14 | 117.46      | 122.60   |
| 1   | A     | 154 | LEU  | CA-C-N     | 5.13  | 127.41      | 120.44   |
| 1   | A     | 154 | LEU  | C-N-CA     | 5.13  | 127.41      | 120.44   |
| 1   | A     | 66  | GLU  | CB-CG-CD   | 5.12  | 121.31      | 112.60   |
| 1   | A     | 156 | ARG  | CA-C-N     | 5.12  | 127.10      | 120.44   |
| 1   | A     | 156 | ARG  | C-N-CA     | 5.12  | 127.10      | 120.44   |
| 1   | B     | 156 | ARG  | NH1-CZ-NH2 | -5.12 | 112.64      | 119.30   |
| 1   | B     | 99  | LYS  | CA-C-O     | -5.12 | 114.31      | 120.10   |
| 1   | B     | 394 | ARG  | NE-CZ-NH2  | -5.12 | 114.59      | 119.20   |
| 1   | B     | 320 | GLU  | CA-C-O     | -5.11 | 115.43      | 120.70   |
| 1   | A     | 333 | GLU  | CG-CD-OE1  | -5.11 | 106.65      | 118.40   |
| 1   | A     | 311 | ASN  | CA-C-N     | 5.11  | 127.13      | 120.28   |
| 1   | A     | 311 | ASN  | C-N-CA     | 5.11  | 127.13      | 120.28   |
| 1   | B     | 148 | LYS  | O-C-N      | 5.11  | 129.79      | 123.15   |
| 1   | B     | 268 | PHE  | CA-CB-CG   | 5.10  | 118.90      | 113.80   |
| 1   | B     | 16  | THR  | CA-CB-OG1  | -5.10 | 101.95      | 109.60   |
| 1   | B     | 117 | LYS  | CA-CB-CG   | 5.09  | 124.29      | 114.10   |
| 1   | B     | 104 | THR  | O-C-N      | -5.09 | 116.00      | 122.26   |
| 1   | B     | 263 | ASP  | N-CA-CB    | -5.09 | 103.23      | 110.46   |
| 1   | A     | 346 | THR  | CA-CB-OG1  | -5.09 | 101.97      | 109.60   |
| 1   | A     | 77  | ALA  | CA-C-N     | 5.08  | 127.05      | 120.44   |
| 1   | A     | 77  | ALA  | C-N-CA     | 5.08  | 127.05      | 120.44   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 323 | LEU  | N-CA-C    | -5.07 | 105.66      | 111.14   |
| 1   | B     | 234 | ALA  | CA-C-N    | 5.07  | 127.03      | 120.44   |
| 1   | B     | 234 | ALA  | C-N-CA    | 5.07  | 127.03      | 120.44   |
| 1   | B     | 187 | ARG  | CA-C-O    | -5.06 | 115.65      | 121.47   |
| 1   | B     | 153 | ALA  | CA-C-N    | 5.05  | 127.05      | 120.28   |
| 1   | B     | 153 | ALA  | C-N-CA    | 5.05  | 127.05      | 120.28   |
| 1   | A     | 11  | THR  | CB-CA-C   | 5.05  | 119.27      | 109.33   |
| 1   | A     | 190 | ILE  | CA-C-O    | -5.05 | 114.97      | 120.72   |
| 1   | B     | 321 | ARG  | CA-C-N    | 5.05  | 127.46      | 120.29   |
| 1   | B     | 321 | ARG  | C-N-CA    | 5.05  | 127.46      | 120.29   |
| 1   | A     | 266 | SER  | CA-C-O    | -5.04 | 115.20      | 120.55   |
| 1   | A     | 356 | ASP  | CA-C-N    | 5.04  | 127.00      | 120.44   |
| 1   | A     | 356 | ASP  | C-N-CA    | 5.04  | 127.00      | 120.44   |
| 1   | B     | 131 | GLU  | CA-C-O    | 5.03  | 124.68      | 119.14   |
| 1   | A     | 393 | SER  | O-C-N     | 5.03  | 129.50      | 122.36   |
| 1   | B     | 5   | THR  | O-C-N     | -5.02 | 118.31      | 121.88   |
| 1   | A     | 201 | PHE  | CA-C-N    | 5.02  | 127.33      | 120.46   |
| 1   | A     | 201 | PHE  | C-N-CA    | 5.02  | 127.33      | 120.46   |
| 1   | B     | 183 | PRO  | CA-C-N    | 5.02  | 130.38      | 121.80   |
| 1   | B     | 183 | PRO  | C-N-CA    | 5.02  | 130.38      | 121.80   |
| 1   | B     | 228 | THR  | CA-CB-OG1 | -5.01 | 102.09      | 109.60   |
| 1   | B     | 138 | GLY  | N-CA-C    | 5.01  | 119.80      | 113.24   |
| 1   | B     | 393 | SER  | CA-C-O    | -5.01 | 113.36      | 119.32   |
| 1   | A     | 106 | ASN  | CA-CB-CG  | 5.00  | 117.61      | 112.60   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3026  | 0        | 2888     | 25      | 0            |
| 1   | B     | 3026  | 0        | 2888     | 25      | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 298   | 0        | 0        | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | B     | 288   | 0        | 0        | 1       | 1            |
| All | All   | 6640  | 0        | 5776     | 49      | 1            |

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 4.

All (49) 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:95:HIS:HD2   | 1:A:97:VAL:H     | 1.36                     | 0.73              |
| 1:B:184:ASN:HA   | 1:B:190:ILE:HG13 | 1.77                     | 0.66              |
| 1:B:95:HIS:HD2   | 1:B:97:VAL:H     | 1.46                     | 0.63              |
| 1:B:275:GLU:HG3  | 1:B:319:LYS:HG3  | 1.79                     | 0.63              |
| 1:B:148:LYS:HG3  | 1:B:191:PHE:HZ   | 1.69                     | 0.57              |
| 1:B:11:THR:HG21  | 1:B:86:PRO:HG2   | 1.87                     | 0.56              |
| 1:B:182:LYS:HE2  | 1:B:184:ASN:O    | 2.07                     | 0.56              |
| 1:A:215:PRO:HG2  | 1:A:231:ILE:HG22 | 1.88                     | 0.55              |
| 1:A:11:THR:HG21  | 1:A:86:PRO:HG2   | 1.88                     | 0.55              |
| 1:A:249:ARG:O    | 1:A:252:LYS:HE3  | 2.08                     | 0.53              |
| 1:B:319:LYS:O    | 1:B:323:LEU:HG   | 2.09                     | 0.53              |
| 1:A:2:VAL:HG13   | 1:A:316:LEU:HB2  | 1.90                     | 0.51              |
| 1:B:140:GLU:HG3  | 1:B:157:MET:HE1  | 1.92                     | 0.51              |
| 1:B:235:LEU:HD12 | 1:B:273:LEU:HD11 | 1.93                     | 0.51              |
| 1:A:299:ASP:HB3  | 1:A:303:GLY:HA3  | 1.93                     | 0.50              |
| 1:A:195:VAL:HG22 | 1:A:213:LEU:HD12 | 1.93                     | 0.50              |
| 1:B:35:PRO:O     | 1:B:39:VAL:HG23  | 2.11                     | 0.49              |
| 1:B:55:ASN:HA    | 1:B:58:ILE:O     | 2.13                     | 0.49              |
| 1:A:58:ILE:HD11  | 1:A:71:LEU:HD21  | 1.93                     | 0.49              |
| 1:B:43:ALA:HA    | 1:B:83:LEU:HD21  | 1.94                     | 0.48              |
| 1:A:273:LEU:HD23 | 3:A:584(A):HOH:O | 2.15                     | 0.47              |
| 1:A:363:SER:HB2  | 3:A:619(A):HOH:O | 2.14                     | 0.47              |
| 1:A:328:ASP:HA   | 1:A:329:PRO:HD3  | 1.74                     | 0.46              |
| 1:A:289:ARG:HD3  | 3:A:404(A):HOH:O | 2.15                     | 0.46              |
| 1:B:182:LYS:HA   | 1:B:183:PRO:HD3  | 1.74                     | 0.46              |
| 1:A:55:ASN:HA    | 1:A:58:ILE:O     | 2.16                     | 0.45              |
| 1:A:216:GLU:HB2  | 1:A:244:ASP:HB2  | 1.98                     | 0.45              |
| 1:B:39:VAL:HG13  | 1:B:83:LEU:HD12  | 1.97                     | 0.45              |
| 1:A:95:HIS:CD2   | 1:A:97:VAL:H     | 2.25                     | 0.45              |
| 1:B:124:LEU:HD11 | 1:B:128:MET:HE3  | 1.98                     | 0.44              |
| 1:A:221:GLN:HE21 | 1:A:248:GLN:HB3  | 1.82                     | 0.44              |
| 1:B:328:ASP:HA   | 1:B:329:PRO:HD3  | 1.78                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:275:GLU:OE1  | 1:B:319:LYS:HE3  | 2.17                     | 0.43              |
| 1:A:261:HIS:NE2  | 1:B:384:GLN:NE2  | 2.67                     | 0.43              |
| 1:B:294:LYS:HA   | 1:B:295:PRO:HD3  | 1.85                     | 0.43              |
| 1:B:179:LEU:O    | 1:B:181:PRO:HD3  | 2.19                     | 0.42              |
| 1:B:273:LEU:HD12 | 1:B:273:LEU:O    | 2.19                     | 0.42              |
| 1:A:185:GLU:HA   | 1:A:186:PRO:HA   | 1.73                     | 0.42              |
| 1:B:208:GLY:HA3  | 3:B:572(B):HOH:O | 2.19                     | 0.42              |
| 1:B:278:PHE:HA   | 1:B:279:PRO:HD3  | 1.91                     | 0.41              |
| 1:B:195:VAL:HG23 | 1:B:220:GLU:CD   | 2.46                     | 0.41              |
| 1:A:53:HIS:CD2   | 1:A:89:THR:HG23  | 2.55                     | 0.41              |
| 1:A:192:LEU:N    | 1:A:193:PRO:CD   | 2.83                     | 0.41              |
| 1:A:135:MET:HE3  | 1:A:177:ILE:HD13 | 2.03                     | 0.41              |
| 1:A:122:ILE:HG23 | 1:A:175:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:217:THR:HA   | 1:A:227:PHE:CD1  | 2.56                     | 0.41              |
| 1:A:51:THR:CG2   | 1:A:87:MET:HB3   | 2.51                     | 0.40              |
| 1:A:235:LEU:HG   | 1:A:240:LEU:HD23 | 2.03                     | 0.40              |
| 1:B:235:LEU:HD22 | 1:B:283:PRO:HB2  | 2.04                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1           | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------------|--------------------------|-------------------|
| 3:B:573(B):HOH:O | 3:B:614(B):HOH:O[4_555] | 2.15                     | 0.05              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | A     | 391/394 (99%) | 375 (96%) | 15 (4%) | 1 (0%)   | 36          | 55 |
| 1   | B     | 391/394 (99%) | 379 (97%) | 10 (3%) | 2 (0%)   | 24          | 43 |
| All | All   | 782/788 (99%) | 754 (96%) | 25 (3%) | 3 (0%)   | 30          | 49 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 185 | GLU  |
| 1   | B     | 185 | GLU  |
| 1   | B     | 6   | PRO  |

### 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     | 305/310 (98%) | 290 (95%) | 15 (5%)  | 22          | 45 |
| 1   | B     | 305/310 (98%) | 294 (96%) | 11 (4%)  | 31          | 58 |
| All | All   | 610/620 (98%) | 584 (96%) | 26 (4%)  | 26          | 51 |

All (26) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | VAL  |
| 1   | A     | 68  | GLU  |
| 1   | A     | 90  | THR  |
| 1   | A     | 94  | SER  |
| 1   | A     | 149 | ASP  |
| 1   | A     | 184 | ASN  |
| 1   | A     | 195 | VAL  |
| 1   | A     | 213 | LEU  |
| 1   | A     | 273 | LEU  |
| 1   | A     | 289 | ARG  |
| 1   | A     | 313 | SER  |
| 1   | A     | 333 | GLU  |
| 1   | A     | 361 | SER  |
| 1   | A     | 370 | GLU  |
| 1   | A     | 393 | SER  |
| 1   | B     | 41  | LYS  |
| 1   | B     | 68  | GLU  |
| 1   | B     | 79  | LYS  |
| 1   | B     | 174 | ASN  |
| 1   | B     | 193 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 235 | LEU  |
| 1   | B     | 273 | LEU  |
| 1   | B     | 320 | GLU  |
| 1   | B     | 333 | GLU  |
| 1   | B     | 336 | LYS  |
| 1   | B     | 357 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 75  | ASN  |
| 1   | A     | 95  | HIS  |
| 1   | A     | 221 | GLN  |
| 1   | A     | 233 | GLN  |
| 1   | A     | 384 | GLN  |
| 1   | B     | 9   | HIS  |
| 1   | B     | 32  | ASN  |
| 1   | B     | 75  | ASN  |
| 1   | B     | 95  | HIS  |
| 1   | B     | 174 | ASN  |
| 1   | B     | 221 | GLN  |
| 1   | B     | 384 | GLN  |

### 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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

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.