



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:03 PM UTC

PDB ID : 1J4S / pdb\_00001j4s  
Title : Structure of Artocarpin: a Lectin with Mannose Specificity (Form 1)  
Authors : Pratap, J.V.; Jeyaprakash, A.A.; Rani, P.G.; Sekar, K.; Surolia, A.; Vijayan, M.  
Deposited on : 2001-10-30  
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)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

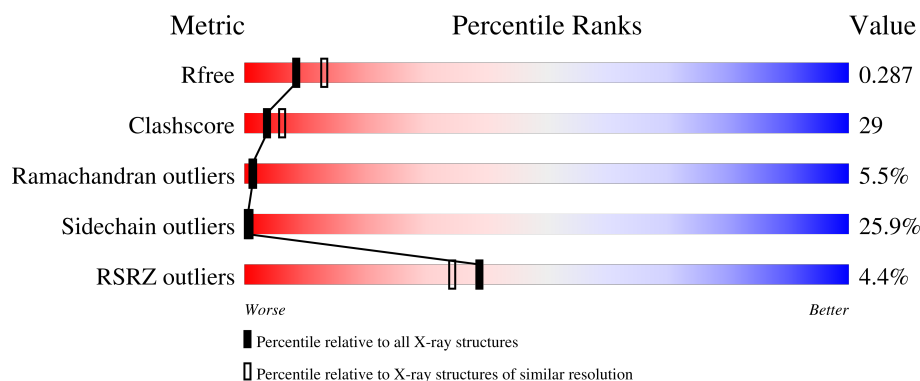
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 5829 (2.50-2.50)                                      |
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |
| RSRZ outliers         | 180081                      | 5833 (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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                      |
|-----|-------|--------|---------------------------------------------------------------------------------------|
| 1   | A     | 149    | <div> <div>10%</div> <div>38%</div> <div>38%</div> <div>15%</div> </div>              |
| 1   | B     | 149    | <div> <div>5%</div> <div>9%</div> <div>43%</div> <div>34%</div> <div>14%</div> </div> |
| 1   | C     | 149    | <div> <div>5%</div> <div>7%</div> <div>56%</div> <div>28%</div> <div>10%</div> </div> |
| 1   | D     | 149    | <div> <div>7%</div> <div>7%</div> <div>44%</div> <div>37%</div> <div>12%</div> </div> |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4917 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 Artocarpin.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1119  | 718 | 181 | 219 | 1 |         |         |       |
| 1   | B     | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1118  | 717 | 181 | 219 | 1 |         |         |       |
| 1   | C     | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1126  | 722 | 182 | 221 | 1 |         |         |       |
| 1   | D     | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1123  | 720 | 181 | 221 | 1 |         |         |       |

There are 28 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 9       | SER      | PRO    | conflict | UNP Q7M1T4 |
| A     | 20      | GLU      | ASP    | conflict | UNP Q7M1T4 |
| A     | 49      | ASP      | GLU    | conflict | UNP Q7M1T4 |
| A     | 70      | LYS      | ARG    | conflict | UNP Q7M1T4 |
| A     | 84      | GLY      | ALA    | conflict | UNP Q7M1T4 |
| A     | 145     | ILE      | VAL    | conflict | UNP Q7M1T4 |
| A     | 148     | SER      | ALA    | conflict | UNP Q7M1T4 |
| B     | 9       | SER      | PRO    | conflict | UNP Q7M1T4 |
| B     | 20      | GLU      | ASP    | conflict | UNP Q7M1T4 |
| B     | 49      | ASP      | GLU    | conflict | UNP Q7M1T4 |
| B     | 70      | LYS      | ARG    | conflict | UNP Q7M1T4 |
| B     | 84      | GLY      | ALA    | conflict | UNP Q7M1T4 |
| B     | 145     | ILE      | VAL    | conflict | UNP Q7M1T4 |
| B     | 148     | SER      | ALA    | conflict | UNP Q7M1T4 |
| C     | 9       | SER      | PRO    | conflict | UNP Q7M1T4 |
| C     | 20      | GLU      | ASP    | conflict | UNP Q7M1T4 |
| C     | 49      | ASP      | GLU    | conflict | UNP Q7M1T4 |
| C     | 70      | LYS      | ARG    | conflict | UNP Q7M1T4 |
| C     | 84      | GLY      | ALA    | conflict | UNP Q7M1T4 |
| C     | 145     | ILE      | VAL    | conflict | UNP Q7M1T4 |
| C     | 148     | SER      | ALA    | conflict | UNP Q7M1T4 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 9       | SER      | PRO    | conflict | UNP Q7M1T4 |
| D     | 20      | GLU      | ASP    | conflict | UNP Q7M1T4 |
| D     | 49      | ASP      | GLU    | conflict | UNP Q7M1T4 |
| D     | 70      | LYS      | ARG    | conflict | UNP Q7M1T4 |
| D     | 84      | GLY      | ALA    | conflict | UNP Q7M1T4 |
| D     | 145     | ILE      | VAL    | conflict | UNP Q7M1T4 |
| D     | 148     | SER      | ALA    | conflict | UNP Q7M1T4 |

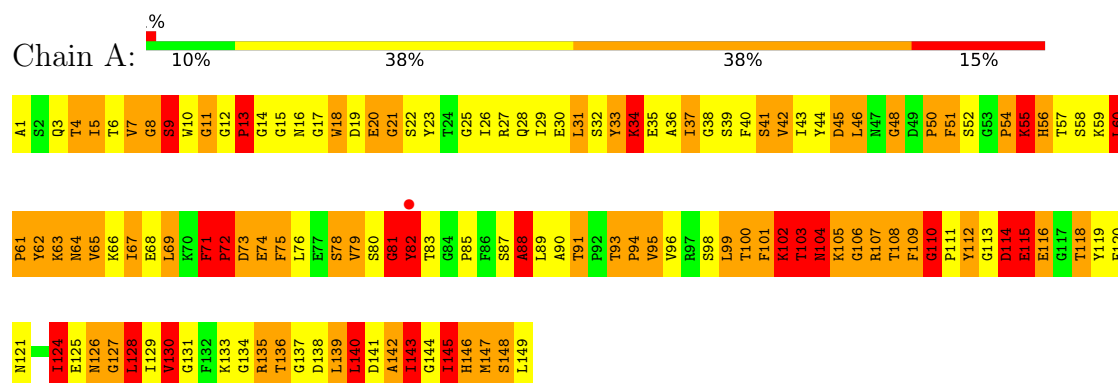
- Molecule 2 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 2   | A     | 102      | Total O<br>102 102 | 0       | 0       |
| 2   | B     | 112      | Total O<br>112 112 | 0       | 0       |
| 2   | C     | 105      | Total O<br>105 105 | 0       | 0       |
| 2   | D     | 112      | Total O<br>112 112 | 0       | 0       |

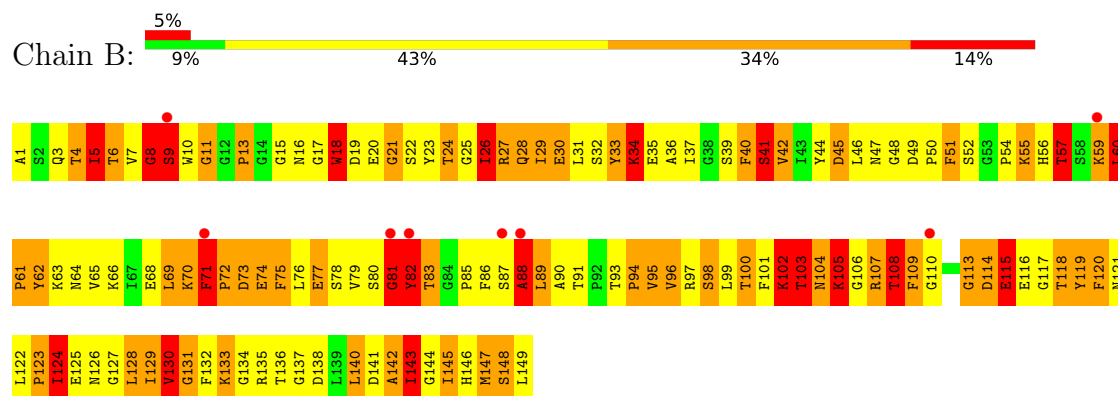
### 3 Residue-property plots [i](#)

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

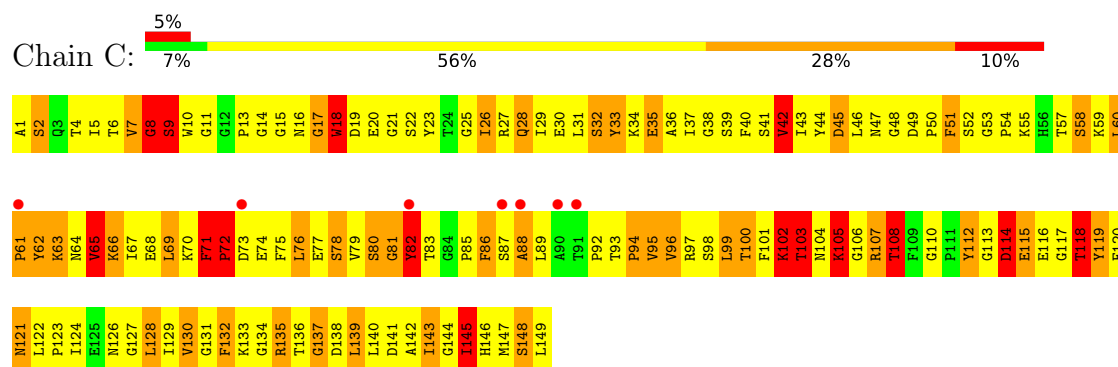
#### • Molecule 1: Artocarpin



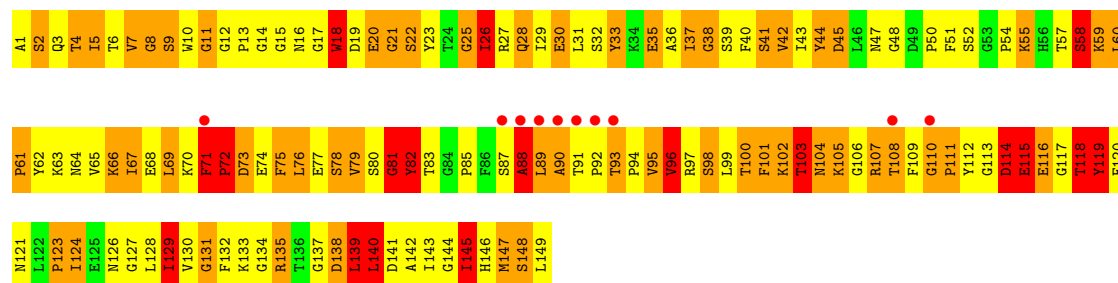
#### • Molecule 1: Artocarpin



#### • Molecule 1: Artocarpin



Chain D: 



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 69.88Å 73.74Å 60.64Å<br>90.00° 95.06° 90.00°                | Depositor        |
| Resolution (Å)                                                          | 20.00 – 2.50<br>20.00 – 2.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (20.00-2.50)<br>81.5 (20.00-2.50)           | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.96 (at 2.44Å)                                             | Xtriage          |
| Refinement program                                                      | X-PLOR 3.1                                                  | Depositor        |
| R, $R_{free}$                                                           | 0.199 , 0.262<br>0.237 , 0.287                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1036 reflections (5.89%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 19.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.610                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.25 , 62.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.87                                                        | EDS              |
| Total number of atoms                                                   | 4917                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 11.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$      |
| 1   | A     | 3.33         | 8/1149 (0.7%)  | 3.30        | 151/1561 (9.7%)  |
| 1   | B     | 1.38         | 10/1149 (0.9%) | 3.49        | 163/1563 (10.4%) |
| 1   | C     | 1.08         | 4/1157 (0.3%)  | 2.79        | 152/1572 (9.7%)  |
| 1   | D     | 3.14         | 5/1153 (0.4%)  | 3.30        | 143/1566 (9.1%)  |
| All | All   | 2.45         | 27/4608 (0.6%) | 3.23        | 609/6262 (9.7%)  |

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     | 1                   | 5                   |
| 1   | B     | 1                   | 7                   |
| 1   | C     | 1                   | 5                   |
| 1   | D     | 1                   | 4                   |
| All | All   | 4                   | 21                  |

All (27) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | A     | 1   | ALA  | C-O   | 104.17 | 3.31        | 1.23     |
| 1   | D     | 1   | ALA  | C-O   | 99.95  | 3.23        | 1.23     |
| 1   | B     | 70  | LYS  | C-N   | 22.98  | 1.75        | 1.33     |
| 1   | A     | 82  | TYR  | C-N   | -20.60 | 1.07        | 1.33     |
| 1   | B     | 9   | SER  | C-N   | 12.06  | 1.48        | 1.33     |
| 1   | D     | 82  | TYR  | C-N   | -11.91 | 1.15        | 1.33     |
| 1   | B     | 33  | TYR  | C-N   | 11.54  | 1.49        | 1.33     |
| 1   | C     | 81  | GLY  | C-N   | 10.05  | 1.47        | 1.33     |
| 1   | C     | 96  | VAL  | CA-CB | 9.53   | 1.65        | 1.53     |
| 1   | A     | 9   | SER  | C-N   | 9.38   | 1.49        | 1.33     |
| 1   | B     | 26  | ILE  | CA-CB | 9.37   | 1.65        | 1.54     |
| 1   | A     | 96  | VAL  | CA-CB | 7.61   | 1.61        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 81  | GLY  | C-N   | -7.31 | 1.23        | 1.33     |
| 1   | B     | 108 | THR  | CA-CB | 7.23  | 1.63        | 1.53     |
| 1   | B     | 81  | GLY  | C-N   | -6.97 | 1.24        | 1.33     |
| 1   | D     | 26  | ILE  | CA-CB | 6.32  | 1.61        | 1.54     |
| 1   | D     | 8   | GLY  | C-N   | -6.22 | 1.26        | 1.33     |
| 1   | B     | 82  | TYR  | C-N   | 5.96  | 1.41        | 1.33     |
| 1   | A     | 71  | PHE  | CA-C  | 5.55  | 1.59        | 1.52     |
| 1   | A     | 130 | VAL  | CA-CB | 5.53  | 1.61        | 1.54     |
| 1   | D     | 71  | PHE  | N-CA  | 5.39  | 1.53        | 1.46     |
| 1   | C     | 26  | ILE  | CA-CB | 5.22  | 1.60        | 1.54     |
| 1   | C     | 108 | THR  | CA-CB | 5.19  | 1.61        | 1.53     |
| 1   | A     | 129 | ILE  | CA-CB | 5.19  | 1.60        | 1.54     |
| 1   | B     | 96  | VAL  | CA-CB | 5.16  | 1.59        | 1.53     |
| 1   | B     | 71  | PHE  | N-CA  | 5.00  | 1.54        | 1.46     |
| 1   | B     | 79  | VAL  | CA-CB | 5.00  | 1.60        | 1.54     |

All (609) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 1   | ALA  | CA-C-O  | -53.24 | 30.29       | 120.80   |
| 1   | D     | 1   | ALA  | CA-C-O  | -52.20 | 32.06       | 120.80   |
| 1   | B     | 71  | PHE  | O-C-N   | -46.35 | 74.93       | 121.28   |
| 1   | A     | 82  | TYR  | O-C-N   | -38.40 | 71.51       | 122.59   |
| 1   | B     | 81  | GLY  | O-C-N   | -35.30 | 76.81       | 122.70   |
| 1   | A     | 81  | GLY  | O-C-N   | -32.87 | 79.97       | 122.70   |
| 1   | D     | 8   | GLY  | CA-C-N  | 29.11  | 166.88      | 122.93   |
| 1   | D     | 8   | GLY  | C-N-CA  | 29.11  | 166.88      | 122.93   |
| 1   | B     | 71  | PHE  | CA-C-N  | 25.07  | 151.18      | 119.84   |
| 1   | B     | 71  | PHE  | C-N-CA  | 25.07  | 151.18      | 119.84   |
| 1   | A     | 1   | ALA  | CB-CA-C | 22.65  | 144.48      | 110.50   |
| 1   | D     | 82  | TYR  | O-C-N   | -21.27 | 94.30       | 122.59   |
| 1   | C     | 8   | GLY  | O-C-N   | -20.97 | 101.89      | 122.86   |
| 1   | D     | 1   | ALA  | CB-CA-C | 20.85  | 141.77      | 110.50   |
| 1   | B     | 34  | LYS  | O-C-N   | -20.73 | 95.02       | 122.59   |
| 1   | D     | 9   | SER  | O-C-N   | -20.45 | 98.38       | 123.33   |
| 1   | B     | 1   | ALA  | CB-CA-C | 20.20  | 140.80      | 110.50   |
| 1   | A     | 1   | ALA  | N-CA-CB | -19.94 | 80.49       | 110.40   |
| 1   | D     | 8   | GLY  | O-C-N   | -19.10 | 88.59       | 123.16   |
| 1   | B     | 81  | GLY  | CA-C-N  | 18.24  | 156.38      | 121.54   |
| 1   | B     | 81  | GLY  | C-N-CA  | 18.24  | 156.38      | 121.54   |
| 1   | C     | 1   | ALA  | CB-CA-C | 18.18  | 137.78      | 110.50   |
| 1   | D     | 1   | ALA  | N-CA-CB | -16.97 | 84.95       | 110.40   |

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| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | B     | 9   | SER  | O-C-N    | 16.47  | 144.50      | 122.59   |
| 1   | B     | 71  | PHE  | C-N-CD   | -15.62 | 60.95       | 125.00   |
| 1   | B     | 82  | TYR  | O-C-N    | 15.47  | 143.16      | 122.59   |
| 1   | B     | 102 | LYS  | CG-CD-CE | 15.39  | 146.71      | 111.30   |
| 1   | B     | 33  | TYR  | CA-C-N   | -14.70 | 93.47       | 121.54   |
| 1   | B     | 33  | TYR  | C-N-CA   | -14.70 | 93.47       | 121.54   |
| 1   | C     | 81  | GLY  | O-C-N    | -14.55 | 103.79      | 122.70   |
| 1   | B     | 1   | ALA  | N-CA-CB  | 14.16  | 131.63      | 110.40   |
| 1   | B     | 82  | TYR  | CA-C-N   | -13.69 | 103.83      | 122.72   |
| 1   | B     | 82  | TYR  | C-N-CA   | -13.69 | 103.83      | 122.72   |
| 1   | C     | 1   | ALA  | N-CA-CB  | 13.59  | 130.78      | 110.40   |
| 1   | C     | 1   | ALA  | CA-C-O   | -13.05 | 98.61       | 120.80   |
| 1   | D     | 81  | GLY  | O-C-N    | -13.02 | 105.77      | 122.70   |
| 1   | C     | 129 | ILE  | N-CA-C   | -12.33 | 93.89       | 109.30   |
| 1   | D     | 71  | PHE  | O-C-N    | -11.36 | 108.25      | 121.32   |
| 1   | C     | 71  | PHE  | N-CA-C   | 11.30  | 134.78      | 109.81   |
| 1   | B     | 1   | ALA  | CA-C-O   | -11.04 | 102.04      | 120.80   |
| 1   | B     | 138 | ASP  | N-CA-C   | -11.00 | 100.35      | 113.88   |
| 1   | A     | 15  | GLY  | O-C-N    | -10.93 | 113.81      | 122.88   |
| 1   | C     | 71  | PHE  | CA-C-N   | -10.69 | 106.47      | 119.84   |
| 1   | C     | 71  | PHE  | C-N-CA   | -10.69 | 106.47      | 119.84   |
| 1   | D     | 25  | GLY  | O-C-N    | -10.62 | 113.72      | 123.92   |
| 1   | B     | 89  | LEU  | N-CA-C   | -10.49 | 100.43      | 113.02   |
| 1   | A     | 144 | GLY  | O-C-N    | -10.47 | 114.52      | 123.73   |
| 1   | C     | 17  | GLY  | O-C-N    | -10.26 | 112.77      | 122.93   |
| 1   | C     | 48  | GLY  | O-C-N    | -10.14 | 114.60      | 122.71   |
| 1   | C     | 106 | GLY  | O-C-N    | -9.83  | 114.84      | 122.71   |
| 1   | B     | 127 | GLY  | O-C-N    | -9.83  | 114.49      | 123.92   |
| 1   | D     | 17  | GLY  | O-C-N    | -9.73  | 113.03      | 122.96   |
| 1   | B     | 17  | GLY  | O-C-N    | -9.71  | 113.32      | 122.93   |
| 1   | A     | 12  | GLY  | CA-C-N   | 9.56   | 129.22      | 119.56   |
| 1   | A     | 12  | GLY  | C-N-CA   | 9.56   | 129.22      | 119.56   |
| 1   | C     | 127 | GLY  | O-C-N    | -9.52  | 114.01      | 123.06   |
| 1   | C     | 134 | GLY  | O-C-N    | -9.40  | 112.96      | 123.58   |
| 1   | B     | 95  | VAL  | O-C-N    | -9.16  | 112.84      | 122.82   |
| 1   | C     | 89  | LEU  | N-CA-C   | -9.12  | 102.30      | 113.15   |
| 1   | B     | 21  | GLY  | O-C-N    | -9.12  | 113.66      | 123.05   |
| 1   | A     | 138 | ASP  | N-CA-C   | -9.07  | 102.12      | 113.55   |
| 1   | D     | 118 | THR  | O-C-N    | -8.99  | 112.73      | 123.16   |
| 1   | C     | 133 | LYS  | O-C-N    | -8.95  | 112.23      | 123.24   |
| 1   | D     | 142 | ALA  | O-C-N    | -8.95  | 114.60      | 123.46   |
| 1   | A     | 95  | VAL  | O-C-N    | -8.90  | 113.12      | 122.82   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 145 | ILE  | N-CA-C   | 8.85  | 119.61      | 108.82   |
| 1   | C     | 93  | THR  | N-CA-C   | 8.83  | 121.05      | 109.83   |
| 1   | B     | 79  | VAL  | O-C-N    | -8.76 | 114.07      | 123.18   |
| 1   | B     | 70  | LYS  | N-CA-C   | -8.70 | 95.19       | 108.67   |
| 1   | D     | 55  | LYS  | O-C-N    | -8.66 | 113.35      | 123.22   |
| 1   | B     | 26  | ILE  | O-C-N    | -8.64 | 114.11      | 123.18   |
| 1   | D     | 81  | GLY  | CA-C-N   | 8.64  | 138.04      | 121.54   |
| 1   | D     | 81  | GLY  | C-N-CA   | 8.64  | 138.04      | 121.54   |
| 1   | B     | 108 | THR  | O-C-N    | -8.62 | 113.39      | 123.22   |
| 1   | A     | 78  | SER  | O-C-N    | -8.62 | 114.04      | 123.52   |
| 1   | C     | 95  | VAL  | O-C-N    | -8.62 | 113.52      | 123.00   |
| 1   | D     | 29  | ILE  | O-C-N    | -8.58 | 114.39      | 123.14   |
| 1   | A     | 1   | ALA  | N-CA-C   | 8.57  | 135.00      | 111.00   |
| 1   | D     | 124 | ILE  | O-C-N    | -8.54 | 113.55      | 123.03   |
| 1   | A     | 71  | PHE  | O-C-N    | -8.54 | 111.50      | 121.32   |
| 1   | C     | 33  | TYR  | O-C-N    | -8.52 | 115.02      | 123.46   |
| 1   | A     | 26  | ILE  | O-C-N    | -8.52 | 113.90      | 122.93   |
| 1   | B     | 11  | GLY  | O-C-N    | -8.52 | 114.55      | 123.58   |
| 1   | A     | 80  | SER  | O-C-N    | -8.51 | 112.97      | 122.92   |
| 1   | D     | 95  | VAL  | O-C-N    | -8.50 | 113.64      | 123.00   |
| 1   | C     | 144 | GLY  | O-C-N    | -8.49 | 115.70      | 123.42   |
| 1   | B     | 1   | ALA  | N-CA-C   | -8.39 | 87.52       | 111.00   |
| 1   | A     | 89  | LEU  | N-CA-C   | -8.38 | 103.06      | 113.20   |
| 1   | B     | 102 | LYS  | CB-CG-CD | -8.38 | 92.03       | 111.30   |
| 1   | D     | 32  | SER  | O-C-N    | -8.37 | 113.06      | 123.27   |
| 1   | A     | 129 | ILE  | N-CA-C   | -8.35 | 98.10       | 109.37   |
| 1   | A     | 5   | ILE  | O-C-N    | -8.34 | 113.49      | 122.83   |
| 1   | B     | 113 | GLY  | O-C-N    | -8.33 | 112.98      | 122.56   |
| 1   | B     | 146 | HIS  | O-C-N    | -8.33 | 112.36      | 123.19   |
| 1   | C     | 5   | ILE  | O-C-N    | -8.32 | 113.09      | 122.66   |
| 1   | D     | 100 | THR  | O-C-N    | -8.29 | 113.65      | 123.27   |
| 1   | D     | 143 | ILE  | O-C-N    | -8.29 | 114.22      | 123.10   |
| 1   | A     | 79  | VAL  | O-C-N    | -8.24 | 114.28      | 123.10   |
| 1   | D     | 45  | ASP  | O-C-N    | -8.24 | 113.96      | 123.27   |
| 1   | D     | 129 | ILE  | O-C-N    | -8.23 | 114.27      | 122.67   |
| 1   | A     | 145 | ILE  | O-C-N    | -8.22 | 114.29      | 122.92   |
| 1   | D     | 127 | GLY  | O-C-N    | -8.22 | 114.87      | 123.58   |
| 1   | C     | 117 | GLY  | O-C-N    | -8.20 | 115.06      | 122.85   |
| 1   | B     | 7   | VAL  | O-C-N    | -8.19 | 114.25      | 122.93   |
| 1   | A     | 134 | GLY  | O-C-N    | -8.19 | 114.90      | 123.58   |
| 1   | D     | 40  | PHE  | O-C-N    | -8.19 | 114.15      | 123.40   |
| 1   | C     | 6   | THR  | O-C-N    | -8.18 | 113.63      | 123.29   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 48  | GLY  | O-C-N    | -8.16 | 113.87      | 122.52   |
| 1   | A     | 55  | LYS  | O-C-N    | -8.14 | 113.73      | 123.10   |
| 1   | D     | 41  | SER  | O-C-N    | -8.09 | 113.30      | 123.24   |
| 1   | A     | 63  | LYS  | O-C-N    | -8.08 | 113.03      | 122.89   |
| 1   | B     | 98  | SER  | O-C-N    | -8.05 | 112.69      | 123.15   |
| 1   | A     | 58  | SER  | O-C-N    | -8.04 | 113.94      | 123.03   |
| 1   | D     | 10  | TRP  | O-C-N    | -8.04 | 114.05      | 123.22   |
| 1   | C     | 112 | TYR  | O-C-N    | -8.03 | 113.95      | 123.27   |
| 1   | D     | 35  | GLU  | N-CA-C   | -8.03 | 103.61      | 113.41   |
| 1   | A     | 142 | ALA  | O-C-N    | -8.02 | 114.26      | 123.33   |
| 1   | D     | 22  | SER  | O-C-N    | -8.02 | 113.81      | 123.19   |
| 1   | A     | 113 | GLY  | O-C-N    | -8.02 | 113.34      | 122.64   |
| 1   | D     | 145 | ILE  | O-C-N    | -8.02 | 114.54      | 123.20   |
| 1   | D     | 9   | SER  | N-CA-C   | -8.00 | 101.55      | 110.91   |
| 1   | B     | 69  | LEU  | O-C-N    | -7.98 | 114.12      | 123.06   |
| 1   | A     | 56  | HIS  | CA-CB-CG | -7.98 | 105.82      | 113.80   |
| 1   | A     | 21  | GLY  | O-C-N    | -7.96 | 116.06      | 122.90   |
| 1   | B     | 83  | THR  | O-C-N    | -7.96 | 114.28      | 123.27   |
| 1   | D     | 1   | ALA  | N-CA-C   | 7.94  | 133.24      | 111.00   |
| 1   | C     | 1   | ALA  | N-CA-C   | -7.91 | 88.86       | 111.00   |
| 1   | D     | 89  | LEU  | N-CA-C   | -7.90 | 103.64      | 113.20   |
| 1   | B     | 133 | LYS  | O-C-N    | -7.89 | 113.53      | 123.24   |
| 1   | D     | 80  | SER  | O-C-N    | -7.89 | 115.40      | 123.29   |
| 1   | C     | 29  | ILE  | O-C-N    | -7.88 | 114.75      | 123.03   |
| 1   | D     | 38  | GLY  | O-C-N    | -7.88 | 112.45      | 122.70   |
| 1   | B     | 40  | PHE  | O-C-N    | -7.83 | 113.81      | 123.44   |
| 1   | A     | 73  | ASP  | O-C-N    | -7.81 | 113.08      | 122.22   |
| 1   | B     | 32  | SER  | O-C-N    | -7.80 | 113.33      | 123.16   |
| 1   | D     | 98  | SER  | O-C-N    | -7.79 | 113.02      | 123.15   |
| 1   | A     | 29  | ILE  | O-C-N    | -7.78 | 114.85      | 123.26   |
| 1   | D     | 28  | GLN  | O-C-N    | -7.76 | 114.57      | 123.42   |
| 1   | D     | 63  | LYS  | O-C-N    | -7.71 | 113.49      | 122.89   |
| 1   | B     | 68  | GLU  | O-C-N    | -7.70 | 114.19      | 123.27   |
| 1   | A     | 64  | ASN  | O-C-N    | -7.69 | 113.47      | 123.16   |
| 1   | C     | 103 | THR  | O-C-N    | -7.69 | 112.81      | 123.11   |
| 1   | B     | 134 | GLY  | O-C-N    | -7.68 | 114.70      | 123.61   |
| 1   | A     | 148 | SER  | O-C-N    | -7.66 | 115.63      | 123.29   |
| 1   | D     | 3   | GLN  | O-C-N    | -7.66 | 112.33      | 122.97   |
| 1   | B     | 57  | THR  | N-CA-C   | 7.63  | 122.45      | 110.32   |
| 1   | C     | 63  | LYS  | O-C-N    | -7.63 | 114.09      | 122.79   |
| 1   | D     | 108 | THR  | O-C-N    | -7.62 | 113.23      | 123.14   |
| 1   | C     | 36  | ALA  | O-C-N    | -7.61 | 114.34      | 123.10   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 114 | ASP  | N-CA-C   | 7.61  | 121.64      | 109.24   |
| 1   | C     | 9   | SER  | N-CA-C   | -7.59 | 94.63       | 110.80   |
| 1   | B     | 19  | ASP  | O-C-N    | -7.59 | 114.11      | 123.44   |
| 1   | B     | 88  | ALA  | N-CA-C   | -7.59 | 94.64       | 110.80   |
| 1   | B     | 144 | GLY  | O-C-N    | -7.59 | 116.69      | 123.29   |
| 1   | C     | 55  | LYS  | O-C-N    | -7.57 | 114.59      | 123.22   |
| 1   | C     | 38  | GLY  | O-C-N    | -7.57 | 112.87      | 122.70   |
| 1   | C     | 81  | GLY  | N-CA-C   | 7.56  | 131.10      | 113.18   |
| 1   | A     | 75  | PHE  | O-C-N    | -7.52 | 114.83      | 123.33   |
| 1   | A     | 17  | GLY  | O-C-N    | -7.52 | 112.93      | 122.70   |
| 1   | C     | 102 | LYS  | O-C-N    | -7.48 | 114.50      | 123.10   |
| 1   | C     | 54  | PRO  | O-C-N    | -7.48 | 113.74      | 123.01   |
| 1   | D     | 144 | GLY  | O-C-N    | -7.48 | 112.98      | 122.70   |
| 1   | B     | 63  | LYS  | O-C-N    | -7.47 | 114.05      | 122.86   |
| 1   | D     | 113 | GLY  | O-C-N    | -7.47 | 114.19      | 123.37   |
| 1   | B     | 123 | PRO  | O-C-N    | -7.46 | 113.73      | 123.13   |
| 1   | A     | 33  | TYR  | O-C-N    | -7.45 | 114.53      | 123.10   |
| 1   | C     | 67  | ILE  | O-C-N    | -7.45 | 113.91      | 122.62   |
| 1   | B     | 62  | TYR  | O-C-N    | -7.44 | 114.62      | 123.03   |
| 1   | B     | 124 | ILE  | O-C-N    | -7.43 | 115.18      | 123.20   |
| 1   | B     | 117 | GLY  | O-C-N    | -7.42 | 113.05      | 122.70   |
| 1   | D     | 72  | PRO  | CA-N-CD  | -7.42 | 101.61      | 112.00   |
| 1   | D     | 42  | VAL  | O-C-N    | -7.42 | 115.06      | 123.00   |
| 1   | C     | 57  | THR  | O-C-N    | -7.41 | 114.64      | 122.94   |
| 1   | A     | 140 | LEU  | O-C-N    | -7.36 | 113.96      | 123.02   |
| 1   | B     | 18  | TRP  | O-C-N    | -7.36 | 114.73      | 123.27   |
| 1   | D     | 65  | VAL  | O-C-N    | -7.36 | 114.55      | 123.09   |
| 1   | D     | 119 | TYR  | O-C-N    | -7.35 | 114.34      | 123.01   |
| 1   | B     | 86  | PHE  | O-C-N    | -7.34 | 113.74      | 123.14   |
| 1   | D     | 26  | ILE  | O-C-N    | -7.34 | 115.47      | 123.18   |
| 1   | D     | 119 | TYR  | CA-CB-CG | 7.34  | 127.11      | 113.90   |
| 1   | C     | 48  | GLY  | CA-C-O   | 7.33  | 126.06      | 119.83   |
| 1   | B     | 5   | ILE  | O-C-N    | -7.33 | 114.69      | 122.68   |
| 1   | C     | 40  | PHE  | O-C-N    | -7.33 | 114.57      | 123.36   |
| 1   | A     | 37  | ILE  | O-C-N    | -7.30 | 115.19      | 122.93   |
| 1   | C     | 7   | VAL  | O-C-N    | -7.30 | 115.30      | 123.18   |
| 1   | C     | 138 | ASP  | N-CA-C   | -7.29 | 104.36      | 113.55   |
| 1   | B     | 118 | THR  | O-C-N    | -7.29 | 114.18      | 122.93   |
| 1   | D     | 18  | TRP  | O-C-N    | -7.29 | 114.38      | 123.27   |
| 1   | B     | 42  | VAL  | O-C-N    | -7.29 | 115.71      | 123.14   |
| 1   | D     | 94  | PRO  | O-C-N    | -7.28 | 114.36      | 123.10   |
| 1   | B     | 78  | SER  | O-C-N    | -7.27 | 115.19      | 123.48   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 60  | LEU  | CA-C-N | 7.25  | 128.91      | 119.84   |
| 1   | A     | 60  | LEU  | C-N-CA | 7.25  | 128.91      | 119.84   |
| 1   | B     | 64  | ASN  | O-C-N  | -7.25 | 113.80      | 123.23   |
| 1   | C     | 15  | GLY  | O-C-N  | -7.23 | 116.03      | 122.90   |
| 1   | D     | 146 | HIS  | O-C-N  | -7.21 | 114.80      | 123.10   |
| 1   | A     | 107 | ARG  | O-C-N  | -7.21 | 113.95      | 122.89   |
| 1   | C     | 113 | GLY  | O-C-N  | -7.21 | 113.94      | 122.87   |
| 1   | B     | 74  | GLU  | O-C-N  | -7.20 | 114.73      | 123.30   |
| 1   | D     | 11  | GLY  | O-C-N  | -7.18 | 113.37      | 122.70   |
| 1   | C     | 77  | GLU  | O-C-N  | -7.15 | 113.97      | 122.27   |
| 1   | A     | 135 | ARG  | O-C-N  | -7.15 | 113.85      | 123.15   |
| 1   | A     | 8   | GLY  | CA-C-N | 7.14  | 135.18      | 121.54   |
| 1   | A     | 8   | GLY  | C-N-CA | 7.14  | 135.18      | 121.54   |
| 1   | D     | 103 | THR  | O-C-N  | -7.14 | 113.89      | 123.10   |
| 1   | A     | 119 | TYR  | N-CA-C | 7.13  | 120.66      | 109.96   |
| 1   | D     | 96  | VAL  | O-C-N  | -7.12 | 114.86      | 122.83   |
| 1   | D     | 57  | THR  | O-C-N  | -7.10 | 114.92      | 123.16   |
| 1   | C     | 82  | TYR  | O-C-N  | 7.09  | 132.01      | 122.59   |
| 1   | B     | 106 | GLY  | O-C-N  | -7.07 | 114.06      | 122.33   |
| 1   | D     | 75  | PHE  | O-C-N  | -7.06 | 115.20      | 123.25   |
| 1   | B     | 115 | GLU  | O-C-N  | -7.05 | 113.21      | 122.59   |
| 1   | C     | 148 | SER  | O-C-N  | -7.05 | 115.86      | 123.26   |
| 1   | A     | 143 | ILE  | O-C-N  | -7.04 | 115.57      | 123.10   |
| 1   | B     | 126 | ASN  | O-C-N  | -7.04 | 116.44      | 123.62   |
| 1   | D     | 78  | SER  | O-C-N  | -7.04 | 115.37      | 123.33   |
| 1   | C     | 142 | ALA  | O-C-N  | -7.04 | 115.38      | 123.33   |
| 1   | D     | 135 | ARG  | O-C-N  | -7.03 | 114.69      | 123.27   |
| 1   | A     | 8   | GLY  | N-CA-C | 7.01  | 118.50      | 111.21   |
| 1   | A     | 28  | GLN  | O-C-N  | -7.00 | 114.85      | 123.33   |
| 1   | A     | 31  | LEU  | O-C-N  | -7.00 | 113.72      | 123.11   |
| 1   | B     | 28  | GLN  | O-C-N  | -7.00 | 115.44      | 123.42   |
| 1   | C     | 20  | GLU  | O-C-N  | -7.00 | 113.66      | 122.27   |
| 1   | A     | 10  | TRP  | O-C-N  | -7.00 | 114.72      | 123.05   |
| 1   | B     | 22  | SER  | O-C-N  | -7.00 | 114.13      | 123.23   |
| 1   | A     | 131 | GLY  | O-C-N  | -7.00 | 116.80      | 123.87   |
| 1   | D     | 47  | ASN  | O-C-N  | -6.99 | 114.19      | 122.58   |
| 1   | C     | 10  | TRP  | O-C-N  | -6.97 | 114.56      | 122.93   |
| 1   | C     | 146 | HIS  | O-C-N  | -6.97 | 114.37      | 123.16   |
| 1   | B     | 65  | VAL  | O-C-N  | -6.96 | 115.55      | 123.00   |
| 1   | C     | 137 | GLY  | O-C-N  | -6.95 | 113.66      | 122.70   |
| 1   | C     | 28  | GLN  | O-C-N  | -6.95 | 115.48      | 123.33   |
| 1   | B     | 4   | THR  | O-C-N  | -6.93 | 113.82      | 123.11   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | C     | 79  | VAL  | O-C-N    | -6.93 | 115.69      | 123.10   |
| 1   | C     | 34  | LYS  | O-C-N    | -6.92 | 113.38      | 122.59   |
| 1   | B     | 33  | TYR  | O-C-N    | 6.91  | 130.81      | 123.42   |
| 1   | C     | 45  | ASP  | O-C-N    | -6.91 | 115.14      | 123.29   |
| 1   | C     | 78  | SER  | O-C-N    | -6.87 | 113.45      | 122.59   |
| 1   | B     | 71  | PHE  | CA-CB-CG | -6.86 | 106.94      | 113.80   |
| 1   | C     | 101 | PHE  | O-C-N    | -6.86 | 115.31      | 123.27   |
| 1   | D     | 33  | TYR  | O-C-N    | -6.86 | 115.44      | 123.25   |
| 1   | D     | 37  | ILE  | O-C-N    | -6.83 | 115.18      | 122.83   |
| 1   | D     | 54  | PRO  | O-C-N    | -6.83 | 113.42      | 122.64   |
| 1   | B     | 31  | LEU  | O-C-N    | -6.83 | 115.62      | 123.33   |
| 1   | B     | 81  | GLY  | N-CA-C   | 6.80  | 129.31      | 113.18   |
| 1   | A     | 88  | ALA  | N-CA-C   | -6.80 | 96.31       | 110.80   |
| 1   | A     | 124 | ILE  | O-C-N    | -6.80 | 113.97      | 122.88   |
| 1   | B     | 80  | SER  | O-C-N    | -6.79 | 113.37      | 122.74   |
| 1   | A     | 68  | GLU  | O-C-N    | -6.78 | 115.45      | 122.64   |
| 1   | C     | 39  | SER  | O-C-N    | -6.78 | 115.12      | 122.85   |
| 1   | A     | 82  | TYR  | CA-C-N   | 6.78  | 134.64      | 121.63   |
| 1   | A     | 82  | TYR  | C-N-CA   | 6.78  | 134.64      | 121.63   |
| 1   | D     | 82  | TYR  | N-CA-C   | 6.78  | 125.23      | 110.80   |
| 1   | C     | 2   | SER  | O-C-N    | -6.77 | 115.35      | 122.94   |
| 1   | B     | 50  | PRO  | O-C-N    | -6.77 | 114.62      | 123.01   |
| 1   | D     | 50  | PRO  | O-C-N    | -6.77 | 113.50      | 122.64   |
| 1   | A     | 32  | SER  | O-C-N    | -6.77 | 114.62      | 123.21   |
| 1   | C     | 129 | ILE  | O-C-N    | -6.76 | 115.30      | 122.67   |
| 1   | A     | 34  | LYS  | O-C-N    | -6.76 | 113.60      | 122.59   |
| 1   | C     | 32  | SER  | O-C-N    | -6.76 | 114.37      | 123.15   |
| 1   | C     | 67  | ILE  | N-CA-C   | 6.75  | 117.48      | 107.15   |
| 1   | C     | 19  | ASP  | O-C-N    | -6.74 | 114.34      | 123.24   |
| 1   | D     | 14  | GLY  | O-C-N    | -6.73 | 114.23      | 122.71   |
| 1   | C     | 58  | SER  | O-C-N    | -6.73 | 115.15      | 123.36   |
| 1   | A     | 81  | GLY  | N-CA-C   | 6.70  | 129.07      | 113.18   |
| 1   | A     | 45  | ASP  | O-C-N    | -6.70 | 115.38      | 123.29   |
| 1   | B     | 85  | PRO  | O-C-N    | -6.68 | 114.69      | 122.71   |
| 1   | D     | 69  | LEU  | O-C-N    | -6.68 | 115.23      | 122.85   |
| 1   | A     | 40  | PHE  | O-C-N    | -6.68 | 114.19      | 123.34   |
| 1   | C     | 37  | ILE  | O-C-N    | -6.68 | 115.35      | 122.83   |
| 1   | A     | 108 | THR  | O-C-N    | -6.67 | 115.41      | 123.29   |
| 1   | D     | 82  | TYR  | CA-C-N   | 6.66  | 133.51      | 122.73   |
| 1   | D     | 82  | TYR  | C-N-CA   | 6.66  | 133.51      | 122.73   |
| 1   | B     | 101 | PHE  | O-C-N    | -6.65 | 114.58      | 123.23   |
| 1   | C     | 41  | SER  | O-C-N    | -6.65 | 115.16      | 123.27   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 142 | ALA  | O-C-N  | -6.64 | 115.46      | 123.10   |
| 1   | C     | 131 | GLY  | O-C-N  | -6.64 | 114.06      | 122.70   |
| 1   | D     | 4   | THR  | O-C-N  | -6.64 | 113.58      | 122.74   |
| 1   | D     | 7   | VAL  | O-C-N  | -6.64 | 115.12      | 122.69   |
| 1   | D     | 51  | PHE  | O-C-N  | -6.63 | 115.28      | 123.44   |
| 1   | D     | 5   | ILE  | O-C-N  | -6.63 | 115.41      | 122.83   |
| 1   | C     | 64  | ASN  | O-C-N  | -6.62 | 114.38      | 123.12   |
| 1   | A     | 94  | PRO  | O-C-N  | -6.62 | 114.81      | 123.01   |
| 1   | B     | 25  | GLY  | O-C-N  | -6.61 | 115.69      | 123.55   |
| 1   | D     | 66  | LYS  | O-C-N  | -6.61 | 115.61      | 123.27   |
| 1   | A     | 51  | PHE  | O-C-N  | -6.59 | 115.60      | 123.31   |
| 1   | D     | 76  | LEU  | O-C-N  | -6.59 | 114.65      | 122.96   |
| 1   | D     | 116 | GLU  | O-C-N  | -6.59 | 115.60      | 123.31   |
| 1   | A     | 25  | GLY  | O-C-N  | -6.59 | 116.04      | 123.61   |
| 1   | B     | 57  | THR  | O-C-N  | -6.59 | 115.68      | 123.06   |
| 1   | A     | 30  | GLU  | O-C-N  | -6.58 | 114.43      | 123.12   |
| 1   | A     | 36  | ALA  | O-C-N  | -6.57 | 115.23      | 122.92   |
| 1   | A     | 66  | LYS  | O-C-N  | -6.57 | 114.87      | 123.28   |
| 1   | A     | 81  | GLY  | CA-C-N | 6.57  | 134.08      | 121.54   |
| 1   | A     | 81  | GLY  | C-N-CA | 6.57  | 134.08      | 121.54   |
| 1   | D     | 67  | ILE  | O-C-N  | -6.56 | 113.11      | 122.76   |
| 1   | C     | 60  | LEU  | CA-C-N | 6.56  | 128.04      | 119.84   |
| 1   | C     | 60  | LEU  | C-N-CA | 6.56  | 128.04      | 119.84   |
| 1   | C     | 21  | GLY  | O-C-N  | -6.55 | 115.71      | 122.98   |
| 1   | D     | 58  | SER  | O-C-N  | -6.55 | 115.87      | 123.27   |
| 1   | C     | 51  | PHE  | O-C-N  | -6.55 | 114.90      | 123.28   |
| 1   | B     | 119 | TYR  | O-C-N  | -6.54 | 114.76      | 122.81   |
| 1   | C     | 9   | SER  | CA-C-N | -6.54 | 113.72      | 122.42   |
| 1   | C     | 9   | SER  | C-N-CA | -6.54 | 113.72      | 122.42   |
| 1   | B     | 121 | ASN  | O-C-N  | -6.52 | 115.42      | 123.44   |
| 1   | B     | 36  | ALA  | O-C-N  | -6.52 | 114.75      | 122.96   |
| 1   | D     | 39  | SER  | O-C-N  | -6.52 | 115.60      | 123.10   |
| 1   | C     | 106 | GLY  | CA-C-O | 6.51  | 125.37      | 119.83   |
| 1   | C     | 83  | THR  | O-C-N  | -6.51 | 115.72      | 123.27   |
| 1   | A     | 120 | PHE  | O-C-N  | -6.50 | 115.34      | 123.27   |
| 1   | C     | 115 | GLU  | O-C-N  | -6.46 | 114.00      | 122.59   |
| 1   | C     | 120 | PHE  | O-C-N  | -6.46 | 115.77      | 123.27   |
| 1   | C     | 75  | PHE  | O-C-N  | -6.46 | 115.35      | 123.17   |
| 1   | C     | 108 | THR  | O-C-N  | -6.46 | 114.59      | 123.12   |
| 1   | B     | 73  | ASP  | O-C-N  | -6.46 | 113.00      | 122.43   |
| 1   | D     | 77  | GLU  | O-C-N  | -6.46 | 114.43      | 122.24   |
| 1   | B     | 24  | THR  | O-C-N  | -6.45 | 115.24      | 122.34   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | B     | 102 | LYS  | O-C-N    | -6.45 | 115.76      | 123.31   |
| 1   | D     | 85  | PRO  | O-C-N    | -6.44 | 115.12      | 122.91   |
| 1   | C     | 136 | THR  | O-C-N    | -6.43 | 114.49      | 123.11   |
| 1   | D     | 131 | GLY  | O-C-N    | -6.42 | 114.35      | 122.70   |
| 1   | A     | 109 | PHE  | CA-CB-CG | -6.42 | 107.38      | 113.80   |
| 1   | B     | 8   | GLY  | N-CA-C   | 6.42  | 119.34      | 111.45   |
| 1   | C     | 119 | TYR  | O-C-N    | -6.41 | 115.88      | 123.06   |
| 1   | A     | 125 | GLU  | O-C-N    | -6.41 | 113.61      | 122.46   |
| 1   | A     | 9   | SER  | CA-C-N   | -6.41 | 114.51      | 122.84   |
| 1   | A     | 9   | SER  | C-N-CA   | -6.41 | 114.51      | 122.84   |
| 1   | B     | 135 | ARG  | O-C-N    | -6.41 | 114.86      | 123.19   |
| 1   | A     | 140 | LEU  | N-CA-C   | -6.40 | 99.46       | 109.25   |
| 1   | A     | 110 | GLY  | N-CA-C   | 6.40  | 125.39      | 112.34   |
| 1   | D     | 15  | GLY  | O-C-N    | -6.39 | 116.83      | 122.90   |
| 1   | C     | 94  | PRO  | O-C-N    | -6.39 | 115.30      | 123.03   |
| 1   | A     | 16  | ASN  | O-C-N    | -6.37 | 115.82      | 123.27   |
| 1   | D     | 73  | ASP  | O-C-N    | -6.37 | 115.37      | 122.12   |
| 1   | B     | 130 | VAL  | O-C-N    | -6.37 | 115.15      | 122.09   |
| 1   | B     | 99  | LEU  | O-C-N    | -6.36 | 114.62      | 123.34   |
| 1   | A     | 147 | MET  | O-C-N    | -6.36 | 114.90      | 123.10   |
| 1   | B     | 15  | GLY  | O-C-N    | -6.36 | 114.56      | 123.02   |
| 1   | A     | 100 | THR  | O-C-N    | -6.36 | 115.79      | 123.10   |
| 1   | D     | 43  | ILE  | O-C-N    | -6.36 | 114.58      | 122.97   |
| 1   | C     | 128 | LEU  | O-C-N    | -6.35 | 115.61      | 123.36   |
| 1   | A     | 65  | VAL  | O-C-N    | -6.35 | 115.85      | 123.02   |
| 1   | A     | 48  | GLY  | O-C-N    | -6.33 | 115.72      | 122.56   |
| 1   | C     | 145 | ILE  | O-C-N    | -6.32 | 116.24      | 123.00   |
| 1   | B     | 66  | LYS  | O-C-N    | -6.32 | 115.81      | 123.27   |
| 1   | D     | 101 | PHE  | O-C-N    | -6.31 | 116.14      | 123.27   |
| 1   | D     | 137 | GLY  | O-C-N    | -6.30 | 114.51      | 122.70   |
| 1   | B     | 107 | ARG  | O-C-N    | -6.30 | 116.15      | 123.27   |
| 1   | C     | 22  | SER  | O-C-N    | -6.30 | 115.22      | 123.16   |
| 1   | B     | 34  | LYS  | CA-C-N   | 6.29  | 133.15      | 122.26   |
| 1   | B     | 34  | LYS  | C-N-CA   | 6.29  | 133.15      | 122.26   |
| 1   | C     | 42  | VAL  | O-C-N    | -6.29 | 116.37      | 123.10   |
| 1   | C     | 116 | GLU  | O-C-N    | -6.29 | 115.05      | 123.23   |
| 1   | D     | 129 | ILE  | N-CA-C   | -6.29 | 100.88      | 109.37   |
| 1   | A     | 35  | GLU  | O-C-N    | -6.29 | 114.19      | 122.42   |
| 1   | B     | 61  | PRO  | O-C-N    | -6.28 | 114.17      | 122.64   |
| 1   | B     | 103 | THR  | O-C-N    | -6.28 | 116.03      | 123.06   |
| 1   | A     | 72  | PRO  | CA-N-CD  | -6.27 | 103.22      | 112.00   |
| 1   | D     | 19  | ASP  | O-C-N    | -6.27 | 114.84      | 123.12   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 88  | ALA  | N-CA-C   | -6.27 | 97.45       | 110.80   |
| 1   | B     | 136 | THR  | O-C-N    | -6.26 | 116.08      | 123.41   |
| 1   | B     | 141 | ASP  | O-C-N    | -6.26 | 115.48      | 122.12   |
| 1   | C     | 86  | PHE  | O-C-N    | -6.26 | 114.54      | 123.06   |
| 1   | A     | 105 | LYS  | O-C-N    | -6.26 | 113.12      | 122.39   |
| 1   | A     | 42  | VAL  | O-C-N    | -6.26 | 116.30      | 123.00   |
| 1   | B     | 8   | GLY  | CA-C-O   | 6.25  | 126.14      | 120.64   |
| 1   | B     | 148 | SER  | O-C-N    | -6.24 | 116.71      | 123.26   |
| 1   | A     | 102 | LYS  | O-C-N    | -6.24 | 115.96      | 122.94   |
| 1   | D     | 16  | ASN  | O-C-N    | -6.24 | 115.12      | 123.23   |
| 1   | D     | 105 | LYS  | O-C-N    | -6.24 | 113.33      | 122.43   |
| 1   | D     | 126 | ASN  | O-C-N    | -6.23 | 114.80      | 123.34   |
| 1   | B     | 55  | LYS  | O-C-N    | -6.23 | 115.92      | 122.96   |
| 1   | A     | 130 | VAL  | O-C-N    | -6.23 | 114.79      | 122.57   |
| 1   | D     | 123 | PRO  | O-C-N    | -6.22 | 114.24      | 122.64   |
| 1   | C     | 96  | VAL  | N-CA-CB  | 6.22  | 118.09      | 112.06   |
| 1   | C     | 96  | VAL  | O-C-N    | -6.21 | 115.47      | 122.36   |
| 1   | A     | 74  | GLU  | O-C-N    | -6.21 | 115.91      | 123.30   |
| 1   | B     | 120 | PHE  | O-C-N    | -6.20 | 115.82      | 123.33   |
| 1   | C     | 80  | SER  | O-C-N    | -6.20 | 115.14      | 122.96   |
| 1   | A     | 35  | GLU  | CA-C-O   | 6.19  | 126.21      | 119.15   |
| 1   | B     | 37  | ILE  | O-C-N    | -6.18 | 114.81      | 122.97   |
| 1   | C     | 85  | PRO  | O-C-N    | -6.17 | 114.31      | 122.64   |
| 1   | B     | 118 | THR  | CA-C-O   | 6.17  | 127.18      | 120.58   |
| 1   | D     | 30  | GLU  | O-C-N    | -6.17 | 113.62      | 122.99   |
| 1   | C     | 120 | PHE  | CA-CB-CG | 6.15  | 119.95      | 113.80   |
| 1   | C     | 139 | LEU  | CA-CB-CG | 6.15  | 137.83      | 116.30   |
| 1   | B     | 72  | PRO  | O-C-N    | -6.15 | 114.34      | 122.64   |
| 1   | B     | 91  | THR  | CA-C-N   | 6.14  | 126.03      | 119.28   |
| 1   | B     | 91  | THR  | C-N-CA   | 6.14  | 126.03      | 119.28   |
| 1   | A     | 71  | PHE  | N-CA-C   | 6.14  | 123.37      | 109.81   |
| 1   | C     | 59  | LYS  | O-C-N    | -6.13 | 114.21      | 122.43   |
| 1   | A     | 19  | ASP  | O-C-N    | -6.13 | 115.03      | 123.12   |
| 1   | D     | 134 | GLY  | O-C-N    | -6.13 | 117.89      | 123.96   |
| 1   | C     | 44  | TYR  | N-CA-C   | 6.11  | 117.93      | 110.41   |
| 1   | C     | 132 | PHE  | O-C-N    | -6.11 | 115.45      | 123.21   |
| 1   | A     | 62  | TYR  | O-C-N    | -6.10 | 115.77      | 122.84   |
| 1   | A     | 14  | GLY  | O-C-N    | -6.08 | 116.83      | 122.79   |
| 1   | D     | 44  | TYR  | O-C-N    | -6.07 | 115.58      | 122.68   |
| 1   | B     | 94  | PRO  | O-C-N    | -6.07 | 115.73      | 123.14   |
| 1   | A     | 104 | ASN  | O-C-N    | -6.07 | 114.81      | 122.27   |
| 1   | C     | 69  | LEU  | O-C-N    | -6.06 | 115.94      | 122.85   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 67  | ILE  | O-C-N    | -6.05 | 114.99      | 122.97   |
| 1   | D     | 36  | ALA  | O-C-N    | -6.05 | 115.34      | 122.96   |
| 1   | B     | 9   | SER  | CA-C-N   | -6.04 | 113.44      | 122.39   |
| 1   | B     | 9   | SER  | C-N-CA   | -6.04 | 113.44      | 122.39   |
| 1   | A     | 112 | TYR  | O-C-N    | -6.04 | 116.26      | 123.27   |
| 1   | A     | 4   | THR  | O-C-N    | -6.04 | 115.35      | 122.96   |
| 1   | C     | 100 | THR  | O-C-N    | -6.04 | 115.91      | 123.27   |
| 1   | A     | 41  | SER  | O-C-N    | -6.03 | 116.52      | 123.33   |
| 1   | A     | 103 | THR  | O-C-N    | -6.02 | 115.33      | 123.15   |
| 1   | B     | 39  | SER  | O-C-N    | -6.02 | 116.16      | 122.96   |
| 1   | B     | 3   | GLN  | O-C-N    | -6.00 | 115.36      | 123.10   |
| 1   | B     | 147 | MET  | N-CA-C   | 6.00  | 118.30      | 109.24   |
| 1   | D     | 23  | TYR  | O-C-N    | -6.00 | 114.61      | 122.59   |
| 1   | C     | 46  | LEU  | O-C-N    | -6.00 | 113.85      | 122.96   |
| 1   | C     | 114 | ASP  | O-C-N    | -5.99 | 116.19      | 122.96   |
| 1   | D     | 64  | ASN  | O-C-N    | -5.99 | 115.61      | 123.16   |
| 1   | A     | 71  | PHE  | C-N-CD   | -5.99 | 100.44      | 125.00   |
| 1   | B     | 10  | TRP  | O-C-N    | -5.99 | 115.61      | 123.28   |
| 1   | B     | 16  | ASN  | O-C-N    | -5.99 | 116.50      | 123.27   |
| 1   | B     | 45  | ASP  | O-C-N    | -5.99 | 116.33      | 123.27   |
| 1   | A     | 35  | GLU  | N-CA-C   | -5.96 | 106.05      | 113.38   |
| 1   | B     | 114 | ASP  | N-CA-C   | 5.96  | 118.36      | 109.25   |
| 1   | C     | 53  | GLY  | N-CA-C   | -5.94 | 104.79      | 112.10   |
| 1   | B     | 116 | GLU  | O-C-N    | -5.94 | 116.36      | 123.31   |
| 1   | D     | 117 | GLY  | O-C-N    | -5.93 | 113.68      | 122.70   |
| 1   | D     | 140 | LEU  | O-C-N    | -5.93 | 115.82      | 122.93   |
| 1   | B     | 71  | PHE  | N-CA-C   | 5.92  | 118.20      | 109.50   |
| 1   | C     | 44  | TYR  | O-C-N    | -5.92 | 115.43      | 122.65   |
| 1   | C     | 18  | TRP  | O-C-N    | -5.91 | 115.47      | 123.15   |
| 1   | C     | 141 | ASP  | O-C-N    | -5.90 | 114.42      | 122.33   |
| 1   | C     | 16  | ASN  | O-C-N    | -5.89 | 115.71      | 123.13   |
| 1   | B     | 125 | GLU  | O-C-N    | -5.87 | 114.02      | 122.36   |
| 1   | D     | 73  | ASP  | N-CA-C   | 5.87  | 117.68      | 111.28   |
| 1   | A     | 11  | GLY  | O-C-N    | -5.87 | 115.07      | 122.70   |
| 1   | B     | 27  | ARG  | O-C-N    | -5.87 | 113.33      | 122.13   |
| 1   | A     | 69  | LEU  | O-C-N    | -5.87 | 115.60      | 122.81   |
| 1   | C     | 25  | GLY  | O-C-N    | -5.85 | 116.88      | 123.61   |
| 1   | C     | 121 | ASN  | O-C-N    | -5.85 | 115.52      | 123.24   |
| 1   | B     | 100 | THR  | O-C-N    | -5.85 | 116.34      | 123.30   |
| 1   | A     | 126 | ASN  | O-C-N    | -5.85 | 116.01      | 123.26   |
| 1   | B     | 109 | PHE  | CA-CB-CG | -5.85 | 107.95      | 113.80   |
| 1   | C     | 8   | GLY  | N-CA-C   | 5.84  | 123.35      | 112.77   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 127 | GLY  | O-C-N  | -5.83 | 115.63      | 123.67   |
| 1   | D     | 52  | SER  | O-C-N  | -5.82 | 116.43      | 123.13   |
| 1   | A     | 39  | SER  | O-C-N  | -5.82 | 116.54      | 123.06   |
| 1   | B     | 70  | LYS  | O-C-N  | 5.81  | 130.38      | 122.82   |
| 1   | B     | 71  | PHE  | CA-C-O | -5.81 | 113.99      | 119.80   |
| 1   | A     | 133 | LYS  | O-C-N  | -5.81 | 114.63      | 122.94   |
| 1   | B     | 29  | ILE  | O-C-N  | -5.81 | 115.39      | 122.36   |
| 1   | B     | 51  | PHE  | O-C-N  | -5.81 | 115.59      | 123.14   |
| 1   | B     | 41  | SER  | O-C-N  | -5.81 | 116.06      | 123.26   |
| 1   | D     | 145 | ILE  | N-CA-C | 5.80  | 116.48      | 108.12   |
| 1   | B     | 60  | LEU  | CA-C-N | 5.80  | 127.09      | 119.84   |
| 1   | B     | 60  | LEU  | C-N-CA | 5.80  | 127.09      | 119.84   |
| 1   | D     | 107 | ARG  | O-C-N  | -5.80 | 115.90      | 122.97   |
| 1   | C     | 17  | GLY  | CA-C-O | 5.79  | 126.50      | 121.41   |
| 1   | A     | 121 | ASN  | O-C-N  | -5.79 | 116.64      | 123.41   |
| 1   | C     | 135 | ARG  | O-C-N  | -5.78 | 116.33      | 123.44   |
| 1   | B     | 138 | ASP  | O-C-N  | -5.78 | 114.61      | 122.36   |
| 1   | A     | 61  | PRO  | O-C-N  | -5.78 | 114.84      | 122.64   |
| 1   | D     | 102 | LYS  | O-C-N  | -5.78 | 116.43      | 123.19   |
| 1   | A     | 96  | VAL  | O-C-N  | -5.78 | 115.86      | 122.62   |
| 1   | C     | 50  | PRO  | O-C-N  | -5.78 | 115.96      | 123.06   |
| 1   | C     | 4   | THR  | O-C-N  | -5.75 | 116.21      | 123.17   |
| 1   | B     | 6   | THR  | O-C-N  | -5.71 | 115.42      | 122.68   |
| 1   | B     | 88  | ALA  | O-C-N  | -5.71 | 114.99      | 122.59   |
| 1   | C     | 107 | ARG  | O-C-N  | -5.71 | 115.87      | 122.95   |
| 1   | C     | 143 | ILE  | O-C-N  | -5.71 | 116.91      | 123.07   |
| 1   | B     | 52  | SER  | O-C-N  | -5.70 | 115.78      | 122.96   |
| 1   | A     | 56  | HIS  | N-CA-C | -5.70 | 101.74      | 109.54   |
| 1   | C     | 15  | GLY  | N-CA-C | 5.69  | 122.84      | 112.37   |
| 1   | B     | 30  | GLU  | O-C-N  | -5.68 | 116.43      | 123.36   |
| 1   | C     | 105 | LYS  | O-C-N  | -5.67 | 114.15      | 122.43   |
| 1   | A     | 50  | PRO  | O-C-N  | -5.67 | 115.92      | 123.06   |
| 1   | D     | 99  | LEU  | O-C-N  | -5.66 | 116.25      | 123.26   |
| 1   | D     | 121 | ASN  | O-C-N  | -5.65 | 115.60      | 123.34   |
| 1   | A     | 3   | GLN  | O-C-N  | -5.64 | 115.21      | 122.20   |
| 1   | A     | 18  | TRP  | O-C-N  | -5.64 | 116.48      | 123.36   |
| 1   | C     | 14  | GLY  | O-C-N  | -5.63 | 114.35      | 122.69   |
| 1   | A     | 76  | LEU  | O-C-N  | -5.62 | 116.23      | 122.86   |
| 1   | B     | 87  | SER  | O-C-N  | -5.62 | 115.13      | 122.43   |
| 1   | C     | 66  | LYS  | O-C-N  | -5.61 | 115.95      | 123.14   |
| 1   | B     | 143 | ILE  | O-C-N  | -5.61 | 117.01      | 123.07   |
| 1   | D     | 119 | TYR  | N-CA-C | 5.61  | 119.06      | 110.20   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 115 | GLU  | O-C-N   | -5.61 | 115.14      | 122.59   |
| 1   | B     | 137 | GLY  | O-C-N   | -5.60 | 115.42      | 122.70   |
| 1   | B     | 105 | LYS  | O-C-N   | -5.60 | 114.64      | 122.37   |
| 1   | A     | 13  | PRO  | O-C-N   | -5.60 | 114.69      | 122.30   |
| 1   | B     | 131 | GLY  | O-C-N   | -5.59 | 115.43      | 122.70   |
| 1   | B     | 35  | GLU  | N-CA-C  | -5.59 | 106.50      | 113.38   |
| 1   | C     | 126 | ASN  | O-C-N   | -5.59 | 116.57      | 123.44   |
| 1   | C     | 52  | SER  | O-C-N   | -5.59 | 116.15      | 123.02   |
| 1   | D     | 62  | TYR  | O-C-N   | -5.58 | 114.96      | 122.94   |
| 1   | D     | 70  | LYS  | N-CA-C  | -5.57 | 98.19       | 107.99   |
| 1   | D     | 43  | ILE  | CA-C-O  | 5.57  | 126.66      | 120.59   |
| 1   | A     | 136 | THR  | O-C-N   | -5.56 | 115.72      | 123.34   |
| 1   | C     | 31  | LEU  | O-C-N   | -5.56 | 115.07      | 122.74   |
| 1   | B     | 114 | ASP  | O-C-N   | -5.55 | 116.19      | 123.02   |
| 1   | C     | 11  | GLY  | O-C-N   | -5.54 | 115.49      | 122.70   |
| 1   | B     | 59  | LYS  | O-C-N   | -5.54 | 115.00      | 122.43   |
| 1   | A     | 128 | LEU  | O-C-N   | -5.53 | 116.40      | 123.26   |
| 1   | A     | 71  | PHE  | CA-C-N  | 5.52  | 126.74      | 119.84   |
| 1   | A     | 71  | PHE  | C-N-CA  | 5.52  | 126.74      | 119.84   |
| 1   | D     | 148 | SER  | O-C-N   | -5.51 | 115.62      | 122.73   |
| 1   | A     | 146 | HIS  | O-C-N   | -5.51 | 116.22      | 123.28   |
| 1   | A     | 82  | TYR  | N-CA-C  | 5.50  | 122.52      | 110.80   |
| 1   | B     | 130 | VAL  | N-CA-CB | -5.50 | 105.01      | 112.16   |
| 1   | D     | 79  | VAL  | O-C-N   | -5.50 | 116.95      | 123.05   |
| 1   | D     | 90  | ALA  | N-CA-C  | -5.49 | 104.65      | 111.90   |
| 1   | A     | 64  | ASN  | N-CA-C  | 5.48  | 118.67      | 109.95   |
| 1   | C     | 140 | LEU  | O-C-N   | -5.48 | 116.53      | 123.05   |
| 1   | A     | 116 | GLU  | O-C-N   | -5.48 | 116.25      | 123.21   |
| 1   | C     | 72  | PRO  | O-C-N   | -5.47 | 115.25      | 122.64   |
| 1   | A     | 20  | GLU  | O-C-N   | -5.46 | 114.92      | 122.46   |
| 1   | B     | 89  | LEU  | O-C-N   | -5.46 | 115.34      | 122.39   |
| 1   | D     | 21  | GLY  | O-C-N   | -5.46 | 116.71      | 123.21   |
| 1   | A     | 118 | THR  | O-C-N   | -5.46 | 117.10      | 123.27   |
| 1   | A     | 44  | TYR  | O-C-N   | -5.45 | 115.94      | 122.65   |
| 1   | C     | 65  | VAL  | CB-CA-C | -5.45 | 103.75      | 111.38   |
| 1   | C     | 30  | GLU  | O-C-N   | -5.45 | 116.05      | 123.24   |
| 1   | A     | 38  | GLY  | O-C-N   | -5.44 | 115.62      | 122.70   |
| 1   | B     | 128 | LEU  | O-C-N   | -5.44 | 115.89      | 123.34   |
| 1   | C     | 23  | TYR  | O-C-N   | -5.44 | 115.36      | 122.59   |
| 1   | A     | 52  | SER  | O-C-N   | -5.44 | 116.41      | 122.93   |
| 1   | B     | 46  | LEU  | O-C-N   | -5.44 | 116.86      | 123.27   |
| 1   | A     | 46  | LEU  | O-C-N   | -5.43 | 114.83      | 122.87   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 54  | PRO  | O-C-N   | -5.43 | 116.34      | 122.91   |
| 1   | C     | 26  | ILE  | O-C-N   | -5.43 | 115.81      | 122.97   |
| 1   | D     | 114 | ASP  | CA-C-O  | 5.42  | 126.34      | 120.43   |
| 1   | D     | 67  | ILE  | CA-C-N  | -5.42 | 115.35      | 122.99   |
| 1   | D     | 67  | ILE  | C-N-CA  | -5.42 | 115.35      | 122.99   |
| 1   | A     | 137 | GLY  | O-C-N   | -5.40 | 115.68      | 122.70   |
| 1   | B     | 103 | THR  | N-CA-C  | 5.39  | 118.89      | 110.32   |
| 1   | C     | 123 | PRO  | O-C-N   | -5.39 | 115.36      | 122.64   |
| 1   | D     | 112 | TYR  | O-C-N   | -5.38 | 116.36      | 123.13   |
| 1   | D     | 111 | PRO  | O-C-N   | -5.38 | 115.38      | 122.64   |
| 1   | D     | 61  | PRO  | O-C-N   | -5.37 | 115.39      | 122.64   |
| 1   | A     | 119 | TYR  | O-C-N   | -5.37 | 116.33      | 122.93   |
| 1   | A     | 34  | LYS  | N-CA-C  | -5.36 | 99.39       | 110.80   |
| 1   | D     | 77  | GLU  | N-CA-C  | -5.35 | 106.13      | 113.30   |
| 1   | A     | 114 | ASP  | N-CA-CB | 5.34  | 118.57      | 109.87   |
| 1   | C     | 9   | SER  | O-C-N   | -5.32 | 115.51      | 122.59   |
| 1   | C     | 27  | ARG  | O-C-N   | -5.32 | 114.43      | 122.20   |
| 1   | D     | 20  | GLU  | O-C-N   | -5.30 | 115.33      | 122.43   |
| 1   | A     | 129 | ILE  | O-C-N   | -5.30 | 117.27      | 122.67   |
| 1   | D     | 138 | ASP  | N-CA-C  | -5.28 | 104.44      | 112.04   |
| 1   | C     | 97  | ARG  | O-C-N   | -5.27 | 116.64      | 122.07   |
| 1   | D     | 120 | PHE  | O-C-N   | -5.27 | 116.05      | 123.11   |
| 1   | B     | 64  | ASN  | N-CA-C  | 5.26  | 117.98      | 109.40   |
| 1   | D     | 6   | THR  | O-C-N   | -5.26 | 116.17      | 123.01   |
| 1   | A     | 59  | LYS  | N-CA-C  | -5.25 | 106.02      | 112.90   |
| 1   | A     | 106 | GLY  | O-C-N   | -5.24 | 115.89      | 122.70   |
| 1   | C     | 35  | GLU  | O-C-N   | -5.24 | 115.56      | 122.42   |
| 1   | C     | 118 | THR  | O-C-N   | -5.24 | 117.04      | 122.96   |
| 1   | B     | 77  | GLU  | O-C-N   | -5.24 | 115.90      | 122.24   |
| 1   | A     | 87  | SER  | O-C-N   | -5.23 | 115.36      | 122.48   |
| 1   | C     | 76  | LEU  | O-C-N   | -5.23 | 116.44      | 122.87   |
| 1   | A     | 83  | THR  | O-C-N   | -5.22 | 117.63      | 123.48   |
| 1   | C     | 70  | LYS  | O-C-N   | -5.22 | 116.24      | 122.46   |
| 1   | B     | 8   | GLY  | CA-C-N  | -5.20 | 111.61      | 121.54   |
| 1   | B     | 8   | GLY  | C-N-CA  | -5.20 | 111.61      | 121.54   |
| 1   | C     | 113 | GLY  | N-CA-C  | -5.20 | 106.04      | 112.33   |
| 1   | D     | 139 | LEU  | O-C-N   | -5.19 | 115.58      | 122.59   |
| 1   | B     | 145 | ILE  | O-C-N   | -5.19 | 117.08      | 123.00   |
| 1   | B     | 140 | LEU  | O-C-N   | -5.18 | 115.26      | 122.41   |
| 1   | D     | 57  | THR  | N-CA-C  | 5.18  | 118.66      | 109.96   |
| 1   | D     | 81  | GLY  | N-CA-C  | 5.18  | 125.45      | 113.18   |
| 1   | A     | 9   | SER  | O-C-N   | 5.17  | 129.47      | 122.59   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 48  | GLY  | CA-C-O  | 5.17  | 124.65      | 119.27   |
| 1   | B     | 48  | GLY  | O-C-N   | -5.16 | 116.11      | 122.46   |
| 1   | B     | 3   | GLN  | N-CA-C  | 5.16  | 118.13      | 110.14   |
| 1   | B     | 75  | PHE  | O-C-N   | -5.16 | 117.37      | 123.25   |
| 1   | D     | 143 | ILE  | N-CA-C  | 5.15  | 116.14      | 108.46   |
| 1   | D     | 2   | SER  | O-C-N   | -5.15 | 114.77      | 123.00   |
| 1   | B     | 129 | ILE  | N-CA-C  | -5.14 | 102.05      | 108.84   |
| 1   | C     | 65  | VAL  | O-C-N   | -5.14 | 116.19      | 122.36   |
| 1   | B     | 9   | SER  | CB-CA-C | 5.14  | 120.64      | 110.42   |
| 1   | B     | 9   | SER  | CA-C-O  | -5.13 | 113.17      | 120.51   |
| 1   | D     | 12  | GLY  | CA-C-N  | 5.13  | 125.82      | 120.12   |
| 1   | D     | 12  | GLY  | C-N-CA  | 5.13  | 125.82      | 120.12   |
| 1   | C     | 99  | LEU  | O-C-N   | -5.13 | 115.77      | 122.59   |
| 1   | C     | 62  | TYR  | O-C-N   | -5.13 | 115.84      | 122.97   |
| 1   | A     | 85  | PRO  | O-C-N   | -5.12 | 115.72      | 122.64   |
| 1   | D     | 97  | ARG  | O-C-N   | -5.12 | 114.75      | 122.28   |
| 1   | C     | 13  | PRO  | CA-C-O  | 5.12  | 125.23      | 118.98   |
| 1   | B     | 13  | PRO  | O-C-N   | -5.12 | 114.34      | 122.52   |
| 1   | C     | 17  | GLY  | N-CA-C  | 5.11  | 117.34      | 111.36   |
| 1   | B     | 24  | THR  | N-CA-C  | -5.11 | 107.72      | 114.31   |
| 1   | D     | 147 | MET  | O-C-N   | -5.08 | 117.37      | 123.27   |
| 1   | A     | 57  | THR  | N-CA-C  | 5.08  | 117.79      | 110.28   |
| 1   | A     | 101 | PHE  | N-CA-C  | 5.07  | 117.05      | 108.02   |
| 1   | A     | 133 | LYS  | N-CA-CB | -5.07 | 103.44      | 111.05   |
| 1   | A     | 6   | THR  | O-C-N   | -5.07 | 116.76      | 122.84   |
| 1   | D     | 114 | ASP  | N-CA-CB | 5.06  | 118.68      | 110.43   |
| 1   | C     | 92  | PRO  | CA-C-N  | 5.06  | 127.68      | 120.49   |
| 1   | C     | 92  | PRO  | C-N-CA  | 5.06  | 127.68      | 120.49   |
| 1   | A     | 88  | ALA  | O-C-N   | -5.05 | 115.87      | 122.59   |
| 1   | D     | 115 | GLU  | O-C-N   | -5.05 | 115.88      | 122.59   |
| 1   | C     | 8   | GLY  | CA-C-N  | 5.04  | 131.17      | 121.54   |
| 1   | C     | 8   | GLY  | C-N-CA  | 5.04  | 131.17      | 121.54   |
| 1   | A     | 72  | PRO  | O-C-N   | -5.04 | 115.84      | 122.64   |
| 1   | C     | 82  | TYR  | N-CA-C  | 5.04  | 121.53      | 110.80   |
| 1   | D     | 106 | GLY  | O-C-N   | -5.04 | 116.15      | 122.70   |
| 1   | C     | 61  | PRO  | O-C-N   | -5.03 | 115.85      | 122.64   |
| 1   | C     | 130 | VAL  | O-C-N   | -5.02 | 116.29      | 122.57   |
| 1   | C     | 34  | LYS  | N-CA-C  | -5.01 | 100.13      | 110.80   |
| 1   | B     | 47  | ASN  | O-C-N   | -5.00 | 116.86      | 122.86   |
| 1   | B     | 47  | ASN  | N-CA-C  | 5.00  | 118.22      | 111.17   |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 1   | ALA  | CA   |
| 1   | B     | 1   | ALA  | CA   |
| 1   | C     | 1   | ALA  | CA   |
| 1   | D     | 1   | ALA  | CA   |

All (21) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 114 | ASP  | Mainchain         |
| 1   | A     | 81  | GLY  | Mainchain,Peptide |
| 1   | A     | 82  | TYR  | Mainchain         |
| 1   | A     | 9   | SER  | Mainchain         |
| 1   | B     | 109 | PHE  | Mainchain         |
| 1   | B     | 34  | LYS  | Mainchain         |
| 1   | B     | 71  | PHE  | Mainchain,Peptide |
| 1   | B     | 8   | GLY  | Peptide           |
| 1   | B     | 81  | GLY  | Mainchain,Peptide |
| 1   | C     | 72  | PRO  | Mainchain         |
| 1   | C     | 8   | GLY  | Mainchain,Peptide |
| 1   | C     | 9   | SER  | Mainchain         |
| 1   | C     | 94  | PRO  | Mainchain         |
| 1   | D     | 119 | TYR  | Sidechain         |
| 1   | D     | 71  | PHE  | Mainchain         |
| 1   | D     | 8   | GLY  | Mainchain,Peptide |

## 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     | 1119  | 0        | 1061     | 77      | 0            |
| 1   | B     | 1118  | 0        | 1059     | 73      | 0            |
| 1   | C     | 1126  | 0        | 1076     | 48      | 0            |
| 1   | D     | 1123  | 0        | 1064     | 69      | 0            |
| 2   | A     | 102   | 0        | 0        | 9       | 0            |
| 2   | B     | 112   | 0        | 0        | 7       | 0            |
| 2   | C     | 105   | 0        | 0        | 6       | 0            |
| 2   | D     | 112   | 0        | 0        | 9       | 0            |
| All | All   | 4917  | 0        | 4260     | 253     | 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 29.

All (253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:70:LYS:C     | 1:B:71:PHE:N     | 1.75                     | 1.44              |
| 1:B:82:TYR:HE2   | 1:B:115:GLU:HG3  | 1.10                     | 1.14              |
| 1:B:82:TYR:CE2   | 1:B:115:GLU:HG3  | 1.92                     | 1.05              |
| 1:C:72:PRO:HD3   | 2:C:171:HOH:O    | 1.62                     | 0.99              |
| 1:A:82:TYR:N     | 1:A:82:TYR:CD1   | 2.26                     | 0.99              |
| 1:A:55:LYS:HG2   | 2:A:166:HOH:O    | 1.66                     | 0.95              |
| 1:A:20:GLU:HG2   | 1:A:54:PRO:HD2   | 1.54                     | 0.88              |
| 1:A:82:TYR:N     | 1:A:82:TYR:HD1   | 1.67                     | 0.87              |
| 1:A:22:SER:H     | 1:C:47:ASN:HD21  | 1.23                     | 0.86              |
| 1:A:82:TYR:CE1   | 1:A:115:GLU:HG3  | 2.09                     | 0.86              |
| 1:A:82:TYR:HD1   | 1:A:82:TYR:H     | 0.88                     | 0.85              |
| 1:B:57:THR:HG23  | 2:B:170:HOH:O    | 1.80                     | 0.82              |
| 1:A:27:ARG:HG2   | 1:A:27:ARG:HH11  | 1.44                     | 0.81              |
| 1:D:74:GLU:HA    | 1:D:104:ASN:HD21 | 1.47                     | 0.80              |
| 1:B:20:GLU:HG2   | 1:B:54:PRO:HD2   | 1.65                     | 0.78              |
| 1:A:23:TYR:O     | 1:A:130:VAL:HG22 | 1.83                     | 0.77              |
| 1:C:102:LYS:CE   | 1:C:108:THR:HB   | 2.14                     | 0.77              |
| 1:B:140:LEU:HD21 | 1:B:143:ILE:HD12 | 1.66                     | 0.77              |
| 1:D:45:ASP:CG    | 1:D:71:PHE:CE2   | 2.63                     | 0.77              |
| 1:A:82:TYR:CZ    | 1:A:115:GLU:HG3  | 2.21                     | 0.76              |
| 1:B:74:GLU:HA    | 1:B:104:ASN:HD21 | 1.48                     | 0.76              |
| 1:D:78:SER:HB3   | 1:D:102:LYS:HB2  | 1.68                     | 0.75              |
| 1:B:82:TYR:CE1   | 1:B:119:TYR:HB2  | 2.22                     | 0.75              |
| 1:C:102:LYS:HE2  | 1:C:108:THR:HB   | 1.70                     | 0.73              |
| 1:D:11:GLY:HA2   | 1:D:83:THR:HG21  | 1.71                     | 0.73              |
| 1:D:45:ASP:CG    | 1:D:71:PHE:HE2   | 1.96                     | 0.73              |
| 1:C:107:ARG:HD2  | 2:C:248:HOH:O    | 1.89                     | 0.73              |
| 1:B:103:THR:HG22 | 1:B:105:LYS:H    | 1.55                     | 0.71              |
| 1:B:45:ASP:OD2   | 1:B:71:PHE:CE2   | 2.44                     | 0.71              |
| 1:D:74:GLU:OE2   | 1:D:103:THR:HG21 | 1.91                     | 0.69              |
| 1:B:75:PHE:H     | 1:B:104:ASN:ND2  | 1.91                     | 0.69              |
| 1:C:8:GLY:HA2    | 1:D:123:PRO:HD2  | 1.75                     | 0.68              |
| 1:B:41:SER:CB    | 1:B:55:LYS:HD2   | 2.23                     | 0.68              |
| 1:A:27:ARG:HG2   | 1:A:27:ARG:NH1   | 2.07                     | 0.68              |
| 1:C:74:GLU:OE2   | 1:C:103:THR:HG21 | 1.94                     | 0.68              |
| 1:A:18:TRP:HH2   | 1:A:140:LEU:HD13 | 1.59                     | 0.67              |
| 1:A:75:PHE:HA    | 2:A:158:HOH:O    | 1.95                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:37:ILE:O     | 1:A:139:LEU:HB3  | 1.94                     | 0.67              |
| 1:A:9:SER:O      | 2:A:154:HOH:O    | 2.13                     | 0.67              |
| 1:A:74:GLU:OE2   | 1:A:107:ARG:HD3  | 1.95                     | 0.66              |
| 1:B:74:GLU:OE2   | 1:B:103:THR:HG21 | 1.94                     | 0.66              |
| 1:A:41:SER:HB2   | 1:A:55:LYS:HD2   | 1.75                     | 0.66              |
| 1:C:73:ASP:HB3   | 1:C:105:LYS:HE2  | 1.77                     | 0.66              |
| 1:C:66:LYS:HD2   | 2:C:240:HOH:O    | 1.94                     | 0.65              |
| 1:D:83:THR:HB    | 2:D:200:HOH:O    | 1.96                     | 0.65              |
| 1:D:58:SER:HB2   | 1:D:138:ASP:O    | 1.97                     | 0.65              |
| 1:D:67:ILE:HG23  | 1:D:109:PHE:CE2  | 2.31                     | 0.65              |
| 1:D:71:PHE:O     | 1:D:72:PRO:HG2   | 1.97                     | 0.65              |
| 1:D:129:ILE:HG23 | 2:D:216:HOH:O    | 1.96                     | 0.65              |
| 1:B:45:ASP:CG    | 1:B:71:PHE:CE2   | 2.77                     | 0.63              |
| 1:D:60:LEU:HD23  | 1:D:139:LEU:HD13 | 1.78                     | 0.63              |
| 1:D:26:ILE:HD12  | 1:D:26:ILE:N     | 2.13                     | 0.63              |
| 1:B:124:ILE:HG21 | 1:B:147:MET:HE1  | 1.80                     | 0.63              |
| 1:B:8:GLY:O      | 1:B:9:SER:CB     | 2.48                     | 0.62              |
| 1:A:18:TRP:CH2   | 1:A:140:LEU:HD13 | 2.35                     | 0.61              |
| 1:A:71:PHE:O     | 1:A:72:PRO:HG2   | 2.01                     | 0.61              |
| 1:A:141:ASP:HB3  | 2:A:173:HOH:O    | 1.99                     | 0.60              |
| 1:D:95:VAL:HG13  | 1:D:140:LEU:O    | 2.01                     | 0.60              |
| 1:C:147:MET:HB3  | 1:D:5:ILE:HD13   | 1.82                     | 0.60              |
| 1:D:71:PHE:CG    | 1:D:72:PRO:HD2   | 2.37                     | 0.60              |
| 1:A:13:PRO:HD2   | 1:A:94:PRO:HD2   | 1.83                     | 0.59              |
| 1:A:98:SER:O     | 1:A:99:LEU:HB2   | 2.02                     | 0.59              |
| 1:A:135:ARG:HG3  | 1:A:142:ALA:HB3  | 1.85                     | 0.59              |
| 1:C:82:TYR:HA    | 1:C:118:THR:O    | 2.02                     | 0.58              |
| 1:D:135:ARG:HG3  | 2:D:171:HOH:O    | 2.02                     | 0.58              |
| 1:C:65:VAL:HG11  | 1:C:112:TYR:CZ   | 2.39                     | 0.58              |
| 1:C:18:TRP:CD1   | 1:C:18:TRP:C     | 2.81                     | 0.58              |
| 1:D:71:PHE:O     | 1:D:72:PRO:CG    | 2.52                     | 0.58              |
| 1:A:74:GLU:OE2   | 1:A:103:THR:HG21 | 2.04                     | 0.58              |
| 1:C:82:TYR:CE1   | 1:C:119:TYR:HB2  | 2.39                     | 0.58              |
| 1:A:31:LEU:HD13  | 1:A:37:ILE:HD12  | 1.85                     | 0.57              |
| 1:C:28:GLN:O     | 1:C:42:VAL:HG23  | 2.05                     | 0.57              |
| 1:D:82:TYR:CE1   | 1:D:115:GLU:HG3  | 2.39                     | 0.57              |
| 1:C:103:THR:HG23 | 1:C:105:LYS:H    | 1.70                     | 0.56              |
| 1:C:102:LYS:HE3  | 1:C:108:THR:HB   | 1.86                     | 0.56              |
| 1:D:71:PHE:O     | 1:D:73:ASP:N     | 2.39                     | 0.56              |
| 1:C:98:SER:HB2   | 1:C:114:ASP:O    | 2.06                     | 0.56              |
| 1:A:103:THR:HB   | 1:A:107:ARG:O    | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:35:GLU:HA    | 1:C:114:ASP:OD1  | 2.06                     | 0.56              |
| 1:D:30:GLU:HG3   | 1:D:66:LYS:HG3   | 1.87                     | 0.55              |
| 1:D:107:ARG:HD2  | 2:D:190:HOH:O    | 2.06                     | 0.55              |
| 1:D:59:LYS:HE3   | 2:D:183:HOH:O    | 2.06                     | 0.55              |
| 1:A:71:PHE:CG    | 1:A:72:PRO:CD    | 2.90                     | 0.55              |
| 1:D:90:ALA:O     | 1:D:92:PRO:HD3   | 2.07                     | 0.55              |
| 1:C:60:LEU:HD22  | 1:C:60:LEU:H     | 1.72                     | 0.55              |
| 1:C:71:PHE:CG    | 1:C:71:PHE:O     | 2.60                     | 0.55              |
| 1:C:74:GLU:HA    | 1:C:104:ASN:HD21 | 1.72                     | 0.55              |
| 1:D:95:VAL:HG22  | 1:D:141:ASP:HA   | 1.88                     | 0.55              |
| 1:A:91:THR:HG23  | 2:A:172:HOH:O    | 2.07                     | 0.55              |
| 1:D:37:ILE:HG13  | 1:D:96:VAL:HG23  | 1.89                     | 0.55              |
| 1:B:82:TYR:O     | 1:B:97:ARG:HB2   | 2.07                     | 0.54              |
| 1:C:71:PHE:O     | 1:C:71:PHE:CD1   | 2.59                     | 0.54              |
| 1:A:23:TYR:CE2   | 1:A:51:PHE:CD2   | 2.95                     | 0.54              |
| 1:C:108:THR:HG22 | 2:C:254:HOH:O    | 2.06                     | 0.54              |
| 1:B:128:LEU:HD23 | 1:D:2:SER:HB3    | 1.89                     | 0.54              |
| 1:B:40:PHE:O     | 1:B:56:HIS:HB2   | 2.08                     | 0.54              |
| 1:D:35:GLU:HA    | 1:D:114:ASP:OD1  | 2.07                     | 0.54              |
| 1:D:103:THR:HG23 | 1:D:105:LYS:H    | 1.73                     | 0.54              |
| 1:B:34:LYS:HD3   | 1:B:62:TYR:CD1   | 2.43                     | 0.54              |
| 1:A:41:SER:OG    | 1:A:55:LYS:HE3   | 2.08                     | 0.54              |
| 1:D:67:ILE:HG23  | 1:D:109:PHE:CD2  | 2.43                     | 0.53              |
| 1:B:76:LEU:HD22  | 1:B:76:LEU:H     | 1.74                     | 0.53              |
| 1:A:71:PHE:O     | 1:A:73:ASP:N     | 2.41                     | 0.53              |
| 1:C:17:GLY:HA2   | 1:C:135:ARG:HG2  | 1.90                     | 0.53              |
| 1:A:9:SER:HA     | 1:A:143:ILE:O    | 2.09                     | 0.53              |
| 1:B:123:PRO:HB3  | 2:B:216:HOH:O    | 2.08                     | 0.52              |
| 1:D:88:ALA:H     | 1:D:90:ALA:H     | 1.57                     | 0.52              |
| 1:C:103:THR:CG2  | 1:C:105:LYS:H    | 2.22                     | 0.52              |
| 1:B:18:TRP:CD1   | 1:B:18:TRP:C     | 2.87                     | 0.52              |
| 1:C:32:SER:HA    | 1:C:63:LYS:O     | 2.09                     | 0.52              |
| 1:A:71:PHE:CG    | 1:A:72:PRO:HD2   | 2.45                     | 0.52              |
| 1:D:114:ASP:HB3  | 2:D:258:HOH:O    | 2.10                     | 0.52              |
| 1:A:48:GLY:HA2   | 2:A:241:HOH:O    | 2.09                     | 0.52              |
| 1:C:35:GLU:HB2   | 1:C:86:PHE:CZ    | 2.44                     | 0.51              |
| 1:D:124:ILE:HD13 | 1:D:147:MET:HE3  | 1.93                     | 0.51              |
| 1:A:149:LEU:O    | 1:C:2:SER:HB2    | 2.11                     | 0.51              |
| 1:B:103:THR:CG2  | 1:B:105:LYS:H    | 2.22                     | 0.51              |
| 1:C:118:THR:HA   | 2:C:208:HOH:O    | 2.10                     | 0.51              |
| 1:B:114:ASP:HA   | 2:B:194:HOH:O    | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:25:GLY:C     | 1:D:26:ILE:HD12  | 2.36                     | 0.50              |
| 1:A:7:VAL:HG23   | 1:B:124:ILE:CG2  | 2.42                     | 0.50              |
| 1:D:133:LYS:HE2  | 2:D:170:HOH:O    | 2.09                     | 0.50              |
| 1:A:50:PRO:HD2   | 2:A:165:HOH:O    | 2.11                     | 0.50              |
| 1:B:77:GLU:O     | 1:B:124:ILE:HG12 | 2.12                     | 0.50              |
| 1:A:74:GLU:HA    | 1:A:104:ASN:HD21 | 1.77                     | 0.50              |
| 1:B:8:GLY:O      | 1:B:9:SER:HB3    | 2.12                     | 0.50              |
| 1:D:89:LEU:CB    | 2:D:249:HOH:O    | 2.58                     | 0.50              |
| 1:A:22:SER:H     | 1:C:47:ASN:ND2   | 2.01                     | 0.50              |
| 1:A:8:GLY:HA2    | 1:B:123:PRO:HG2  | 1.94                     | 0.49              |
| 1:A:67:ILE:HG23  | 1:A:109:PHE:CD2  | 2.47                     | 0.49              |
| 1:D:38:GLY:C     | 1:D:58:SER:HB3   | 2.36                     | 0.49              |
| 1:A:45:ASP:CG    | 1:A:71:PHE:CE2   | 2.91                     | 0.49              |
| 1:A:34:LYS:HB2   | 1:A:62:TYR:CD1   | 2.48                     | 0.49              |
| 1:B:41:SER:HB3   | 1:B:55:LYS:HA    | 1.93                     | 0.49              |
| 1:A:64:ASN:HB3   | 2:A:167:HOH:O    | 2.11                     | 0.49              |
| 1:B:59:LYS:HB2   | 2:B:261:HOH:O    | 2.11                     | 0.49              |
| 1:A:71:PHE:CD2   | 1:A:72:PRO:CD    | 2.96                     | 0.49              |
| 1:A:71:PHE:CB    | 1:A:72:PRO:HD2   | 2.42                     | 0.49              |
| 1:D:109:PHE:CD1  | 1:D:109:PHE:N    | 2.80                     | 0.49              |
| 1:B:41:SER:HB2   | 1:B:55:LYS:HD2   | 1.94                     | 0.49              |
| 1:B:82:TYR:CD2   | 1:B:115:GLU:HA   | 2.47                     | 0.49              |
| 1:B:41:SER:HB3   | 1:B:55:LYS:HD2   | 1.93                     | 0.49              |
| 1:C:87:SER:O     | 1:C:88:ALA:HB2   | 2.13                     | 0.48              |
| 1:B:18:TRP:CE2   | 1:B:56:HIS:CD2   | 3.02                     | 0.48              |
| 1:A:71:PHE:O     | 1:A:72:PRO:CG    | 2.62                     | 0.48              |
| 1:D:132:PHE:CE1  | 1:D:145:ILE:HD11 | 2.49                     | 0.48              |
| 1:A:127:GLY:O    | 1:A:128:LEU:CD1  | 2.61                     | 0.48              |
| 1:D:71:PHE:CD2   | 1:D:72:PRO:HD2   | 2.50                     | 0.47              |
| 1:D:75:PHE:H     | 1:D:104:ASN:ND2  | 2.12                     | 0.47              |
| 1:B:26:ILE:HD13  | 1:B:129:ILE:O    | 2.15                     | 0.47              |
| 1:A:106:GLY:O    | 1:A:107:ARG:C    | 2.57                     | 0.47              |
| 1:A:124:ILE:HG23 | 1:A:147:MET:HE1  | 1.95                     | 0.47              |
| 1:A:11:GLY:HA3   | 1:A:142:ALA:HA   | 1.97                     | 0.47              |
| 1:A:145:ILE:HG23 | 1:A:146:HIS:N    | 2.28                     | 0.47              |
| 1:B:29:ILE:HG22  | 1:B:30:GLU:N     | 2.30                     | 0.47              |
| 1:B:81:GLY:HA3   | 1:B:120:PHE:CE2  | 2.50                     | 0.47              |
| 1:B:103:THR:HG22 | 1:B:105:LYS:N    | 2.28                     | 0.47              |
| 1:C:60:LEU:HD22  | 1:C:60:LEU:N     | 2.28                     | 0.47              |
| 1:B:21:GLY:HA2   | 2:B:164:HOH:O    | 2.15                     | 0.47              |
| 1:B:81:GLY:O     | 1:B:98:SER:HB3   | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:88:ALA:H     | 1:A:90:ALA:H     | 1.63                     | 0.46              |
| 1:B:124:ILE:CG2  | 1:B:147:MET:HE1  | 2.45                     | 0.46              |
| 1:D:41:SER:HB3   | 1:D:55:LYS:HA    | 1.96                     | 0.46              |
| 1:D:28:GLN:HG3   | 1:D:68:GLU:HB3   | 1.97                     | 0.46              |
| 1:A:8:GLY:CA     | 1:B:123:PRO:HG2  | 2.45                     | 0.46              |
| 1:A:21:GLY:HA3   | 1:C:47:ASN:ND2   | 2.29                     | 0.46              |
| 1:D:45:ASP:CB    | 1:D:71:PHE:CE2   | 2.99                     | 0.46              |
| 1:A:5:ILE:HD12   | 1:B:5:ILE:HD12   | 1.98                     | 0.46              |
| 1:D:81:GLY:O     | 1:D:98:SER:O     | 2.34                     | 0.46              |
| 1:A:126:ASN:HB3  | 1:B:6:THR:H      | 1.81                     | 0.45              |
| 1:A:91:THR:OG1   | 1:A:93:THR:HG23  | 2.16                     | 0.45              |
| 1:A:33:TYR:O     | 1:A:63:LYS:N     | 2.48                     | 0.45              |
| 1:B:70:LYS:CA    | 1:B:71:PHE:N     | 2.72                     | 0.45              |
| 1:D:82:TYR:CE2   | 1:D:119:TYR:HB2  | 2.51                     | 0.45              |
| 1:D:87:SER:O     | 1:D:88:ALA:HB2   | 2.16                     | 0.45              |
| 1:D:118:THR:HG22 | 2:D:248:HOH:O    | 2.15                     | 0.45              |
| 1:B:102:LYS:HG3  | 1:B:108:THR:HB   | 1.99                     | 0.45              |
| 1:A:46:LEU:HD23  | 1:C:51:PHE:CE2   | 2.52                     | 0.45              |
| 1:D:79:VAL:HG22  | 1:D:101:PHE:CD2  | 2.52                     | 0.45              |
| 1:A:23:TYR:HE2   | 1:A:51:PHE:CD2   | 2.35                     | 0.45              |
| 1:A:114:ASP:C    | 1:A:116:GLU:H    | 2.25                     | 0.45              |
| 1:B:130:VAL:O    | 1:B:130:VAL:HG13 | 2.16                     | 0.45              |
| 1:D:18:TRP:CD1   | 1:D:18:TRP:C     | 2.95                     | 0.45              |
| 1:C:102:LYS:HE3  | 1:C:108:THR:CB   | 2.47                     | 0.45              |
| 1:C:132:PHE:CE1  | 1:C:145:ILE:HD11 | 2.52                     | 0.45              |
| 1:A:79:VAL:HG13  | 1:A:101:PHE:CE1  | 2.52                     | 0.44              |
| 1:D:60:LEU:HD23  | 1:D:139:LEU:CD1  | 2.46                     | 0.44              |
| 1:B:11:GLY:HA3   | 1:B:142:ALA:HA   | 1.98                     | 0.44              |
| 1:B:27:ARG:CZ    | 1:B:71:PHE:CD2   | 3.00                     | 0.44              |
| 1:D:33:TYR:N     | 1:D:33:TYR:CD1   | 2.85                     | 0.44              |
| 1:D:44:TYR:OH    | 1:D:132:PHE:N    | 2.48                     | 0.44              |
| 1:A:114:ASP:C    | 1:A:116:GLU:N    | 2.75                     | 0.44              |
| 1:A:127:GLY:O    | 1:A:128:LEU:HD12 | 2.17                     | 0.44              |
| 1:B:42:VAL:HG11  | 1:B:132:PHE:HD2  | 1.82                     | 0.44              |
| 1:B:33:TYR:CD2   | 1:B:113:GLY:N    | 2.86                     | 0.44              |
| 1:B:45:ASP:OD2   | 1:B:71:PHE:HE2   | 1.98                     | 0.44              |
| 1:C:121:ASN:ND2  | 2:C:210:HOH:O    | 2.50                     | 0.44              |
| 1:D:71:PHE:CG    | 1:D:72:PRO:CD    | 3.00                     | 0.44              |
| 1:A:71:PHE:CD2   | 1:A:72:PRO:HD2   | 2.53                     | 0.44              |
| 1:B:33:TYR:HD2   | 1:B:113:GLY:H    | 1.63                     | 0.44              |
| 1:B:74:GLU:CD    | 1:B:103:THR:HG21 | 2.42                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:82:TYR:O     | 1:B:97:ARG:N     | 2.47                     | 0.44              |
| 1:D:27:ARG:NH1   | 1:D:27:ARG:HG2   | 2.33                     | 0.44              |
| 1:B:124:ILE:HG21 | 1:B:147:MET:CE   | 2.47                     | 0.44              |
| 1:C:33:TYR:CD1   | 1:C:33:TYR:C     | 2.96                     | 0.44              |
| 1:C:33:TYR:N     | 1:C:62:TYR:HB3   | 2.33                     | 0.44              |
| 1:D:45:ASP:HB2   | 1:D:71:PHE:CE2   | 2.53                     | 0.43              |
| 1:D:110:GLY:O    | 1:D:111:PRO:C    | 2.61                     | 0.43              |
| 1:A:78:SER:HB3   | 1:A:102:LYS:CB   | 2.47                     | 0.43              |
| 1:B:89:LEU:O     | 1:B:90:ALA:C     | 2.58                     | 0.43              |
| 1:D:13:PRO:HD2   | 1:D:93:THR:OG1   | 2.19                     | 0.43              |
| 1:B:13:PRO:HD2   | 1:B:94:PRO:HD2   | 2.00                     | 0.43              |
| 1:B:42:VAL:HG11  | 1:B:132:PHE:CD2  | 2.54                     | 0.43              |
| 1:B:60:LEU:HA    | 1:B:61:PRO:HD3   | 1.86                     | 0.43              |
| 1:A:8:GLY:C      | 1:B:123:PRO:HG2  | 2.43                     | 0.43              |
| 1:C:98:SER:O     | 1:C:99:LEU:HB2   | 2.19                     | 0.42              |
| 1:A:98:SER:HA    | 1:A:112:TYR:O    | 2.19                     | 0.42              |
| 1:B:88:ALA:C     | 1:B:90:ALA:H     | 2.27                     | 0.42              |
| 1:D:89:LEU:C     | 1:D:91:THR:N     | 2.76                     | 0.42              |
| 1:B:27:ARG:CZ    | 1:B:71:PHE:HD2   | 2.32                     | 0.42              |
| 1:B:23:TYR:HE2   | 1:B:51:PHE:CD1   | 2.37                     | 0.42              |
| 1:D:26:ILE:N     | 1:D:26:ILE:CD1   | 2.83                     | 0.42              |
| 1:D:27:ARG:HG2   | 1:D:27:ARG:HH11  | 1.85                     | 0.42              |
| 1:B:33:TYR:HD2   | 1:B:113:GLY:N    | 2.18                     | 0.42              |
| 1:A:60:LEU:HD22  | 1:A:60:LEU:H     | 1.85                     | 0.42              |
| 1:C:74:GLU:HA    | 1:C:104:ASN:ND2  | 2.35                     | 0.42              |
| 1:C:45:ASP:CG    | 1:C:71:PHE:CZ    | 2.98                     | 0.42              |
| 1:D:114:ASP:O    | 1:D:116:GLU:N    | 2.50                     | 0.41              |
| 1:C:33:TYR:H     | 1:C:62:TYR:HB3   | 1.86                     | 0.41              |
| 1:C:80:SER:O     | 1:C:99:LEU:HD12  | 2.21                     | 0.41              |
| 1:A:18:TRP:O     | 1:A:18:TRP:CG    | 2.71                     | 0.41              |
| 1:A:103:THR:HG23 | 1:A:105:LYS:H    | 1.84                     | 0.41              |
| 1:A:18:TRP:CD1   | 1:A:56:HIS:NE2   | 2.88                     | 0.41              |
| 1:D:89:LEU:O     | 1:D:90:ALA:C     | 2.62                     | 0.41              |
| 1:A:110:GLY:HA3  | 2:A:181:HOH:O    | 2.21                     | 0.41              |
| 1:B:27:ARG:NH1   | 1:B:71:PHE:HB3   | 2.36                     | 0.41              |
| 1:D:21:GLY:O     | 1:D:131:GLY:HA3  | 2.21                     | 0.41              |
| 1:D:26:ILE:CD1   | 1:D:129:ILE:HG22 | 2.51                     | 0.41              |
| 1:A:110:GLY:O    | 1:A:111:PRO:C    | 2.62                     | 0.41              |
| 1:B:34:LYS:HB2   | 1:B:62:TYR:CD1   | 2.56                     | 0.41              |
| 1:B:88:ALA:H     | 1:B:90:ALA:H     | 1.67                     | 0.41              |
| 1:A:140:LEU:HD21 | 1:A:143:ILE:HD12 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:44:TYR:CE1   | 1:B:131:GLY:HA2 | 2.56                     | 0.41              |
| 1:C:82:TYR:CZ    | 1:C:119:TYR:HB2 | 2.55                     | 0.41              |
| 1:D:82:TYR:CD1   | 1:D:115:GLU:HG3 | 2.55                     | 0.41              |
| 1:C:122:LEU:HD12 | 1:C:122:LEU:HA  | 1.76                     | 0.41              |
| 1:D:41:SER:CB    | 1:D:55:LYS:HA   | 2.50                     | 0.41              |
| 1:B:21:GLY:O     | 1:B:131:GLY:HA3 | 2.21                     | 0.40              |
| 1:B:41:SER:HA    | 2:B:169:HOH:O   | 2.20                     | 0.40              |
| 1:B:119:TYR:HB3  | 2:B:151:HOH:O   | 2.21                     | 0.40              |
| 1:A:60:LEU:HA    | 1:A:61:PRO:HD3  | 1.72                     | 0.40              |
| 1:D:18:TRP:HE1   | 1:D:20:GLU:HG3  | 1.86                     | 0.40              |
| 1:C:26:ILE:HD12  | 1:C:26:ILE:N    | 2.37                     | 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     | 146/149 (98%) | 124 (85%) | 13 (9%) | 9 (6%)   |  |  |
| 1   | B     | 147/149 (99%) | 130 (88%) | 11 (8%) | 6 (4%)   |  |  |
| 1   | C     | 147/149 (99%) | 129 (88%) | 9 (6%)  | 9 (6%)   |  |  |
| 1   | D     | 146/149 (98%) | 128 (88%) | 10 (7%) | 8 (6%)   |  |  |
| All | All   | 586/596 (98%) | 511 (87%) | 43 (7%) | 32 (6%)  |  |  |

All (32) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 71  | PHE  |
| 1   | A     | 72  | PRO  |
| 1   | A     | 82  | TYR  |
| 1   | A     | 99  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 110 | GLY  |
| 1   | A     | 115 | GLU  |
| 1   | B     | 72  | PRO  |
| 1   | B     | 115 | GLU  |
| 1   | C     | 9   | SER  |
| 1   | C     | 71  | PHE  |
| 1   | C     | 82  | TYR  |
| 1   | C     | 88  | ALA  |
| 1   | D     | 72  | PRO  |
| 1   | D     | 82  | TYR  |
| 1   | D     | 115 | GLU  |
| 1   | A     | 88  | ALA  |
| 1   | B     | 82  | TYR  |
| 1   | B     | 110 | GLY  |
| 1   | C     | 72  | PRO  |
| 1   | C     | 110 | GLY  |
| 1   | D     | 71  | PHE  |
| 1   | D     | 81  | GLY  |
| 1   | D     | 88  | ALA  |
| 1   | D     | 110 | GLY  |
| 1   | A     | 34  | LYS  |
| 1   | B     | 88  | ALA  |
| 1   | C     | 81  | GLY  |
| 1   | C     | 137 | GLY  |
| 1   | C     | 61  | PRO  |
| 1   | B     | 9   | SER  |
| 1   | D     | 61  | PRO  |
| 1   | A     | 81  | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|----------|-------------|---|
| 1   | A     | 117/122 (96%) | 87 (74%)  | 30 (26%) | 0           | 1 |
| 1   | B     | 117/122 (96%) | 84 (72%)  | 33 (28%) | 0           | 0 |
| 1   | C     | 119/122 (98%) | 90 (76%)  | 29 (24%) | 1           | 1 |

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| Mol | Chain | Analysed      | Rotameric | Outliers  | Percentiles |   |
|-----|-------|---------------|-----------|-----------|-------------|---|
| 1   | D     | 118/122 (97%) | 88 (75%)  | 30 (25%)  | 0           | 1 |
| All | All   | 471/488 (96%) | 349 (74%) | 122 (26%) | 0           | 1 |

All (122) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | THR  |
| 1   | A     | 7   | VAL  |
| 1   | A     | 9   | SER  |
| 1   | A     | 13  | PRO  |
| 1   | A     | 42  | VAL  |
| 1   | A     | 43  | ILE  |
| 1   | A     | 55  | LYS  |
| 1   | A     | 60  | LEU  |
| 1   | A     | 65  | VAL  |
| 1   | A     | 69  | LEU  |
| 1   | A     | 82  | TYR  |
| 1   | A     | 91  | THR  |
| 1   | A     | 93  | THR  |
| 1   | A     | 95  | VAL  |
| 1   | A     | 100 | THR  |
| 1   | A     | 102 | LYS  |
| 1   | A     | 103 | THR  |
| 1   | A     | 104 | ASN  |
| 1   | A     | 108 | THR  |
| 1   | A     | 115 | GLU  |
| 1   | A     | 118 | THR  |
| 1   | A     | 124 | ILE  |
| 1   | A     | 128 | LEU  |
| 1   | A     | 130 | VAL  |
| 1   | A     | 136 | THR  |
| 1   | A     | 139 | LEU  |
| 1   | A     | 140 | LEU  |
| 1   | A     | 143 | ILE  |
| 1   | A     | 145 | ILE  |
| 1   | A     | 148 | SER  |
| 1   | B     | 4   | THR  |
| 1   | B     | 5   | ILE  |
| 1   | B     | 18  | TRP  |
| 1   | B     | 24  | THR  |
| 1   | B     | 26  | ILE  |
| 1   | B     | 28  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 41  | SER  |
| 1   | B     | 49  | ASP  |
| 1   | B     | 57  | THR  |
| 1   | B     | 60  | LEU  |
| 1   | B     | 69  | LEU  |
| 1   | B     | 73  | ASP  |
| 1   | B     | 83  | THR  |
| 1   | B     | 93  | THR  |
| 1   | B     | 95  | VAL  |
| 1   | B     | 96  | VAL  |
| 1   | B     | 100 | THR  |
| 1   | B     | 102 | LYS  |
| 1   | B     | 103 | THR  |
| 1   | B     | 104 | ASN  |
| 1   | B     | 105 | LYS  |
| 1   | B     | 107 | ARG  |
| 1   | B     | 108 | THR  |
| 1   | B     | 115 | GLU  |
| 1   | B     | 118 | THR  |
| 1   | B     | 122 | LEU  |
| 1   | B     | 124 | ILE  |
| 1   | B     | 130 | VAL  |
| 1   | B     | 133 | LYS  |
| 1   | B     | 143 | ILE  |
| 1   | B     | 145 | ILE  |
| 1   | B     | 148 | SER  |
| 1   | B     | 149 | LEU  |
| 1   | C     | 7   | VAL  |
| 1   | C     | 18  | TRP  |
| 1   | C     | 42  | VAL  |
| 1   | C     | 43  | ILE  |
| 1   | C     | 49  | ASP  |
| 1   | C     | 58  | SER  |
| 1   | C     | 65  | VAL  |
| 1   | C     | 68  | GLU  |
| 1   | C     | 69  | LEU  |
| 1   | C     | 76  | LEU  |
| 1   | C     | 78  | SER  |
| 1   | C     | 95  | VAL  |
| 1   | C     | 96  | VAL  |
| 1   | C     | 100 | THR  |
| 1   | C     | 102 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 103 | THR  |
| 1   | C     | 105 | LYS  |
| 1   | C     | 108 | THR  |
| 1   | C     | 114 | ASP  |
| 1   | C     | 115 | GLU  |
| 1   | C     | 118 | THR  |
| 1   | C     | 124 | ILE  |
| 1   | C     | 128 | LEU  |
| 1   | C     | 130 | VAL  |
| 1   | C     | 139 | LEU  |
| 1   | C     | 143 | ILE  |
| 1   | C     | 145 | ILE  |
| 1   | C     | 148 | SER  |
| 1   | C     | 149 | LEU  |
| 1   | D     | 4   | THR  |
| 1   | D     | 7   | VAL  |
| 1   | D     | 9   | SER  |
| 1   | D     | 18  | TRP  |
| 1   | D     | 22  | SER  |
| 1   | D     | 26  | ILE  |
| 1   | D     | 31  | LEU  |
| 1   | D     | 42  | VAL  |
| 1   | D     | 58  | SER  |
| 1   | D     | 59  | LYS  |
| 1   | D     | 60  | LEU  |
| 1   | D     | 69  | LEU  |
| 1   | D     | 76  | LEU  |
| 1   | D     | 93  | THR  |
| 1   | D     | 96  | VAL  |
| 1   | D     | 100 | THR  |
| 1   | D     | 103 | THR  |
| 1   | D     | 104 | ASN  |
| 1   | D     | 108 | THR  |
| 1   | D     | 114 | ASP  |
| 1   | D     | 115 | GLU  |
| 1   | D     | 118 | THR  |
| 1   | D     | 128 | LEU  |
| 1   | D     | 129 | ILE  |
| 1   | D     | 130 | VAL  |
| 1   | D     | 139 | LEU  |
| 1   | D     | 140 | LEU  |
| 1   | D     | 145 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 148 | SER  |
| 1   | D     | 149 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 28  | GLN  |
| 1   | A     | 47  | ASN  |
| 1   | A     | 104 | ASN  |
| 1   | B     | 47  | ASN  |
| 1   | B     | 104 | ASN  |
| 1   | C     | 16  | ASN  |
| 1   | C     | 47  | ASN  |
| 1   | C     | 104 | ASN  |
| 1   | C     | 121 | ASN  |
| 1   | D     | 28  | GLN  |
| 1   | D     | 47  | ASN  |
| 1   | D     | 64  | ASN  |
| 1   | D     | 104 | 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | D     | 2                |
| 1   | A     | 2                |
| 1   | B     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | D     | 1:ALA     | C      | 2:SER     | N      | 3.92         |
| 1     | A     | 1:ALA     | C      | 2:SER     | N      | 3.83         |
| 1     | B     | 70:LYS    | C      | 71:PHE    | N      | 1.75         |
| 1     | D     | 82:TYR    | C      | 83:THR    | N      | 1.15         |
| 1     | A     | 82:TYR    | C      | 83:THR    | N      | 1.08         |

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 149/149 (100%) | 0.14   | 1 (0%) 84 81  | 2, 7, 20, 47          | 0     |
| 1   | B     | 149/149 (100%) | 0.29   | 8 (5%) 31 27  | 2, 9, 28, 51          | 0     |
| 1   | C     | 149/149 (100%) | 0.24   | 7 (4%) 36 32  | 2, 7, 26, 48          | 0     |
| 1   | D     | 149/149 (100%) | 0.32   | 10 (6%) 24 21 | 2, 9, 30, 56          | 0     |
| All | All   | 596/596 (100%) | 0.25   | 26 (4%) 39 34 | 2, 8, 27, 56          | 0     |

All (26) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 91  | THR  | 7.7  |
| 1   | C     | 91  | THR  | 6.1  |
| 1   | B     | 9   | SER  | 4.3  |
| 1   | D     | 87  | SER  | 4.1  |
| 1   | B     | 87  | SER  | 3.9  |
| 1   | B     | 81  | GLY  | 3.5  |
| 1   | D     | 88  | ALA  | 3.5  |
| 1   | D     | 90  | ALA  | 3.4  |
| 1   | C     | 82  | TYR  | 3.2  |
| 1   | C     | 87  | SER  | 3.1  |
| 1   | D     | 71  | PHE  | 3.1  |
| 1   | C     | 88  | ALA  | 3.0  |
| 1   | C     | 90  | ALA  | 2.8  |
| 1   | B     | 110 | GLY  | 2.8  |
| 1   | A     | 82  | TYR  | 2.7  |
| 1   | D     | 89  | LEU  | 2.6  |
| 1   | D     | 110 | GLY  | 2.3  |
| 1   | D     | 92  | PRO  | 2.3  |
| 1   | B     | 88  | ALA  | 2.2  |
| 1   | B     | 82  | TYR  | 2.2  |
| 1   | D     | 93  | THR  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 73  | ASP  | 2.2  |
| 1   | B     | 71  | PHE  | 2.1  |
| 1   | D     | 108 | THR  | 2.1  |
| 1   | C     | 61  | PRO  | 2.1  |
| 1   | B     | 59  | LYS  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.