



# Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:08 AM EDT

PDB ID : 3REQ / pdb\_00003req  
Title : METHYLMALONYL-COA MUTASE, SUBSTRATE-FREE STATE (POOR QUALITY STRUCTURE)  
Authors : Evans, P.R.; Mancina, F.  
Deposited on : 1997-12-04  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

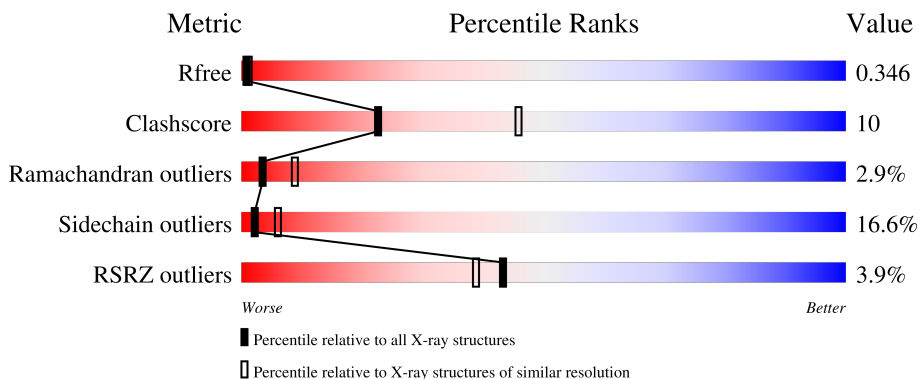
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.70 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 180053                      | 3538 (2.70-2.70)                                      |
| Clashscore            | 190562                      | 3843 (2.70-2.70)                                      |
| Ramachandran outliers | 187476                      | 3778 (2.70-2.70)                                      |
| Sidechain outliers    | 187428                      | 3778 (2.70-2.70)                                      |
| RSRZ outliers         | 180081                      | 3538 (2.70-2.70)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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     | 727    |  |
| 2   | B     | 637    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | B12  | A     | 800 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10285 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 METHYLMALONYL-COA MUTASE.

| Mol | Chain | Residues | Atoms |      |     |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
|     |       |          | Total | C    | N   | O    | S  |         |         |       |
| 1   | A     | 725      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5552  | 3508 | 964 | 1056 | 24 |         |         |       |

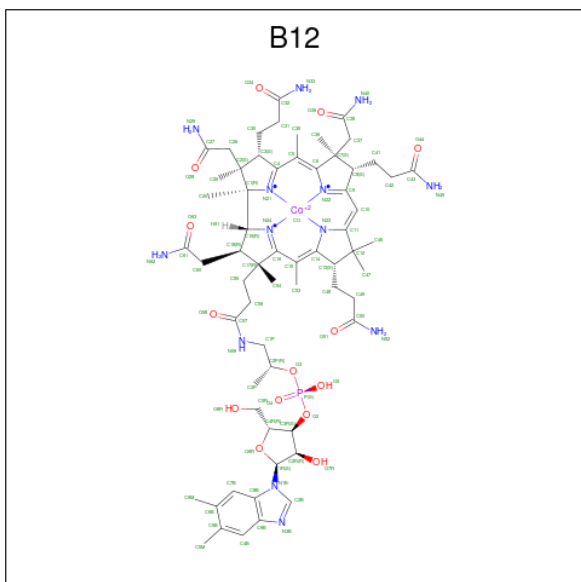
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |         |       |
| 2   | B     | 620      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4624  | 2918 | 796 | 897 | 13 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

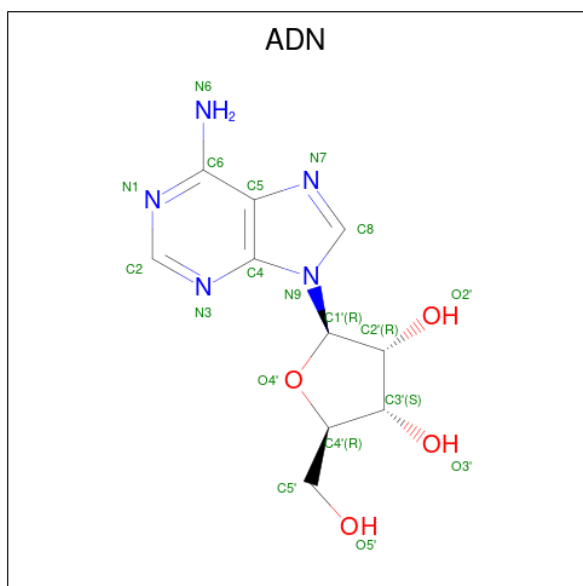
| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 203     | GLY      | ALA    | conflict | UNP P11652 |
| B     | 330     | GLU      | ASP    | conflict | UNP P11652 |
| B     | 331     | LEU      | VAL    | conflict | UNP P11652 |

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



| Mol | Chain | Residues | Atoms |    |    |    |    | ZeroOcc | AltConf |   |
|-----|-------|----------|-------|----|----|----|----|---------|---------|---|
|     |       |          | Total | C  | Co | N  | O  |         |         | P |
| 3   | A     | 1        | 91    | 62 | 1  | 13 | 14 | 1       | 0       | 0 |

- Molecule 4 is ADENOSINE (CCD ID: ADN) (formula:  $C_{10}H_{13}N_5O_4$ ).

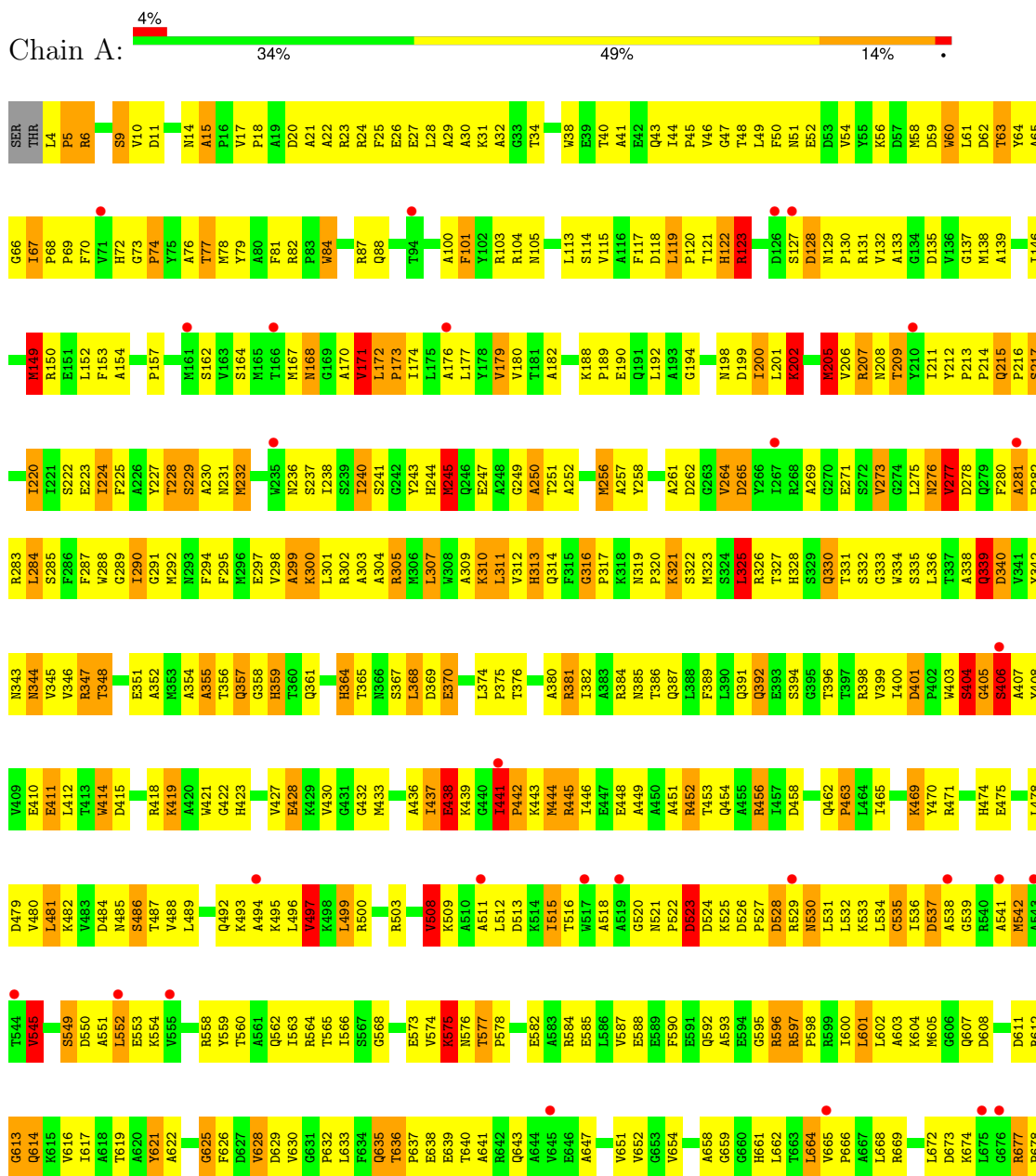


| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
|     |       |          | Total | C  | N | O |         |         |
| 4   | A     | 1        | 18    | 10 | 5 | 3 | 0       | 0       |

### 3 Residue-property plots

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

#### • Molecule 1: METHYLMALONYL-COA MUTASE





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 41 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 110.91Å 110.91Å 257.74Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 20.00 – 2.70<br>20.00 – 2.70                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.6 (20.00-2.70)<br>97.4 (20.00-2.70)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.07  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.98 (at 2.68Å)   | Xtrriage         |
| Refinement program  | REFMAC  | Depositor        |
| R, $R_{free}$   | 0.313 , 0.393<br>0.277 , 0.346                              | Depositor<br>DCC |
| $R_{free}$ test set   | 2225 reflections (4.94%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 70.1  | Xtrriage         |
| Anisotropy  | 0.125   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 50.3   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 10285   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 68.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: B12, ADN

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     | 0.88         | 1/5667 (0.0%)  | 2.82        | 643/7699 (8.4%)   |
| 2   | B     | 0.82         | 1/4714 (0.0%)  | 2.69        | 455/6425 (7.1%)   |
| All | All   | 0.85         | 2/10381 (0.0%) | 2.76        | 1098/14124 (7.8%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 12                  |
| 2   | B     | 0                   | 8                   |
| All | All   | 0                   | 20                  |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | B     | 458 | GLN  | N-CA  | -6.06 | 1.39        | 1.46     |
| 1   | A     | 47  | GLY  | N-CA  | 5.40  | 1.48        | 1.44     |

All (1098) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 77  | ARG  | CD-NE-CZ | 18.90 | 150.87      | 124.40   |
| 1   | A     | 380 | ALA  | CA-C-N   | 16.80 | 143.29      | 120.44   |
| 1   | A     | 380 | ALA  | C-N-CA   | 16.80 | 143.29      | 120.44   |
| 2   | B     | 457 | LYS  | CA-C-N   | 16.59 | 143.57      | 123.16   |
| 2   | B     | 457 | LYS  | C-N-CA   | 16.59 | 143.57      | 123.16   |
| 2   | B     | 363 | PHE  | CA-CB-CG | 16.32 | 130.12      | 113.80   |
| 1   | A     | 206 | VAL  | N-CA-C   | 14.91 | 124.63      | 111.81   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 2   | B     | 493 | ASP  | CA-CB-CG  | 14.81  | 127.41      | 112.60   |
| 1   | A     | 299 | ALA  | O-C-N     | -14.51 | 107.00      | 122.09   |
| 1   | A     | 406 | SER  | CA-C-O    | 14.43  | 141.14      | 120.51   |
| 1   | A     | 131 | ARG  | CD-NE-CZ  | 14.37  | 144.52      | 124.40   |
| 2   | B     | 115 | ASP  | CA-C-O    | 14.24  | 131.67      | 119.71   |
| 1   | A     | 23  | ARG  | CD-NE-CZ  | 13.91  | 143.88      | 124.40   |
| 2   | B     | 503 | ARG  | CD-NE-CZ  | 13.57  | 143.40      | 124.40   |
| 1   | A     | 118 | ASP  | CA-CB-CG  | 13.39  | 125.99      | 112.60   |
| 2   | B     | 278 | ASP  | CA-CB-CG  | 13.20  | 125.80      | 112.60   |
| 1   | A     | 529 | ARG  | CD-NE-CZ  | 13.15  | 142.81      | 124.40   |
| 1   | A     | 612 | ARG  | NE-CZ-NH2 | 12.98  | 130.89      | 119.20   |
| 1   | A     | 241 | SER  | CA-C-O    | 12.83  | 134.41      | 120.43   |
| 1   | A     | 381 | ARG  | CD-NE-CZ  | 12.36  | 141.70      | 124.40   |
| 1   | A     | 391 | GLN  | CB-CG-CD  | 12.28  | 133.47      | 112.60   |
| 2   | B     | 147 | PRO  | CA-C-N    | 11.99  | 140.75      | 120.72   |
| 2   | B     | 147 | PRO  | C-N-CA    | 11.99  | 140.75      | 120.72   |
| 1   | A     | 537 | ASP  | CA-CB-CG  | 11.88  | 124.48      | 112.60   |
| 2   | B     | 460 | ILE  | CB-CA-C   | 11.43  | 123.44      | 110.41   |
| 2   | B     | 38  | GLU  | CA-C-N    | 11.39  | 138.99      | 120.30   |
| 2   | B     | 38  | GLU  | C-N-CA    | 11.39  | 138.99      | 120.30   |
| 1   | A     | 319 | ASN  | CA-CB-CG  | 11.22  | 123.82      | 112.60   |
| 1   | A     | 708 | GLY  | CA-C-O    | 10.94  | 129.05      | 118.77   |
| 2   | B     | 394 | ARG  | CD-NE-CZ  | 10.80  | 139.52      | 124.40   |
| 1   | A     | 597 | ARG  | CD-NE-CZ  | 10.62  | 139.26      | 124.40   |
| 2   | B     | 384 | ILE  | CA-C-O    | -10.56 | 109.97      | 121.17   |
| 2   | B     | 342 | ARG  | CD-NE-CZ  | 10.56  | 139.18      | 124.40   |
| 2   | B     | 239 | ASN  | CA-CB-CG  | 10.51  | 123.11      | 112.60   |
| 1   | A     | 287 | PHE  | CA-CB-CG  | 10.50  | 124.30      | 113.80   |
| 1   | A     | 486 | SER  | CA-C-N    | 10.48  | 135.37      | 120.28   |
| 1   | A     | 486 | SER  | C-N-CA    | 10.48  | 135.37      | 120.28   |
| 2   | B     | 420 | PHE  | CA-CB-CG  | 10.46  | 124.26      | 113.80   |
| 1   | A     | 225 | PHE  | CA-CB-CG  | 10.37  | 124.17      | 113.80   |
| 1   | A     | 452 | ARG  | CD-NE-CZ  | 10.34  | 138.87      | 124.40   |
| 1   | A     | 669 | ARG  | CD-NE-CZ  | 10.30  | 138.82      | 124.40   |
| 2   | B     | 60  | LYS  | CA-C-N    | 10.24  | 135.88      | 120.31   |
| 2   | B     | 60  | LYS  | C-N-CA    | 10.24  | 135.88      | 120.31   |
| 1   | A     | 224 | ILE  | N-CA-C    | -10.21 | 103.16      | 113.47   |
| 1   | A     | 241 | SER  | O-C-N     | -10.04 | 111.93      | 123.27   |
| 1   | A     | 73  | GLY  | CA-C-N    | 10.04  | 129.70      | 119.56   |
| 1   | A     | 73  | GLY  | C-N-CA    | 10.04  | 129.70      | 119.56   |
| 1   | A     | 269 | ALA  | CA-C-N    | 10.02  | 132.97      | 120.34   |
| 1   | A     | 269 | ALA  | C-N-CA    | 10.02  | 132.97      | 120.34   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 578 | PRO  | CA-C-N     | 10.00 | 133.69      | 120.28   |
| 1   | A     | 578 | PRO  | C-N-CA     | 10.00 | 133.69      | 120.28   |
| 1   | A     | 84  | TRP  | CA-C-N     | 9.91  | 136.76      | 122.09   |
| 1   | A     | 84  | TRP  | C-N-CA     | 9.91  | 136.76      | 122.09   |
| 1   | A     | 612 | ARG  | CD-NE-CZ   | 9.89  | 138.24      | 124.40   |
| 1   | A     | 223 | GLU  | CA-C-N     | 9.79  | 133.00      | 122.14   |
| 1   | A     | 223 | GLU  | C-N-CA     | 9.79  | 133.00      | 122.14   |
| 2   | B     | 375 | PRO  | CA-C-N     | 9.62  | 134.13      | 120.28   |
| 2   | B     | 375 | PRO  | C-N-CA     | 9.62  | 134.13      | 120.28   |
| 1   | A     | 357 | GLN  | OE1-CD-NE2 | -9.59 | 113.01      | 122.60   |
| 1   | A     | 170 | ALA  | CA-C-N     | 9.54  | 135.54      | 120.47   |
| 1   | A     | 170 | ALA  | C-N-CA     | 9.54  | 135.54      | 120.47   |
| 1   | A     | 356 | THR  | CA-C-O     | -9.50 | 110.74      | 120.90   |
| 1   | A     | 88  | GLN  | CA-C-O     | -9.46 | 109.51      | 120.49   |
| 1   | A     | 340 | ASP  | CA-C-N     | 9.43  | 136.61      | 120.86   |
| 1   | A     | 340 | ASP  | C-N-CA     | 9.43  | 136.61      | 120.86   |
| 1   | A     | 367 | SER  | O-C-N      | -9.32 | 112.62      | 123.06   |
| 2   | B     | 100 | ARG  | CD-NE-CZ   | 9.31  | 137.43      | 124.40   |
| 2   | B     | 38  | GLU  | N-CA-C     | 9.29  | 122.39      | 111.71   |
| 1   | A     | 465 | ILE  | CA-C-O     | 9.28  | 132.38      | 120.78   |
| 1   | A     | 693 | PHE  | CA-CB-CG   | 9.23  | 123.03      | 113.80   |
| 1   | A     | 406 | SER  | CA-C-N     | 9.20  | 132.96      | 120.54   |
| 1   | A     | 406 | SER  | C-N-CA     | 9.20  | 132.96      | 120.54   |
| 1   | A     | 79  | TYR  | CA-C-N     | 9.16  | 133.48      | 120.28   |
| 1   | A     | 79  | TYR  | C-N-CA     | 9.16  | 133.48      | 120.28   |
| 2   | B     | 72  | ILE  | CA-C-O     | 9.14  | 130.53      | 120.48   |
| 2   | B     | 403 | TYR  | CA-C-N     | 9.12  | 133.46      | 120.79   |
| 2   | B     | 403 | TYR  | C-N-CA     | 9.12  | 133.46      | 120.79   |
| 1   | A     | 128 | ASP  | CA-CB-CG   | 9.11  | 121.71      | 112.60   |
| 1   | A     | 262 | ASP  | CA-C-O     | -9.00 | 110.91      | 120.63   |
| 1   | A     | 276 | ASN  | CA-CB-CG   | 8.98  | 121.58      | 112.60   |
| 1   | A     | 299 | ALA  | CA-C-O     | 8.98  | 130.51      | 120.90   |
| 1   | A     | 258 | TYR  | CA-C-N     | 8.97  | 132.64      | 120.44   |
| 1   | A     | 258 | TYR  | C-N-CA     | 8.97  | 132.64      | 120.44   |
| 2   | B     | 327 | SER  | CA-C-N     | 8.96  | 133.01      | 120.29   |
| 2   | B     | 327 | SER  | C-N-CA     | 8.96  | 133.01      | 120.29   |
| 1   | A     | 20  | ASP  | CA-CB-CG   | 8.94  | 121.54      | 112.60   |
| 1   | A     | 300 | LYS  | CA-C-N     | 8.94  | 135.63      | 120.71   |
| 1   | A     | 300 | LYS  | C-N-CA     | 8.94  | 135.63      | 120.71   |
| 1   | A     | 354 | ALA  | CA-C-O     | -8.81 | 111.57      | 120.82   |
| 1   | A     | 243 | TYR  | CA-C-N     | 8.81  | 132.96      | 120.28   |
| 1   | A     | 243 | TYR  | C-N-CA     | 8.81  | 132.96      | 120.28   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 612 | ARG  | NH1-CZ-NH2 | -8.80 | 107.86      | 119.30   |
| 2   | B     | 115 | ASP  | O-C-N      | -8.77 | 114.19      | 121.38   |
| 2   | B     | 337 | TYR  | CA-C-N     | 8.76  | 134.39      | 121.77   |
| 2   | B     | 337 | TYR  | C-N-CA     | 8.76  | 134.39      | 121.77   |
| 1   | A     | 101 | PHE  | CA-CB-CG   | 8.76  | 122.56      | 113.80   |
| 2   | B     | 632 | ASP  | CA-C-N     | 8.72  | 134.34      | 120.82   |
| 2   | B     | 632 | ASP  | C-N-CA     | 8.72  | 134.34      | 120.82   |
| 2   | B     | 632 | ASP  | CA-CB-CG   | 8.67  | 121.27      | 112.60   |
| 2   | B     | 391 | ASN  | OD1-CG-ND2 | -8.64 | 113.96      | 122.60   |
| 2   | B     | 211 | GLU  | CA-C-O     | 8.62  | 126.32      | 119.59   |
| 2   | B     | 585 | LEU  | CA-C-O     | -8.62 | 111.59      | 121.07   |
| 1   | A     | 530 | ASN  | CA-CB-CG   | 8.56  | 121.16      | 112.60   |
| 1   | A     | 403 | TRP  | CA-C-O     | -8.55 | 111.36      | 120.42   |
| 1   | A     | 407 | ALA  | N-CA-CB    | -8.55 | 97.20       | 109.94   |
| 1   | A     | 303 | ALA  | O-C-N      | -8.47 | 111.32      | 122.59   |
| 1   | A     | 622 | ALA  | CA-C-N     | 8.40  | 132.22      | 120.29   |
| 1   | A     | 622 | ALA  | C-N-CA     | 8.40  | 132.22      | 120.29   |
| 1   | A     | 46  | VAL  | CA-C-O     | -8.36 | 111.30      | 120.67   |
| 1   | A     | 294 | PHE  | CA-C-O     | 8.35  | 132.45      | 120.51   |
| 2   | B     | 382 | THR  | O-C-N      | 8.35  | 131.11      | 122.09   |
| 2   | B     | 78  | PRO  | O-C-N      | -8.34 | 112.08      | 122.17   |
| 1   | A     | 727 | ASP  | CA-CB-CG   | 8.33  | 120.93      | 112.60   |
| 1   | A     | 415 | ASP  | CA-CB-CG   | 8.32  | 120.92      | 112.60   |
| 2   | B     | 171 | ASP  | CA-CB-CG   | 8.31  | 120.92      | 112.60   |
| 1   | A     | 25  | PHE  | CA-C-N     | 8.29  | 131.74      | 120.54   |
| 1   | A     | 25  | PHE  | C-N-CA     | 8.29  | 131.74      | 120.54   |
| 1   | A     | 326 | ARG  | CA-C-O     | 8.29  | 129.44      | 120.32   |
| 2   | B     | 524 | PHE  | CA-CB-CG   | 8.29  | 122.09      | 113.80   |
| 1   | A     | 247 | GLU  | CA-C-N     | 8.28  | 132.90      | 120.31   |
| 1   | A     | 247 | GLU  | C-N-CA     | 8.28  | 132.90      | 120.31   |
| 1   | A     | 41  | ALA  | CA-C-N     | 8.24  | 135.56      | 121.14   |
| 1   | A     | 41  | ALA  | C-N-CA     | 8.24  | 135.56      | 121.14   |
| 1   | A     | 17  | VAL  | CA-C-O     | 8.22  | 125.20      | 119.20   |
| 2   | B     | 512 | LYS  | O-C-N      | -8.17 | 113.28      | 123.17   |
| 1   | A     | 484 | ASP  | CA-CB-CG   | 8.17  | 120.77      | 112.60   |
| 2   | B     | 457 | LYS  | CA-C-O     | 8.15  | 128.44      | 119.15   |
| 1   | A     | 358 | GLY  | CA-C-N     | 8.10  | 137.02      | 121.54   |
| 1   | A     | 358 | GLY  | C-N-CA     | 8.10  | 137.02      | 121.54   |
| 2   | B     | 367 | LEU  | N-CA-C     | 8.10  | 119.89      | 111.14   |
| 1   | A     | 21  | ALA  | CA-C-N     | 8.08  | 131.45      | 120.54   |
| 1   | A     | 21  | ALA  | C-N-CA     | 8.08  | 131.45      | 120.54   |
| 2   | B     | 56  | ALA  | O-C-N      | -8.07 | 113.37      | 122.09   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 381 | ARG  | CB-CG-CD  | 8.07  | 129.86      | 111.30   |
| 1   | A     | 177 | LEU  | CA-C-N    | 8.05  | 134.34      | 120.58   |
| 1   | A     | 177 | LEU  | C-N-CA    | 8.05  | 134.34      | 120.58   |
| 2   | B     | 408 | LEU  | O-C-N     | -8.04 | 112.87      | 122.11   |
| 1   | A     | 231 | ASN  | N-CA-C    | 8.03  | 122.70      | 113.15   |
| 1   | A     | 278 | ASP  | CA-C-N    | 8.03  | 134.83      | 122.23   |
| 1   | A     | 278 | ASP  | C-N-CA    | 8.03  | 134.83      | 122.23   |
| 1   | A     | 608 | ASP  | CA-CB-CG  | 8.02  | 120.61      | 112.60   |
| 2   | B     | 132 | GLY  | CA-C-O    | -7.99 | 109.93      | 119.03   |
| 1   | A     | 66  | GLY  | CA-C-N    | 7.98  | 130.38      | 123.04   |
| 1   | A     | 66  | GLY  | C-N-CA    | 7.98  | 130.38      | 123.04   |
| 1   | A     | 313 | HIS  | O-C-N     | -7.97 | 113.86      | 122.07   |
| 1   | A     | 619 | THR  | O-C-N     | -7.95 | 111.68      | 122.33   |
| 2   | B     | 366 | ALA  | CA-C-N    | 7.94  | 131.24      | 120.44   |
| 2   | B     | 366 | ALA  | C-N-CA    | 7.94  | 131.24      | 120.44   |
| 1   | A     | 60  | TRP  | CA-C-N    | 7.91  | 138.13      | 122.31   |
| 1   | A     | 60  | TRP  | C-N-CA    | 7.91  | 138.13      | 122.31   |
| 1   | A     | 330 | GLN  | CA-C-O    | -7.91 | 110.55      | 120.28   |
| 2   | B     | 52  | GLN  | CA-CB-CG  | 7.91  | 129.91      | 114.10   |
| 1   | A     | 677 | ARG  | N-CA-C    | 7.91  | 124.99      | 108.39   |
| 2   | B     | 631 | LEU  | CA-C-N    | 7.90  | 131.91      | 120.38   |
| 2   | B     | 631 | LEU  | C-N-CA    | 7.90  | 131.91      | 120.38   |
| 2   | B     | 111 | ALA  | CA-C-N    | 7.90  | 133.27      | 122.77   |
| 2   | B     | 111 | ALA  | C-N-CA    | 7.90  | 133.27      | 122.77   |
| 2   | B     | 289 | ASP  | CA-CB-CG  | -7.89 | 104.71      | 112.60   |
| 2   | B     | 106 | ALA  | CA-C-N    | 7.89  | 136.62      | 121.54   |
| 2   | B     | 106 | ALA  | C-N-CA    | 7.89  | 136.62      | 121.54   |
| 2   | B     | 380 | ARG  | CD-NE-CZ  | 7.89  | 135.44      | 124.40   |
| 2   | B     | 314 | ASP  | CA-C-N    | 7.88  | 133.22      | 120.60   |
| 2   | B     | 314 | ASP  | C-N-CA    | 7.88  | 133.22      | 120.60   |
| 1   | A     | 577 | THR  | CA-C-N    | 7.88  | 129.69      | 119.84   |
| 1   | A     | 577 | THR  | C-N-CA    | 7.88  | 129.69      | 119.84   |
| 1   | A     | 428 | GLU  | CA-C-N    | 7.86  | 135.70      | 122.65   |
| 1   | A     | 428 | GLU  | C-N-CA    | 7.86  | 135.70      | 122.65   |
| 1   | A     | 495 | LYS  | N-CA-C    | -7.86 | 103.82      | 113.41   |
| 1   | A     | 726 | LEU  | N-CA-C    | 7.86  | 120.93      | 111.82   |
| 1   | A     | 320 | PRO  | CA-C-N    | 7.83  | 135.17      | 122.65   |
| 1   | A     | 320 | PRO  | C-N-CA    | 7.83  | 135.17      | 122.65   |
| 1   | A     | 597 | ARG  | NE-CZ-NH1 | 7.82  | 129.32      | 121.50   |
| 1   | A     | 40  | THR  | CA-C-N    | 7.81  | 133.09      | 120.60   |
| 1   | A     | 40  | THR  | C-N-CA    | 7.81  | 133.09      | 120.60   |
| 1   | A     | 228 | THR  | N-CA-CB   | 7.80  | 121.30      | 109.91   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 408 | LEU  | CA-C-N    | 7.78  | 131.61      | 120.79   |
| 2   | B     | 408 | LEU  | C-N-CA    | 7.78  | 131.61      | 120.79   |
| 2   | B     | 306 | ARG  | CD-NE-CZ  | 7.77  | 135.28      | 124.40   |
| 2   | B     | 52  | GLN  | N-CA-CB   | 7.72  | 124.27      | 110.83   |
| 2   | B     | 365 | GLN  | N-CA-C    | 7.72  | 122.28      | 113.01   |
| 1   | A     | 277 | VAL  | O-C-N     | -7.72 | 114.34      | 121.91   |
| 2   | B     | 385 | VAL  | O-C-N     | -7.72 | 114.35      | 121.91   |
| 1   | A     | 578 | PRO  | N-CA-CB   | 7.71  | 111.34      | 103.25   |
| 1   | A     | 310 | LYS  | O-C-N     | -7.70 | 112.35      | 122.59   |
| 1   | A     | 593 | ALA  | N-CA-C    | 7.70  | 122.11      | 112.87   |
| 1   | A     | 613 | GLY  | O-C-N     | -7.70 | 112.69      | 122.70   |
| 1   | A     | 115 | VAL  | CB-CA-C   | -7.67 | 100.70      | 111.21   |
| 2   | B     | 456 | ARG  | NE-CZ-NH2 | 7.67  | 126.10      | 119.20   |
| 1   | A     | 68  | PRO  | N-CA-CB   | 7.64  | 110.49      | 103.08   |
| 2   | B     | 264 | ARG  | CD-NE-CZ  | 7.64  | 135.10      | 124.40   |
| 2   | B     | 68  | ASP  | CA-CB-CG  | 7.64  | 120.24      | 112.60   |
| 2   | B     | 358 | ILE  | N-CA-CB   | 7.62  | 121.55      | 111.64   |
| 1   | A     | 51  | ASN  | N-CA-C    | 7.62  | 118.30      | 108.24   |
| 1   | A     | 31  | LYS  | O-C-N     | -7.62 | 112.22      | 122.43   |
| 1   | A     | 614 | GLN  | CA-C-N    | 7.62  | 131.89      | 120.31   |
| 1   | A     | 614 | GLN  | C-N-CA    | 7.62  | 131.89      | 120.31   |
| 1   | A     | 389 | PHE  | CA-CB-CG  | 7.61  | 121.41      | 113.80   |
| 2   | B     | 534 | VAL  | CA-C-N    | 7.59  | 131.07      | 120.29   |
| 2   | B     | 534 | VAL  | C-N-CA    | 7.59  | 131.07      | 120.29   |
| 1   | A     | 392 | GLN  | CA-C-O    | -7.58 | 111.82      | 120.24   |
| 1   | A     | 215 | GLN  | CA-C-N    | 7.58  | 127.22      | 119.56   |
| 1   | A     | 215 | GLN  | C-N-CA    | 7.58  | 127.22      | 119.56   |
| 2   | B     | 433 | VAL  | CA-C-N    | 7.58  | 130.77      | 120.38   |
| 2   | B     | 433 | VAL  | C-N-CA    | 7.58  | 130.77      | 120.38   |
| 1   | A     | 626 | PHE  | CA-CB-CG  | 7.55  | 121.35      | 113.80   |
| 2   | B     | 242 | HIS  | CA-C-N    | 7.55  | 130.40      | 120.28   |
| 2   | B     | 242 | HIS  | C-N-CA    | 7.55  | 130.40      | 120.28   |
| 2   | B     | 152 | GLU  | CA-C-O    | -7.55 | 112.89      | 120.82   |
| 2   | B     | 626 | THR  | CA-C-O    | -7.54 | 112.90      | 120.82   |
| 2   | B     | 286 | ALA  | CA-C-O    | 7.54  | 128.32      | 120.40   |
| 2   | B     | 521 | ARG  | N-CA-C    | 7.53  | 121.39      | 111.75   |
| 1   | A     | 469 | LYS  | O-C-N     | -7.52 | 114.83      | 123.33   |
| 1   | A     | 437 | ILE  | CA-C-N    | 7.52  | 130.57      | 120.65   |
| 1   | A     | 437 | ILE  | C-N-CA    | 7.52  | 130.57      | 120.65   |
| 2   | B     | 443 | ASP  | CA-C-N    | 7.51  | 130.96      | 120.29   |
| 2   | B     | 443 | ASP  | C-N-CA    | 7.51  | 130.96      | 120.29   |
| 1   | A     | 528 | ASP  | CA-CB-CG  | 7.50  | 120.10      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 684 | VAL  | CA-C-O     | 7.50  | 127.84      | 120.27   |
| 2   | B     | 536 | HIS  | CA-C-N     | 7.49  | 131.06      | 120.42   |
| 2   | B     | 536 | HIS  | C-N-CA     | 7.49  | 131.06      | 120.42   |
| 1   | A     | 496 | LEU  | CA-C-N     | 7.49  | 130.06      | 120.70   |
| 1   | A     | 496 | LEU  | C-N-CA     | 7.49  | 130.06      | 120.70   |
| 1   | A     | 352 | ALA  | CA-C-N     | 7.48  | 130.91      | 120.29   |
| 1   | A     | 352 | ALA  | C-N-CA     | 7.48  | 130.91      | 120.29   |
| 2   | B     | 606 | ALA  | N-CA-C     | 7.46  | 120.28      | 111.71   |
| 1   | A     | 678 | PRO  | CA-C-N     | 7.45  | 130.13      | 120.44   |
| 1   | A     | 678 | PRO  | C-N-CA     | 7.45  | 130.13      | 120.44   |
| 1   | A     | 74  | PRO  | CA-C-N     | 7.45  | 134.51      | 122.81   |
| 1   | A     | 74  | PRO  | C-N-CA     | 7.45  | 134.51      | 122.81   |
| 1   | A     | 333 | GLY  | CA-C-N     | 7.45  | 130.87      | 120.29   |
| 1   | A     | 333 | GLY  | C-N-CA     | 7.45  | 130.87      | 120.29   |
| 2   | B     | 462 | ALA  | CA-C-N     | 7.45  | 135.38      | 121.97   |
| 2   | B     | 462 | ALA  | C-N-CA     | 7.45  | 135.38      | 121.97   |
| 1   | A     | 340 | ASP  | O-C-N      | -7.44 | 113.71      | 122.86   |
| 2   | B     | 382 | THR  | CA-C-O     | -7.42 | 113.06      | 120.70   |
| 2   | B     | 32  | GLU  | CA-C-N     | 7.42  | 130.82      | 120.29   |
| 2   | B     | 32  | GLU  | C-N-CA     | 7.42  | 130.82      | 120.29   |
| 1   | A     | 673 | ASP  | CA-CB-CG   | 7.41  | 120.01      | 112.60   |
| 2   | B     | 115 | ASP  | CA-C-N     | 7.39  | 127.02      | 119.19   |
| 2   | B     | 115 | ASP  | C-N-CA     | 7.39  | 127.02      | 119.19   |
| 2   | B     | 120 | PHE  | N-CA-C     | -7.39 | 102.85      | 112.68   |
| 1   | A     | 320 | PRO  | O-C-N      | -7.39 | 112.67      | 122.64   |
| 1   | A     | 241 | SER  | N-CA-C     | 7.38  | 121.26      | 109.24   |
| 2   | B     | 146 | ALA  | CA-C-N     | 7.36  | 129.04      | 119.84   |
| 2   | B     | 146 | ALA  | C-N-CA     | 7.36  | 129.04      | 119.84   |
| 2   | B     | 34  | GLN  | OE1-CD-NE2 | 7.36  | 129.96      | 122.60   |
| 2   | B     | 176 | ALA  | CA-C-N     | 7.36  | 134.65      | 121.92   |
| 2   | B     | 176 | ALA  | C-N-CA     | 7.36  | 134.65      | 121.92   |
| 1   | A     | 470 | TYR  | CA-C-N     | 7.36  | 131.86      | 120.75   |
| 1   | A     | 470 | TYR  | C-N-CA     | 7.36  | 131.86      | 120.75   |
| 1   | A     | 139 | ALA  | CA-C-N     | 7.35  | 130.50      | 120.72   |
| 1   | A     | 139 | ALA  | C-N-CA     | 7.35  | 130.50      | 120.72   |
| 1   | A     | 182 | ALA  | CA-C-N     | 7.33  | 132.96      | 120.72   |
| 1   | A     | 182 | ALA  | C-N-CA     | 7.33  | 132.96      | 120.72   |
| 2   | B     | 160 | GLU  | CA-C-N     | 7.32  | 130.69      | 120.29   |
| 2   | B     | 160 | GLU  | C-N-CA     | 7.32  | 130.69      | 120.29   |
| 2   | B     | 69  | GLY  | N-CA-C     | 7.32  | 124.71      | 115.42   |
| 2   | B     | 260 | ALA  | CA-C-N     | 7.32  | 130.40      | 120.38   |
| 2   | B     | 260 | ALA  | C-N-CA     | 7.32  | 130.40      | 120.38   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 455 | ASN  | OD1-CG-ND2 | -7.31 | 115.29      | 122.60   |
| 2   | B     | 105 | ASP  | CA-CB-CG   | 7.31  | 119.91      | 112.60   |
| 1   | A     | 465 | ILE  | CA-C-N     | 7.28  | 133.94      | 122.51   |
| 1   | A     | 465 | ILE  | C-N-CA     | 7.28  | 133.94      | 122.51   |
| 1   | A     | 168 | ASN  | CA-CB-CG   | 7.28  | 119.88      | 112.60   |
| 1   | A     | 469 | LYS  | CA-C-N     | 7.28  | 132.72      | 122.46   |
| 1   | A     | 469 | LYS  | C-N-CA     | 7.28  | 132.72      | 122.46   |
| 2   | B     | 446 | ASN  | CA-C-N     | 7.28  | 133.03      | 120.58   |
| 2   | B     | 446 | ASN  | C-N-CA     | 7.28  | 133.03      | 120.58   |
| 2   | B     | 557 | PHE  | CA-CB-CG   | 7.28  | 121.08      | 113.80   |
| 1   | A     | 206 | VAL  | CB-CA-C    | -7.27 | 103.19      | 111.55   |
| 2   | B     | 35  | TRP  | N-CA-C     | -7.27 | 102.75      | 111.69   |
| 1   | A     | 290 | ILE  | N-CA-CB    | 7.24  | 121.36      | 112.10   |
| 1   | A     | 332 | SER  | O-C-N      | -7.23 | 114.03      | 122.93   |
| 2   | B     | 323 | ASN  | CA-CB-CG   | 7.22  | 119.82      | 112.60   |
| 1   | A     | 295 | PHE  | CA-C-O     | -7.22 | 112.89      | 120.55   |
| 1   | A     | 410 | GLU  | CA-CB-CG   | 7.22  | 128.53      | 114.10   |
| 1   | A     | 545 | VAL  | CA-C-N     | 7.22  | 127.95      | 119.94   |
| 1   | A     | 545 | VAL  | C-N-CA     | 7.22  | 127.95      | 119.94   |
| 1   | A     | 541 | ALA  | CA-C-N     | 7.21  | 135.31      | 121.54   |
| 1   | A     | 541 | ALA  | C-N-CA     | 7.21  | 135.31      | 121.54   |
| 2   | B     | 152 | GLU  | CB-CG-CD   | 7.20  | 124.84      | 112.60   |
| 2   | B     | 382 | THR  | CA-C-N     | 7.19  | 127.91      | 120.00   |
| 2   | B     | 382 | THR  | C-N-CA     | 7.19  | 127.91      | 120.00   |
| 1   | A     | 61  | LEU  | N-CA-C     | 7.19  | 121.71      | 113.15   |
| 1   | A     | 135 | ASP  | CA-C-O     | 7.19  | 126.66      | 118.97   |
| 1   | A     | 132 | VAL  | N-CA-C     | 7.18  | 122.23      | 111.89   |
| 2   | B     | 543 | PRO  | N-CA-CB    | 7.18  | 110.00      | 103.33   |
| 2   | B     | 159 | LEU  | N-CA-C     | 7.16  | 120.91      | 111.75   |
| 2   | B     | 288 | HIS  | CA-CB-CG   | 7.16  | 120.96      | 113.80   |
| 1   | A     | 344 | ASN  | CA-CB-CG   | 7.15  | 119.75      | 112.60   |
| 1   | A     | 463 | PRO  | N-CA-CB    | 7.15  | 110.76      | 103.25   |
| 1   | A     | 22  | ALA  | CA-C-N     | 7.14  | 129.73      | 120.44   |
| 1   | A     | 22  | ALA  | C-N-CA     | 7.14  | 129.73      | 120.44   |
| 1   | A     | 41  | ALA  | CA-C-O     | 7.14  | 128.13      | 119.49   |
| 2   | B     | 629 | SER  | O-C-N      | -7.14 | 114.72      | 122.07   |
| 2   | B     | 277 | PHE  | N-CA-C     | 7.14  | 121.68      | 113.19   |
| 1   | A     | 123 | ARG  | CA-C-N     | 7.12  | 130.87      | 120.11   |
| 1   | A     | 123 | ARG  | C-N-CA     | 7.12  | 130.87      | 120.11   |
| 1   | A     | 384 | ARG  | NE-CZ-NH1  | -7.11 | 114.39      | 121.50   |
| 2   | B     | 167 | PHE  | CA-CB-CG   | 7.11  | 120.91      | 113.80   |
| 2   | B     | 176 | ALA  | O-C-N      | -7.11 | 112.65      | 122.46   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 577 | GLN  | N-CA-C   | 7.10  | 121.66      | 112.92   |
| 1   | A     | 121 | THR  | CA-C-O   | -7.10 | 113.26      | 121.07   |
| 2   | B     | 474 | ILE  | O-C-N    | -7.09 | 114.91      | 123.00   |
| 1   | A     | 725 | SER  | CA-C-N   | 7.08  | 131.08      | 120.31   |
| 1   | A     | 725 | SER  | C-N-CA   | 7.08  | 131.08      | 120.31   |
| 1   | A     | 658 | ALA  | CA-C-N   | 7.08  | 135.80      | 121.78   |
| 1   | A     | 658 | ALA  | C-N-CA   | 7.08  | 135.80      | 121.78   |
| 1   | A     | 720 | LYS  | CA-C-N   | 7.08  | 130.08      | 120.38   |
| 1   | A     | 720 | LYS  | C-N-CA   | 7.08  | 130.08      | 120.38   |
| 2   | B     | 372 | ASP  | CA-CB-CG | 7.08  | 119.67      | 112.60   |
| 1   | A     | 40  | THR  | O-C-N    | -7.07 | 113.18      | 122.59   |
| 1   | A     | 392 | GLN  | N-CA-C   | 7.07  | 120.39      | 111.69   |
| 2   | B     | 220 | TRP  | CA-C-N   | 7.07  | 131.89      | 120.30   |
| 2   | B     | 220 | TRP  | C-N-CA   | 7.07  | 131.89      | 120.30   |
| 2   | B     | 467 | PRO  | N-CA-CB  | 7.07  | 109.90      | 103.33   |
| 1   | A     | 252 | ALA  | CA-C-N   | 7.06  | 129.74      | 120.28   |
| 1   | A     | 252 | ALA  | C-N-CA   | 7.06  | 129.74      | 120.28   |
| 2   | B     | 381 | ASN  | CA-C-N   | 7.05  | 130.02      | 120.44   |
| 2   | B     | 381 | ASN  | C-N-CA   | 7.05  | 130.02      | 120.44   |
| 2   | B     | 113 | HIS  | CA-CB-CG | -7.03 | 106.77      | 113.80   |
| 1   | A     | 271 | GLU  | CA-C-N   | 7.01  | 133.24      | 122.23   |
| 1   | A     | 271 | GLU  | C-N-CA   | 7.01  | 133.24      | 122.23   |
| 1   | A     | 711 | ILE  | CA-C-N   | 7.01  | 128.60      | 119.84   |
| 1   | A     | 711 | ILE  | C-N-CA   | 7.01  | 128.60      | 119.84   |
| 2   | B     | 342 | ARG  | O-C-N    | -7.01 | 114.85      | 122.07   |
| 2   | B     | 314 | ASP  | CA-CB-CG | 7.01  | 119.61      | 112.60   |
| 1   | A     | 278 | ASP  | O-C-N    | -7.00 | 113.28      | 122.59   |
| 2   | B     | 315 | GLU  | N-CA-C   | 6.99  | 120.91      | 112.38   |
| 2   | B     | 338 | VAL  | O-C-N    | -6.99 | 115.21      | 122.20   |
| 1   | A     | 622 | ALA  | O-C-N    | -6.98 | 114.72      | 122.12   |
| 1   | A     | 677 | ARG  | CA-C-N   | 6.96  | 126.57      | 119.19   |
| 1   | A     | 677 | ARG  | C-N-CA   | 6.96  | 126.57      | 119.19   |
| 1   | A     | 419 | LYS  | CA-C-N   | 6.96  | 130.17      | 120.29   |
| 1   | A     | 419 | LYS  | C-N-CA   | 6.96  | 130.17      | 120.29   |
| 1   | A     | 438 | GLU  | CA-C-N   | 6.95  | 131.82      | 120.63   |
| 1   | A     | 438 | GLU  | C-N-CA   | 6.95  | 131.82      | 120.63   |
| 2   | B     | 201 | PRO  | O-C-N    | -6.94 | 114.25      | 122.24   |
| 2   | B     | 617 | LEU  | N-CA-CB  | 6.94  | 121.48      | 110.65   |
| 2   | B     | 109 | VAL  | N-CA-CB  | 6.93  | 119.84      | 111.31   |
| 2   | B     | 434 | MET  | N-CA-C   | 6.93  | 119.72      | 111.33   |
| 2   | B     | 380 | ARG  | N-CA-CB  | 6.93  | 120.31      | 110.12   |
| 1   | A     | 598 | PRO  | N-CA-CB  | 6.93  | 109.43      | 103.19   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 15  | ALA  | CA-C-O     | 6.91  | 129.63      | 120.16   |
| 1   | A     | 228 | THR  | CA-C-O     | -6.91 | 113.75      | 121.00   |
| 1   | A     | 100 | ALA  | CA-C-N     | 6.90  | 129.85      | 120.54   |
| 1   | A     | 100 | ALA  | C-N-CA     | 6.90  | 129.85      | 120.54   |
| 1   | A     | 52  | GLU  | O-C-N      | -6.88 | 113.44      | 122.39   |
| 1   | A     | 348 | THR  | CA-C-N     | 6.88  | 130.77      | 120.31   |
| 1   | A     | 348 | THR  | C-N-CA     | 6.88  | 130.77      | 120.31   |
| 1   | A     | 38  | TRP  | CA-C-N     | -6.88 | 112.59      | 122.77   |
| 1   | A     | 38  | TRP  | C-N-CA     | -6.88 | 112.59      | 122.77   |
| 1   | A     | 595 | GLY  | CA-C-N     | 6.88  | 134.67      | 121.54   |
| 1   | A     | 595 | GLY  | C-N-CA     | 6.88  | 134.67      | 121.54   |
| 1   | A     | 382 | ILE  | CA-C-N     | 6.87  | 129.37      | 120.44   |
| 1   | A     | 382 | ILE  | C-N-CA     | 6.87  | 129.37      | 120.44   |
| 1   | A     | 643 | GLN  | CA-C-N     | 6.87  | 129.48      | 120.28   |
| 1   | A     | 643 | GLN  | C-N-CA     | 6.87  | 129.48      | 120.28   |
| 2   | B     | 63  | THR  | CA-C-O     | -6.86 | 113.23      | 121.05   |
| 2   | B     | 349 | SER  | CA-C-O     | -6.85 | 113.23      | 120.63   |
| 2   | B     | 501 | MET  | CA-C-N     | 6.83  | 129.99      | 120.29   |
| 2   | B     | 501 | MET  | C-N-CA     | 6.83  | 129.99      | 120.29   |
| 2   | B     | 26  | ASP  | CA-C-O     | 6.83  | 126.93      | 119.15   |
| 2   | B     | 122 | ARG  | CA-C-O     | -6.81 | 113.61      | 120.90   |
| 2   | B     | 391 | ASN  | CA-CB-CG   | 6.81  | 119.41      | 112.60   |
| 1   | A     | 405 | GLY  | CA-C-O     | -6.80 | 117.15      | 122.52   |
| 1   | A     | 334 | TRP  | CA-C-O     | -6.78 | 113.24      | 120.42   |
| 2   | B     | 143 | ASP  | CA-C-N     | 6.77  | 133.49      | 122.39   |
| 2   | B     | 143 | ASP  | C-N-CA     | 6.77  | 133.49      | 122.39   |
| 1   | A     | 328 | HIS  | CA-CB-CG   | 6.76  | 120.56      | 113.80   |
| 1   | A     | 322 | SER  | CA-C-N     | 6.75  | 134.62      | 122.06   |
| 1   | A     | 322 | SER  | C-N-CA     | 6.75  | 134.62      | 122.06   |
| 1   | A     | 281 | ALA  | N-CA-C     | 6.75  | 121.39      | 112.35   |
| 1   | A     | 127 | SER  | CA-C-N     | 6.74  | 132.16      | 121.44   |
| 1   | A     | 127 | SER  | C-N-CA     | 6.74  | 132.16      | 121.44   |
| 2   | B     | 76  | TYR  | CB-CA-C    | 6.74  | 120.89      | 109.50   |
| 2   | B     | 86  | GLY  | O-C-N      | -6.74 | 114.82      | 122.64   |
| 2   | B     | 403 | TYR  | CA-C-O     | 6.72  | 128.89      | 121.02   |
| 1   | A     | 67  | ILE  | CA-C-N     | 6.71  | 127.30      | 120.38   |
| 1   | A     | 67  | ILE  | C-N-CA     | 6.71  | 127.30      | 120.38   |
| 1   | A     | 321 | LYS  | CA-C-O     | 6.71  | 127.42      | 119.56   |
| 2   | B     | 289 | ASP  | CA-C-O     | 6.71  | 127.90      | 120.92   |
| 1   | A     | 497 | VAL  | CA-CB-CG1  | 6.71  | 121.80      | 110.40   |
| 1   | A     | 635 | GLN  | OE1-CD-NE2 | -6.70 | 115.90      | 122.60   |
| 2   | B     | 169 | ARG  | NE-CZ-NH2  | 6.70  | 125.23      | 119.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 280 | ILE  | CB-CG1-CD1 | 6.70  | 127.86      | 113.80   |
| 1   | A     | 375 | PRO  | N-CA-CB    | 6.68  | 109.56      | 103.34   |
| 2   | B     | 381 | ASN  | O-C-N      | -6.68 | 112.68      | 122.43   |
| 2   | B     | 535 | TRP  | O-C-N      | -6.67 | 114.55      | 122.15   |
| 1   | A     | 647 | ALA  | CA-C-O     | 6.67  | 127.52      | 119.78   |
| 1   | A     | 389 | PHE  | CA-C-O     | -6.67 | 113.48      | 120.55   |
| 2   | B     | 70  | ILE  | CB-CG1-CD1 | 6.66  | 127.79      | 113.80   |
| 1   | A     | 713 | GLU  | O-C-N      | -6.65 | 115.07      | 122.12   |
| 1   | A     | 245 | MET  | CA-C-N     | 6.65  | 129.85      | 120.28   |
| 1   | A     | 245 | MET  | C-N-CA     | 6.65  | 129.85      | 120.28   |
| 2   | B     | 340 | ILE  | CA-C-N     | 6.64  | 129.17      | 120.28   |
| 2   | B     | 340 | ILE  | C-N-CA     | 6.64  | 129.17      | 120.28   |
| 1   | A     | 357 | GLN  | CB-CG-CD   | 6.62  | 123.86      | 112.60   |
| 1   | A     | 368 | LEU  | N-CA-C     | 6.62  | 119.32      | 111.71   |
| 1   | A     | 405 | GLY  | N-CA-C     | -6.62 | 104.33      | 112.33   |
| 1   | A     | 673 | ASP  | O-C-N      | -6.61 | 114.20      | 122.20   |
| 1   | A     | 443 | LYS  | CA-C-N     | 6.60  | 129.42      | 120.44   |
| 1   | A     | 443 | LYS  | C-N-CA     | 6.60  | 129.42      | 120.44   |
| 2   | B     | 336 | PRO  | O-C-N      | -6.60 | 113.32      | 122.30   |
| 2   | B     | 388 | GLU  | OE1-CD-OE2 | -6.60 | 107.05      | 122.90   |
| 2   | B     | 239 | ASN  | CA-C-O     | -6.60 | 113.56      | 120.55   |
| 1   | A     | 82  | ARG  | CA-C-O     | 6.58  | 126.54      | 120.09   |
| 2   | B     | 555 | GLU  | N-CA-C     | 6.58  | 119.45      | 111.82   |
| 1   | A     | 52  | GLU  | CA-CB-CG   | 6.58  | 127.26      | 114.10   |
| 1   | A     | 5   | PRO  | N-CA-CB    | 6.58  | 109.04      | 103.25   |
| 1   | A     | 307 | LEU  | N-CA-CB    | 6.58  | 120.70      | 110.44   |
| 1   | A     | 31  | LYS  | CA-C-O     | 6.56  | 127.45      | 119.38   |
| 1   | A     | 28  | LEU  | CA-C-O     | 6.56  | 127.53      | 119.79   |
| 1   | A     | 513 | ASP  | CA-C-N     | 6.55  | 131.82      | 120.68   |
| 1   | A     | 513 | ASP  | C-N-CA     | 6.55  | 131.82      | 120.68   |
| 2   | B     | 558 | LYS  | CA-C-N     | 6.55  | 129.35      | 120.44   |
| 2   | B     | 558 | LYS  | C-N-CA     | 6.55  | 129.35      | 120.44   |
| 1   | A     | 49  | LEU  | N-CA-CB    | 6.55  | 121.39      | 110.59   |
| 2   | B     | 497 | PHE  | CA-C-N     | 6.54  | 128.94      | 120.44   |
| 2   | B     | 497 | PHE  | C-N-CA     | 6.54  | 128.94      | 120.44   |
| 2   | B     | 77  | ARG  | NE-CZ-NH1  | -6.53 | 114.97      | 121.50   |
| 1   | A     | 617 | ILE  | O-C-N      | -6.53 | 113.22      | 121.84   |
| 1   | A     | 200 | ILE  | CB-CG1-CD1 | 6.53  | 127.51      | 113.80   |
| 2   | B     | 627 | LEU  | N-CA-C     | 6.53  | 118.40      | 111.28   |
| 1   | A     | 327 | THR  | N-CA-C     | 6.53  | 119.81      | 109.50   |
| 2   | B     | 379 | ALA  | CA-C-N     | 6.53  | 129.03      | 120.28   |
| 2   | B     | 379 | ALA  | C-N-CA     | 6.53  | 129.03      | 120.28   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 566 | ASP  | CA-CB-CG | 6.53  | 119.12      | 112.60   |
| 1   | A     | 398 | ARG  | CB-CA-C  | 6.52  | 121.06      | 110.95   |
| 2   | B     | 465 | GLU  | O-C-N    | -6.52 | 114.94      | 123.28   |
| 1   | A     | 66  | GLY  | O-C-N    | -6.52 | 114.23      | 122.70   |
| 1   | A     | 146 | ILE  | N-CA-C   | 6.50  | 117.25      | 110.62   |
| 2   | B     | 295 | ALA  | N-CA-C   | 6.50  | 119.19      | 111.33   |
| 1   | A     | 487 | THR  | N-CA-C   | 6.49  | 119.17      | 111.71   |
| 1   | A     | 288 | TRP  | CA-C-N   | 6.49  | 128.66      | 122.36   |
| 1   | A     | 288 | TRP  | C-N-CA   | 6.49  | 128.66      | 122.36   |
| 1   | A     | 603 | ALA  | N-CA-C   | 6.49  | 120.03      | 109.59   |
| 1   | A     | 480 | VAL  | N-CA-C   | 6.48  | 116.58      | 107.37   |
| 1   | A     | 303 | ALA  | CA-C-N   | 6.47  | 128.95      | 120.28   |
| 1   | A     | 303 | ALA  | C-N-CA   | 6.47  | 128.95      | 120.28   |
| 2   | B     | 182 | VAL  | CB-CA-C  | -6.47 | 103.60      | 111.88   |
| 2   | B     | 243 | ASN  | O-C-N    | -6.47 | 115.26      | 122.12   |
| 1   | A     | 527 | PRO  | N-CA-C   | 6.47  | 122.25      | 113.84   |
| 1   | A     | 31  | LYS  | CA-C-N   | 6.47  | 134.19      | 121.58   |
| 1   | A     | 31  | LYS  | C-N-CA   | 6.47  | 134.19      | 121.58   |
| 1   | A     | 568 | GLY  | CA-C-N   | 6.47  | 128.61      | 120.72   |
| 1   | A     | 568 | GLY  | C-N-CA   | 6.47  | 128.61      | 120.72   |
| 1   | A     | 441 | ILE  | CA-C-N   | 6.46  | 125.89      | 118.85   |
| 1   | A     | 441 | ILE  | C-N-CA   | 6.46  | 125.89      | 118.85   |
| 2   | B     | 200 | ASP  | CA-C-N   | 6.46  | 126.68      | 119.32   |
| 2   | B     | 200 | ASP  | C-N-CA   | 6.46  | 126.68      | 119.32   |
| 1   | A     | 407 | ALA  | CA-C-O   | -6.45 | 114.00      | 120.90   |
| 1   | A     | 232 | MET  | CA-C-N   | 6.45  | 126.21      | 119.05   |
| 1   | A     | 232 | MET  | C-N-CA   | 6.45  | 126.21      | 119.05   |
| 2   | B     | 578 | GLY  | CA-C-O   | -6.44 | 112.05      | 119.65   |
| 2   | B     | 578 | GLY  | N-CA-C   | 6.44  | 122.23      | 113.99   |
| 2   | B     | 369 | LEU  | CA-C-O   | 6.44  | 127.72      | 120.70   |
| 2   | B     | 128 | GLY  | O-C-N    | -6.43 | 114.34      | 122.70   |
| 1   | A     | 526 | ASP  | CA-C-N   | 6.43  | 126.12      | 119.56   |
| 1   | A     | 526 | ASP  | C-N-CA   | 6.43  | 126.12      | 119.56   |
| 1   | A     | 54  | VAL  | CA-C-N   | 6.43  | 129.42      | 120.29   |
| 1   | A     | 54  | VAL  | C-N-CA   | 6.43  | 129.42      | 120.29   |
| 1   | A     | 611 | ASP  | CA-CB-CG | 6.43  | 119.03      | 112.60   |
| 2   | B     | 370 | PRO  | N-CA-CB  | 6.43  | 109.05      | 103.27   |
| 2   | B     | 628 | SER  | CA-C-N   | 6.42  | 128.78      | 120.44   |
| 2   | B     | 628 | SER  | C-N-CA   | 6.42  | 128.78      | 120.44   |
| 1   | A     | 74  | PRO  | CB-CA-C  | -6.42 | 102.31      | 111.68   |
| 2   | B     | 142 | PRO  | CA-C-N   | 6.42  | 135.14      | 122.31   |
| 2   | B     | 142 | PRO  | C-N-CA   | 6.42  | 135.14      | 122.31   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 472 | ARG  | NE-CZ-NH2  | 6.42  | 124.97      | 119.20   |
| 1   | A     | 294 | PHE  | CA-CB-CG   | -6.41 | 107.39      | 113.80   |
| 2   | B     | 388 | GLU  | CG-CD-OE1  | 6.41  | 133.15      | 118.40   |
| 1   | A     | 418 | ARG  | O-C-N      | -6.41 | 115.17      | 122.09   |
| 1   | A     | 63  | THR  | N-CA-CB    | 6.41  | 119.16      | 110.38   |
| 2   | B     | 328 | TRP  | O-C-N      | -6.41 | 114.85      | 122.15   |
| 1   | A     | 201 | LEU  | O-C-N      | -6.40 | 114.45      | 122.20   |
| 2   | B     | 382 | THR  | CA-CB-OG1  | -6.40 | 100.00      | 109.60   |
| 1   | A     | 573 | GLU  | N-CA-C     | 6.40  | 118.25      | 111.28   |
| 2   | B     | 377 | ARG  | CA-C-N     | 6.39  | 129.50      | 120.42   |
| 2   | B     | 377 | ARG  | C-N-CA     | 6.39  | 129.50      | 120.42   |
| 1   | A     | 558 | ARG  | CD-NE-CZ   | 6.39  | 133.35      | 124.40   |
| 1   | A     | 641 | ALA  | CA-C-N     | 6.39  | 129.67      | 120.79   |
| 1   | A     | 641 | ALA  | C-N-CA     | 6.39  | 129.67      | 120.79   |
| 1   | A     | 637 | PRO  | CA-C-N     | 6.39  | 132.41      | 122.26   |
| 1   | A     | 637 | PRO  | C-N-CA     | 6.39  | 132.41      | 122.26   |
| 2   | B     | 60  | LYS  | O-C-N      | -6.38 | 115.35      | 122.12   |
| 1   | A     | 525 | LYS  | CA-C-O     | 6.38  | 126.07      | 119.05   |
| 1   | A     | 66  | GLY  | CA-C-O     | 6.38  | 131.66      | 120.57   |
| 1   | A     | 398 | ARG  | CA-C-N     | 6.38  | 131.28      | 121.71   |
| 1   | A     | 398 | ARG  | C-N-CA     | 6.38  | 131.28      | 121.71   |
| 1   | A     | 122 | HIS  | N-CA-C     | 6.38  | 119.04      | 111.33   |
| 2   | B     | 345 | ILE  | CB-CG1-CD1 | 6.37  | 127.17      | 113.80   |
| 1   | A     | 129 | ASN  | CA-C-O     | 6.36  | 125.53      | 120.19   |
| 1   | A     | 677 | ARG  | N-CA-CB    | -6.34 | 101.89      | 111.21   |
| 2   | B     | 607 | ALA  | CA-C-N     | 6.34  | 131.42      | 120.58   |
| 2   | B     | 607 | ALA  | C-N-CA     | 6.34  | 131.42      | 120.58   |
| 1   | A     | 370 | GLU  | N-CA-CB    | -6.34 | 101.31      | 110.56   |
| 2   | B     | 466 | PHE  | CA-C-N     | 6.33  | 126.25      | 119.85   |
| 2   | B     | 466 | PHE  | C-N-CA     | 6.33  | 126.25      | 119.85   |
| 2   | B     | 77  | ARG  | CA-C-N     | 6.33  | 126.81      | 119.47   |
| 2   | B     | 77  | ARG  | C-N-CA     | 6.33  | 126.81      | 119.47   |
| 2   | B     | 335 | ASP  | CA-C-N     | 6.32  | 125.95      | 119.56   |
| 2   | B     | 335 | ASP  | C-N-CA     | 6.32  | 125.95      | 119.56   |
| 1   | A     | 439 | LYS  | N-CA-C     | 6.32  | 120.55      | 112.34   |
| 1   | A     | 358 | GLY  | O-C-N      | -6.31 | 114.50      | 122.70   |
| 2   | B     | 318 | ARG  | CD-NE-CZ   | 6.31  | 133.24      | 124.40   |
| 1   | A     | 213 | PRO  | CA-C-N     | 6.31  | 127.72      | 119.84   |
| 1   | A     | 213 | PRO  | C-N-CA     | 6.31  | 127.72      | 119.84   |
| 2   | B     | 451 | LYS  | CA-C-O     | -6.30 | 113.87      | 120.55   |
| 2   | B     | 390 | VAL  | CA-C-O     | 6.30  | 127.45      | 120.46   |
| 1   | A     | 241 | SER  | CA-C-N     | 6.29  | 133.75      | 121.41   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 241 | SER  | C-N-CA   | 6.29  | 133.75      | 121.41   |
| 2   | B     | 48  | PRO  | CA-C-N   | 6.29  | 126.03      | 119.05   |
| 2   | B     | 48  | PRO  | C-N-CA   | 6.29  | 126.03      | 119.05   |
| 1   | A     | 280 | PHE  | CA-C-N   | 6.28  | 127.57      | 119.78   |
| 1   | A     | 280 | PHE  | C-N-CA   | 6.28  | 127.57      | 119.78   |
| 1   | A     | 697 | ARG  | O-C-N    | -6.28 | 114.99      | 122.15   |
| 1   | A     | 213 | PRO  | N-CA-CB  | 6.26  | 109.15      | 103.08   |
| 1   | A     | 289 | GLY  | O-C-N    | -6.26 | 116.97      | 123.48   |
| 2   | B     | 397 | ASP  | CA-C-N   | 6.26  | 125.83      | 119.19   |
| 2   | B     | 397 | ASP  | C-N-CA   | 6.26  | 125.83      | 119.19   |
| 1   | A     | 385 | ASN  | CA-CB-CG | 6.26  | 118.86      | 112.60   |
| 1   | A     | 518 | ALA  | CA-C-N   | 6.26  | 128.95      | 120.44   |
| 1   | A     | 518 | ALA  | C-N-CA   | 6.26  | 128.95      | 120.44   |
| 1   | A     | 41  | ALA  | N-CA-C   | 6.25  | 120.00      | 112.38   |
| 1   | A     | 523 | ASP  | CA-CB-CG | 6.25  | 118.85      | 112.60   |
| 1   | A     | 105 | ASN  | CA-C-N   | 6.25  | 129.47      | 120.79   |
| 1   | A     | 105 | ASN  | C-N-CA   | 6.25  | 129.47      | 120.79   |
| 1   | A     | 18  | PRO  | N-CA-CB  | 6.23  | 109.80      | 103.25   |
| 1   | A     | 628 | VAL  | CA-C-O   | 6.23  | 127.09      | 120.48   |
| 2   | B     | 394 | ARG  | CA-C-O   | 6.23  | 127.15      | 119.79   |
| 2   | B     | 440 | LYS  | CA-C-N   | 6.23  | 128.41      | 120.56   |
| 2   | B     | 440 | LYS  | C-N-CA   | 6.23  | 128.41      | 120.56   |
| 1   | A     | 121 | THR  | CA-C-N   | 6.23  | 128.92      | 120.38   |
| 1   | A     | 121 | THR  | C-N-CA   | 6.23  | 128.92      | 120.38   |
| 1   | A     | 84  | TRP  | O-C-N    | -6.23 | 114.31      | 122.59   |
| 1   | A     | 343 | ASN  | CA-C-N   | 6.23  | 131.12      | 120.72   |
| 1   | A     | 343 | ASN  | C-N-CA   | 6.23  | 131.12      | 120.72   |
| 2   | B     | 43  | LEU  | N-CA-C   | 6.23  | 119.04      | 111.82   |
| 1   | A     | 387 | GLN  | CA-C-N   | 6.22  | 128.94      | 120.54   |
| 1   | A     | 387 | GLN  | C-N-CA   | 6.22  | 128.94      | 120.54   |
| 2   | B     | 20  | THR  | N-CA-CB  | 6.22  | 120.60      | 110.90   |
| 2   | B     | 18  | PRO  | CA-C-O   | -6.22 | 113.85      | 121.31   |
| 2   | B     | 146 | ALA  | CA-C-O   | 6.22  | 127.48      | 120.70   |
| 1   | A     | 322 | SER  | CA-C-O   | 6.21  | 126.87      | 119.60   |
| 2   | B     | 319 | GLY  | CA-C-O   | -6.21 | 115.73      | 120.76   |
| 1   | A     | 319 | ASN  | CB-CA-C  | 6.21  | 119.17      | 109.42   |
| 1   | A     | 304 | ALA  | CA-C-N   | 6.21  | 128.92      | 120.54   |
| 1   | A     | 304 | ALA  | C-N-CA   | 6.21  | 128.92      | 120.54   |
| 1   | A     | 14  | ASN  | CA-C-O   | 6.21  | 125.96      | 119.51   |
| 1   | A     | 553 | GLU  | CA-CB-CG | 6.20  | 126.51      | 114.10   |
| 1   | A     | 551 | ALA  | CA-C-N   | 6.20  | 131.99      | 121.14   |
| 1   | A     | 551 | ALA  | C-N-CA   | 6.20  | 131.99      | 121.14   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 364 | THR  | O-C-N     | -6.20 | 114.63      | 122.26   |
| 1   | A     | 339 | GLN  | O-C-N     | -6.20 | 115.35      | 123.16   |
| 2   | B     | 350 | ALA  | CA-C-N    | 6.20  | 128.87      | 120.44   |
| 2   | B     | 350 | ALA  | C-N-CA    | 6.20  | 128.87      | 120.44   |
| 2   | B     | 529 | GLY  | N-CA-C    | 6.19  | 121.92      | 113.99   |
| 1   | A     | 81  | PHE  | CA-CB-CG  | 6.18  | 119.98      | 113.80   |
| 1   | A     | 194 | GLY  | CA-C-O    | 6.18  | 127.84      | 121.35   |
| 2   | B     | 384 | ILE  | N-CA-CB   | 6.18  | 117.78      | 110.55   |
| 1   | A     | 332 | SER  | CA-C-O    | 6.17  | 127.91      | 120.81   |
| 2   | B     | 352 | VAL  | CA-C-N    | 6.17  | 133.51      | 121.41   |
| 2   | B     | 352 | VAL  | C-N-CA    | 6.17  | 133.51      | 121.41   |
| 1   | A     | 357 | GLN  | CA-C-N    | 6.17  | 133.50      | 121.41   |
| 1   | A     | 357 | GLN  | C-N-CA    | 6.17  | 133.50      | 121.41   |
| 2   | B     | 238 | ALA  | CA-C-N    | 6.17  | 128.54      | 120.28   |
| 2   | B     | 238 | ALA  | C-N-CA    | 6.17  | 128.54      | 120.28   |
| 2   | B     | 230 | ASP  | CA-CB-CG  | 6.16  | 118.76      | 112.60   |
| 1   | A     | 692 | ASP  | CA-CB-CG  | 6.16  | 118.76      | 112.60   |
| 1   | A     | 171 | VAL  | CB-CA-C   | -6.15 | 102.62      | 112.16   |
| 1   | A     | 687 | VAL  | O-C-N     | -6.14 | 114.89      | 122.57   |
| 1   | A     | 171 | VAL  | CA-C-O    | -6.14 | 114.00      | 120.57   |
| 1   | A     | 659 | GLY  | N-CA-C    | 6.14  | 123.51      | 115.47   |
| 1   | A     | 355 | ALA  | O-C-N     | -6.13 | 114.44      | 122.59   |
| 1   | A     | 521 | ASN  | CA-C-N    | 6.13  | 127.34      | 120.66   |
| 1   | A     | 521 | ASN  | C-N-CA    | 6.13  | 127.34      | 120.66   |
| 1   | A     | 421 | TRP  | CA-C-N    | 6.13  | 126.91      | 119.99   |
| 1   | A     | 421 | TRP  | C-N-CA    | 6.13  | 126.91      | 119.99   |
| 1   | A     | 590 | PHE  | CA-C-O    | -6.13 | 113.85      | 121.02   |
| 1   | A     | 44  | ILE  | N-CA-CB   | 6.12  | 119.78      | 111.21   |
| 1   | A     | 597 | ARG  | NE-CZ-NH2 | -6.12 | 113.69      | 119.20   |
| 1   | A     | 345 | VAL  | CA-C-O    | -6.11 | 114.69      | 121.17   |
| 1   | A     | 492 | GLN  | CA-C-N    | 6.11  | 128.47      | 120.28   |
| 1   | A     | 492 | GLN  | C-N-CA    | 6.11  | 128.47      | 120.28   |
| 1   | A     | 444 | MET  | CA-C-O    | -6.11 | 114.41      | 120.70   |
| 1   | A     | 28  | LEU  | CA-C-N    | 6.11  | 128.38      | 120.44   |
| 1   | A     | 28  | LEU  | C-N-CA    | 6.11  | 128.38      | 120.44   |
| 2   | B     | 469 | ILE  | N-CA-C    | -6.11 | 101.67      | 109.30   |
| 1   | A     | 247 | GLU  | O-C-N     | -6.10 | 114.76      | 122.27   |
| 1   | A     | 633 | LEU  | O-C-N     | -6.10 | 116.07      | 122.96   |
| 2   | B     | 47  | ARG  | CD-NE-CZ  | 6.10  | 132.94      | 124.40   |
| 2   | B     | 147 | PRO  | O-C-N     | -6.09 | 114.41      | 122.64   |
| 1   | A     | 297 | GLU  | CA-C-O    | -6.09 | 112.97      | 119.97   |
| 2   | B     | 385 | VAL  | CA-C-N    | 6.09  | 128.76      | 120.54   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 385 | VAL  | C-N-CA     | 6.09  | 128.76      | 120.54   |
| 1   | A     | 384 | ARG  | NH1-CZ-NH2 | 6.06  | 127.18      | 119.30   |
| 2   | B     | 330 | GLU  | CA-C-O     | -6.06 | 111.93      | 119.38   |
| 1   | A     | 344 | ASN  | O-C-N      | -6.05 | 114.32      | 122.43   |
| 2   | B     | 345 | ILE  | CA-C-O     | -6.05 | 113.94      | 120.47   |
| 2   | B     | 498 | GLU  | CA-C-N     | 6.05  | 128.99      | 120.28   |
| 2   | B     | 498 | GLU  | C-N-CA     | 6.05  | 128.99      | 120.28   |
| 1   | A     | 415 | ASP  | CA-C-O     | -6.04 | 114.14      | 120.55   |
| 2   | B     | 324 | ALA  | N-CA-C     | 6.04  | 119.37      | 109.76   |
| 1   | A     | 257 | ALA  | CA-C-O     | -6.04 | 113.95      | 121.02   |
| 1   | A     | 351 | GLU  | O-C-N      | -6.03 | 115.27      | 122.15   |
| 2   | B     | 39  | VAL  | CA-C-N     | 6.03  | 130.94      | 120.68   |
| 2   | B     | 39  | VAL  | C-N-CA     | 6.03  | 130.94      | 120.68   |
| 2   | B     | 26  | ASP  | CA-CB-CG   | 6.03  | 118.63      | 112.60   |
| 1   | A     | 703 | GLU  | CA-C-O     | 6.03  | 127.49      | 120.80   |
| 1   | A     | 340 | ASP  | OD1-CG-OD2 | -6.02 | 108.44      | 122.90   |
| 1   | A     | 637 | PRO  | N-CA-CB    | 6.01  | 109.20      | 103.19   |
| 1   | A     | 194 | GLY  | O-C-N      | -6.01 | 118.15      | 123.92   |
| 1   | A     | 549 | SER  | CA-C-N     | 6.01  | 128.61      | 120.38   |
| 1   | A     | 549 | SER  | C-N-CA     | 6.01  | 128.61      | 120.38   |
| 1   | A     | 664 | LEU  | CA-C-O     | -6.01 | 114.69      | 121.00   |
| 1   | A     | 48  | THR  | CA-C-O     | 6.00  | 126.29      | 119.27   |
| 1   | A     | 685 | GLY  | N-CA-C     | 6.00  | 121.66      | 111.04   |
| 1   | A     | 20  | ASP  | N-CA-C     | 6.00  | 120.11      | 113.21   |
| 1   | A     | 171 | VAL  | N-CA-C     | 5.99  | 118.54      | 111.05   |
| 1   | A     | 683 | THR  | O-C-N      | 5.98  | 130.97      | 123.19   |
| 1   | A     | 216 | PRO  | N-CA-CB    | 5.98  | 109.25      | 103.51   |
| 2   | B     | 192 | ASP  | N-CA-C     | 5.98  | 120.30      | 112.89   |
| 2   | B     | 478 | PRO  | N-CA-CB    | 5.97  | 108.57      | 103.19   |
| 2   | B     | 63  | THR  | CA-CB-CG2  | 5.97  | 120.65      | 110.50   |
| 1   | A     | 44  | ILE  | CA-C-O     | 5.97  | 127.95      | 119.95   |
| 1   | A     | 441 | ILE  | CB-CG1-CD1 | 5.97  | 126.33      | 113.80   |
| 1   | A     | 524 | ASP  | N-CA-C     | 5.97  | 119.30      | 112.97   |
| 2   | B     | 632 | ASP  | N-CA-C     | 5.96  | 119.39      | 111.75   |
| 2   | B     | 169 | ARG  | CD-NE-CZ   | 5.96  | 132.75      | 124.40   |
| 2   | B     | 341 | LEU  | CA-C-N     | 5.96  | 128.19      | 120.44   |
| 2   | B     | 341 | LEU  | C-N-CA     | 5.96  | 128.19      | 120.44   |
| 1   | A     | 625 | GLY  | CA-C-N     | 5.96  | 129.58      | 120.82   |
| 1   | A     | 625 | GLY  | C-N-CA     | 5.96  | 129.58      | 120.82   |
| 2   | B     | 178 | ALA  | N-CA-C     | -5.96 | 104.17      | 112.45   |
| 2   | B     | 619 | MET  | CA-CB-CG   | 5.96  | 126.01      | 114.10   |
| 2   | B     | 188 | LYS  | CA-C-O     | 5.95  | 128.31      | 120.16   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 122 | HIS  | CA-CB-CG  | 5.93  | 119.73      | 113.80   |
| 2   | B     | 129 | LEU  | O-C-N     | -5.93 | 114.70      | 122.59   |
| 2   | B     | 319 | GLY  | O-C-N     | 5.93  | 127.74      | 123.35   |
| 1   | A     | 576 | ASN  | N-CA-C    | 5.92  | 117.27      | 107.20   |
| 2   | B     | 86  | GLY  | CA-C-O    | 5.92  | 126.32      | 122.23   |
| 2   | B     | 534 | VAL  | O-C-N     | -5.92 | 115.73      | 121.83   |
| 2   | B     | 600 | LYS  | O-C-N     | -5.92 | 114.75      | 122.39   |
| 1   | A     | 249 | GLY  | O-C-N     | 5.92  | 130.39      | 122.70   |
| 2   | B     | 522 | ARG  | CA-C-O    | 5.92  | 126.22      | 119.18   |
| 2   | B     | 404 | TYR  | CB-CG-CD1 | 5.92  | 129.67      | 120.80   |
| 1   | A     | 516 | THR  | O-C-N     | -5.91 | 115.98      | 122.07   |
| 1   | A     | 677 | ARG  | O-C-N     | -5.91 | 116.05      | 121.37   |
| 2   | B     | 143 | ASP  | CA-CB-CG  | 5.91  | 118.51      | 112.60   |
| 1   | A     | 559 | TYR  | CA-C-O    | 5.91  | 127.78      | 121.16   |
| 1   | A     | 146 | ILE  | CA-C-N    | 5.90  | 128.11      | 120.44   |
| 1   | A     | 146 | ILE  | C-N-CA    | 5.90  | 128.11      | 120.44   |
| 2   | B     | 19  | THR  | CA-C-N    | 5.89  | 130.98      | 122.44   |
| 2   | B     | 19  | THR  | C-N-CA    | 5.89  | 130.98      | 122.44   |
| 2   | B     | 632 | ASP  | O-C-N     | -5.88 | 115.50      | 122.20   |
| 2   | B     | 447 | ALA  | CA-C-O    | 5.88  | 126.77      | 120.24   |
| 1   | A     | 493 | LYS  | CA-C-N    | 5.88  | 133.01      | 122.38   |
| 1   | A     | 493 | LYS  | C-N-CA    | 5.88  | 133.01      | 122.38   |
| 1   | A     | 347 | ARG  | NE-CZ-NH2 | -5.87 | 113.91      | 119.20   |
| 2   | B     | 218 | GLY  | CA-C-N    | 5.87  | 128.43      | 120.38   |
| 2   | B     | 218 | GLY  | C-N-CA    | 5.87  | 128.43      | 120.38   |
| 2   | B     | 303 | ALA  | N-CA-C    | 5.87  | 120.30      | 113.20   |
| 2   | B     | 397 | ASP  | CA-C-O    | 5.87  | 128.20      | 120.16   |
| 2   | B     | 465 | GLU  | CA-C-O    | 5.87  | 127.36      | 120.20   |
| 1   | A     | 211 | ILE  | N-CA-CB   | 5.87  | 120.91      | 111.23   |
| 1   | A     | 539 | GLY  | CA-C-N    | 5.86  | 128.41      | 120.38   |
| 1   | A     | 539 | GLY  | C-N-CA    | 5.86  | 128.41      | 120.38   |
| 1   | A     | 119 | LEU  | CA-C-N    | 5.86  | 127.17      | 119.84   |
| 1   | A     | 119 | LEU  | C-N-CA    | 5.86  | 127.17      | 119.84   |
| 2   | B     | 552 | GLU  | N-CA-C    | -5.86 | 106.47      | 113.97   |
| 1   | A     | 497 | VAL  | CA-C-N    | 5.85  | 128.60      | 120.29   |
| 1   | A     | 497 | VAL  | C-N-CA    | 5.85  | 128.60      | 120.29   |
| 1   | A     | 597 | ARG  | CA-C-O    | 5.85  | 124.97      | 119.76   |
| 1   | A     | 399 | VAL  | CA-C-N    | 5.85  | 129.68      | 122.37   |
| 1   | A     | 399 | VAL  | C-N-CA    | 5.85  | 129.68      | 122.37   |
| 1   | A     | 458 | ASP  | O-C-N     | -5.85 | 115.38      | 122.22   |
| 1   | A     | 281 | ALA  | CA-C-N    | 5.85  | 125.47      | 119.56   |
| 1   | A     | 281 | ALA  | C-N-CA    | 5.85  | 125.47      | 119.56   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 453 | THR  | CA-C-O     | -5.85 | 114.68      | 120.70   |
| 2   | B     | 199 | LEU  | CA-C-O     | 5.84  | 127.71      | 121.16   |
| 2   | B     | 100 | ARG  | CG-CD-NE   | 5.84  | 124.85      | 112.00   |
| 1   | A     | 375 | PRO  | CA-C-O     | 5.84  | 128.31      | 121.31   |
| 2   | B     | 307 | ILE  | O-C-N      | -5.84 | 116.21      | 121.87   |
| 2   | B     | 411 | SER  | O-C-N      | -5.83 | 116.03      | 122.09   |
| 1   | A     | 462 | GLN  | CG-CD-NE2  | 5.83  | 125.14      | 116.40   |
| 1   | A     | 11  | ASP  | CA-CB-CG   | 5.82  | 118.42      | 112.60   |
| 1   | A     | 152 | LEU  | CA-C-N     | 5.82  | 132.56      | 122.56   |
| 1   | A     | 152 | LEU  | C-N-CA     | 5.82  | 132.56      | 122.56   |
| 1   | A     | 607 | GLN  | CA-C-N     | 5.82  | 129.98      | 121.31   |
| 1   | A     | 607 | GLN  | C-N-CA     | 5.82  | 129.98      | 121.31   |
| 1   | A     | 62  | ASP  | N-CA-C     | -5.81 | 104.36      | 113.02   |
| 1   | A     | 245 | MET  | O-C-N      | -5.81 | 115.98      | 122.03   |
| 2   | B     | 529 | GLY  | O-C-N      | -5.79 | 116.17      | 122.54   |
| 1   | A     | 575 | LYS  | CA-CB-CG   | 5.79  | 125.68      | 114.10   |
| 1   | A     | 364 | HIS  | CA-C-O     | -5.78 | 113.96      | 120.32   |
| 1   | A     | 636 | THR  | CA-C-N     | 5.78  | 126.54      | 120.12   |
| 1   | A     | 636 | THR  | C-N-CA     | 5.78  | 126.54      | 120.12   |
| 1   | A     | 509 | LYS  | N-CA-C     | 5.78  | 118.32      | 111.33   |
| 1   | A     | 314 | GLN  | N-CA-C     | 5.77  | 123.10      | 110.80   |
| 2   | B     | 27  | PHE  | CA-C-N     | 5.77  | 125.72      | 119.78   |
| 2   | B     | 27  | PHE  | C-N-CA     | 5.77  | 125.72      | 119.78   |
| 1   | A     | 340 | ASP  | CB-CG-OD2  | 5.77  | 131.67      | 118.40   |
| 1   | A     | 157 | PRO  | CA-C-O     | -5.76 | 114.18      | 120.92   |
| 1   | A     | 535 | CYS  | CA-C-N     | 5.76  | 127.82      | 120.56   |
| 1   | A     | 535 | CYS  | C-N-CA     | 5.76  | 127.82      | 120.56   |
| 1   | A     | 428 | GLU  | O-C-N      | -5.76 | 114.51      | 122.46   |
| 1   | A     | 6   | ARG  | CA-CB-CG   | 5.75  | 125.60      | 114.10   |
| 1   | A     | 251 | THR  | CA-C-N     | 5.75  | 128.26      | 120.38   |
| 1   | A     | 251 | THR  | C-N-CA     | 5.75  | 128.26      | 120.38   |
| 2   | B     | 536 | HIS  | CB-CG-CD2  | 5.75  | 138.67      | 131.20   |
| 1   | A     | 347 | ARG  | NH1-CZ-NH2 | 5.74  | 126.77      | 119.30   |
| 2   | B     | 59  | LEU  | CA-C-N     | 5.74  | 128.25      | 120.38   |
| 2   | B     | 59  | LEU  | C-N-CA     | 5.74  | 128.25      | 120.38   |
| 2   | B     | 72  | ILE  | O-C-N      | -5.74 | 116.85      | 122.99   |
| 2   | B     | 323 | ASN  | CA-C-N     | 5.74  | 129.71      | 121.50   |
| 2   | B     | 323 | ASN  | C-N-CA     | 5.74  | 129.71      | 121.50   |
| 2   | B     | 552 | GLU  | CA-C-N     | 5.74  | 130.16      | 120.29   |
| 2   | B     | 552 | GLU  | C-N-CA     | 5.74  | 130.16      | 120.29   |
| 2   | B     | 580 | GLU  | CA-C-N     | 5.74  | 128.00      | 120.60   |
| 2   | B     | 580 | GLU  | C-N-CA     | 5.74  | 128.00      | 120.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 133 | VAL  | CA-CB-CG1  | 5.73  | 120.14      | 110.40   |
| 2   | B     | 520 | THR  | CA-C-O     | 5.73  | 128.70      | 120.51   |
| 2   | B     | 22  | SER  | CA-CB-OG   | 5.73  | 122.56      | 111.10   |
| 1   | A     | 693 | PHE  | CA-C-N     | 5.73  | 127.95      | 120.28   |
| 1   | A     | 693 | PHE  | C-N-CA     | 5.73  | 127.95      | 120.28   |
| 1   | A     | 391 | GLN  | OE1-CD-NE2 | -5.72 | 116.88      | 122.60   |
| 2   | B     | 149 | HIS  | CA-C-N     | 5.72  | 128.41      | 120.29   |
| 2   | B     | 149 | HIS  | C-N-CA     | 5.72  | 128.41      | 120.29   |
| 2   | B     | 377 | ARG  | CD-NE-CZ   | -5.72 | 116.40      | 124.40   |
| 2   | B     | 467 | PRO  | CB-CA-C    | -5.72 | 103.49      | 110.98   |
| 2   | B     | 328 | TRP  | CA-C-N     | 5.71  | 127.94      | 120.28   |
| 2   | B     | 328 | TRP  | C-N-CA     | 5.71  | 127.94      | 120.28   |
| 1   | A     | 662 | LEU  | N-CA-C     | 5.71  | 119.86      | 113.01   |
| 1   | A     | 600 | ILE  | CA-C-O     | 5.71  | 126.41      | 120.36   |
| 2   | B     | 76  | TYR  | O-C-N      | -5.71 | 116.54      | 123.10   |
| 2   | B     | 197 | LEU  | CA-C-O     | -5.71 | 114.43      | 120.71   |
| 1   | A     | 313 | HIS  | CA-C-N     | 5.70  | 132.44      | 121.54   |
| 1   | A     | 313 | HIS  | C-N-CA     | 5.70  | 132.44      | 121.54   |
| 2   | B     | 18  | PRO  | N-CA-CB    | 5.70  | 108.64      | 103.34   |
| 2   | B     | 294 | ILE  | CA-C-N     | 5.70  | 128.19      | 120.38   |
| 2   | B     | 294 | ILE  | C-N-CA     | 5.70  | 128.19      | 120.38   |
| 2   | B     | 518 | LEU  | N-CA-C     | 5.70  | 117.50      | 108.67   |
| 1   | A     | 406 | SER  | N-CA-CB    | 5.69  | 120.10      | 110.49   |
| 1   | A     | 411 | GLU  | CB-CG-CD   | 5.68  | 122.26      | 112.60   |
| 2   | B     | 600 | LYS  | CA-C-N     | 5.68  | 131.97      | 121.52   |
| 2   | B     | 600 | LYS  | C-N-CA     | 5.68  | 131.97      | 121.52   |
| 2   | B     | 279 | THR  | N-CA-C     | -5.68 | 106.99      | 114.31   |
| 2   | B     | 338 | VAL  | N-CA-C     | -5.68 | 106.24      | 113.22   |
| 2   | B     | 580 | GLU  | CA-CB-CG   | 5.68  | 125.45      | 114.10   |
| 1   | A     | 358 | GLY  | CA-C-O     | 5.68  | 130.45      | 120.57   |
| 2   | B     | 204 | PHE  | CA-C-O     | 5.67  | 126.95      | 121.00   |
| 2   | B     | 614 | ASP  | CA-CB-CG   | -5.67 | 106.93      | 112.60   |
| 1   | A     | 70  | PHE  | O-C-N      | -5.67 | 114.81      | 122.41   |
| 1   | A     | 621 | TYR  | CA-C-O     | -5.67 | 114.87      | 120.82   |
| 1   | A     | 273 | VAL  | O-C-N      | 5.67  | 127.97      | 122.25   |
| 1   | A     | 361 | GLN  | CG-CD-OE1  | 5.66  | 132.13      | 120.80   |
| 1   | A     | 59  | ASP  | CA-C-O     | 5.66  | 126.33      | 119.31   |
| 2   | B     | 505 | THR  | CA-C-N     | 5.66  | 128.18      | 120.54   |
| 2   | B     | 505 | THR  | C-N-CA     | 5.66  | 128.18      | 120.54   |
| 2   | B     | 115 | ASP  | N-CA-CB    | -5.66 | 99.84       | 109.57   |
| 1   | A     | 9   | SER  | CA-C-N     | 5.65  | 132.15      | 121.97   |
| 1   | A     | 9   | SER  | C-N-CA     | 5.65  | 132.15      | 121.97   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 327 | SER  | N-CA-C    | 5.65  | 118.75      | 109.76   |
| 1   | A     | 32  | ALA  | CA-C-N    | 5.65  | 129.28      | 121.26   |
| 1   | A     | 32  | ALA  | C-N-CA    | 5.65  | 129.28      | 121.26   |
| 2   | B     | 84  | LYS  | CA-C-O    | -5.65 | 114.42      | 120.92   |
| 2   | B     | 492 | ARG  | NE-CZ-NH2 | 5.65  | 124.28      | 119.20   |
| 1   | A     | 499 | LEU  | N-CA-C    | 5.65  | 118.21      | 111.71   |
| 2   | B     | 36  | GLU  | CA-C-N    | 5.65  | 127.78      | 120.44   |
| 2   | B     | 36  | GLU  | C-N-CA    | 5.65  | 127.78      | 120.44   |
| 1   | A     | 291 | GLY  | O-C-N     | -5.65 | 116.83      | 122.82   |
| 1   | A     | 168 | ASN  | N-CA-C    | -5.64 | 107.04      | 114.04   |
| 1   | A     | 20  | ASP  | CA-C-N    | 5.64  | 132.31      | 121.54   |
| 1   | A     | 20  | ASP  | C-N-CA    | 5.64  | 132.31      | 121.54   |
| 1   | A     | 632 | PRO  | N-CA-CB   | 5.64  | 108.69      | 103.39   |
| 1   | A     | 311 | LEU  | N-CA-C    | 5.63  | 119.66      | 112.34   |
| 1   | A     | 220 | ILE  | CA-C-N    | 5.63  | 128.41      | 120.42   |
| 1   | A     | 220 | ILE  | C-N-CA    | 5.63  | 128.41      | 120.42   |
| 2   | B     | 219 | ASP  | CA-C-N    | 5.63  | 128.09      | 120.44   |
| 2   | B     | 219 | ASP  | C-N-CA    | 5.63  | 128.09      | 120.44   |
| 1   | A     | 346 | VAL  | CB-CA-C   | -5.62 | 104.77      | 111.97   |
| 1   | A     | 601 | LEU  | N-CA-CB   | 5.62  | 119.38      | 110.55   |
| 1   | A     | 194 | GLY  | N-CA-C    | 5.62  | 118.17      | 110.69   |
| 2   | B     | 35  | TRP  | N-CA-CB   | 5.62  | 118.57      | 110.20   |
| 2   | B     | 445 | CYS  | N-CA-CB   | 5.61  | 119.54      | 110.40   |
| 1   | A     | 342 | TYR  | CA-C-N    | 5.60  | 130.94      | 121.14   |
| 1   | A     | 342 | TYR  | C-N-CA    | 5.60  | 130.94      | 121.14   |
| 1   | A     | 451 | ALA  | O-C-N     | -5.60 | 116.30      | 122.07   |
| 2   | B     | 296 | ARG  | NE-CZ-NH2 | 5.60  | 124.24      | 119.20   |
| 2   | B     | 240 | ILE  | CA-C-N    | 5.60  | 127.78      | 120.28   |
| 2   | B     | 240 | ILE  | C-N-CA    | 5.60  | 127.78      | 120.28   |
| 1   | A     | 436 | ALA  | O-C-N     | -5.59 | 116.19      | 122.12   |
| 2   | B     | 403 | TYR  | O-C-N     | -5.59 | 115.43      | 122.20   |
| 2   | B     | 439 | THR  | CA-C-N    | 5.59  | 128.09      | 120.54   |
| 2   | B     | 439 | THR  | C-N-CA    | 5.59  | 128.09      | 120.54   |
| 1   | A     | 617 | ILE  | CA-C-O    | 5.59  | 126.69      | 120.71   |
| 2   | B     | 377 | ARG  | NE-CZ-NH1 | 5.59  | 127.09      | 121.50   |
| 2   | B     | 457 | LYS  | O-C-N     | -5.58 | 115.10      | 122.42   |
| 1   | A     | 432 | GLY  | CA-C-O    | -5.58 | 115.99      | 120.79   |
| 1   | A     | 679 | ASP  | CA-C-O    | -5.58 | 114.96      | 120.82   |
| 2   | B     | 302 | GLU  | CA-C-N    | 5.58  | 133.10      | 121.94   |
| 2   | B     | 302 | GLU  | C-N-CA    | 5.58  | 133.10      | 121.94   |
| 2   | B     | 480 | PRO  | N-CA-CB   | 5.58  | 108.21      | 103.19   |
| 2   | B     | 536 | HIS  | O-C-N     | -5.58 | 114.76      | 122.46   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 38  | GLU  | CA-CB-CG   | -5.57 | 102.95      | 114.10   |
| 2   | B     | 380 | ARG  | CA-C-O     | -5.57 | 114.64      | 120.55   |
| 2   | B     | 74  | PRO  | N-CA-CB    | 5.57  | 109.43      | 103.52   |
| 1   | A     | 298 | VAL  | CA-C-N     | 5.57  | 128.06      | 120.54   |
| 1   | A     | 298 | VAL  | C-N-CA     | 5.57  | 128.06      | 120.54   |
| 1   | A     | 442 | PRO  | N-CA-C     | 5.57  | 120.86      | 113.40   |
| 1   | A     | 628 | VAL  | N-CA-C     | 5.57  | 115.97      | 108.17   |
| 1   | A     | 381 | ARG  | CB-CA-C    | -5.57 | 102.11      | 110.90   |
| 1   | A     | 208 | ASN  | N-CA-C     | 5.56  | 119.31      | 111.52   |
| 1   | A     | 419 | LYS  | O-C-N      | -5.56 | 115.71      | 122.22   |
| 1   | A     | 265 | ASP  | CA-CB-CG   | 5.56  | 118.16      | 112.60   |
| 2   | B     | 500 | LEU  | CA-C-O     | 5.56  | 125.78      | 119.27   |
| 1   | A     | 633 | LEU  | CA-C-N     | 5.54  | 132.13      | 121.54   |
| 1   | A     | 633 | LEU  | C-N-CA     | 5.54  | 132.13      | 121.54   |
| 1   | A     | 244 | HIS  | CA-C-N     | 5.54  | 127.97      | 120.65   |
| 1   | A     | 244 | HIS  | C-N-CA     | 5.54  | 127.97      | 120.65   |
| 1   | A     | 135 | ASP  | CA-C-N     | 5.53  | 128.77      | 120.69   |
| 1   | A     | 135 | ASP  | C-N-CA     | 5.53  | 128.77      | 120.69   |
| 1   | A     | 285 | SER  | CA-C-O     | 5.53  | 126.67      | 120.70   |
| 1   | A     | 392 | GLN  | OE1-CD-NE2 | -5.53 | 117.07      | 122.60   |
| 1   | A     | 720 | LYS  | O-C-N      | -5.53 | 116.28      | 122.03   |
| 1   | A     | 129 | ASN  | CA-CB-CG   | 5.53  | 118.13      | 112.60   |
| 1   | A     | 132 | VAL  | CB-CA-C    | -5.53 | 101.23      | 111.79   |
| 1   | A     | 311 | LEU  | CA-C-N     | 5.52  | 129.36      | 121.02   |
| 1   | A     | 311 | LEU  | C-N-CA     | 5.52  | 129.36      | 121.02   |
| 1   | A     | 11  | ASP  | CA-C-N     | 5.52  | 128.14      | 120.63   |
| 1   | A     | 11  | ASP  | C-N-CA     | 5.52  | 128.14      | 120.63   |
| 2   | B     | 375 | PRO  | O-C-N      | -5.52 | 116.22      | 122.18   |
| 1   | A     | 250 | ALA  | CA-C-O     | -5.52 | 114.46      | 120.81   |
| 1   | A     | 212 | TYR  | CA-C-N     | 5.51  | 126.06      | 120.38   |
| 1   | A     | 212 | TYR  | C-N-CA     | 5.51  | 126.06      | 120.38   |
| 1   | A     | 512 | LEU  | CA-C-N     | 5.51  | 128.69      | 120.31   |
| 1   | A     | 512 | LEU  | C-N-CA     | 5.51  | 128.69      | 120.31   |
| 2   | B     | 397 | ASP  | O-C-N      | -5.51 | 114.99      | 121.32   |
| 2   | B     | 243 | ASN  | CA-C-O     | 5.50  | 126.38      | 120.55   |
| 1   | A     | 698 | LYS  | N-CA-C     | 5.50  | 118.03      | 111.71   |
| 2   | B     | 292 | LEU  | CB-CA-C    | 5.49  | 120.19      | 110.85   |
| 1   | A     | 529 | ARG  | N-CA-C     | -5.49 | 104.82      | 112.45   |
| 1   | A     | 284 | LEU  | O-C-N      | 5.49  | 129.74      | 123.27   |
| 2   | B     | 482 | ALA  | CA-C-O     | 5.49  | 126.62      | 120.04   |
| 1   | A     | 188 | LYS  | CA-C-N     | 5.48  | 126.69      | 119.84   |
| 1   | A     | 188 | LYS  | C-N-CA     | 5.48  | 126.69      | 119.84   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 454 | GLN  | N-CA-C     | 5.48  | 117.25      | 111.28   |
| 1   | A     | 436 | ALA  | CA-C-N     | 5.48  | 128.20      | 120.42   |
| 1   | A     | 436 | ALA  | C-N-CA     | 5.48  | 128.20      | 120.42   |
| 1   | A     | 117 | PHE  | CA-C-O     | 5.47  | 127.34      | 121.16   |
| 1   | A     | 582 | GLU  | CA-C-O     | -5.47 | 115.08      | 120.82   |
| 1   | A     | 63  | THR  | CA-C-N     | -5.47 | 113.87      | 122.73   |
| 1   | A     | 63  | THR  | C-N-CA     | -5.47 | 113.87      | 122.73   |
| 2   | B     | 267 | VAL  | CA-C-N     | 5.47  | 128.15      | 120.28   |
| 2   | B     | 267 | VAL  | C-N-CA     | 5.47  | 128.15      | 120.28   |
| 2   | B     | 377 | ARG  | CG-CD-NE   | 5.46  | 124.01      | 112.00   |
| 1   | A     | 678 | PRO  | N-CA-CB    | 5.46  | 109.31      | 103.52   |
| 1   | A     | 52  | GLU  | N-CA-C     | 5.45  | 119.03      | 112.38   |
| 1   | A     | 357 | GLN  | N-CA-C     | 5.45  | 119.55      | 113.01   |
| 2   | B     | 531 | SER  | CA-C-O     | -5.44 | 113.50      | 120.31   |
| 2   | B     | 251 | GLU  | CA-C-N     | 5.44  | 128.02      | 120.29   |
| 2   | B     | 251 | GLU  | C-N-CA     | 5.44  | 128.02      | 120.29   |
| 2   | B     | 120 | PHE  | CA-CB-CG   | -5.44 | 108.36      | 113.80   |
| 2   | B     | 532 | SER  | CA-C-O     | 5.43  | 123.62      | 118.63   |
| 2   | B     | 511 | PRO  | N-CA-CB    | 5.42  | 108.94      | 103.25   |
| 1   | A     | 256 | MET  | CB-CG-SD   | -5.42 | 96.43       | 112.70   |
| 1   | A     | 528 | ASP  | CA-C-O     | 5.42  | 125.99      | 119.59   |
| 1   | A     | 527 | PRO  | CA-C-N     | 5.42  | 131.05      | 122.60   |
| 1   | A     | 527 | PRO  | C-N-CA     | 5.42  | 131.05      | 122.60   |
| 2   | B     | 398 | PRO  | CA-C-N     | 5.42  | 127.81      | 120.44   |
| 2   | B     | 398 | PRO  | C-N-CA     | 5.42  | 127.81      | 120.44   |
| 2   | B     | 563 | GLN  | CA-C-N     | 5.42  | 131.77      | 122.67   |
| 2   | B     | 563 | GLN  | C-N-CA     | 5.42  | 131.77      | 122.67   |
| 1   | A     | 128 | ASP  | CA-C-O     | 5.41  | 124.91      | 118.79   |
| 1   | A     | 82  | ARG  | CD-NE-CZ   | 5.41  | 131.98      | 124.40   |
| 1   | A     | 224 | ILE  | CA-C-O     | 5.41  | 123.85      | 118.98   |
| 1   | A     | 292 | MET  | N-CA-C     | 5.41  | 119.75      | 113.20   |
| 2   | B     | 496 | VAL  | O-C-N      | -5.41 | 116.41      | 121.87   |
| 2   | B     | 558 | LYS  | CA-C-O     | 5.41  | 126.25      | 120.24   |
| 1   | A     | 105 | ASN  | O-C-N      | -5.41 | 116.39      | 122.12   |
| 2   | B     | 615 | GLY  | CA-C-N     | -5.41 | 113.35      | 123.03   |
| 2   | B     | 615 | GLY  | C-N-CA     | -5.41 | 113.35      | 123.03   |
| 1   | A     | 485 | ASN  | OD1-CG-ND2 | -5.40 | 117.20      | 122.60   |
| 1   | A     | 638 | GLU  | N-CA-C     | -5.40 | 106.70      | 113.72   |
| 2   | B     | 280 | ILE  | CA-C-O     | 5.40  | 127.34      | 120.75   |
| 1   | A     | 621 | TYR  | O-C-N      | -5.40 | 116.51      | 122.07   |
| 1   | A     | 135 | ASP  | CA-CB-CG   | 5.39  | 117.99      | 112.60   |
| 1   | A     | 361 | GLN  | CB-CA-C    | 5.38  | 118.44      | 109.56   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 318 | ARG  | CA-CB-CG   | 5.38  | 124.87      | 114.10   |
| 2   | B     | 460 | ILE  | N-CA-CB    | -5.38 | 105.34      | 112.34   |
| 1   | A     | 347 | ARG  | O-C-N      | -5.38 | 116.50      | 122.09   |
| 2   | B     | 406 | GLU  | CA-C-O     | -5.38 | 114.73      | 121.02   |
| 2   | B     | 424 | GLU  | CA-C-N     | 5.38  | 132.07      | 122.06   |
| 2   | B     | 424 | GLU  | C-N-CA     | 5.38  | 132.07      | 122.06   |
| 1   | A     | 214 | PRO  | CA-C-N     | 5.38  | 128.93      | 120.97   |
| 1   | A     | 214 | PRO  | C-N-CA     | 5.38  | 128.93      | 120.97   |
| 1   | A     | 684 | VAL  | CA-CB-CG1  | 5.38  | 119.54      | 110.40   |
| 2   | B     | 213 | ASP  | CA-CB-CG   | -5.37 | 107.23      | 112.60   |
| 2   | B     | 202 | ILE  | CA-C-N     | 5.36  | 125.90      | 120.00   |
| 2   | B     | 202 | ILE  | C-N-CA     | 5.36  | 125.90      | 120.00   |
| 2   | B     | 243 | ASN  | CA-CB-CG   | 5.36  | 117.96      | 112.60   |
| 2   | B     | 75  | MET  | N-CA-C     | 5.36  | 117.13      | 108.34   |
| 2   | B     | 503 | ARG  | CA-C-O     | -5.36 | 114.87      | 120.55   |
| 2   | B     | 492 | ARG  | CD-NE-CZ   | 5.35  | 131.89      | 124.40   |
| 1   | A     | 150 | ARG  | NE-CZ-NH1  | -5.35 | 116.15      | 121.50   |
| 1   | A     | 335 | SER  | N-CA-C     | 5.34  | 119.06      | 112.54   |
| 1   | A     | 347 | ARG  | CG-CD-NE   | -5.34 | 100.24      | 112.00   |
| 1   | A     | 331 | THR  | CA-CB-OG1  | -5.34 | 101.60      | 109.60   |
| 1   | A     | 364 | HIS  | CG-CD2-NE2 | 5.34  | 112.54      | 107.20   |
| 2   | B     | 37  | ARG  | CA-C-O     | -5.34 | 115.22      | 120.82   |
| 1   | A     | 77  | THR  | N-CA-C     | -5.33 | 106.90      | 113.41   |
| 1   | A     | 180 | VAL  | CA-C-N     | 5.33  | 127.74      | 120.54   |
| 1   | A     | 180 | VAL  | C-N-CA     | 5.33  | 127.74      | 120.54   |
| 1   | A     | 74  | PRO  | N-CA-C     | 5.33  | 120.52      | 113.86   |
| 1   | A     | 401 | ASP  | CA-C-O     | 5.33  | 127.46      | 120.16   |
| 2   | B     | 338 | VAL  | CA-C-N     | 5.33  | 130.46      | 121.14   |
| 2   | B     | 338 | VAL  | C-N-CA     | 5.33  | 130.46      | 121.14   |
| 1   | A     | 137 | GLY  | N-CA-C     | 5.33  | 121.25      | 113.48   |
| 1   | A     | 454 | GLN  | CG-CD-NE2  | 5.33  | 124.39      | 116.40   |
| 2   | B     | 413 | ALA  | CA-C-O     | -5.32 | 115.41      | 121.00   |
| 1   | A     | 351 | GLU  | CB-CG-CD   | 5.32  | 121.64      | 112.60   |
| 2   | B     | 160 | GLU  | CB-CG-CD   | 5.32  | 121.64      | 112.60   |
| 1   | A     | 520 | GLY  | CA-C-N     | 5.32  | 130.26      | 122.98   |
| 1   | A     | 520 | GLY  | C-N-CA     | 5.32  | 130.26      | 122.98   |
| 2   | B     | 126 | LEU  | O-C-N      | -5.32 | 116.56      | 122.09   |
| 1   | A     | 697 | ARG  | CA-C-N     | 5.31  | 127.93      | 120.28   |
| 1   | A     | 697 | ARG  | C-N-CA     | 5.31  | 127.93      | 120.28   |
| 2   | B     | 563 | GLN  | OE1-CD-NE2 | -5.31 | 117.29      | 122.60   |
| 1   | A     | 325 | LEU  | CA-C-O     | -5.31 | 115.40      | 120.92   |
| 2   | B     | 316 | ASP  | CA-C-N     | 5.30  | 132.55      | 121.94   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 316 | ASP  | C-N-CA   | 5.30  | 132.55      | 121.94   |
| 1   | A     | 385 | ASN  | CA-C-N   | 5.30  | 127.65      | 120.44   |
| 1   | A     | 385 | ASN  | C-N-CA   | 5.30  | 127.65      | 120.44   |
| 2   | B     | 414 | ASP  | CA-C-N   | 5.30  | 127.69      | 120.54   |
| 2   | B     | 414 | ASP  | C-N-CA   | 5.30  | 127.69      | 120.54   |
| 2   | B     | 351 | SER  | CA-C-N   | 5.30  | 129.43      | 120.64   |
| 2   | B     | 351 | SER  | C-N-CA   | 5.30  | 129.43      | 120.64   |
| 1   | A     | 202 | LYS  | CA-C-N   | 5.29  | 129.55      | 120.71   |
| 1   | A     | 202 | LYS  | C-N-CA   | 5.29  | 129.55      | 120.71   |
| 1   | A     | 281 | ALA  | CA-C-O   | 5.29  | 123.87      | 118.79   |
| 2   | B     | 236 | ILE  | CB-CA-C  | -5.29 | 105.52      | 111.23   |
| 1   | A     | 325 | LEU  | CA-CB-CG | 5.29  | 134.80      | 116.30   |
| 1   | A     | 316 | GLY  | CA-C-N   | 5.28  | 126.44      | 119.84   |
| 1   | A     | 316 | GLY  | C-N-CA   | 5.28  | 126.44      | 119.84   |
| 1   | A     | 224 | ILE  | O-C-N    | -5.28 | 115.28      | 122.03   |
| 1   | A     | 422 | GLY  | O-C-N    | -5.28 | 116.91      | 122.13   |
| 1   | A     | 449 | ALA  | O-C-N    | -5.27 | 115.54      | 122.39   |
| 2   | B     | 374 | PHE  | CA-C-N   | 5.27  | 124.72      | 119.24   |
| 2   | B     | 374 | PHE  | C-N-CA   | 5.27  | 124.72      | 119.24   |
| 1   | A     | 497 | VAL  | CB-CA-C  | 5.26  | 118.39      | 111.81   |
| 2   | B     | 280 | ILE  | N-CA-C   | 5.26  | 115.94      | 107.73   |
| 2   | B     | 576 | GLN  | CB-CG-CD | 5.26  | 121.55      | 112.60   |
| 2   | B     | 376 | LEU  | O-C-N    | -5.26 | 116.06      | 122.22   |
| 1   | A     | 258 | TYR  | N-CA-C   | 5.26  | 117.92      | 111.82   |
| 2   | B     | 92  | PRO  | N-CA-CB  | 5.25  | 108.38      | 102.60   |
| 2   | B     | 342 | ARG  | CA-C-N   | 5.25  | 125.78      | 120.00   |
| 2   | B     | 342 | ARG  | C-N-CA   | 5.25  | 125.78      | 120.00   |
| 2   | B     | 329 | ARG  | CA-CB-CG | 5.24  | 124.58      | 114.10   |
| 1   | A     | 319 | ASN  | N-CA-CB  | -5.24 | 101.74      | 110.02   |
| 1   | A     | 357 | GLN  | O-C-N    | -5.24 | 115.23      | 122.46   |
| 1   | A     | 479 | ASP  | N-CA-C   | 5.24  | 116.84      | 108.41   |
| 1   | A     | 582 | GLU  | CB-CG-CD | 5.24  | 121.50      | 112.60   |
| 2   | B     | 220 | TRP  | O-C-N    | -5.24 | 116.44      | 122.09   |
| 2   | B     | 389 | GLU  | CA-CB-CG | 5.23  | 124.57      | 114.10   |
| 1   | A     | 179 | VAL  | CA-C-N   | 5.23  | 127.62      | 120.77   |
| 1   | A     | 179 | VAL  | C-N-CA   | 5.23  | 127.62      | 120.77   |
| 2   | B     | 300 | LEU  | CA-C-N   | 5.23  | 127.60      | 120.54   |
| 2   | B     | 300 | LEU  | C-N-CA   | 5.23  | 127.60      | 120.54   |
| 2   | B     | 306 | ARG  | CA-C-O   | -5.23 | 115.30      | 120.90   |
| 1   | A     | 46  | VAL  | CA-C-N   | -5.23 | 117.25      | 122.69   |
| 1   | A     | 46  | VAL  | C-N-CA   | -5.23 | 117.25      | 122.69   |
| 2   | B     | 176 | ALA  | N-CA-C   | 5.22  | 119.28      | 113.01   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 51  | ASN  | O-C-N     | -5.22 | 116.72      | 122.72   |
| 1   | A     | 380 | ALA  | O-C-N     | -5.22 | 116.11      | 122.22   |
| 2   | B     | 103 | ASP  | CA-CB-CG  | 5.22  | 117.82      | 112.60   |
| 2   | B     | 538 | ALA  | CA-C-N    | 5.22  | 128.68      | 121.26   |
| 2   | B     | 538 | ALA  | C-N-CA    | 5.22  | 128.68      | 121.26   |
| 1   | A     | 588 | GLU  | O-C-N     | -5.22 | 115.65      | 122.59   |
| 1   | A     | 613 | GLY  | CA-C-N    | 5.21  | 128.64      | 120.82   |
| 1   | A     | 613 | GLY  | C-N-CA    | 5.21  | 128.64      | 120.82   |
| 1   | A     | 309 | ALA  | N-CA-CB   | -5.21 | 101.68      | 110.49   |
| 1   | A     | 149 | MET  | CA-CB-CG  | -5.20 | 103.69      | 114.10   |
| 1   | A     | 305 | ARG  | CA-C-O    | -5.20 | 115.33      | 120.90   |
| 1   | A     | 374 | LEU  | CA-C-O    | 5.20  | 125.29      | 120.50   |
| 1   | A     | 133 | ALA  | N-CA-C    | 5.20  | 121.88      | 110.80   |
| 1   | A     | 638 | GLU  | CA-CB-CG  | 5.20  | 124.49      | 114.10   |
| 2   | B     | 161 | MET  | CB-CA-C   | -5.20 | 102.02      | 110.85   |
| 1   | A     | 238 | ILE  | N-CA-C    | 5.19  | 114.71      | 108.06   |
| 1   | A     | 524 | ASP  | CA-CB-CG  | 5.19  | 117.79      | 112.60   |
| 1   | A     | 588 | GLU  | CA-C-N    | 5.19  | 129.44      | 121.19   |
| 1   | A     | 588 | GLU  | C-N-CA    | 5.19  | 129.44      | 121.19   |
| 1   | A     | 511 | ALA  | N-CA-C    | -5.18 | 106.11      | 112.90   |
| 2   | B     | 417 | TRP  | CA-C-N    | 5.18  | 128.60      | 120.82   |
| 2   | B     | 417 | TRP  | C-N-CA    | 5.18  | 128.60      | 120.82   |
| 1   | A     | 719 | VAL  | CA-C-O    | -5.18 | 115.56      | 120.95   |
| 2   | B     | 48  | PRO  | N-CA-CB   | 5.18  | 108.11      | 103.08   |
| 2   | B     | 302 | GLU  | O-C-N     | -5.18 | 115.93      | 122.20   |
| 1   | A     | 321 | LYS  | O-C-N     | -5.17 | 116.13      | 122.34   |
| 1   | A     | 495 | LYS  | CA-C-O    | 5.17  | 125.25      | 119.41   |
| 1   | A     | 76  | ALA  | N-CA-C    | 5.17  | 119.64      | 113.23   |
| 2   | B     | 555 | GLU  | CA-C-N    | 5.17  | 130.18      | 121.14   |
| 2   | B     | 555 | GLU  | C-N-CA    | 5.17  | 130.18      | 121.14   |
| 2   | B     | 465 | GLU  | CG-CD-OE1 | 5.16  | 130.28      | 118.40   |
| 1   | A     | 596 | ARG  | N-CA-CB   | 5.16  | 119.21      | 110.49   |
| 2   | B     | 541 | ASP  | O-C-N     | -5.16 | 116.97      | 122.85   |
| 2   | B     | 159 | LEU  | CA-C-N    | 5.15  | 127.61      | 120.29   |
| 2   | B     | 159 | LEU  | C-N-CA    | 5.15  | 127.61      | 120.29   |
| 2   | B     | 106 | ALA  | CA-C-O    | 5.15  | 126.28      | 120.92   |
| 2   | B     | 389 | GLU  | CB-CG-CD  | 5.15  | 121.36      | 112.60   |
| 2   | B     | 331 | LEU  | N-CA-CB   | 5.15  | 117.54      | 109.97   |
| 1   | A     | 654 | VAL  | N-CA-C    | 5.15  | 116.10      | 108.23   |
| 2   | B     | 44  | ASN  | O-C-N     | -5.15 | 115.27      | 122.37   |
| 2   | B     | 361 | LEU  | CA-C-O    | 5.14  | 124.03      | 119.71   |
| 2   | B     | 393 | GLY  | CA-C-N    | 5.14  | 129.43      | 120.68   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 393 | GLY  | C-N-CA   | 5.14  | 129.43      | 120.68   |
| 1   | A     | 182 | ALA  | O-C-N    | -5.14 | 116.29      | 122.15   |
| 1   | A     | 508 | VAL  | N-CA-C   | 5.14  | 115.28      | 110.30   |
| 1   | A     | 565 | THR  | CA-C-O   | 5.14  | 126.78      | 120.92   |
| 1   | A     | 584 | ARG  | CA-C-N   | 5.14  | 127.42      | 120.44   |
| 1   | A     | 584 | ARG  | C-N-CA   | 5.14  | 127.42      | 120.44   |
| 2   | B     | 73  | VAL  | CA-C-N   | 5.14  | 124.63      | 119.19   |
| 2   | B     | 73  | VAL  | C-N-CA   | 5.14  | 124.63      | 119.19   |
| 2   | B     | 368 | GLY  | CA-C-O   | -5.14 | 115.96      | 121.35   |
| 1   | A     | 301 | LEU  | CA-C-O   | -5.13 | 115.06      | 120.55   |
| 2   | B     | 510 | ARG  | CA-C-O   | 5.13  | 124.33      | 119.76   |
| 1   | A     | 300 | LYS  | CA-CB-CG | -5.13 | 103.84      | 114.10   |
| 2   | B     | 619 | MET  | CB-CA-C  | 5.13  | 120.62      | 110.42   |
| 1   | A     | 27  | GLU  | CA-C-N   | 5.12  | 129.39      | 120.68   |
| 1   | A     | 27  | GLU  | C-N-CA   | 5.12  | 129.39      | 120.68   |
| 1   | A     | 122 | HIS  | O-C-N    | -5.12 | 116.69      | 122.12   |
| 1   | A     | 608 | ASP  | CA-C-O   | 5.12  | 126.60      | 121.07   |
| 1   | A     | 718 | LEU  | CA-C-N   | 5.12  | 127.48      | 120.46   |
| 1   | A     | 718 | LEU  | C-N-CA   | 5.12  | 127.48      | 120.46   |
| 2   | B     | 332 | THR  | N-CA-CB  | 5.12  | 119.50      | 111.20   |
| 1   | A     | 445 | ARG  | CD-NE-CZ | 5.12  | 131.56      | 124.40   |
| 1   | A     | 592 | GLN  | O-C-N    | -5.12 | 115.79      | 122.59   |
| 1   | A     | 637 | PRO  | N-CA-C   | 5.11  | 120.33      | 114.20   |
| 2   | B     | 155 | SER  | CA-C-N   | 5.11  | 128.08      | 120.31   |
| 2   | B     | 155 | SER  | C-N-CA   | 5.11  | 128.08      | 120.31   |
| 2   | B     | 528 | GLU  | CA-C-N   | 5.11  | 129.53      | 120.74   |
| 2   | B     | 528 | GLU  | C-N-CA   | 5.11  | 129.53      | 120.74   |
| 2   | B     | 491 | HIS  | N-CA-C   | 5.11  | 117.30      | 109.07   |
| 1   | A     | 240 | ILE  | N-CA-C   | 5.11  | 114.64      | 106.88   |
| 1   | A     | 684 | VAL  | CB-CA-C  | 5.10  | 117.31      | 110.42   |
| 1   | A     | 45  | PRO  | N-CA-C   | -5.10 | 103.18      | 111.14   |
| 1   | A     | 34  | THR  | N-CA-CB  | 5.10  | 117.57      | 109.51   |
| 1   | A     | 59  | ASP  | CA-CB-CG | 5.10  | 117.70      | 112.60   |
| 1   | A     | 480 | VAL  | CB-CA-C  | -5.10 | 106.39      | 111.80   |
| 2   | B     | 200 | ASP  | CA-C-O   | 5.10  | 127.15      | 120.16   |
| 1   | A     | 690 | GLU  | CB-CG-CD | 5.10  | 121.27      | 112.60   |
| 1   | A     | 481 | LEU  | CA-C-N   | 5.09  | 129.90      | 122.41   |
| 1   | A     | 481 | LEU  | C-N-CA   | 5.09  | 129.90      | 122.41   |
| 2   | B     | 307 | ILE  | N-CA-C   | 5.09  | 115.82      | 110.62   |
| 2   | B     | 425 | LYS  | CA-C-N   | 5.09  | 130.20      | 122.87   |
| 2   | B     | 425 | LYS  | C-N-CA   | 5.09  | 130.20      | 122.87   |
| 2   | B     | 456 | ARG  | CG-CD-NE | 5.09  | 123.20      | 112.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 687 | VAL  | CA-C-O     | -5.09 | 114.42      | 120.78   |
| 2   | B     | 364 | THR  | CA-C-O     | 5.09  | 125.95      | 119.95   |
| 1   | A     | 180 | VAL  | CA-C-O     | -5.08 | 116.13      | 121.41   |
| 1   | A     | 538 | ALA  | CA-C-O     | -5.08 | 115.17      | 120.55   |
| 2   | B     | 403 | TYR  | CB-CG-CD1  | 5.08  | 128.42      | 120.80   |
| 1   | A     | 261 | ALA  | O-C-N      | -5.08 | 116.84      | 122.07   |
| 1   | A     | 401 | ASP  | CA-CB-CG   | 5.07  | 117.67      | 112.60   |
| 1   | A     | 669 | ARG  | CA-CB-CG   | 5.07  | 124.24      | 114.10   |
| 2   | B     | 491 | HIS  | CA-CB-CG   | -5.07 | 108.73      | 113.80   |
| 2   | B     | 512 | LYS  | CB-CA-C    | 5.07  | 121.22      | 110.07   |
| 2   | B     | 398 | PRO  | O-C-N      | -5.06 | 115.44      | 122.27   |
| 1   | A     | 448 | GLU  | O-C-N      | -5.05 | 116.67      | 122.08   |
| 2   | B     | 389 | GLU  | CA-C-O     | 5.05  | 124.95      | 119.24   |
| 2   | B     | 349 | SER  | O-C-N      | -5.05 | 116.77      | 122.12   |
| 1   | A     | 550 | ASP  | N-CA-C     | 5.05  | 117.44      | 111.33   |
| 1   | A     | 154 | ALA  | N-CA-C     | -5.04 | 102.40      | 109.96   |
| 1   | A     | 376 | THR  | CA-CB-OG1  | 5.04  | 117.16      | 109.60   |
| 1   | A     | 452 | ARG  | NH1-CZ-NH2 | 5.04  | 125.86      | 119.30   |
| 1   | A     | 685 | GLY  | O-C-N      | -5.04 | 118.74      | 123.48   |
| 2   | B     | 600 | LYS  | CA-C-O     | 5.04  | 125.53      | 119.43   |
| 2   | B     | 250 | ALA  | O-C-N      | -5.04 | 116.85      | 122.09   |
| 1   | A     | 369 | ASP  | CA-CB-CG   | 5.03  | 117.63      | 112.60   |
| 1   | A     | 404 | SER  | CA-C-O     | 5.03  | 127.71      | 120.51   |
| 1   | A     | 453 | THR  | O-C-N      | 5.03  | 127.53      | 122.09   |
| 2   | B     | 532 | SER  | O-C-N      | -5.03 | 115.77      | 120.55   |
| 1   | A     | 123 | ARG  | CB-CG-CD   | 5.03  | 122.87      | 111.30   |
| 2   | B     | 94  | THR  | CA-CB-OG1  | -5.03 | 102.06      | 109.60   |
| 2   | B     | 519 | GLY  | CA-C-O     | -5.02 | 116.18      | 122.61   |
| 2   | B     | 614 | ASP  | N-CA-C     | 5.02  | 119.26      | 113.18   |
| 2   | B     | 570 | SER  | N-CA-CB    | -5.02 | 102.73      | 110.56   |
| 1   | A     | 452 | ARG  | NE-CZ-NH2  | -5.02 | 114.68      | 119.20   |
| 1   | A     | 707 | PRO  | N-CA-CB    | 5.01  | 108.51      | 103.25   |
| 2   | B     | 158 | LEU  | CA-C-N     | 5.01  | 127.70      | 120.38   |
| 2   | B     | 158 | LEU  | C-N-CA     | 5.01  | 127.70      | 120.38   |
| 1   | A     | 59  | ASP  | N-CA-CB    | -5.01 | 102.23      | 110.40   |
| 1   | A     | 385 | ASN  | N-CA-CB    | 5.01  | 118.33      | 110.46   |
| 2   | B     | 412 | LEU  | N-CA-C     | 5.01  | 116.74      | 111.28   |
| 1   | A     | 173 | PRO  | N-CA-CB    | 5.00  | 108.33      | 102.88   |
| 1   | A     | 207 | ARG  | NE-CZ-NH1  | -5.00 | 116.50      | 121.50   |
| 1   | A     | 677 | ARG  | CA-CB-CG   | 5.00  | 124.10      | 114.10   |
| 2   | B     | 189 | PRO  | N-CA-CB    | 5.00  | 108.50      | 103.25   |

There are no chirality outliers.

All (20) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 172 | LEU  | Mainchain |
| 1   | A     | 215 | GLN  | Mainchain |
| 1   | A     | 264 | VAL  | Mainchain |
| 1   | A     | 277 | VAL  | Mainchain |
| 1   | A     | 30  | ALA  | Mainchain |
| 1   | A     | 339 | GLN  | Mainchain |
| 1   | A     | 340 | ASP  | Mainchain |
| 1   | A     | 438 | GLU  | Mainchain |
| 1   | A     | 621 | TYR  | Mainchain |
| 1   | A     | 640 | THR  | Mainchain |
| 1   | A     | 687 | VAL  | Mainchain |
| 1   | A     | 74  | PRO  | Mainchain |
| 2   | B     | 336 | PRO  | Mainchain |
| 2   | B     | 338 | VAL  | Mainchain |
| 2   | B     | 35  | TRP  | Mainchain |
| 2   | B     | 362 | PRO  | Mainchain |
| 2   | B     | 451 | LYS  | Mainchain |
| 2   | B     | 535 | TRP  | Mainchain |
| 2   | B     | 599 | PHE  | Mainchain |
| 2   | B     | 86  | GLY  | Mainchain |

## 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     | 5552  | 0        | 5449     | 109     | 0            |
| 2   | B     | 4624  | 0        | 4439     | 107     | 0            |
| 3   | A     | 91    | 0        | 88       | 22      | 0            |
| 4   | A     | 18    | 0        | 10       | 0       | 0            |
| All | All   | 10285 | 0        | 9986     | 212     | 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 10.

All (212) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:406:SER:HB2  | 2:B:400:GLY:O    | 1.34                     | 1.22              |
| 3:A:800:B12:H362 | 3:A:800:B12:H351 | 1.35                     | 1.06              |
| 3:A:800:B12:H353 | 3:A:800:B12:H302 | 1.37                     | 1.06              |
| 1:A:406:SER:CB   | 2:B:400:GLY:O    | 2.02                     | 1.05              |
| 3:A:800:B12:H312 | 3:A:800:B12:C25  | 1.90                     | 1.01              |
| 1:A:406:SER:N    | 2:B:401:GLY:O    | 2.04                     | 0.91              |
| 2:B:374:PHE:HB3  | 2:B:375:PRO:HD3  | 1.55                     | 0.87              |
| 1:A:405:GLY:C    | 2:B:401:GLY:O    | 2.18                     | 0.86              |
| 1:A:406:SER:HA   | 2:B:400:GLY:O    | 1.76                     | 0.85              |
| 3:A:800:B12:H312 | 3:A:800:B12:H251 | 1.58                     | 0.85              |
| 1:A:706:THR:HB   | 1:A:707:PRO:HD2  | 1.61                     | 0.83              |
| 1:A:316:GLY:H    | 1:A:317:PRO:HD3  | 1.43                     | 0.81              |
| 3:A:800:B12:O28  | 3:A:800:B12:H3   | 1.80                     | 0.79              |
| 3:A:800:B12:H312 | 3:A:800:B12:H253 | 1.65                     | 0.78              |
| 2:B:564:VAL:HG22 | 2:B:592:ALA:HB3  | 1.69                     | 0.75              |
| 1:A:305:ARG:HG2  | 1:A:325:LEU:HB3  | 1.69                     | 0.75              |
| 3:A:800:B12:H302 | 3:A:800:B12:C35  | 2.15                     | 0.74              |
| 1:A:224:ILE:HG12 | 1:A:532:LEU:HD22 | 1.70                     | 0.74              |
| 1:A:665:VAL:HG13 | 1:A:682:ILE:HG21 | 1.70                     | 0.73              |
| 3:A:800:B12:H482 | 3:A:800:B12:H533 | 1.72                     | 0.72              |
| 1:A:200:ILE:HG21 | 1:A:217:SER:HB3  | 1.71                     | 0.72              |
| 2:B:361:LEU:HD22 | 2:B:365:GLN:HG2  | 1.71                     | 0.71              |
| 1:A:173:PRO:HB2  | 1:A:545:VAL:HG22 | 1.71                     | 0.71              |
| 1:A:406:SER:CA   | 2:B:400:GLY:O    | 2.37                     | 0.71              |
| 3:A:800:B12:H531 | 3:A:800:B12:H552 | 1.73                     | 0.71              |
| 1:A:205:MET:HG2  | 1:A:437:ILE:HD11 | 1.73                     | 0.70              |
| 2:B:331:LEU:HD13 | 2:B:365:GLN:HB3  | 1.75                     | 0.68              |
| 1:A:406:SER:HB2  | 2:B:400:GLY:C    | 2.18                     | 0.68              |
| 3:A:800:B12:H353 | 3:A:800:B12:C30  | 2.21                     | 0.68              |
| 1:A:601:LEU:HA   | 1:A:629:ASP:HB2  | 1.75                     | 0.68              |
| 2:B:202:ILE:HD13 | 2:B:429:MET:HB3  | 1.76                     | 0.67              |
| 1:A:406:SER:CB   | 2:B:399:ALA:O    | 2.42                     | 0.67              |
| 1:A:101:PHE:HA   | 1:A:104:ARG:HD2  | 1.76                     | 0.67              |
| 2:B:284:VAL:HG11 | 2:B:322:GLN:HE21 | 1.60                     | 0.67              |
| 2:B:332:THR:HG21 | 2:B:460:ILE:HD11 | 1.76                     | 0.66              |
| 1:A:406:SER:N    | 2:B:401:GLY:C    | 2.53                     | 0.66              |
| 2:B:391:ASN:ND2  | 2:B:394:ARG:HE   | 1.93                     | 0.66              |
| 2:B:386:LEU:HD23 | 2:B:390:VAL:HG21 | 1.78                     | 0.65              |
| 1:A:172:LEU:HB2  | 1:A:173:PRO:HD3  | 1.78                     | 0.65              |
| 2:B:391:ASN:HD22 | 2:B:394:ARG:HE   | 1.45                     | 0.65              |
| 1:A:441:ILE:HB   | 1:A:442:PRO:HD3  | 1.78                     | 0.65              |
| 1:A:15:ALA:HB1   | 2:B:92:PRO:HB3   | 1.78                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:800:B12:H362 | 3:A:800:B12:C35  | 2.21                     | 0.63              |
| 2:B:550:THR:HG21 | 2:B:580:GLU:HG2  | 1.80                     | 0.63              |
| 1:A:405:GLY:CA   | 2:B:401:GLY:O    | 2.46                     | 0.63              |
| 2:B:91:ALA:HA    | 2:B:92:PRO:C     | 2.22                     | 0.63              |
| 2:B:104:MET:HG3  | 2:B:388:GLU:HG2  | 1.81                     | 0.63              |
| 1:A:171:VAL:HG11 | 1:A:198:ASN:HD22 | 1.65                     | 0.62              |
| 1:A:406:SER:HB3  | 2:B:399:ALA:O    | 2.00                     | 0.61              |
| 1:A:63:THR:HG21  | 1:A:69:PRO:HD2   | 1.82                     | 0.61              |
| 1:A:316:GLY:N    | 1:A:317:PRO:HD3  | 2.15                     | 0.60              |
| 3:A:800:B12:O7R  | 3:A:800:B12:C2B  | 2.49                     | 0.60              |
| 2:B:254:TRP:HA   | 2:B:257:ALA:HB3  | 1.82                     | 0.60              |
| 1:A:172:LEU:HD11 | 1:A:220:ILE:HG12 | 1.83                     | 0.60              |
| 3:A:800:B12:O7R  | 3:A:800:B12:H2B  | 2.01                     | 0.60              |
| 2:B:92:PRO:O     | 2:B:93:PHE:HB2   | 2.01                     | 0.60              |
| 2:B:202:ILE:HG21 | 2:B:429:MET:HG3  | 1.85                     | 0.58              |
| 1:A:290:ILE:HG13 | 1:A:355:ALA:HB2  | 1.84                     | 0.58              |
| 1:A:405:GLY:HA3  | 2:B:401:GLY:O    | 2.04                     | 0.58              |
| 1:A:437:ILE:HG13 | 1:A:442:PRO:HG2  | 1.85                     | 0.58              |
| 2:B:460:ILE:HG23 | 2:B:464:SER:H    | 1.69                     | 0.58              |
| 3:A:800:B12:H351 | 3:A:800:B12:C36  | 2.17                     | 0.58              |
| 2:B:150:LEU:HD21 | 2:B:166:VAL:HG11 | 1.85                     | 0.58              |
| 1:A:406:SER:HB3  | 2:B:401:GLY:C    | 2.29                     | 0.57              |
| 1:A:665:VAL:HB   | 1:A:666:PRO:HD3  | 1.86                     | 0.57              |
| 2:B:141:ASP:HB3  | 2:B:142:PRO:HD2  | 1.86                     | 0.57              |
| 1:A:250:ALA:HB2  | 1:A:446:ILE:HG12 | 1.86                     | 0.57              |
| 1:A:494:ALA:HA   | 1:A:497:VAL:HB   | 1.87                     | 0.57              |
| 1:A:240:ILE:HD11 | 1:A:284:LEU:HD22 | 1.86                     | 0.56              |
| 2:B:234:VAL:HB   | 2:B:280:ILE:HG12 | 1.86                     | 0.56              |
| 1:A:406:SER:HB3  | 2:B:402:SER:N    | 2.21                     | 0.56              |
| 3:A:800:B12:C25  | 3:A:800:B12:C31  | 2.72                     | 0.56              |
| 3:A:800:B12:H2B  | 3:A:800:B12:O2   | 2.06                     | 0.56              |
| 1:A:64:TYR:HB3   | 2:B:35:TRP:HB2   | 1.88                     | 0.55              |
| 2:B:534:VAL:HA   | 2:B:537:ILE:HD12 | 1.88                     | 0.54              |
| 2:B:424:GLU:HA   | 2:B:428:GLY:HA2  | 1.89                     | 0.54              |
| 1:A:587:VAL:HG11 | 1:A:625:GLY:HA3  | 1.89                     | 0.53              |
| 2:B:617:LEU:HD22 | 2:B:621:MET:HE1  | 1.89                     | 0.53              |
| 1:A:665:VAL:HB   | 1:A:666:PRO:CD   | 2.38                     | 0.53              |
| 1:A:123:ARG:HD2  | 1:A:209:THR:HA   | 1.89                     | 0.53              |
| 1:A:705:TYR:HB3  | 1:A:709:THR:HG21 | 1.90                     | 0.53              |
| 2:B:390:VAL:O    | 2:B:391:ASN:HB2  | 2.08                     | 0.53              |
| 1:A:406:SER:CB   | 2:B:400:GLY:C    | 2.81                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:602:PHE:HB3  | 2:B:605:ASP:HB2  | 1.91                     | 0.52              |
| 1:A:672:LEU:HD22 | 1:A:680:ILE:HD12 | 1.91                     | 0.52              |
| 1:A:406:SER:HA   | 2:B:401:GLY:HA3  | 1.91                     | 0.52              |
| 2:B:460:ILE:HD12 | 2:B:463:VAL:HB   | 1.91                     | 0.52              |
| 1:A:281:ALA:N    | 1:A:282:PRO:HD2  | 2.25                     | 0.52              |
| 2:B:595:LEU:HD23 | 2:B:616:ARG:HG2  | 1.90                     | 0.52              |
| 1:A:58:MET:HE2   | 1:A:414:TRP:HB2  | 1.91                     | 0.51              |
| 1:A:264:VAL:HG21 | 1:A:311:LEU:HD22 | 1.92                     | 0.51              |
| 2:B:154:LEU:HD21 | 2:B:164:VAL:HG11 | 1.91                     | 0.51              |
| 1:A:522:PRO:O    | 1:A:523:ASP:HB2  | 2.09                     | 0.51              |
| 3:A:800:B12:H541 | 3:A:800:B12:H621 | 1.75                     | 0.51              |
| 1:A:503:ARG:NH1  | 1:A:508:VAL:HG11 | 2.26                     | 0.51              |
| 1:A:344:ASN:HA   | 1:A:347:ARG:HB2  | 1.93                     | 0.51              |
| 3:A:800:B12:H541 | 3:A:800:B12:N62  | 2.25                     | 0.51              |
| 2:B:374:PHE:HB3  | 2:B:375:PRO:CD   | 2.34                     | 0.51              |
| 2:B:166:VAL:HG13 | 2:B:179:LEU:HD22 | 1.92                     | 0.50              |
| 2:B:81:ALA:HA    | 2:B:406:GLU:HB3  | 1.93                     | 0.50              |
| 2:B:364:THR:HG22 | 2:B:474:ILE:HG21 | 1.93                     | 0.50              |
| 1:A:299:ALA:O    | 1:A:300:LYS:C    | 2.54                     | 0.50              |
| 2:B:281:ASN:HD22 | 2:B:323:ASN:HD21 | 1.59                     | 0.49              |
| 1:A:515:ILE:HG23 | 1:A:552:LEU:HG   | 1.94                     | 0.49              |
| 2:B:534:VAL:HG13 | 2:B:623:VAL:HG12 | 1.93                     | 0.49              |
| 2:B:253:ALA:HB2  | 2:B:416:ALA:HA   | 1.94                     | 0.49              |
| 1:A:202:LYS:HA   | 1:A:205:MET:HG3  | 1.93                     | 0.49              |
| 2:B:399:ALA:HB1  | 2:B:405:VAL:HG11 | 1.93                     | 0.49              |
| 1:A:122:HIS:HA   | 1:A:167:MET:HE1  | 1.95                     | 0.49              |
| 1:A:67:ILE:HG21  | 2:B:30:ALA:HB2   | 1.95                     | 0.49              |
| 1:A:330:GLN:HG3  | 1:A:364:HIS:HB3  | 1.95                     | 0.49              |
| 2:B:201:PRO:HB2  | 2:B:214:LEU:HD12 | 1.95                     | 0.49              |
| 1:A:563:ILE:HG21 | 1:A:630:VAL:HB   | 1.94                     | 0.48              |
| 2:B:370:PRO:HB3  | 2:B:375:PRO:HG2  | 1.95                     | 0.48              |
| 1:A:574:VAL:O    | 1:A:575:LYS:HB2  | 2.13                     | 0.48              |
| 1:A:338:ALA:HB3  | 1:A:339:GLN:NE2  | 2.30                     | 0.47              |
| 1:A:503:ARG:HD2  | 1:A:508:VAL:HG21 | 1.97                     | 0.47              |
| 2:B:328:TRP:HA   | 2:B:331:LEU:HG   | 1.96                     | 0.46              |
| 2:B:274:THR:HA   | 2:B:313:VAL:HG13 | 1.98                     | 0.46              |
| 2:B:292:LEU:HD23 | 2:B:408:LEU:HD21 | 1.97                     | 0.46              |
| 1:A:605:MET:HE3  | 1:A:664:LEU:HD13 | 1.98                     | 0.46              |
| 2:B:518:LEU:HB2  | 2:B:569:SER:HB2  | 1.96                     | 0.46              |
| 2:B:100:ARG:HD3  | 2:B:393:GLY:O    | 2.15                     | 0.46              |
| 2:B:532:SER:HB2  | 2:B:533:PRO:CD   | 2.46                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:48:PRO:CB    | 2:B:49:PRO:HD2   | 2.46                     | 0.45              |
| 2:B:572:LYS:HE2  | 2:B:573:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:149:MET:HE3  | 1:A:153:PHE:HE2  | 1.80                     | 0.45              |
| 2:B:564:VAL:HG11 | 2:B:630:THR:HG23 | 1.98                     | 0.45              |
| 1:A:172:LEU:HD23 | 1:A:224:ILE:HD11 | 1.99                     | 0.45              |
| 2:B:399:ALA:O    | 2:B:400:GLY:C    | 2.60                     | 0.45              |
| 1:A:441:ILE:HB   | 1:A:442:PRO:CD   | 2.47                     | 0.45              |
| 2:B:361:LEU:HD23 | 2:B:362:PRO:HD2  | 1.99                     | 0.44              |
| 1:A:65:ALA:HA    | 1:A:72:HIS:HB2   | 1.98                     | 0.44              |
| 1:A:499:LEU:HD11 | 1:A:542:MET:HG2  | 1.98                     | 0.44              |
| 1:A:531:LEU:HD22 | 1:A:552:LEU:HD21 | 1.99                     | 0.44              |
| 3:A:800:B12:C2B  | 3:A:800:B12:O2   | 2.65                     | 0.44              |
| 2:B:163:LYS:HE2  | 2:B:194:ALA:HB1  | 1.98                     | 0.44              |
| 1:A:338:ALA:HB3  | 1:A:339:GLN:HE21 | 1.81                     | 0.44              |
| 1:A:359:HIS:CE1  | 1:A:401:ASP:H    | 2.35                     | 0.44              |
| 1:A:503:ARG:HH11 | 1:A:508:VAL:HG11 | 1.81                     | 0.44              |
| 2:B:281:ASN:ND2  | 2:B:323:ASN:HD21 | 2.15                     | 0.44              |
| 2:B:396:ASN:O    | 2:B:397:ASP:C    | 2.61                     | 0.44              |
| 2:B:77:ARG:HB3   | 2:B:78:PRO:HD2   | 1.99                     | 0.44              |
| 2:B:115:ASP:HA   | 2:B:116:PRO:HD2  | 1.83                     | 0.44              |
| 1:A:119:LEU:N    | 1:A:120:PRO:HD2  | 2.32                     | 0.44              |
| 1:A:500:ARG:HG3  | 1:A:503:ARG:HH21 | 1.83                     | 0.44              |
| 2:B:553:ILE:HG22 | 2:B:585:LEU:HD21 | 1.99                     | 0.44              |
| 2:B:517:CYS:HB2  | 2:B:545:VAL:O    | 2.18                     | 0.44              |
| 2:B:94:THR:OG1   | 2:B:302:GLU:HG3  | 2.18                     | 0.44              |
| 1:A:167:MET:HE3  | 1:A:174:ILE:HG13 | 2.00                     | 0.44              |
| 1:A:605:MET:HB2  | 1:A:664:LEU:HD13 | 2.00                     | 0.43              |
| 2:B:278:ASP:HA   | 2:B:321:ARG:HH22 | 1.83                     | 0.43              |
| 2:B:141:ASP:CB   | 2:B:142:PRO:HD2  | 2.48                     | 0.43              |
| 2:B:110:ARG:HA   | 2:B:135:SER:O    | 2.17                     | 0.43              |
| 1:A:77:THR:OG1   | 2:B:42:VAL:HG11  | 2.19                     | 0.43              |
| 1:A:392:GLN:HB3  | 2:B:459:PRO:HG2  | 2.00                     | 0.43              |
| 1:A:29:ALA:HA    | 2:B:99:VAL:HG11  | 2.00                     | 0.43              |
| 1:A:302:ARG:O    | 1:A:305:ARG:HB2  | 2.18                     | 0.43              |
| 2:B:298:ARG:HH11 | 2:B:405:VAL:HG12 | 1.84                     | 0.43              |
| 2:B:585:LEU:O    | 2:B:586:LYS:C    | 2.61                     | 0.43              |
| 1:A:227:TYR:HB2  | 1:A:530:ASN:HD21 | 1.84                     | 0.42              |
| 1:A:652:VAL:HG11 | 1:A:668:LEU:HD21 | 2.01                     | 0.42              |
| 2:B:245:GLY:HA3  | 2:B:446:ASN:HD21 | 1.85                     | 0.42              |
| 2:B:504:SER:HB3  | 2:B:511:PRO:HG2  | 2.01                     | 0.42              |
| 1:A:4:LEU:HB3    | 1:A:5:PRO:HD2    | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:404:SER:O    | 2:B:402:SER:HA   | 2.20                     | 0.42              |
| 1:A:205:MET:SD   | 1:A:245:MET:HE2  | 2.59                     | 0.42              |
| 3:A:800:B12:H262 | 3:A:800:B12:H91  | 1.70                     | 0.42              |
| 1:A:394:SER:HB2  | 1:A:396:THR:HG23 | 2.02                     | 0.42              |
| 2:B:532:SER:HB2  | 2:B:533:PRO:HD3  | 2.01                     | 0.42              |
| 1:A:613:GLY:HA2  | 1:A:616:VAL:HG22 | 2.00                     | 0.42              |
| 2:B:455:ASN:O    | 2:B:456:ARG:HB2  | 2.19                     | 0.42              |
| 1:A:172:LEU:HB2  | 1:A:173:PRO:CD   | 2.47                     | 0.41              |
| 3:A:800:B12:H472 | 3:A:800:B12:H10  | 1.88                     | 0.41              |
| 2:B:47:ARG:HA    | 2:B:48:PRO:HD3   | 1.88                     | 0.41              |
| 2:B:589:GLY:O    | 2:B:590:ALA:C    | 2.63                     | 0.41              |
| 1:A:50:PHE:HE2   | 1:A:411:GLU:HG2  | 1.85                     | 0.41              |
| 1:A:176:ALA:HB1  | 1:A:536:ILE:HG13 | 2.02                     | 0.41              |
| 1:A:613:GLY:O    | 1:A:614:GLN:C    | 2.62                     | 0.41              |
| 2:B:48:PRO:HB3   | 2:B:49:PRO:HD2   | 2.02                     | 0.41              |
| 2:B:176:ALA:HB1  | 2:B:197:LEU:HD13 | 2.02                     | 0.41              |
| 1:A:307:LEU:O    | 1:A:311:LEU:HD12 | 2.21                     | 0.41              |
| 2:B:339:ASN:HA   | 2:B:342:ARG:HB2  | 2.02                     | 0.41              |
| 1:A:386:THR:HA   | 2:B:341:LEU:HD13 | 2.01                     | 0.41              |
| 3:A:800:B12:C35  | 3:A:800:B12:C36  | 2.90                     | 0.41              |
| 2:B:126:LEU:HG   | 2:B:130:GLU:OE2  | 2.20                     | 0.41              |
| 2:B:332:THR:CG2  | 2:B:460:ILE:HD11 | 2.49                     | 0.41              |
| 1:A:179:VAL:HG11 | 1:A:536:ILE:HD13 | 2.02                     | 0.41              |
| 1:A:228:THR:O    | 1:A:229:SER:C    | 2.62                     | 0.41              |
| 1:A:305:ARG:HG2  | 1:A:325:LEU:HG   | 2.02                     | 0.41              |
| 1:A:414:TRP:HE3  | 1:A:414:TRP:HA   | 1.84                     | 0.41              |
| 2:B:377:ARG:HG3  | 2:B:380:ARG:NH2  | 2.36                     | 0.41              |
| 1:A:357:GLN:HE22 | 2:B:290:GLN:HE22 | 1.69                     | 0.41              |
| 2:B:58:CYS:O     | 2:B:59:LEU:C     | 2.64                     | 0.41              |
| 1:A:58:MET:HG2   | 1:A:60:TRP:CH2   | 2.56                     | 0.41              |
| 1:A:199:ASP:HB3  | 1:A:202:LYS:HZ2  | 1.85                     | 0.41              |
| 1:A:406:SER:HB2  | 2:B:399:ALA:O    | 2.21                     | 0.41              |
| 1:A:414:TRP:HA   | 1:A:414:TRP:CE3  | 2.55                     | 0.41              |
| 2:B:33:GLU:HA    | 2:B:36:GLU:HB2   | 2.02                     | 0.41              |
| 1:A:463:PRO:HB3  | 1:A:469:LYS:HD2  | 2.02                     | 0.41              |
| 1:A:661:HIS:NE2  | 1:A:689:PRO:HD2  | 2.36                     | 0.41              |
| 1:A:172:LEU:HD21 | 1:A:220:ILE:HG23 | 2.01                     | 0.40              |
| 1:A:176:ALA:HB2  | 1:A:532:LEU:HD12 | 2.03                     | 0.40              |
| 2:B:350:ALA:HB3  | 2:B:358:ILE:HD13 | 2.02                     | 0.40              |
| 1:A:408:TYR:CE1  | 1:A:412:LEU:HD11 | 2.56                     | 0.40              |
| 2:B:195:LEU:HD11 | 2:B:224:LEU:HD11 | 2.02                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:452:ARG:O    | 1:A:456:ARG:HG3 | 2.21                     | 0.40              |
| 2:B:158:LEU:HD12 | 2:B:161:MET:HE2 | 2.03                     | 0.40              |
| 1:A:277:VAL:HG22 | 1:A:281:ALA:HB2 | 2.03                     | 0.40              |
| 1:A:471:ARG:HE   | 1:A:471:ARG:HB2 | 1.77                     | 0.40              |
| 2:B:297:LEU:HD23 | 2:B:322:GLN:NE2 | 2.37                     | 0.40              |
| 2:B:368:GLY:HA2  | 2:B:479:PHE:CD2 | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|-----------|----------|-------------|---|
| 1   | A     | 723/727 (99%)   | 615 (85%)  | 87 (12%)  | 21 (3%)  | 3           | 9 |
| 2   | B     | 616/637 (97%)   | 521 (85%)  | 77 (12%)  | 18 (3%)  | 3           | 9 |
| All | All   | 1339/1364 (98%) | 1136 (85%) | 164 (12%) | 39 (3%)  | 3           | 9 |

All (39) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 474 | HIS  |
| 1   | A     | 523 | ASP  |
| 1   | A     | 596 | ARG  |
| 2   | B     | 93  | PHE  |
| 1   | A     | 56  | LYS  |
| 1   | A     | 205 | MET  |
| 1   | A     | 486 | SER  |
| 2   | B     | 400 | GLY  |
| 2   | B     | 525 | GLY  |
| 2   | B     | 586 | LYS  |
| 1   | A     | 43  | GLN  |
| 1   | A     | 230 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 359 | HIS  |
| 1   | A     | 475 | GLU  |
| 1   | A     | 542 | MET  |
| 2   | B     | 50  | GLU  |
| 2   | B     | 240 | ILE  |
| 2   | B     | 245 | GLY  |
| 2   | B     | 371 | GLU  |
| 2   | B     | 576 | GLN  |
| 1   | A     | 192 | LEU  |
| 1   | A     | 229 | SER  |
| 1   | A     | 404 | SER  |
| 1   | A     | 575 | LYS  |
| 2   | B     | 244 | ALA  |
| 1   | A     | 10  | VAL  |
| 1   | A     | 84  | TRP  |
| 1   | A     | 406 | SER  |
| 2   | B     | 259 | GLY  |
| 2   | B     | 520 | THR  |
| 1   | A     | 130 | PRO  |
| 2   | B     | 145 | ILE  |
| 2   | B     | 228 | SER  |
| 2   | B     | 590 | ALA  |
| 2   | B     | 374 | PHE  |
| 1   | A     | 189 | PRO  |
| 1   | A     | 680 | ILE  |
| 2   | B     | 397 | ASP  |
| 2   | B     | 511 | PRO  |

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

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

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

| Mol | Chain | Analysed        | Rotameric | Outliers  | Percentiles       |
|-----|-------|-----------------|-----------|-----------|-------------------|
| 1   | A     | 568/590 (96%)   | 467 (82%) | 101 (18%) | <b>2</b> <b>5</b> |
| 2   | B     | 458/509 (90%)   | 389 (85%) | 69 (15%)  | <b>3</b> <b>7</b> |
| All | All   | 1026/1099 (93%) | 856 (83%) | 170 (17%) | <b>2</b> <b>6</b> |

All (170) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | ARG  |
| 1   | A     | 9   | SER  |
| 1   | A     | 24  | ARG  |
| 1   | A     | 26  | GLU  |
| 1   | A     | 78  | MET  |
| 1   | A     | 87  | ARG  |
| 1   | A     | 103 | ARG  |
| 1   | A     | 113 | LEU  |
| 1   | A     | 114 | SER  |
| 1   | A     | 123 | ARG  |
| 1   | A     | 128 | ASP  |
| 1   | A     | 138 | MET  |
| 1   | A     | 149 | MET  |
| 1   | A     | 162 | SER  |
| 1   | A     | 164 | SER  |
| 1   | A     | 168 | ASN  |
| 1   | A     | 171 | VAL  |
| 1   | A     | 190 | GLU  |
| 1   | A     | 202 | LYS  |
| 1   | A     | 205 | MET  |
| 1   | A     | 207 | ARG  |
| 1   | A     | 209 | THR  |
| 1   | A     | 217 | SER  |
| 1   | A     | 222 | SER  |
| 1   | A     | 232 | MET  |
| 1   | A     | 236 | ASN  |
| 1   | A     | 237 | SER  |
| 1   | A     | 245 | MET  |
| 1   | A     | 256 | MET  |
| 1   | A     | 265 | ASP  |
| 1   | A     | 273 | VAL  |
| 1   | A     | 275 | LEU  |
| 1   | A     | 276 | ASN  |
| 1   | A     | 283 | ARG  |
| 1   | A     | 310 | LYS  |
| 1   | A     | 312 | VAL  |
| 1   | A     | 313 | HIS  |
| 1   | A     | 321 | LYS  |
| 1   | A     | 323 | MET  |
| 1   | A     | 325 | LEU  |
| 1   | A     | 336 | LEU  |
| 1   | A     | 348 | THR  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 365        | THR         |
| 1          | A            | 368        | LEU         |
| 1          | A            | 370        | GLU         |
| 1          | A            | 381        | ARG         |
| 1          | A            | 400        | ILE         |
| 1          | A            | 414        | TRP         |
| 1          | A            | 419        | LYS         |
| 1          | A            | 423        | HIS         |
| 1          | A            | 427        | VAL         |
| 1          | A            | 428        | GLU         |
| 1          | A            | 430        | VAL         |
| 1          | A            | 433        | MET         |
| 1          | A            | 438        | GLU         |
| 1          | A            | 441        | ILE         |
| 1          | A            | 444        | MET         |
| 1          | A            | 445        | ARG         |
| 1          | A            | 456        | ARG         |
| 1          | A            | 478        | LEU         |
| 1          | A            | 481        | LEU         |
| 1          | A            | 482        | LYS         |
| 1          | A            | 488        | VAL         |
| 1          | A            | 489        | LEU         |
| 1          | A            | 497        | VAL         |
| 1          | A            | 508        | VAL         |
| 1          | A            | 515        | ILE         |
| 1          | A            | 528        | ASP         |
| 1          | A            | 533        | LYS         |
| 1          | A            | 534        | LEU         |
| 1          | A            | 535        | CYS         |
| 1          | A            | 537        | ASP         |
| 1          | A            | 545        | VAL         |
| 1          | A            | 549        | SER         |
| 1          | A            | 552        | LEU         |
| 1          | A            | 554        | LYS         |
| 1          | A            | 560        | THR         |
| 1          | A            | 562        | GLN         |
| 1          | A            | 564        | ARG         |
| 1          | A            | 566        | ILE         |
| 1          | A            | 577        | THR         |
| 1          | A            | 585        | GLU         |
| 1          | A            | 597        | ARG         |
| 1          | A            | 602        | LEU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 604        | LYS         |
| 1          | A            | 628        | VAL         |
| 1          | A            | 635        | GLN         |
| 1          | A            | 636        | THR         |
| 1          | A            | 639        | GLU         |
| 1          | A            | 651        | VAL         |
| 1          | A            | 674        | LYS         |
| 1          | A            | 677        | ARG         |
| 1          | A            | 684        | VAL         |
| 1          | A            | 688        | ILE         |
| 1          | A            | 691        | GLN         |
| 1          | A            | 694        | ASP         |
| 1          | A            | 698        | LYS         |
| 1          | A            | 702        | VAL         |
| 1          | A            | 709        | THR         |
| 1          | A            | 714        | SER         |
| 1          | A            | 717        | SER         |
| 2          | B            | 16         | LEU         |
| 2          | B            | 19         | THR         |
| 2          | B            | 21         | LEU         |
| 2          | B            | 41         | LYS         |
| 2          | B            | 61         | ARG         |
| 2          | B            | 68         | ASP         |
| 2          | B            | 70         | ILE         |
| 2          | B            | 73         | VAL         |
| 2          | B            | 75         | MET         |
| 2          | B            | 83         | LYS         |
| 2          | B            | 90         | VAL         |
| 2          | B            | 104        | MET         |
| 2          | B            | 130        | GLU         |
| 2          | B            | 136        | LEU         |
| 2          | B            | 153        | VAL         |
| 2          | B            | 155        | SER         |
| 2          | B            | 161        | MET         |
| 2          | B            | 162        | THR         |
| 2          | B            | 163        | LYS         |
| 2          | B            | 182        | VAL         |
| 2          | B            | 193        | LEU         |
| 2          | B            | 215        | THR         |
| 2          | B            | 217        | LEU         |
| 2          | B            | 224        | LEU         |
| 2          | B            | 226        | LYS         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | B            | 228        | SER         |
| 2          | B            | 230        | ASP         |
| 2          | B            | 256        | LEU         |
| 2          | B            | 261        | GLU         |
| 2          | B            | 266        | LEU         |
| 2          | B            | 274        | THR         |
| 2          | B            | 287        | THR         |
| 2          | B            | 294        | ILE         |
| 2          | B            | 300        | LEU         |
| 2          | B            | 301        | ARG         |
| 2          | B            | 314        | ASP         |
| 2          | B            | 358        | ILE         |
| 2          | B            | 369        | LEU         |
| 2          | B            | 371        | GLU         |
| 2          | B            | 408        | LEU         |
| 2          | B            | 411        | SER         |
| 2          | B            | 412        | LEU         |
| 2          | B            | 420        | PHE         |
| 2          | B            | 426        | LEU         |
| 2          | B            | 429        | MET         |
| 2          | B            | 430        | SER         |
| 2          | B            | 438        | VAL         |
| 2          | B            | 445        | CYS         |
| 2          | B            | 451        | LYS         |
| 2          | B            | 460        | ILE         |
| 2          | B            | 498        | GLU         |
| 2          | B            | 504        | SER         |
| 2          | B            | 520        | THR         |
| 2          | B            | 521        | ARG         |
| 2          | B            | 541        | ASP         |
| 2          | B            | 542        | THR         |
| 2          | B            | 550        | THR         |
| 2          | B            | 559        | LYS         |
| 2          | B            | 564        | VAL         |
| 2          | B            | 569        | SER         |
| 2          | B            | 573        | VAL         |
| 2          | B            | 579        | LEU         |
| 2          | B            | 595        | LEU         |
| 2          | B            | 601        | GLU         |
| 2          | B            | 616        | ARG         |
| 2          | B            | 619        | MET         |
| 2          | B            | 623        | VAL         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 628 | SER  |
| 2   | B     | 636 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 122 | HIS  |
| 1   | A     | 197 | GLN  |
| 1   | A     | 198 | ASN  |
| 1   | A     | 215 | GLN  |
| 1   | A     | 339 | GLN  |
| 1   | A     | 385 | ASN  |
| 1   | A     | 425 | GLN  |
| 1   | A     | 485 | ASN  |
| 1   | A     | 635 | GLN  |
| 1   | A     | 643 | GLN  |
| 2   | B     | 113 | HIS  |
| 2   | B     | 290 | GLN  |
| 2   | B     | 322 | GLN  |
| 2   | B     | 323 | ASN  |
| 2   | B     | 391 | ASN  |
| 2   | B     | 446 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 4   | ADN  | A     | 801 | 3    | 20,20,21     | 0.53 | 0           | 28,30,31    | 1.87 | 9 (32%)     |
| 3   | B12  | A     | 800 | 4,1  | 94,101,101   | 0.94 | 3 (3%)      | 149,166,166 | 1.87 | 37 (24%)    |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings     |
|-----|------|-------|-----|------|---------|---------------|-----------|
| 4   | ADN  | A     | 801 | 3    | -       | 3/4/20/22     | 0/3/3/3   |
| 3   | B12  | A     | 800 | 4,1  | -       | 19/56/223/223 | 0/3/11/11 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | A     | 800 | B12  | C14-N23 | 2.71 | 1.38        | 1.35     |
| 3   | A     | 800 | B12  | C55-C56 | 2.57 | 1.58        | 1.53     |
| 3   | A     | 800 | B12  | C56-C57 | 2.14 | 1.55        | 1.51     |

All (46) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 800 | B12  | C54-C17-C18 | -5.47 | 105.14      | 112.99   |
| 3   | A     | 800 | B12  | C56-C57-N59 | -5.29 | 106.70      | 116.34   |
| 4   | A     | 801 | ADN  | O2'-C2'-C3' | -5.25 | 94.99       | 111.82   |
| 3   | A     | 800 | B12  | C25-C2-C1   | 5.15  | 121.45      | 113.75   |
| 3   | A     | 800 | B12  | C55-C56-C57 | -4.52 | 101.18      | 111.25   |
| 3   | A     | 800 | B12  | C13-C14-C15 | -3.85 | 118.45      | 124.32   |
| 3   | A     | 800 | B12  | C53-C15-C16 | 3.74  | 126.71      | 120.36   |
| 3   | A     | 800 | B12  | O34-C32-C31 | -3.65 | 110.03      | 121.04   |
| 3   | A     | 800 | B12  | O34-C32-N33 | 3.63  | 132.23      | 122.53   |
| 3   | A     | 800 | B12  | O58-C57-N59 | 3.59  | 130.08      | 123.03   |
| 4   | A     | 801 | ADN  | C2'-C1'-N9  | 3.41  | 121.78      | 113.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | A     | 801 | ADN  | C2'-C3'-C4' | -3.41 | 97.33       | 102.36   |
| 3   | A     | 800 | B12  | C53-C15-C14 | -3.38 | 111.71      | 118.42   |
| 3   | A     | 800 | B12  | C36-C7-C8   | 3.30  | 118.14      | 112.05   |
| 4   | A     | 801 | ADN  | O3'-C3'-C2' | -3.30 | 101.24      | 111.82   |
| 3   | A     | 800 | B12  | C7-C6-N22   | 3.24  | 113.84      | 107.94   |
| 3   | A     | 800 | B12  | C2P-C1P-N59 | 3.16  | 117.57      | 112.92   |
| 3   | A     | 800 | B12  | C30-C31-C32 | -2.92 | 102.62      | 112.55   |
| 3   | A     | 800 | B12  | C26-C2-C3   | -2.92 | 102.33      | 107.42   |
| 3   | A     | 800 | B12  | C7-C6-C5    | -2.81 | 123.69      | 128.07   |
| 3   | A     | 800 | B12  | C26-C2-C1   | -2.78 | 105.71      | 110.00   |
| 3   | A     | 800 | B12  | C4B-C9B-C8B | -2.78 | 117.61      | 120.16   |
| 3   | A     | 800 | B12  | C4B-C5B-C6B | 2.75  | 123.72      | 119.69   |
| 3   | A     | 800 | B12  | O8R-C5R-C4R | -2.74 | 102.00      | 111.33   |
| 3   | A     | 800 | B12  | C31-C30-C3  | -2.72 | 106.95      | 114.65   |
| 3   | A     | 800 | B12  | C17-C16-C15 | 2.71  | 130.55      | 126.26   |
| 3   | A     | 800 | B12  | C15-C14-N23 | 2.70  | 129.51      | 126.26   |
| 4   | A     | 801 | ADN  | O4'-C1'-N9  | -2.58 | 103.14      | 108.09   |
| 3   | A     | 800 | B12  | C7B-C6B-C5B | -2.57 | 115.92      | 119.69   |
| 3   | A     | 800 | B12  | C55-C17-C16 | 2.53  | 121.55      | 116.59   |
| 3   | A     | 800 | B12  | C19-N24-C16 | 2.49  | 110.01      | 107.29   |
| 3   | A     | 800 | B12  | C19-C1-N21  | 2.43  | 104.64      | 102.14   |
| 3   | A     | 800 | B12  | C7B-C8B-C9B | 2.42  | 125.38      | 122.47   |
| 3   | A     | 800 | B12  | C17-C16-N24 | -2.41 | 107.49      | 111.17   |
| 3   | A     | 800 | B12  | C17-C18-C19 | -2.39 | 98.74       | 102.36   |
| 3   | A     | 800 | B12  | C36-C7-C37  | 2.38  | 114.78      | 110.74   |
| 3   | A     | 800 | B12  | C4R-O6R-C1R | 2.35  | 114.65      | 109.47   |
| 4   | A     | 801 | ADN  | O4'-C1'-C2' | -2.30 | 101.70      | 106.62   |
| 3   | A     | 800 | B12  | C2-C1-C19   | -2.25 | 115.12      | 118.61   |
| 4   | A     | 801 | ADN  | C5'-C4'-C3' | 2.24  | 118.05      | 115.70   |
| 3   | A     | 800 | B12  | C46-C12-C11 | 2.17  | 117.83      | 110.08   |
| 3   | A     | 800 | B12  | C13-C14-N23 | 2.15  | 112.01      | 109.09   |
| 3   | A     | 800 | B12  | C18-C19-N24 | 2.15  | 105.55      | 102.33   |
| 4   | A     | 801 | ADN  | O3'-C3'-C4' | -2.11 | 105.30      | 110.47   |
| 4   | A     | 801 | ADN  | N3-C4-N9    | 2.02  | 130.60      | 127.17   |
| 3   | A     | 800 | B12  | C3-C4-C5    | -2.01 | 120.46      | 123.82   |

There are no chirality outliers.

All (22) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | A     | 800 | B12  | C2P-O3-P-O4 |
| 3   | A     | 800 | B12  | C2P-O3-P-O2 |

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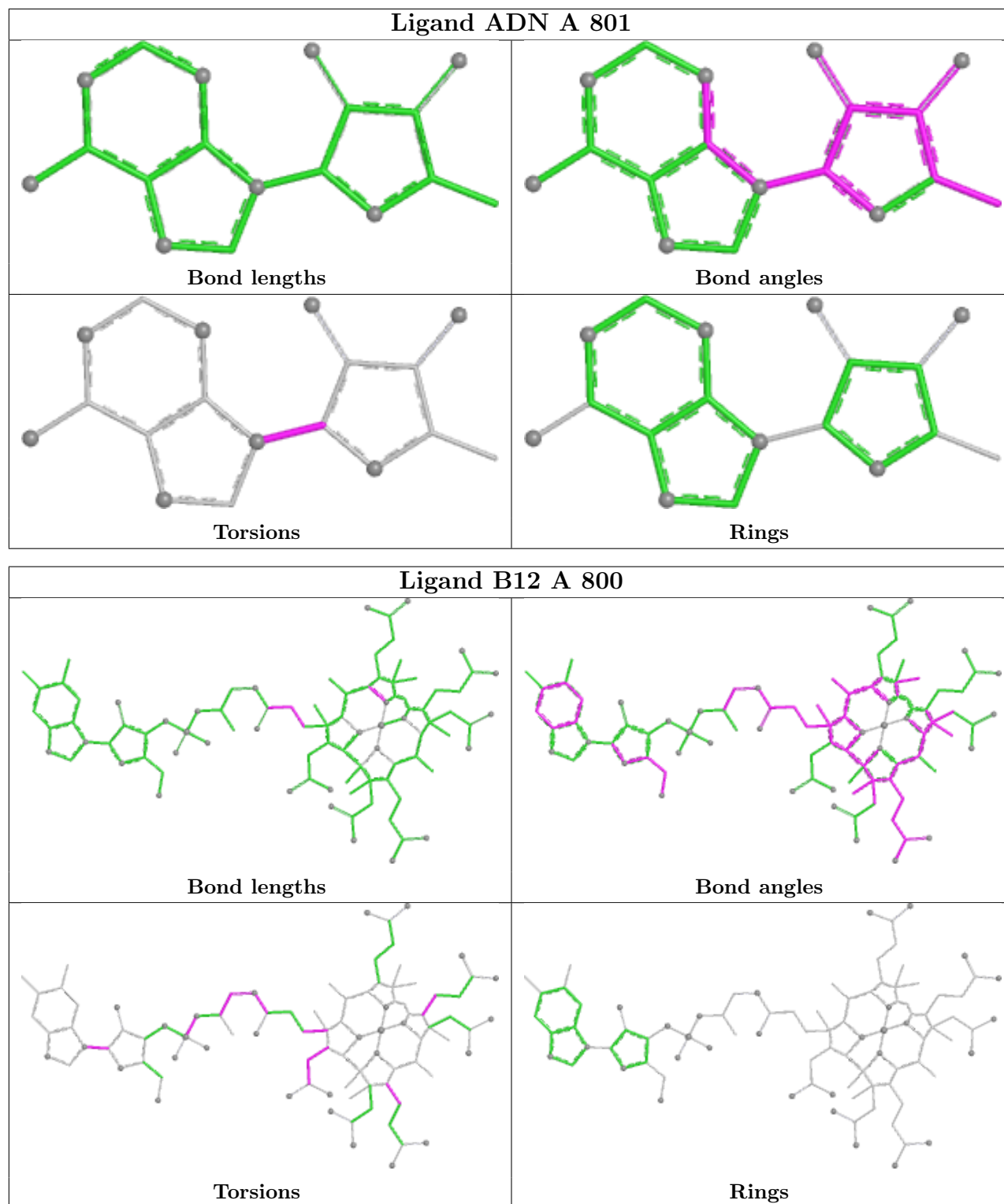
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | A     | 800 | B12  | C2P-C1P-N59-C57 |
| 3   | A     | 800 | B12  | C18-C17-C55-C56 |
| 3   | A     | 800 | B12  | C16-C17-C55-C56 |
| 3   | A     | 800 | B12  | C17-C18-C60-C61 |
| 3   | A     | 800 | B12  | C2R-C1R-N1B-C8B |
| 3   | A     | 800 | B12  | C2R-C1R-N1B-C2B |
| 3   | A     | 800 | B12  | C42-C41-C8-C9   |
| 4   | A     | 801 | ADN  | C2'-C1'-N9-C4   |
| 4   | A     | 801 | ADN  | C2'-C1'-N9-C8   |
| 3   | A     | 800 | B12  | N59-C1P-C2P-O3  |
| 3   | A     | 800 | B12  | O58-C57-N59-C1P |
| 3   | A     | 800 | B12  | C42-C41-C8-C7   |
| 3   | A     | 800 | B12  | C18-C60-C61-O63 |
| 3   | A     | 800 | B12  | C18-C60-C61-N62 |
| 3   | A     | 800 | B12  | O6R-C1R-N1B-C8B |
| 3   | A     | 800 | B12  | C2-C3-C30-C31   |
| 4   | A     | 801 | ADN  | O4'-C1'-N9-C8   |
| 3   | A     | 800 | B12  | C2P-O3-P-O5     |
| 3   | A     | 800 | B12  | O6R-C1R-N1B-C2B |
| 3   | A     | 800 | B12  | C56-C57-N59-C1P |

There are no ring outliers.

1 monomer is involved in 22 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 800 | B12  | 22      | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 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     | 725/727 (99%)   | 0.43   | 30 (4%) 41 37 | 27, 71, 94, 102       | 0     |
| 2   | B     | 620/637 (97%)   | 0.48   | 22 (3%) 47 43 | 29, 72, 94, 109       | 0     |
| All | All   | 1345/1364 (98%) | 0.45   | 52 (3%) 43 39 | 27, 71, 94, 109       | 0     |

All (52) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 581 | VAL  | 4.1  |
| 2   | B     | 311 | PHE  | 3.9  |
| 1   | A     | 235 | TRP  | 3.5  |
| 1   | A     | 544 | THR  | 3.1  |
| 1   | A     | 543 | ALA  | 3.1  |
| 2   | B     | 201 | PRO  | 3.1  |
| 2   | B     | 183 | TYR  | 2.9  |
| 2   | B     | 589 | GLY  | 2.8  |
| 1   | A     | 675 | LEU  | 2.7  |
| 1   | A     | 676 | GLY  | 2.6  |
| 1   | A     | 683 | THR  | 2.6  |
| 1   | A     | 519 | ALA  | 2.6  |
| 1   | A     | 210 | TYR  | 2.6  |
| 2   | B     | 205 | ALA  | 2.5  |
| 1   | A     | 161 | MET  | 2.5  |
| 1   | A     | 71  | VAL  | 2.5  |
| 1   | A     | 552 | LEU  | 2.4  |
| 2   | B     | 176 | ALA  | 2.4  |
| 2   | B     | 259 | GLY  | 2.4  |
| 1   | A     | 529 | ARG  | 2.4  |
| 1   | A     | 517 | TRP  | 2.4  |
| 1   | A     | 176 | ALA  | 2.4  |
| 2   | B     | 190 | ALA  | 2.4  |
| 1   | A     | 126 | ASP  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 94  | THR  | 2.3  |
| 1   | A     | 166 | THR  | 2.3  |
| 2   | B     | 216 | VAL  | 2.3  |
| 1   | A     | 494 | ALA  | 2.3  |
| 1   | A     | 511 | ALA  | 2.3  |
| 1   | A     | 555 | VAL  | 2.3  |
| 1   | A     | 728 | ALA  | 2.3  |
| 2   | B     | 635 | GLY  | 2.3  |
| 2   | B     | 573 | VAL  | 2.3  |
| 2   | B     | 112 | LEU  | 2.2  |
| 1   | A     | 541 | ALA  | 2.2  |
| 2   | B     | 146 | ALA  | 2.2  |
| 1   | A     | 406 | SER  | 2.2  |
| 2   | B     | 595 | LEU  | 2.2  |
| 2   | B     | 246 | ALA  | 2.2  |
| 2   | B     | 411 | SER  | 2.2  |
| 1   | A     | 281 | ALA  | 2.1  |
| 1   | A     | 267 | ILE  | 2.1  |
| 2   | B     | 524 | PHE  | 2.1  |
| 2   | B     | 269 | GLN  | 2.1  |
| 1   | A     | 441 | ILE  | 2.1  |
| 1   | A     | 127 | SER  | 2.1  |
| 2   | B     | 572 | LYS  | 2.0  |
| 2   | B     | 16  | LEU  | 2.0  |
| 2   | B     | 234 | VAL  | 2.0  |
| 1   | A     | 538 | ALA  | 2.0  |
| 1   | A     | 645 | VAL  | 2.0  |
| 1   | A     | 665 | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

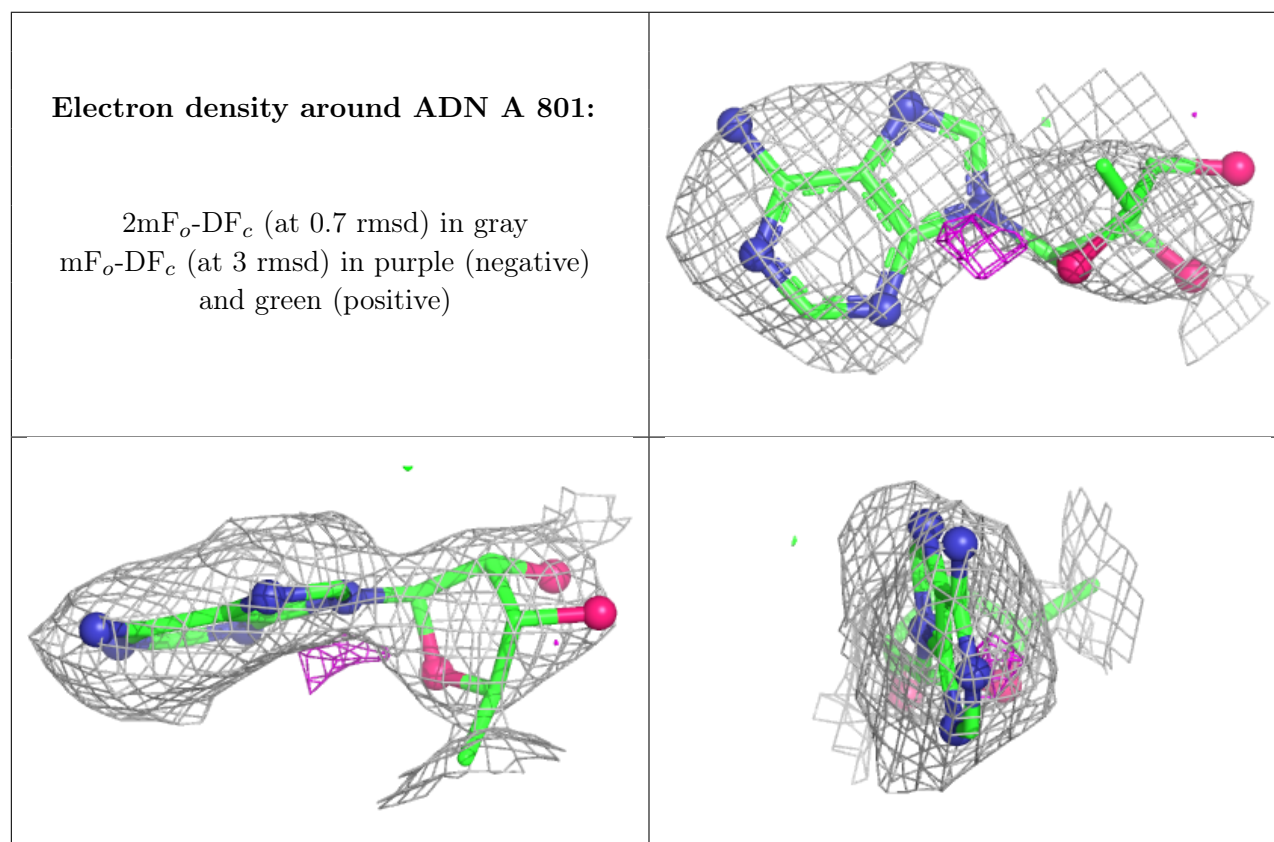
## 6.4 Ligands [i](#)

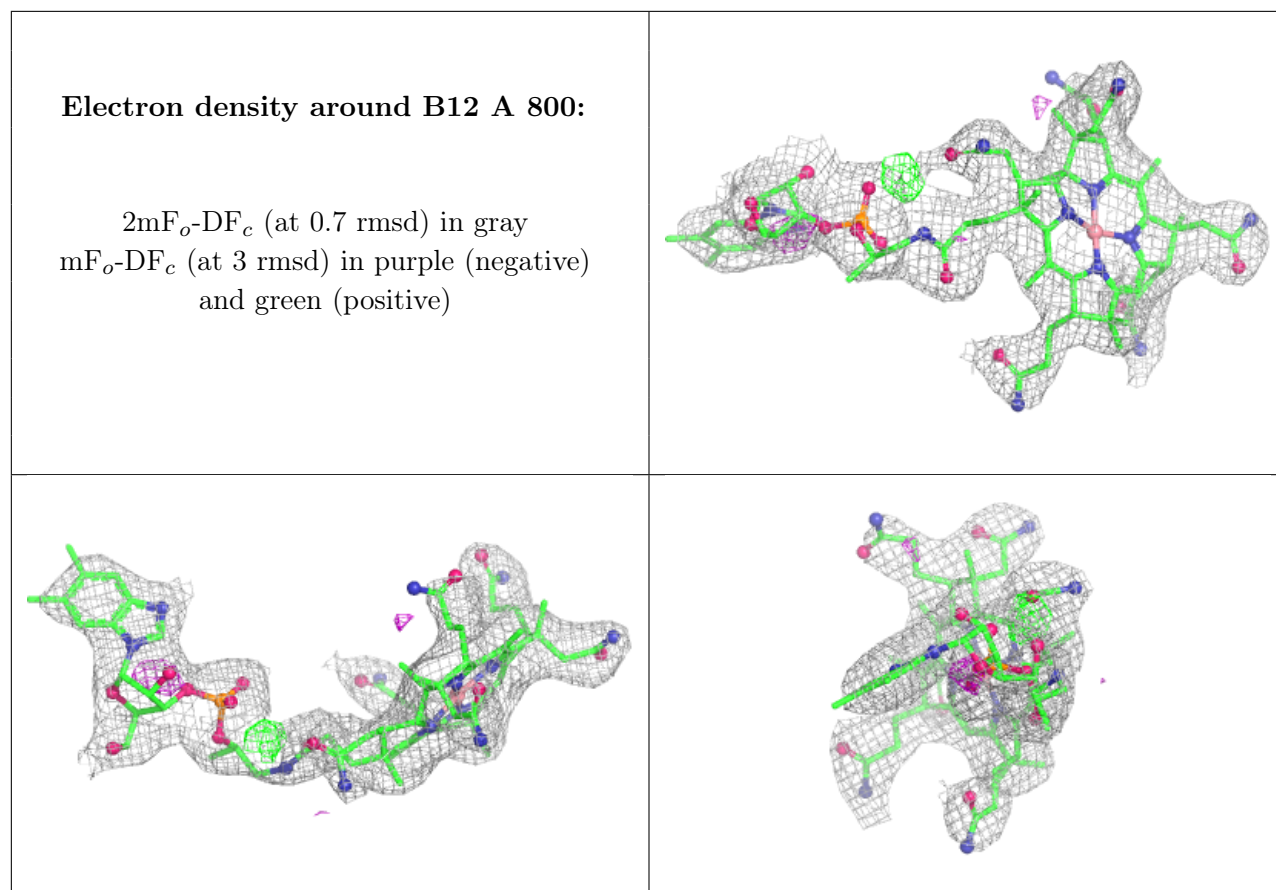
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | ADN  | A     | 801 | 18/19 | 0.83 | 0.13 | 56,79,82,83                | 0     |
| 3   | B12  | A     | 800 | 91/91 | 0.94 | 0.10 | 26,48,67,75                | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.