



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:50 AM UTC

PDB ID : 1UK0 / pdb\_00001uk0  
Title : Crystal structure of catalytic domain of human poly(ADP-ribose) polymerase with a novel inhibitor  
Authors : Kinoshita, T.  
Deposited on : 2003-08-13  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 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                                                             |

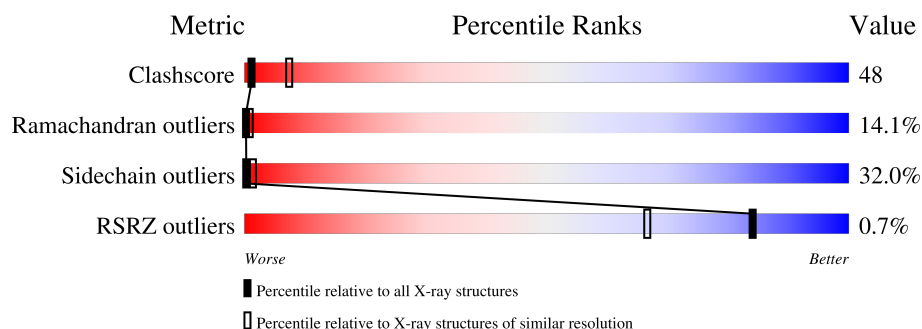
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |
| RSRZ outliers         | 180081                      | 2671 (3.00-3.00)                                      |

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     | 350    | <div> <div>%</div> <div>6% 27% 39% 27%</div> </div> |
| 1   | B     | 350    | <div> <div>%</div> <div>• 20% 44% 33%</div> </div>  |

## 2 Entry composition [i](#)

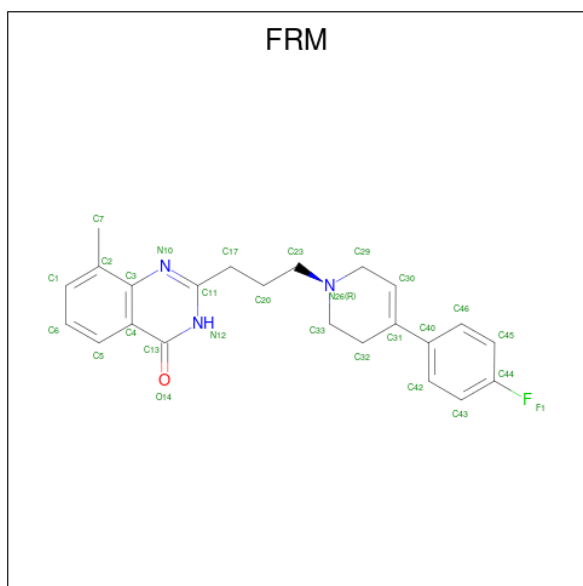
There are 3 unique types of molecules in this entry. The entry contains 5817 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Poly [ADP-ribose] polymerase-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 350      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2754  | 1752 | 465 | 526 | 11 |         |         |       |
| 1   | B     | 350      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2754  | 1752 | 465 | 526 | 11 |         |         |       |

- Molecule 2 is 2-{3-[4-(4-FLUOROPHENYL)-3,6-DIHYDRO-1(2H)-PYRIDINYL]PROPYL}-8-METHYL-4(3H)-QUINAZOLINONE (CCD ID: FRM) (formula: C<sub>23</sub>H<sub>24</sub>FN<sub>3</sub>O).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 28    | 23 | 1 | 3 | 1 |         |         |
| 2   | B     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 28    | 23 | 1 | 3 | 1 |         |         |

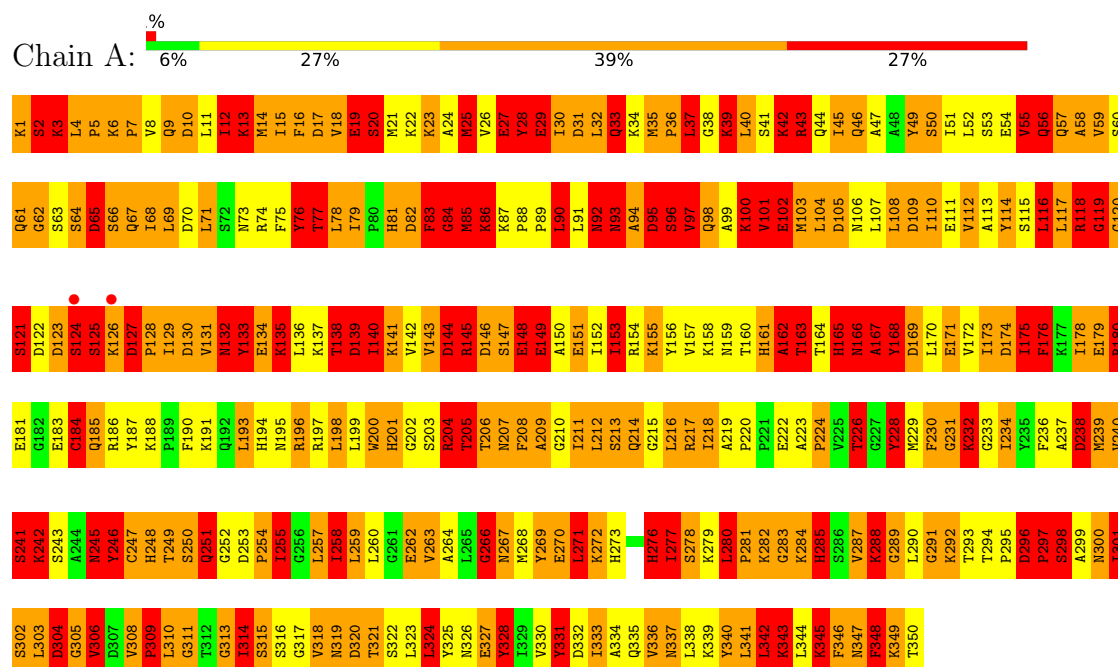
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 3   | A     | 124      | Total<br>124 | O<br>124 | 0       | 0       |
| 3   | B     | 129      | Total<br>129 | O<br>129 | 0       | 0       |

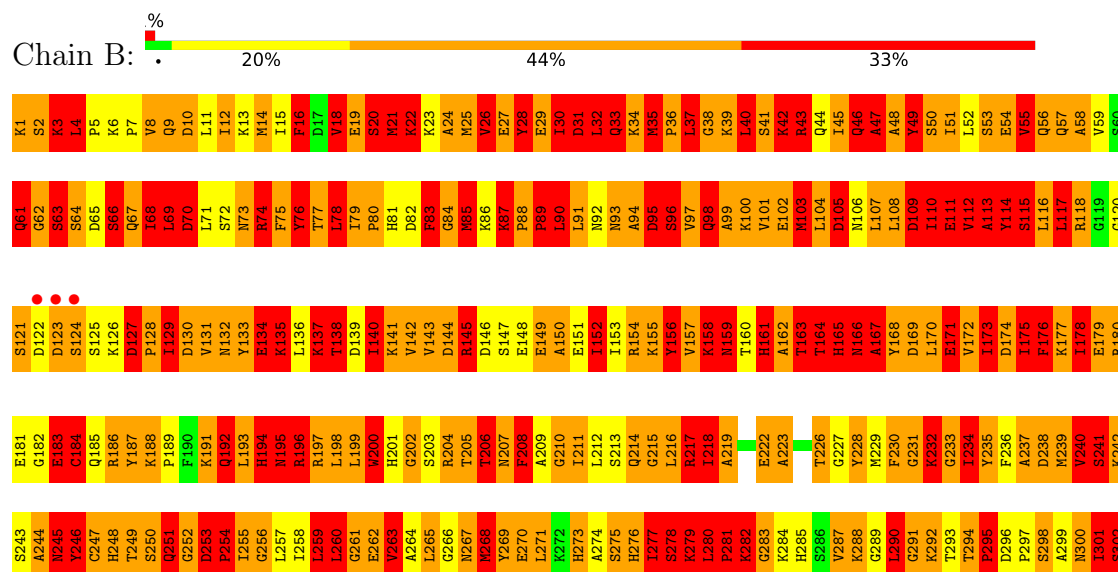
### 3 Residue-property plots

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: Poly [ADP-ribose] polymerase-1



#### • Molecule 1: Poly [ADP-ribose] polymerase-1



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| L303 | D304 | G305 | V306 | D307 | V308 | P309 | L310 | G311 | T312 | G313 | I314 | S315 | S316 | G317 | V318 | N319 | D320 | T321 | S322 | L323 | L324 | Y325 | N326 | E327 | Y328 | I329 | V330 | Y331 | D332 | I333 | A334 | Q335 | V336 | N337 | L338 | K339 | Y340 | L341 | L342 | K343 | L344 | K345 | F346 | K347 | F348 | K349 | T350 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 179.82Å 53.55Å 92.01Å<br>90.00° 114.40° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 50.00 – 3.00<br>50.00 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (50.00-3.00)<br>95.7 (50.00-3.00)           | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.11 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | CNX                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.219 , 0.246<br>0.211 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 39.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.714                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 93.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 5817                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 12.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 2.33         | 121/2806 (4.3%) | 3.60        | 600/3786 (15.8%)  |
| 1   | B     | 2.41         | 135/2806 (4.8%) | 3.72        | 606/3786 (16.0%)  |
| All | All   | 2.37         | 256/5612 (4.6%) | 3.66        | 1206/7572 (15.9%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 47                  |
| 1   | B     | 0                   | 39                  |
| All | All   | 0                   | 86                  |

All (256) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | B     | 282 | LYS  | CA-C  | 17.54  | 1.76        | 1.52     |
| 1   | B     | 282 | LYS  | C-O   | -14.21 | 1.06        | 1.24     |
| 1   | B     | 282 | LYS  | C-N   | 14.13  | 1.54        | 1.33     |
| 1   | A     | 110 | ILE  | CA-CB | -11.66 | 1.41        | 1.54     |
| 1   | A     | 81  | HIS  | CA-C  | 11.61  | 1.68        | 1.52     |
| 1   | B     | 21  | MET  | CA-C  | 11.49  | 1.68        | 1.52     |
| 1   | A     | 288 | LYS  | CA-C  | 11.28  | 1.67        | 1.53     |
| 1   | B     | 304 | ASP  | CA-CB | 11.15  | 1.69        | 1.53     |
| 1   | A     | 109 | ASP  | CA-C  | 10.94  | 1.67        | 1.52     |
| 1   | A     | 122 | ASP  | CA-C  | 10.73  | 1.67        | 1.52     |
| 1   | A     | 241 | SER  | C-N   | 10.47  | 1.48        | 1.33     |
| 1   | B     | 338 | LEU  | CA-C  | 10.06  | 1.65        | 1.52     |
| 1   | B     | 306 | VAL  | C-O   | -10.04 | 1.13        | 1.24     |
| 1   | B     | 288 | LYS  | C-N   | 9.40   | 1.39        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 305 | GLY  | CA-C    | 9.35  | 1.64        | 1.51     |
| 1   | A     | 313 | GLY  | C-N     | 9.30  | 1.46        | 1.33     |
| 1   | A     | 345 | LYS  | CA-C    | -9.14 | 1.41        | 1.52     |
| 1   | A     | 86  | LYS  | CA-C    | 9.11  | 1.65        | 1.52     |
| 1   | B     | 282 | LYS  | N-CA    | 9.11  | 1.57        | 1.46     |
| 1   | A     | 126 | LYS  | CA-C    | 9.06  | 1.65        | 1.52     |
| 1   | B     | 46  | GLN  | CA-C    | 8.89  | 1.64        | 1.52     |
| 1   | B     | 74  | ARG  | CA-C    | -8.84 | 1.40        | 1.52     |
| 1   | A     | 197 | ARG  | CA-C    | -8.76 | 1.41        | 1.52     |
| 1   | A     | 315 | SER  | CA-CB   | -8.32 | 1.42        | 1.53     |
| 1   | B     | 77  | THR  | CA-C    | 8.31  | 1.64        | 1.52     |
| 1   | B     | 304 | ASP  | CB-CG   | 8.30  | 1.72        | 1.52     |
| 1   | B     | 97  | VAL  | C-N     | 8.29  | 1.44        | 1.33     |
| 1   | B     | 248 | HIS  | CE1-NE2 | 8.26  | 1.40        | 1.32     |
| 1   | A     | 273 | HIS  | CA-C    | -8.25 | 1.41        | 1.53     |
| 1   | A     | 200 | TRP  | NE1-CE2 | 8.13  | 1.46        | 1.37     |
| 1   | A     | 78  | LEU  | C-N     | 8.12  | 1.42        | 1.33     |
| 1   | B     | 161 | HIS  | CG-CD2  | 8.12  | 1.44        | 1.35     |
| 1   | B     | 143 | VAL  | CA-C    | -8.07 | 1.42        | 1.52     |
| 1   | B     | 94  | ALA  | CA-C    | -8.07 | 1.41        | 1.52     |
| 1   | B     | 248 | HIS  | ND1-CE1 | 8.07  | 1.40        | 1.32     |
| 1   | A     | 172 | VAL  | CA-CB   | 7.99  | 1.62        | 1.53     |
| 1   | A     | 145 | ARG  | NE-CZ   | 7.88  | 1.41        | 1.33     |
| 1   | A     | 350 | THR  | CA-C    | 7.82  | 1.69        | 1.52     |
| 1   | A     | 263 | VAL  | CA-C    | -7.81 | 1.43        | 1.52     |
| 1   | B     | 79  | ILE  | CA-CB   | 7.79  | 1.61        | 1.54     |
| 1   | A     | 142 | VAL  | C-O     | -7.78 | 1.15        | 1.24     |
| 1   | B     | 154 | ARG  | NE-CZ   | 7.77  | 1.41        | 1.33     |
| 1   | B     | 20  | SER  | N-CA    | 7.76  | 1.56        | 1.46     |
| 1   | A     | 194 | HIS  | ND1-CE1 | 7.71  | 1.40        | 1.32     |
| 1   | A     | 161 | HIS  | CB-CG   | 7.69  | 1.60        | 1.50     |
| 1   | A     | 127 | ASP  | CA-C    | 7.54  | 1.62        | 1.52     |
| 1   | A     | 152 | ILE  | CA-CB   | 7.54  | 1.62        | 1.54     |
| 1   | A     | 320 | ASP  | CA-C    | 7.47  | 1.62        | 1.52     |
| 1   | B     | 306 | VAL  | C-N     | -7.41 | 1.23        | 1.33     |
| 1   | B     | 61  | GLN  | CA-CB   | -7.32 | 1.43        | 1.53     |
| 1   | A     | 142 | VAL  | CA-C    | -7.30 | 1.43        | 1.52     |
| 1   | B     | 139 | ASP  | CA-C    | 7.25  | 1.61        | 1.52     |
| 1   | A     | 35  | MET  | CA-C    | 7.10  | 1.61        | 1.52     |
| 1   | B     | 274 | ALA  | CA-C    | 7.10  | 1.62        | 1.52     |
| 1   | A     | 316 | SER  | CA-C    | -7.07 | 1.43        | 1.53     |
| 1   | B     | 241 | SER  | C-N     | 7.05  | 1.43        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 206 | THR  | CB-OG1  | 7.03  | 1.55        | 1.43     |
| 1   | A     | 129 | ILE  | CA-CB   | -7.03 | 1.46        | 1.54     |
| 1   | B     | 177 | LYS  | C-N     | 6.97  | 1.42        | 1.33     |
| 1   | B     | 275 | SER  | CA-C    | -6.94 | 1.43        | 1.52     |
| 1   | A     | 91  | LEU  | CA-C    | 6.91  | 1.61        | 1.53     |
| 1   | A     | 81  | HIS  | CE1-NE2 | 6.88  | 1.39        | 1.32     |
| 1   | B     | 241 | SER  | CA-C    | 6.88  | 1.61        | 1.52     |
| 1   | B     | 2   | SER  | N-CA    | 6.87  | 1.54        | 1.46     |
| 1   | A     | 242 | LYS  | CG-CD   | 6.82  | 1.73        | 1.52     |
| 1   | A     | 197 | ARG  | NE-CZ   | 6.82  | 1.40        | 1.33     |
| 1   | A     | 101 | VAL  | C-N     | 6.80  | 1.42        | 1.33     |
| 1   | A     | 211 | ILE  | CA-CB   | -6.77 | 1.44        | 1.54     |
| 1   | A     | 99  | ALA  | N-CA    | 6.74  | 1.54        | 1.46     |
| 1   | A     | 181 | GLU  | CA-C    | 6.73  | 1.62        | 1.52     |
| 1   | B     | 35  | MET  | CA-CB   | 6.72  | 1.62        | 1.53     |
| 1   | A     | 251 | GLN  | C-N     | 6.72  | 1.43        | 1.33     |
| 1   | B     | 183 | GLU  | C-N     | 6.69  | 1.43        | 1.33     |
| 1   | B     | 262 | GLU  | CD-OE2  | 6.69  | 1.38        | 1.25     |
| 1   | B     | 227 | GLY  | C-N     | 6.66  | 1.41        | 1.33     |
| 1   | B     | 333 | ILE  | CA-C    | 6.66  | 1.61        | 1.52     |
| 1   | B     | 318 | VAL  | N-CA    | 6.63  | 1.54        | 1.46     |
| 1   | B     | 209 | ALA  | N-CA    | 6.61  | 1.54        | 1.46     |
| 1   | B     | 284 | LYS  | C-O     | -6.60 | 1.16        | 1.24     |
| 1   | A     | 99  | ALA  | CA-C    | -6.58 | 1.44        | 1.52     |
| 1   | B     | 101 | VAL  | CA-CB   | 6.57  | 1.62        | 1.54     |
| 1   | B     | 171 | GLU  | N-CA    | 6.57  | 1.54        | 1.46     |
| 1   | A     | 178 | ILE  | CA-CB   | -6.56 | 1.46        | 1.54     |
| 1   | A     | 41  | SER  | CA-C    | -6.55 | 1.44        | 1.52     |
| 1   | A     | 166 | ASN  | CA-C    | 6.55  | 1.61        | 1.52     |
| 1   | B     | 180 | ARG  | C-N     | 6.54  | 1.42        | 1.33     |
| 1   | A     | 242 | LYS  | N-CA    | 6.54  | 1.54        | 1.46     |
| 1   | B     | 97  | VAL  | CA-CB   | -6.54 | 1.45        | 1.54     |
| 1   | B     | 81  | HIS  | ND1-CE1 | 6.51  | 1.39        | 1.32     |
| 1   | B     | 340 | TYR  | CA-CB   | -6.48 | 1.43        | 1.53     |
| 1   | B     | 40  | LEU  | C-N     | -6.46 | 1.25        | 1.33     |
| 1   | B     | 107 | LEU  | CA-C    | -6.44 | 1.44        | 1.52     |
| 1   | A     | 228 | TYR  | CA-C    | 6.43  | 1.60        | 1.52     |
| 1   | A     | 49  | TYR  | CA-C    | 6.43  | 1.61        | 1.52     |
| 1   | B     | 81  | HIS  | CG-CD2  | 6.42  | 1.43        | 1.35     |
| 1   | B     | 95  | ASP  | CA-C    | 6.42  | 1.61        | 1.52     |
| 1   | B     | 291 | GLY  | CA-C    | 6.42  | 1.58        | 1.51     |
| 1   | A     | 273 | HIS  | CA-CB   | -6.39 | 1.44        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 163 | THR  | CA-C    | 6.37  | 1.61        | 1.52     |
| 1   | B     | 218 | ILE  | CA-C    | -6.36 | 1.45        | 1.52     |
| 1   | A     | 197 | ARG  | N-CA    | 6.35  | 1.53        | 1.46     |
| 1   | B     | 219 | ALA  | C-N     | 6.34  | 1.40        | 1.33     |
| 1   | B     | 283 | GLY  | CA-C    | -6.34 | 1.43        | 1.52     |
| 1   | B     | 81  | HIS  | CE1-NE2 | 6.33  | 1.38        | 1.32     |
| 1   | B     | 242 | LYS  | N-CA    | 6.26  | 1.54        | 1.46     |
| 1   | A     | 194 | HIS  | CE1-NE2 | 6.25  | 1.38        | 1.32     |
| 1   | B     | 152 | ILE  | CA-C    | 6.25  | 1.60        | 1.52     |
| 1   | B     | 242 | LYS  | CD-CE   | 6.22  | 1.71        | 1.52     |
| 1   | B     | 299 | ALA  | CA-C    | -6.20 | 1.44        | 1.52     |
| 1   | A     | 217 | ARG  | NE-CZ   | 6.18  | 1.39        | 1.33     |
| 1   | B     | 273 | HIS  | CG-ND1  | -6.18 | 1.31        | 1.38     |
| 1   | A     | 119 | GLY  | CA-C    | 6.18  | 1.60        | 1.51     |
| 1   | B     | 320 | ASP  | CA-C    | 6.17  | 1.61        | 1.52     |
| 1   | B     | 73  | ASN  | CA-C    | -6.17 | 1.44        | 1.52     |
| 1   | A     | 309 | PRO  | CA-C    | 6.16  | 1.61        | 1.53     |
| 1   | A     | 57  | GLN  | CA-C    | -6.13 | 1.45        | 1.52     |
| 1   | B     | 34  | LYS  | C-N     | 6.11  | 1.41        | 1.33     |
| 1   | A     | 205 | THR  | N-CA    | 6.11  | 1.54        | 1.46     |
| 1   | B     | 287 | VAL  | CA-CB   | 6.08  | 1.62        | 1.54     |
| 1   | B     | 33  | GLN  | C-N     | 6.08  | 1.42        | 1.33     |
| 1   | A     | 29  | GLU  | N-CA    | 6.07  | 1.54        | 1.46     |
| 1   | B     | 85  | MET  | CA-C    | 6.05  | 1.65        | 1.52     |
| 1   | B     | 114 | TYR  | N-CA    | 6.05  | 1.53        | 1.46     |
| 1   | A     | 248 | HIS  | CG-CD2  | 6.04  | 1.42        | 1.35     |
| 1   | B     | 285 | HIS  | CA-CB   | 6.02  | 1.62        | 1.54     |
| 1   | B     | 28  | TYR  | CA-C    | 6.01  | 1.60        | 1.52     |
| 1   | B     | 31  | ASP  | CA-C    | -6.01 | 1.44        | 1.52     |
| 1   | B     | 199 | LEU  | C-N     | 5.97  | 1.42        | 1.33     |
| 1   | A     | 90  | LEU  | CA-C    | 5.97  | 1.60        | 1.52     |
| 1   | B     | 194 | HIS  | CG-CD2  | 5.92  | 1.42        | 1.35     |
| 1   | B     | 85  | MET  | C-N     | 5.91  | 1.41        | 1.33     |
| 1   | B     | 112 | VAL  | CA-CB   | 5.91  | 1.62        | 1.54     |
| 1   | B     | 132 | ASN  | CA-C    | 5.89  | 1.60        | 1.52     |
| 1   | B     | 184 | CYS  | N-CA    | 5.89  | 1.53        | 1.46     |
| 1   | A     | 267 | ASN  | CA-CB   | 5.89  | 1.60        | 1.53     |
| 1   | A     | 285 | HIS  | CD2-NE2 | -5.88 | 1.31        | 1.37     |
| 1   | B     | 133 | TYR  | CA-C    | 5.87  | 1.60        | 1.52     |
| 1   | A     | 74  | ARG  | NE-CZ   | 5.87  | 1.39        | 1.33     |
| 1   | A     | 317 | GLY  | N-CA    | 5.86  | 1.54        | 1.45     |
| 1   | B     | 125 | SER  | CA-C    | 5.86  | 1.60        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 41  | SER  | CA-C   | 5.85  | 1.59        | 1.52     |
| 1   | B     | 322 | SER  | CB-OG  | 5.85  | 1.53        | 1.42     |
| 1   | B     | 267 | ASN  | CA-C   | 5.84  | 1.60        | 1.52     |
| 1   | B     | 138 | THR  | CA-C   | 5.82  | 1.60        | 1.52     |
| 1   | A     | 155 | LYS  | N-CA   | 5.79  | 1.53        | 1.46     |
| 1   | A     | 216 | LEU  | CA-CB  | -5.78 | 1.43        | 1.53     |
| 1   | A     | 143 | VAL  | CA-C   | -5.76 | 1.46        | 1.52     |
| 1   | B     | 130 | ASP  | C-N    | 5.76  | 1.40        | 1.33     |
| 1   | B     | 281 | PRO  | C-O    | -5.75 | 1.17        | 1.23     |
| 1   | B     | 76  | TYR  | CA-C   | 5.75  | 1.60        | 1.52     |
| 1   | B     | 202 | GLY  | N-CA   | 5.74  | 1.52        | 1.45     |
| 1   | A     | 240 | VAL  | CA-C   | -5.72 | 1.43        | 1.52     |
| 1   | A     | 109 | ASP  | C-N    | 5.70  | 1.41        | 1.33     |
| 1   | A     | 269 | TYR  | CA-CB  | 5.70  | 1.60        | 1.53     |
| 1   | B     | 30  | ILE  | N-CA   | 5.70  | 1.53        | 1.46     |
| 1   | A     | 293 | THR  | CA-CB  | 5.70  | 1.60        | 1.53     |
| 1   | A     | 175 | ILE  | CA-CB  | 5.68  | 1.61        | 1.53     |
| 1   | B     | 262 | GLU  | CA-C   | -5.67 | 1.46        | 1.52     |
| 1   | A     | 340 | TYR  | CA-C   | 5.66  | 1.60        | 1.52     |
| 1   | B     | 169 | ASP  | CA-C   | 5.64  | 1.59        | 1.52     |
| 1   | A     | 56  | GLN  | CA-C   | -5.64 | 1.45        | 1.52     |
| 1   | B     | 123 | ASP  | C-N    | 5.63  | 1.41        | 1.33     |
| 1   | B     | 176 | PHE  | CA-C   | 5.63  | 1.60        | 1.52     |
| 1   | B     | 285 | HIS  | CG-CD2 | 5.63  | 1.42        | 1.35     |
| 1   | B     | 207 | ASN  | CA-C   | 5.62  | 1.59        | 1.52     |
| 1   | A     | 13  | LYS  | CA-CB  | 5.61  | 1.62        | 1.53     |
| 1   | A     | 23  | LYS  | CA-C   | 5.61  | 1.60        | 1.52     |
| 1   | B     | 302 | SER  | N-CA   | 5.60  | 1.53        | 1.46     |
| 1   | A     | 248 | HIS  | CB-CG  | 5.59  | 1.57        | 1.50     |
| 1   | B     | 92  | ASN  | CA-C   | 5.55  | 1.60        | 1.53     |
| 1   | A     | 338 | LEU  | CA-C   | 5.54  | 1.60        | 1.52     |
| 1   | A     | 308 | VAL  | CA-CB  | -5.53 | 1.49        | 1.54     |
| 1   | B     | 58  | ALA  | C-O    | -5.53 | 1.17        | 1.24     |
| 1   | B     | 315 | SER  | C-O    | -5.53 | 1.17        | 1.23     |
| 1   | A     | 13  | LYS  | CA-C   | 5.53  | 1.60        | 1.52     |
| 1   | A     | 318 | VAL  | C-N    | 5.53  | 1.40        | 1.33     |
| 1   | A     | 30  | ILE  | CA-C   | -5.52 | 1.46        | 1.52     |
| 1   | A     | 62  | GLY  | C-N    | 5.52  | 1.41        | 1.33     |
| 1   | A     | 108 | LEU  | CA-C   | 5.51  | 1.60        | 1.52     |
| 1   | A     | 284 | LYS  | CA-C   | -5.51 | 1.46        | 1.52     |
| 1   | A     | 33  | GLN  | CA-CB  | 5.50  | 1.62        | 1.53     |
| 1   | A     | 87  | LYS  | N-CA   | 5.49  | 1.52        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 14  | MET  | C-N     | 5.49  | 1.40        | 1.33     |
| 1   | B     | 70  | ASP  | CA-CB   | 5.48  | 1.62        | 1.53     |
| 1   | A     | 196 | ARG  | NE-CZ   | 5.47  | 1.39        | 1.33     |
| 1   | A     | 229 | MET  | CA-C    | -5.46 | 1.45        | 1.52     |
| 1   | B     | 304 | ASP  | CG-OD2  | 5.46  | 1.35        | 1.25     |
| 1   | B     | 246 | TYR  | N-CA    | 5.46  | 1.53        | 1.46     |
| 1   | B     | 135 | LYS  | N-CA    | 5.46  | 1.53        | 1.46     |
| 1   | A     | 141 | LYS  | N-CA    | 5.45  | 1.52        | 1.45     |
| 1   | A     | 81  | HIS  | CD2-NE2 | -5.45 | 1.31        | 1.37     |
| 1   | B     | 312 | THR  | CA-C    | 5.45  | 1.60        | 1.52     |
| 1   | B     | 248 | HIS  | CA-CB   | 5.44  | 1.61        | 1.53     |
| 1   | A     | 110 | ILE  | C-N     | 5.44  | 1.41        | 1.33     |
| 1   | B     | 210 | GLY  | C-N     | 5.44  | 1.40        | 1.33     |
| 1   | B     | 90  | LEU  | CA-C    | 5.43  | 1.59        | 1.52     |
| 1   | A     | 201 | HIS  | CA-C    | 5.43  | 1.59        | 1.53     |
| 1   | A     | 19  | GLU  | CA-C    | -5.42 | 1.46        | 1.52     |
| 1   | B     | 208 | PHE  | C-N     | 5.42  | 1.41        | 1.33     |
| 1   | A     | 187 | TYR  | CA-C    | -5.38 | 1.45        | 1.52     |
| 1   | A     | 258 | ILE  | CA-C    | 5.37  | 1.59        | 1.52     |
| 1   | B     | 57  | GLN  | N-CA    | 5.36  | 1.53        | 1.46     |
| 1   | A     | 132 | ASN  | CA-C    | 5.35  | 1.59        | 1.52     |
| 1   | B     | 226 | THR  | CA-C    | -5.33 | 1.45        | 1.52     |
| 1   | A     | 42  | LYS  | N-CA    | 5.31  | 1.52        | 1.46     |
| 1   | B     | 115 | SER  | N-CA    | 5.31  | 1.52        | 1.46     |
| 1   | B     | 125 | SER  | N-CA    | 5.30  | 1.52        | 1.46     |
| 1   | A     | 128 | PRO  | N-CA    | 5.29  | 1.54        | 1.47     |
| 1   | A     | 332 | ASP  | CA-CB   | -5.26 | 1.45        | 1.53     |
| 1   | A     | 201 | HIS  | CE1-NE2 | 5.25  | 1.37        | 1.32     |
| 1   | B     | 3   | LYS  | CA-C    | 5.25  | 1.60        | 1.52     |
| 1   | B     | 106 | ASN  | C-N     | 5.24  | 1.41        | 1.33     |
| 1   | A     | 138 | THR  | CA-C    | 5.23  | 1.59        | 1.52     |
| 1   | B     | 235 | TYR  | CA-C    | 5.23  | 1.59        | 1.52     |
| 1   | B     | 108 | LEU  | C-O     | -5.22 | 1.18        | 1.24     |
| 1   | B     | 200 | TRP  | CA-C    | -5.22 | 1.46        | 1.52     |
| 1   | A     | 144 | ASP  | C-N     | -5.20 | 1.26        | 1.33     |
| 1   | A     | 162 | ALA  | CA-C    | 5.20  | 1.59        | 1.52     |
| 1   | B     | 276 | HIS  | CE1-NE2 | 5.20  | 1.37        | 1.32     |
| 1   | A     | 230 | PHE  | CA-C    | 5.20  | 1.59        | 1.52     |
| 1   | B     | 121 | SER  | N-CA    | 5.19  | 1.52        | 1.45     |
| 1   | B     | 87  | LYS  | CA-C    | -5.17 | 1.46        | 1.52     |
| 1   | B     | 149 | GLU  | CA-C    | -5.17 | 1.46        | 1.52     |
| 1   | A     | 56  | GLN  | C-N     | 5.17  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 204 | ARG  | CZ-NH2  | 5.16  | 1.40        | 1.33     |
| 1   | A     | 348 | PHE  | CA-CB   | -5.16 | 1.46        | 1.52     |
| 1   | A     | 318 | VAL  | CA-CB   | -5.16 | 1.47        | 1.54     |
| 1   | A     | 65  | ASP  | N-CA    | 5.15  | 1.52        | 1.46     |
| 1   | A     | 62  | GLY  | CA-C    | 5.14  | 1.59        | 1.51     |
| 1   | A     | 165 | HIS  | CE1-NE2 | 5.13  | 1.37        | 1.32     |
| 1   | B     | 276 | HIS  | ND1-CE1 | 5.13  | 1.37        | 1.32     |
| 1   | B     | 201 | HIS  | CB-CG   | 5.12  | 1.57        | 1.50     |
| 1   | A     | 348 | PHE  | CA-C    | -5.11 | 1.46        | 1.52     |
| 1   | A     | 43  | ARG  | CA-C    | 5.09  | 1.59        | 1.52     |
| 1   | A     | 17  | ASP  | C-N     | 5.08  | 1.40        | 1.34     |
| 1   | A     | 68  | ILE  | CA-CB   | -5.07 | 1.49        | 1.54     |
| 1   | A     | 122 | ASP  | N-CA    | 5.07  | 1.52        | 1.46     |
| 1   | B     | 135 | LYS  | CA-CB   | 5.06  | 1.61        | 1.53     |
| 1   | A     | 324 | LEU  | C-O     | -5.06 | 1.17        | 1.24     |
| 1   | B     | 165 | HIS  | ND1-CE1 | 5.06  | 1.37        | 1.32     |
| 1   | A     | 231 | GLY  | CA-C    | 5.05  | 1.59        | 1.51     |
| 1   | B     | 81  | HIS  | C-O     | -5.05 | 1.18        | 1.24     |
| 1   | B     | 184 | CYS  | C-N     | 5.05  | 1.40        | 1.33     |
| 1   | B     | 66  | SER  | CA-C    | -5.04 | 1.46        | 1.52     |
| 1   | B     | 179 | GLU  | CA-C    | 5.04  | 1.58        | 1.52     |
| 1   | B     | 201 | HIS  | C-N     | 5.04  | 1.37        | 1.33     |
| 1   | B     | 322 | SER  | CA-CB   | 5.04  | 1.61        | 1.53     |
| 1   | A     | 259 | LEU  | CA-C    | -5.04 | 1.46        | 1.52     |
| 1   | B     | 204 | ARG  | CA-C    | -5.04 | 1.46        | 1.52     |
| 1   | A     | 165 | HIS  | CG-ND1  | -5.03 | 1.32        | 1.38     |
| 1   | B     | 161 | HIS  | CE1-NE2 | 5.03  | 1.37        | 1.32     |
| 1   | A     | 47  | ALA  | CA-C    | -5.03 | 1.46        | 1.52     |
| 1   | A     | 341 | LEU  | CA-C    | 5.02  | 1.59        | 1.52     |
| 1   | B     | 236 | PHE  | CA-C    | -5.02 | 1.46        | 1.52     |
| 1   | B     | 161 | HIS  | C-N     | 5.01  | 1.40        | 1.33     |
| 1   | B     | 61  | GLN  | CA-C    | 5.00  | 1.60        | 1.52     |

All (1206) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | B     | 304 | ASP  | CA-CB-CG | 19.07  | 131.67      | 112.60   |
| 1   | B     | 346 | PHE  | CA-CB-CG | -18.51 | 95.29       | 113.80   |
| 1   | B     | 318 | VAL  | CA-C-N   | -17.98 | 98.70       | 122.79   |
| 1   | B     | 318 | VAL  | C-N-CA   | -17.98 | 98.70       | 122.79   |
| 1   | B     | 61  | GLN  | N-CA-CB  | -16.61 | 87.06       | 110.65   |
| 1   | B     | 93  | ASN  | N-CA-CB  | -14.98 | 87.56       | 111.22   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | B     | 34  | LYS  | CA-C-N     | -14.88 | 102.59      | 122.98   |
| 1   | B     | 34  | LYS  | C-N-CA     | -14.88 | 102.59      | 122.98   |
| 1   | A     | 201 | HIS  | CA-CB-CG   | -13.82 | 99.98       | 113.80   |
| 1   | B     | 282 | LYS  | O-C-N      | 13.54  | 140.60      | 122.59   |
| 1   | A     | 206 | THR  | CA-C-N     | 13.40  | 138.64      | 120.54   |
| 1   | A     | 206 | THR  | C-N-CA     | 13.40  | 138.64      | 120.54   |
| 1   | B     | 54  | GLU  | CA-CB-CG   | -13.35 | 87.41       | 114.10   |
| 1   | B     | 282 | LYS  | CA-C-N     | -13.33 | 102.38      | 123.31   |
| 1   | B     | 282 | LYS  | C-N-CA     | -13.33 | 102.38      | 123.31   |
| 1   | A     | 178 | ILE  | CB-CA-C    | -13.29 | 90.93       | 110.33   |
| 1   | B     | 172 | VAL  | CA-C-N     | -13.28 | 106.68      | 122.35   |
| 1   | B     | 172 | VAL  | C-N-CA     | -13.28 | 106.68      | 122.35   |
| 1   | A     | 83  | PHE  | N-CA-C     | 13.28  | 129.62      | 113.16   |
| 1   | A     | 40  | LEU  | CA-C-N     | -13.21 | 100.80      | 122.21   |
| 1   | A     | 40  | LEU  | C-N-CA     | -13.21 | 100.80      | 122.21   |
| 1   | B     | 61  | GLN  | CB-CG-CD   | -13.10 | 90.32       | 112.60   |
| 1   | B     | 281 | PRO  | N-CA-CB    | -13.10 | 90.74       | 103.19   |
| 1   | A     | 7   | PRO  | CA-C-N     | -12.96 | 103.88      | 120.60   |
| 1   | A     | 7   | PRO  | C-N-CA     | -12.96 | 103.88      | 120.60   |
| 1   | B     | 179 | GLU  | N-CA-C     | 12.86  | 129.47      | 108.52   |
| 1   | B     | 347 | ASN  | CA-C-N     | -12.78 | 106.23      | 122.84   |
| 1   | B     | 347 | ASN  | C-N-CA     | -12.78 | 106.23      | 122.84   |
| 1   | B     | 28  | TYR  | N-CA-C     | 12.76  | 125.19      | 111.03   |
| 1   | B     | 178 | ILE  | CA-C-N     | -12.67 | 105.31      | 123.05   |
| 1   | B     | 178 | ILE  | C-N-CA     | -12.67 | 105.31      | 123.05   |
| 1   | B     | 337 | ASN  | CA-C-N     | -12.49 | 105.80      | 122.42   |
| 1   | B     | 337 | ASN  | C-N-CA     | -12.49 | 105.80      | 122.42   |
| 1   | B     | 183 | GLU  | N-CA-C     | 12.38  | 124.46      | 110.97   |
| 1   | A     | 292 | LYS  | N-CA-C     | 12.33  | 127.67      | 112.87   |
| 1   | A     | 269 | TYR  | CA-C-N     | -12.24 | 105.82      | 122.72   |
| 1   | A     | 269 | TYR  | C-N-CA     | -12.24 | 105.82      | 122.72   |
| 1   | B     | 169 | ASP  | CA-C-N     | -12.24 | 100.83      | 122.62   |
| 1   | B     | 169 | ASP  | C-N-CA     | -12.24 | 100.83      | 122.62   |
| 1   | A     | 258 | ILE  | CB-CG1-CD1 | -12.21 | 88.17       | 113.80   |
| 1   | B     | 347 | ASN  | N-CA-CB    | -12.15 | 90.97       | 110.77   |
| 1   | A     | 8   | VAL  | N-CA-C     | 12.06  | 123.03      | 110.36   |
| 1   | A     | 171 | GLU  | N-CA-C     | 12.06  | 127.41      | 109.07   |
| 1   | A     | 125 | SER  | N-CA-C     | 12.05  | 124.90      | 110.44   |
| 1   | A     | 58  | ALA  | CA-C-N     | -11.93 | 105.29      | 120.56   |
| 1   | A     | 58  | ALA  | C-N-CA     | -11.93 | 105.29      | 120.56   |
| 1   | B     | 173 | ILE  | N-CA-C     | 11.91  | 122.05      | 111.81   |
| 1   | B     | 306 | VAL  | CA-CB-CG2  | 11.88  | 130.59      | 110.40   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | B     | 229 | MET  | CA-C-O     | 11.86  | 133.48      | 120.20   |
| 1   | B     | 46  | GLN  | N-CA-C     | 11.72  | 126.11      | 111.69   |
| 1   | A     | 302 | SER  | CB-CA-C    | -11.63 | 96.46       | 111.70   |
| 1   | B     | 4   | LEU  | CB-CA-C    | -11.59 | 92.69       | 109.38   |
| 1   | A     | 33  | GLN  | OE1-CD-NE2 | -11.59 | 111.01      | 122.60   |
| 1   | B     | 92  | ASN  | CA-C-O     | 11.37  | 131.34      | 119.51   |
| 1   | A     | 149 | GLU  | CA-CB-CG   | 11.35  | 136.80      | 114.10   |
| 1   | B     | 55  | VAL  | CA-C-N     | -11.32 | 101.74      | 121.66   |
| 1   | B     | 55  | VAL  | C-N-CA     | -11.32 | 101.74      | 121.66   |
| 1   | A     | 90  | LEU  | CA-C-O     | 11.27  | 133.56      | 120.49   |
| 1   | A     | 273 | HIS  | CA-CB-CG   | -11.23 | 102.57      | 113.80   |
| 1   | A     | 231 | GLY  | CA-C-N     | -11.20 | 107.21      | 123.11   |
| 1   | A     | 231 | GLY  | C-N-CA     | -11.20 | 107.21      | 123.11   |
| 1   | B     | 303 | LEU  | N-CA-C     | 11.18  | 126.02      | 109.59   |
| 1   | A     | 118 | ARG  | CB-CG-CD   | 11.18  | 137.00      | 111.30   |
| 1   | A     | 302 | SER  | N-CA-C     | 11.14  | 125.70      | 107.32   |
| 1   | B     | 51  | ILE  | N-CA-C     | 11.12  | 121.09      | 110.42   |
| 1   | A     | 146 | ASP  | CA-CB-CG   | -11.03 | 101.57      | 112.60   |
| 1   | A     | 17  | ASP  | N-CA-C     | 10.97  | 127.13      | 109.24   |
| 1   | B     | 345 | LYS  | CA-C-O     | 10.97  | 132.18      | 120.33   |
| 1   | B     | 259 | LEU  | N-CA-C     | 10.95  | 124.78      | 110.43   |
| 1   | A     | 311 | GLY  | CA-C-N     | -10.91 | 103.72      | 122.92   |
| 1   | A     | 311 | GLY  | C-N-CA     | -10.91 | 103.72      | 122.92   |
| 1   | B     | 277 | ILE  | CA-C-N     | -10.84 | 105.48      | 122.17   |
| 1   | B     | 277 | ILE  | C-N-CA     | -10.84 | 105.48      | 122.17   |
| 1   | B     | 9   | GLN  | CA-CB-CG   | 10.77  | 135.63      | 114.10   |
| 1   | A     | 68  | ILE  | N-CA-C     | 10.74  | 121.39      | 110.23   |
| 1   | A     | 165 | HIS  | CA-CB-CG   | 10.73  | 124.53      | 113.80   |
| 1   | A     | 101 | VAL  | N-CA-C     | 10.72  | 121.56      | 110.62   |
| 1   | B     | 142 | VAL  | N-CA-C     | 10.65  | 122.00      | 106.55   |
| 1   | B     | 178 | ILE  | N-CA-C     | 10.61  | 123.25      | 107.75   |
| 1   | B     | 281 | PRO  | CB-CA-C    | 10.57  | 125.75      | 110.85   |
| 1   | A     | 56  | GLN  | N-CA-CB    | 10.56  | 125.94      | 110.20   |
| 1   | A     | 95  | ASP  | CA-CB-CG   | -10.55 | 102.05      | 112.60   |
| 1   | B     | 248 | HIS  | CA-CB-CG   | -10.55 | 103.25      | 113.80   |
| 1   | A     | 69  | LEU  | CA-C-N     | -10.54 | 103.31      | 122.38   |
| 1   | A     | 69  | LEU  | C-N-CA     | -10.54 | 103.31      | 122.38   |
| 1   | B     | 170 | LEU  | CB-CA-C    | 10.51  | 124.95      | 111.40   |
| 1   | A     | 178 | ILE  | N-CA-C     | 10.46  | 123.19      | 108.12   |
| 1   | B     | 78  | LEU  | CA-C-N     | -10.45 | 111.76      | 123.25   |
| 1   | B     | 78  | LEU  | C-N-CA     | -10.45 | 111.76      | 123.25   |
| 1   | B     | 248 | HIS  | CA-C-N     | -10.41 | 103.79      | 122.74   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | B     | 248 | HIS  | C-N-CA     | -10.41 | 103.79      | 122.74   |
| 1   | B     | 263 | VAL  | CA-C-O     | 10.38  | 131.29      | 120.39   |
| 1   | A     | 175 | ILE  | CA-CB-CG1  | 10.35  | 127.99      | 110.40   |
| 1   | B     | 123 | ASP  | CA-CB-CG   | -10.35 | 102.25      | 112.60   |
| 1   | A     | 123 | ASP  | O-C-N      | -10.34 | 111.31      | 123.41   |
| 1   | A     | 200 | TRP  | CG-CD2-CE3 | -10.31 | 123.58      | 133.90   |
| 1   | B     | 73  | ASN  | CA-CB-CG   | -10.31 | 102.29      | 112.60   |
| 1   | B     | 140 | ILE  | CB-CA-C    | -10.30 | 99.64       | 111.59   |
| 1   | B     | 183 | GLU  | CB-CA-C    | -10.29 | 95.11       | 110.96   |
| 1   | B     | 306 | VAL  | CA-C-O     | 10.15  | 132.54      | 120.66   |
| 1   | B     | 79  | ILE  | CA-CB-CG2  | 10.10  | 127.67      | 110.50   |
| 1   | A     | 165 | HIS  | N-CA-C     | 10.03  | 123.72      | 110.88   |
| 1   | A     | 337 | ASN  | N-CA-CB    | -10.00 | 94.47       | 110.77   |
| 1   | A     | 348 | PHE  | CA-CB-CG   | -9.98  | 103.82      | 113.80   |
| 1   | A     | 146 | ASP  | CA-C-N     | -9.98  | 105.00      | 122.07   |
| 1   | A     | 146 | ASP  | C-N-CA     | -9.98  | 105.00      | 122.07   |
| 1   | B     | 174 | ASP  | CA-CB-CG   | -9.96  | 102.64      | 112.60   |
| 1   | A     | 277 | ILE  | CA-CB-CG1  | 9.95   | 127.31      | 110.40   |
| 1   | B     | 344 | LEU  | N-CA-CB    | -9.91  | 95.10       | 110.46   |
| 1   | A     | 47  | ALA  | CB-CA-C    | -9.89  | 93.87       | 110.68   |
| 1   | B     | 77  | THR  | CA-C-N     | 9.89   | 133.70      | 120.65   |
| 1   | B     | 77  | THR  | C-N-CA     | 9.89   | 133.70      | 120.65   |
| 1   | A     | 134 | GLU  | N-CA-C     | 9.86   | 123.82      | 111.69   |
| 1   | A     | 140 | ILE  | N-CA-C     | 9.86   | 124.15      | 106.61   |
| 1   | A     | 319 | ASN  | OD1-CG-ND2 | -9.78  | 112.82      | 122.60   |
| 1   | B     | 158 | LYS  | N-CA-C     | 9.76   | 127.47      | 111.37   |
| 1   | B     | 138 | THR  | CA-CB-OG1  | -9.75  | 94.98       | 109.60   |
| 1   | A     | 194 | HIS  | CB-CG-CD2  | -9.72  | 118.56      | 131.20   |
| 1   | B     | 208 | PHE  | CA-C-N     | -9.69  | 106.53      | 120.29   |
| 1   | B     | 208 | PHE  | C-N-CA     | -9.69  | 106.53      | 120.29   |
| 1   | B     | 133 | TYR  | N-CA-C     | 9.65   | 123.01      | 111.33   |
| 1   | A     | 140 | ILE  | CA-C-O     | 9.64   | 130.64      | 120.51   |
| 1   | A     | 49  | TYR  | CA-C-O     | 9.63   | 130.63      | 120.42   |
| 1   | B     | 18  | VAL  | N-CA-C     | 9.63   | 125.00      | 112.76   |
| 1   | B     | 288 | LYS  | CA-C-N     | -9.60  | 112.41      | 121.62   |
| 1   | B     | 288 | LYS  | C-N-CA     | -9.60  | 112.41      | 121.62   |
| 1   | B     | 289 | GLY  | O-C-N      | 9.58   | 130.44      | 123.35   |
| 1   | A     | 248 | HIS  | CA-C-O     | 9.57   | 132.85      | 121.65   |
| 1   | A     | 23  | LYS  | N-CA-C     | 9.57   | 122.91      | 111.33   |
| 1   | A     | 17  | ASP  | CA-CB-CG   | -9.53  | 103.07      | 112.60   |
| 1   | B     | 278 | SER  | O-C-N      | 9.52   | 133.09      | 121.95   |
| 1   | B     | 196 | ARG  | N-CA-C     | 9.51   | 122.84      | 109.15   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 258 | ILE  | N-CA-C     | 9.50  | 122.51      | 108.45   |
| 1   | B     | 77  | THR  | OG1-CB-CG2 | 9.47  | 128.25      | 109.30   |
| 1   | B     | 346 | PHE  | CA-C-N     | -9.47 | 108.37      | 122.39   |
| 1   | B     | 346 | PHE  | C-N-CA     | -9.47 | 108.37      | 122.39   |
| 1   | A     | 178 | ILE  | CA-CB-CG1  | 9.47  | 126.50      | 110.40   |
| 1   | A     | 16  | PHE  | CA-C-N     | -9.45 | 109.69      | 122.72   |
| 1   | A     | 16  | PHE  | C-N-CA     | -9.45 | 109.69      | 122.72   |
| 1   | B     | 25  | MET  | CA-CB-CG   | -9.38 | 95.34       | 114.10   |
| 1   | B     | 291 | GLY  | CA-C-O     | 9.38  | 130.49      | 121.49   |
| 1   | B     | 132 | ASN  | CA-CB-CG   | -9.35 | 103.25      | 112.60   |
| 1   | B     | 43  | ARG  | NE-CZ-NH1  | -9.35 | 112.15      | 121.50   |
| 1   | A     | 61  | GLN  | N-CA-C     | 9.31  | 124.48      | 107.73   |
| 1   | B     | 328 | TYR  | CA-C-N     | -9.30 | 107.65      | 122.25   |
| 1   | B     | 328 | TYR  | C-N-CA     | -9.30 | 107.65      | 122.25   |
| 1   | A     | 121 | SER  | CA-C-N     | -9.28 | 103.81      | 121.54   |
| 1   | A     | 121 | SER  | C-N-CA     | -9.28 | 103.81      | 121.54   |
| 1   | B     | 242 | LYS  | CA-C-N     | -9.27 | 105.34      | 121.66   |
| 1   | B     | 242 | LYS  | C-N-CA     | -9.27 | 105.34      | 121.66   |
| 1   | A     | 139 | ASP  | CA-CB-CG   | 9.26  | 121.86      | 112.60   |
| 1   | A     | 167 | ALA  | CA-C-N     | 9.24  | 138.33      | 121.70   |
| 1   | A     | 167 | ALA  | C-N-CA     | 9.24  | 138.33      | 121.70   |
| 1   | B     | 145 | ARG  | CD-NE-CZ   | -9.17 | 111.56      | 124.40   |
| 1   | B     | 271 | LEU  | CA-C-N     | -9.13 | 107.48      | 122.54   |
| 1   | B     | 271 | LEU  | C-N-CA     | -9.13 | 107.48      | 122.54   |
| 1   | B     | 107 | LEU  | CB-CA-C    | -9.10 | 93.79       | 109.07   |
| 1   | B     | 78  | LEU  | N-CA-C     | 9.07  | 120.86      | 110.97   |
| 1   | B     | 70  | ASP  | N-CA-CB    | 9.07  | 123.93      | 110.33   |
| 1   | A     | 180 | ARG  | N-CA-C     | 9.05  | 122.76      | 110.55   |
| 1   | B     | 177 | LYS  | CA-CB-CG   | 9.04  | 132.17      | 114.10   |
| 1   | A     | 301 | ILE  | CA-CB-CG1  | -9.03 | 95.05       | 110.40   |
| 1   | B     | 329 | ILE  | CB-CG1-CD1 | -9.03 | 94.84       | 113.80   |
| 1   | B     | 140 | ILE  | CA-CB-CG1  | 9.02  | 125.74      | 110.40   |
| 1   | A     | 237 | ALA  | CA-C-N     | -9.02 | 107.92      | 122.26   |
| 1   | A     | 237 | ALA  | C-N-CA     | -9.02 | 107.92      | 122.26   |
| 1   | A     | 266 | GLY  | CA-C-N     | -8.99 | 110.46      | 122.42   |
| 1   | A     | 266 | GLY  | C-N-CA     | -8.99 | 110.46      | 122.42   |
| 1   | A     | 57  | GLN  | N-CA-C     | -8.97 | 100.08      | 111.02   |
| 1   | A     | 197 | ARG  | CD-NE-CZ   | -8.96 | 111.86      | 124.40   |
| 1   | A     | 249 | THR  | CA-C-O     | 8.94  | 129.93      | 120.36   |
| 1   | B     | 218 | ILE  | CA-CB-CG1  | 8.91  | 125.56      | 110.40   |
| 1   | B     | 180 | ARG  | CA-C-O     | -8.87 | 110.61      | 120.81   |
| 1   | A     | 140 | ILE  | N-CA-CB    | -8.86 | 101.81      | 112.35   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 284 | LYS  | CA-C-O     | -8.86 | 110.73      | 120.38   |
| 1   | B     | 8   | VAL  | CA-CB-CG2  | -8.85 | 95.36       | 110.40   |
| 1   | B     | 116 | LEU  | CA-C-N     | -8.84 | 108.61      | 120.54   |
| 1   | B     | 116 | LEU  | C-N-CA     | -8.84 | 108.61      | 120.54   |
| 1   | A     | 213 | SER  | N-CA-C     | 8.82  | 120.67      | 111.14   |
| 1   | A     | 262 | GLU  | CA-C-N     | -8.80 | 110.75      | 122.99   |
| 1   | A     | 262 | GLU  | C-N-CA     | -8.80 | 110.75      | 122.99   |
| 1   | B     | 242 | LYS  | CA-CB-CG   | 8.79  | 131.69      | 114.10   |
| 1   | B     | 46  | GLN  | CA-C-O     | 8.69  | 129.89      | 120.24   |
| 1   | B     | 104 | LEU  | CA-C-N     | 8.68  | 138.11      | 121.54   |
| 1   | B     | 104 | LEU  | C-N-CA     | 8.68  | 138.11      | 121.54   |
| 1   | B     | 267 | ASN  | CA-CB-CG   | 8.67  | 121.27      | 112.60   |
| 1   | B     | 176 | PHE  | N-CA-C     | 8.67  | 129.27      | 110.80   |
| 1   | A     | 263 | VAL  | N-CA-CB    | 8.63  | 124.11      | 111.52   |
| 1   | A     | 243 | SER  | CB-CA-C    | -8.62 | 94.94       | 110.70   |
| 1   | B     | 51  | ILE  | CB-CG1-CD1 | -8.61 | 95.71       | 113.80   |
| 1   | A     | 129 | ILE  | CA-C-N     | -8.60 | 105.92      | 122.61   |
| 1   | A     | 129 | ILE  | C-N-CA     | -8.60 | 105.92      | 122.61   |
| 1   | A     | 181 | GLU  | CA-C-N     | -8.60 | 107.55      | 122.09   |
| 1   | A     | 181 | GLU  | C-N-CA     | -8.60 | 107.55      | 122.09   |
| 1   | B     | 346 | PHE  | CD1-CG-CD2 | 8.60  | 131.50      | 118.60   |
| 1   | B     | 209 | ALA  | N-CA-C     | 8.60  | 120.73      | 111.36   |
| 1   | B     | 226 | THR  | CA-CB-CG2  | 8.58  | 125.09      | 110.50   |
| 1   | B     | 107 | LEU  | N-CA-CB    | 8.57  | 122.59      | 110.67   |
| 1   | A     | 102 | GLU  | CA-C-N     | -8.53 | 109.03      | 120.54   |
| 1   | A     | 102 | GLU  | C-N-CA     | -8.53 | 109.03      | 120.54   |
| 1   | A     | 40  | LEU  | CA-C-O     | -8.52 | 110.69      | 120.58   |
| 1   | B     | 8   | VAL  | N-CA-C     | 8.51  | 119.30      | 110.62   |
| 1   | B     | 273 | HIS  | CB-CA-C    | -8.50 | 94.40       | 111.91   |
| 1   | A     | 288 | LYS  | N-CA-CB    | -8.50 | 96.10       | 110.46   |
| 1   | A     | 350 | THR  | N-CA-CB    | -8.49 | 97.07       | 111.50   |
| 1   | A     | 255 | ILE  | CA-CB-CG1  | -8.47 | 96.00       | 110.40   |
| 1   | B     | 209 | ALA  | CB-CA-C    | -8.47 | 96.44       | 110.85   |
| 1   | B     | 32  | LEU  | CA-C-N     | -8.45 | 108.26      | 122.11   |
| 1   | B     | 32  | LEU  | C-N-CA     | -8.45 | 108.26      | 122.11   |
| 1   | A     | 239 | MET  | CA-C-O     | -8.44 | 111.43      | 120.80   |
| 1   | A     | 184 | CYS  | N-CA-C     | 8.44  | 120.40      | 111.03   |
| 1   | A     | 151 | GLU  | N-CA-C     | 8.43  | 121.30      | 111.02   |
| 1   | A     | 238 | ASP  | N-CA-CB    | 8.41  | 123.01      | 110.65   |
| 1   | B     | 244 | ALA  | CA-C-O     | 8.41  | 130.26      | 120.00   |
| 1   | B     | 40  | LEU  | CA-C-N     | -8.41 | 108.59      | 122.21   |
| 1   | B     | 40  | LEU  | C-N-CA     | -8.41 | 108.59      | 122.21   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 126 | LYS  | CA-C-O    | 8.40  | 132.52      | 120.51   |
| 1   | B     | 349 | LYS  | CA-CB-CG  | 8.40  | 130.90      | 114.10   |
| 1   | B     | 140 | ILE  | N-CA-CB   | 8.39  | 122.21      | 112.40   |
| 1   | B     | 266 | GLY  | CA-C-N    | -8.37 | 111.64      | 122.77   |
| 1   | B     | 266 | GLY  | C-N-CA    | -8.37 | 111.64      | 122.77   |
| 1   | A     | 27  | GLU  | N-CA-C    | 8.36  | 123.05      | 113.01   |
| 1   | B     | 54  | GLU  | N-CA-C    | 8.36  | 125.08      | 111.37   |
| 1   | B     | 192 | GLN  | CB-CG-CD  | 8.36  | 126.81      | 112.60   |
| 1   | B     | 191 | LYS  | CA-C-N    | -8.36 | 108.25      | 120.28   |
| 1   | B     | 191 | LYS  | C-N-CA    | -8.36 | 108.25      | 120.28   |
| 1   | A     | 222 | GLU  | N-CA-C    | 8.33  | 123.17      | 112.34   |
| 1   | B     | 343 | LYS  | CA-C-N    | -8.33 | 108.26      | 122.67   |
| 1   | B     | 343 | LYS  | C-N-CA    | -8.33 | 108.26      | 122.67   |
| 1   | B     | 301 | ILE  | CA-CB-CG1 | -8.32 | 96.25       | 110.40   |
| 1   | A     | 282 | LYS  | N-CA-CB   | -8.32 | 97.65       | 110.29   |
| 1   | B     | 227 | GLY  | O-C-N     | 8.30  | 133.49      | 122.70   |
| 1   | A     | 242 | LYS  | CG-CD-CE  | 8.29  | 130.37      | 111.30   |
| 1   | B     | 145 | ARG  | N-CA-CB   | 8.29  | 124.41      | 110.32   |
| 1   | B     | 322 | SER  | CA-CB-OG  | 8.28  | 127.67      | 111.10   |
| 1   | A     | 76  | TYR  | CA-CB-CG  | -8.28 | 99.00       | 113.90   |
| 1   | A     | 332 | ASP  | N-CA-C    | 8.27  | 120.52      | 108.86   |
| 1   | A     | 93  | ASN  | N-CA-CB   | -8.27 | 97.68       | 111.57   |
| 1   | A     | 320 | ASP  | N-CA-C    | 8.27  | 128.40      | 110.80   |
| 1   | B     | 79  | ILE  | O-C-N     | 8.27  | 128.90      | 120.96   |
| 1   | B     | 177 | LYS  | CA-C-O    | -8.27 | 110.68      | 120.60   |
| 1   | A     | 246 | TYR  | CA-C-N    | -8.24 | 106.72      | 121.14   |
| 1   | A     | 246 | TYR  | C-N-CA    | -8.24 | 106.72      | 121.14   |
| 1   | A     | 139 | ASP  | CA-C-N    | -8.23 | 112.64      | 123.17   |
| 1   | A     | 139 | ASP  | C-N-CA    | -8.23 | 112.64      | 123.17   |
| 1   | A     | 204 | ARG  | NE-CZ-NH1 | -8.23 | 113.27      | 121.50   |
| 1   | B     | 93  | ASN  | CA-C-N    | -8.22 | 109.34      | 122.24   |
| 1   | B     | 93  | ASN  | C-N-CA    | -8.22 | 109.34      | 122.24   |
| 1   | B     | 222 | GLU  | N-CA-C    | 8.22  | 128.30      | 110.80   |
| 1   | B     | 110 | ILE  | CA-C-N    | -8.21 | 105.73      | 120.99   |
| 1   | B     | 110 | ILE  | C-N-CA    | -8.21 | 105.73      | 120.99   |
| 1   | A     | 268 | MET  | CA-C-N    | -8.20 | 109.77      | 121.99   |
| 1   | A     | 268 | MET  | C-N-CA    | -8.20 | 109.77      | 121.99   |
| 1   | A     | 90  | LEU  | N-CA-C    | 8.20  | 121.79      | 109.25   |
| 1   | B     | 179 | GLU  | CA-C-N    | -8.20 | 109.48      | 120.95   |
| 1   | B     | 179 | GLU  | C-N-CA    | -8.20 | 109.48      | 120.95   |
| 1   | B     | 199 | LEU  | CA-C-N    | -8.20 | 108.71      | 122.64   |
| 1   | B     | 199 | LEU  | C-N-CA    | -8.20 | 108.71      | 122.64   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 169 | ASP  | CA-C-N   | -8.19 | 109.46      | 122.73   |
| 1   | A     | 169 | ASP  | C-N-CA   | -8.19 | 109.46      | 122.73   |
| 1   | A     | 130 | ASP  | CA-CB-CG | -8.19 | 104.41      | 112.60   |
| 1   | A     | 197 | ARG  | CB-CA-C  | -8.18 | 93.48       | 109.68   |
| 1   | A     | 123 | ASP  | CA-CB-CG | -8.16 | 104.44      | 112.60   |
| 1   | A     | 288 | LYS  | N-CA-C   | 8.16  | 123.69      | 107.62   |
| 1   | A     | 205 | THR  | CA-C-N   | 8.15  | 137.11      | 121.54   |
| 1   | A     | 205 | THR  | C-N-CA   | 8.15  | 137.11      | 121.54   |
| 1   | B     | 74  | ARG  | CB-CG-CD | -8.14 | 92.57       | 111.30   |
| 1   | B     | 327 | GLU  | N-CA-CB  | -8.14 | 97.52       | 111.69   |
| 1   | A     | 203 | SER  | N-CA-CB  | -8.14 | 98.07       | 111.66   |
| 1   | B     | 214 | GLN  | O-C-N    | 8.14  | 133.22      | 122.15   |
| 1   | A     | 57  | GLN  | CB-CG-CD | 8.13  | 126.43      | 112.60   |
| 1   | B     | 139 | ASP  | CA-C-N   | -8.13 | 113.10      | 122.93   |
| 1   | B     | 139 | ASP  | C-N-CA   | -8.13 | 113.10      | 122.93   |
| 1   | A     | 39  | LYS  | CA-C-N   | -8.11 | 109.56      | 121.24   |
| 1   | A     | 39  | LYS  | C-N-CA   | -8.11 | 109.56      | 121.24   |
| 1   | A     | 81  | HIS  | N-CA-C   | 8.11  | 122.13      | 109.96   |
| 1   | A     | 174 | ASP  | CA-C-N   | -8.11 | 112.79      | 123.17   |
| 1   | A     | 174 | ASP  | C-N-CA   | -8.11 | 112.79      | 123.17   |
| 1   | B     | 276 | HIS  | CA-CB-CG | -8.11 | 105.69      | 113.80   |
| 1   | A     | 306 | VAL  | CA-C-N   | -8.10 | 108.21      | 122.07   |
| 1   | A     | 306 | VAL  | C-N-CA   | -8.10 | 108.21      | 122.07   |
| 1   | B     | 1   | LYS  | CB-CA-C  | 8.09  | 125.48      | 110.10   |
| 1   | B     | 211 | ILE  | N-CA-C   | 8.07  | 118.85      | 110.62   |
| 1   | A     | 53  | SER  | N-CA-C   | 8.06  | 120.14      | 111.36   |
| 1   | B     | 21  | MET  | CG-SD-CE | -8.06 | 83.18       | 100.90   |
| 1   | A     | 172 | VAL  | CA-C-N   | -8.05 | 111.06      | 120.88   |
| 1   | A     | 172 | VAL  | C-N-CA   | -8.05 | 111.06      | 120.88   |
| 1   | B     | 300 | ASN  | CA-CB-CG | -8.05 | 104.55      | 112.60   |
| 1   | B     | 285 | HIS  | CA-C-O   | 8.04  | 127.75      | 118.90   |
| 1   | A     | 50  | SER  | CA-C-N   | -8.04 | 110.43      | 120.56   |
| 1   | A     | 50  | SER  | C-N-CA   | -8.04 | 110.43      | 120.56   |
| 1   | B     | 106 | ASN  | CA-C-O   | -8.04 | 109.02      | 120.51   |
| 1   | A     | 195 | ASN  | N-CA-C   | 8.03  | 122.22      | 111.30   |
| 1   | B     | 69  | LEU  | N-CA-CB  | -8.02 | 97.46       | 110.14   |
| 1   | B     | 14  | MET  | CB-CG-SD | -8.02 | 88.65       | 112.70   |
| 1   | A     | 207 | ASN  | N-CA-C   | 8.01  | 120.72      | 111.11   |
| 1   | B     | 319 | ASN  | N-CA-C   | 8.00  | 120.47      | 109.11   |
| 1   | A     | 84  | GLY  | CA-C-N   | -7.96 | 106.33      | 121.54   |
| 1   | A     | 84  | GLY  | C-N-CA   | -7.96 | 106.33      | 121.54   |
| 1   | B     | 35  | MET  | CA-CB-CG | 7.96  | 130.01      | 114.10   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 323 | LEU  | CA-C-N    | -7.95 | 109.75      | 122.24   |
| 1   | A     | 323 | LEU  | C-N-CA    | -7.95 | 109.75      | 122.24   |
| 1   | B     | 20  | SER  | CA-C-O    | 7.94  | 129.10      | 119.49   |
| 1   | A     | 340 | TYR  | N-CA-CB   | -7.94 | 97.47       | 110.41   |
| 1   | B     | 232 | LYS  | CA-C-N    | -7.94 | 108.37      | 123.29   |
| 1   | B     | 232 | LYS  | C-N-CA    | -7.94 | 108.37      | 123.29   |
| 1   | B     | 287 | VAL  | CA-C-N    | -7.94 | 111.94      | 123.05   |
| 1   | B     | 287 | VAL  | C-N-CA    | -7.94 | 111.94      | 123.05   |
| 1   | A     | 70  | ASP  | CA-C-N    | -7.93 | 106.92      | 121.52   |
| 1   | A     | 70  | ASP  | C-N-CA    | -7.93 | 106.92      | 121.52   |
| 1   | A     | 110 | ILE  | N-CA-C    | 7.91  | 118.67      | 110.36   |
| 1   | A     | 86  | LYS  | N-CA-C    | 7.89  | 127.61      | 110.80   |
| 1   | B     | 34  | LYS  | N-CA-CB   | 7.89  | 121.99      | 110.47   |
| 1   | A     | 314 | ILE  | CA-CB-CG2 | 7.89  | 123.91      | 110.50   |
| 1   | B     | 200 | TRP  | N-CA-CB   | 7.88  | 123.47      | 110.63   |
| 1   | B     | 141 | LYS  | CA-C-N    | -7.87 | 113.17      | 122.22   |
| 1   | B     | 141 | LYS  | C-N-CA    | -7.87 | 113.17      | 122.22   |
| 1   | A     | 124 | SER  | CA-C-N    | -7.87 | 109.18      | 123.34   |
| 1   | A     | 124 | SER  | C-N-CA    | -7.87 | 109.18      | 123.34   |
| 1   | B     | 159 | ASN  | N-CA-C    | 7.86  | 122.90      | 113.16   |
| 1   | A     | 161 | HIS  | CA-C-N    | -7.86 | 111.69      | 122.30   |
| 1   | A     | 161 | HIS  | C-N-CA    | -7.86 | 111.69      | 122.30   |
| 1   | B     | 239 | MET  | O-C-N     | -7.82 | 113.06      | 123.23   |
| 1   | B     | 139 | ASP  | N-CA-C    | 7.82  | 121.70      | 108.02   |
| 1   | A     | 123 | ASP  | CA-C-N    | 7.82  | 135.77      | 121.70   |
| 1   | A     | 123 | ASP  | C-N-CA    | 7.82  | 135.77      | 121.70   |
| 1   | B     | 38  | GLY  | N-CA-C    | 7.82  | 123.67      | 113.27   |
| 1   | A     | 93  | ASN  | CA-C-N    | -7.81 | 107.22      | 120.58   |
| 1   | A     | 93  | ASN  | C-N-CA    | -7.81 | 107.22      | 120.58   |
| 1   | A     | 35  | MET  | CA-C-O    | 7.81  | 130.86      | 120.16   |
| 1   | A     | 205 | THR  | N-CA-C    | 7.80  | 127.42      | 110.80   |
| 1   | B     | 31  | ASP  | O-C-N     | 7.79  | 132.96      | 122.59   |
| 1   | A     | 309 | PRO  | N-CA-CB   | -7.78 | 97.60       | 102.81   |
| 1   | B     | 141 | LYS  | N-CA-C    | 7.76  | 121.97      | 110.48   |
| 1   | B     | 61  | GLN  | N-CA-C    | 7.75  | 121.18      | 112.97   |
| 1   | B     | 340 | TYR  | N-CA-CB   | -7.72 | 98.64       | 110.77   |
| 1   | A     | 68  | ILE  | CA-CB-CG1 | -7.72 | 97.28       | 110.40   |
| 1   | B     | 53  | SER  | CA-C-O    | 7.71  | 128.80      | 120.55   |
| 1   | B     | 233 | GLY  | N-CA-C    | 7.71  | 123.66      | 112.55   |
| 1   | B     | 238 | ASP  | N-CA-C    | 7.71  | 121.28      | 112.57   |
| 1   | B     | 248 | HIS  | CB-CG-CD2 | -7.71 | 121.18      | 131.20   |
| 1   | B     | 255 | ILE  | N-CA-C    | 7.70  | 119.94      | 108.54   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 246 | TYR  | CA-C-O     | 7.69  | 131.51      | 120.51   |
| 1   | B     | 12  | ILE  | CA-CB-CG2  | 7.69  | 123.58      | 110.50   |
| 1   | B     | 236 | PHE  | CA-C-N     | -7.68 | 110.16      | 122.53   |
| 1   | B     | 236 | PHE  | C-N-CA     | -7.68 | 110.16      | 122.53   |
| 1   | B     | 251 | GLN  | N-CA-C     | 7.66  | 127.12      | 110.80   |
| 1   | B     | 209 | ALA  | N-CA-CB    | 7.65  | 121.49      | 110.16   |
| 1   | A     | 314 | ILE  | CA-C-N     | -7.65 | 112.60      | 122.77   |
| 1   | A     | 314 | ILE  | C-N-CA     | -7.65 | 112.60      | 122.77   |
| 1   | B     | 110 | ILE  | N-CA-C     | 7.64  | 125.22      | 109.34   |
| 1   | A     | 82  | ASP  | CA-CB-CG   | 7.63  | 120.23      | 112.60   |
| 1   | A     | 267 | ASN  | CA-CB-CG   | 7.59  | 120.19      | 112.60   |
| 1   | A     | 74  | ARG  | NE-CZ-NH1  | 7.59  | 129.09      | 121.50   |
| 1   | B     | 61  | GLN  | CA-CB-CG   | 7.58  | 129.26      | 114.10   |
| 1   | B     | 291 | GLY  | CA-C-N     | -7.57 | 110.53      | 122.65   |
| 1   | B     | 291 | GLY  | C-N-CA     | -7.57 | 110.53      | 122.65   |
| 1   | A     | 315 | SER  | N-CA-CB    | -7.55 | 98.11       | 110.42   |
| 1   | A     | 188 | LYS  | CA-CB-CG   | -7.55 | 99.01       | 114.10   |
| 1   | A     | 123 | ASP  | CA-C-O     | 7.54  | 129.81      | 120.54   |
| 1   | B     | 134 | GLU  | CA-CB-CG   | 7.53  | 129.15      | 114.10   |
| 1   | B     | 69  | LEU  | CA-C-O     | 7.51  | 128.61      | 120.20   |
| 1   | B     | 138 | THR  | N-CA-C     | 7.50  | 121.29      | 109.81   |
| 1   | A     | 74  | ARG  | CA-CB-CG   | -7.50 | 99.11       | 114.10   |
| 1   | B     | 172 | VAL  | N-CA-C     | 7.49  | 118.93      | 107.99   |
| 1   | A     | 175 | ILE  | CB-CA-C    | 7.49  | 119.40      | 111.09   |
| 1   | B     | 324 | LEU  | CB-CA-C    | -7.48 | 98.14       | 110.85   |
| 1   | B     | 92  | ASN  | OD1-CG-ND2 | -7.48 | 115.12      | 122.60   |
| 1   | A     | 282 | LYS  | CA-C-N     | -7.47 | 109.46      | 122.09   |
| 1   | A     | 282 | LYS  | C-N-CA     | -7.47 | 109.46      | 122.09   |
| 1   | A     | 285 | HIS  | N-CA-C     | 7.47  | 121.70      | 112.59   |
| 1   | B     | 234 | ILE  | CA-CB-CG2  | -7.47 | 97.80       | 110.50   |
| 1   | B     | 48  | ALA  | N-CA-C     | 7.47  | 121.49      | 112.38   |
| 1   | A     | 141 | LYS  | CA-C-N     | -7.45 | 113.17      | 122.93   |
| 1   | A     | 141 | LYS  | C-N-CA     | -7.45 | 113.17      | 122.93   |
| 1   | A     | 150 | ALA  | N-CA-C     | 7.44  | 120.33      | 111.33   |
| 1   | A     | 156 | TYR  | N-CA-C     | 7.43  | 119.38      | 111.28   |
| 1   | B     | 261 | GLY  | CA-C-N     | -7.42 | 112.28      | 122.30   |
| 1   | B     | 261 | GLY  | C-N-CA     | -7.42 | 112.28      | 122.30   |
| 1   | B     | 338 | LEU  | N-CA-CB    | -7.42 | 98.41       | 110.21   |
| 1   | B     | 39  | LYS  | N-CA-C     | 7.42  | 121.58      | 112.23   |
| 1   | B     | 83  | PHE  | CA-C-N     | 7.41  | 134.40      | 122.40   |
| 1   | B     | 83  | PHE  | C-N-CA     | 7.41  | 134.40      | 122.40   |
| 1   | A     | 337 | ASN  | OD1-CG-ND2 | 7.40  | 130.00      | 122.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 232 | LYS  | CA-C-O    | 7.39  | 128.37      | 120.46   |
| 1   | B     | 183 | GLU  | CA-C-N    | -7.39 | 107.43      | 121.54   |
| 1   | B     | 183 | GLU  | C-N-CA    | -7.39 | 107.43      | 121.54   |
| 1   | B     | 237 | ALA  | O-C-N     | 7.38  | 132.60      | 122.78   |
| 1   | A     | 208 | PHE  | CA-C-N    | -7.37 | 109.77      | 120.82   |
| 1   | A     | 208 | PHE  | C-N-CA    | -7.37 | 109.77      | 120.82   |
| 1   | A     | 51  | ILE  | N-CA-C    | 7.37  | 117.50      | 110.42   |
| 1   | A     | 340 | TYR  | N-CA-C    | 7.37  | 122.03      | 110.32   |
| 1   | A     | 193 | LEU  | CA-C-N    | -7.36 | 110.11      | 121.74   |
| 1   | A     | 193 | LEU  | C-N-CA    | -7.36 | 110.11      | 121.74   |
| 1   | B     | 2   | SER  | N-CA-C    | 7.36  | 121.40      | 109.40   |
| 1   | A     | 331 | TYR  | CA-C-N    | -7.35 | 110.69      | 122.53   |
| 1   | A     | 331 | TYR  | C-N-CA    | -7.35 | 110.69      | 122.53   |
| 1   | B     | 166 | ASN  | CA-C-O    | 7.35  | 129.51      | 120.25   |
| 1   | A     | 328 | TYR  | N-CA-C    | 7.35  | 121.05      | 110.10   |
| 1   | B     | 290 | LEU  | N-CA-C    | 7.35  | 126.45      | 110.80   |
| 1   | A     | 276 | HIS  | N-CA-C    | 7.34  | 126.42      | 110.80   |
| 1   | B     | 64  | SER  | CA-C-O    | 7.33  | 129.41      | 121.05   |
| 1   | A     | 345 | LYS  | N-CA-C    | -7.33 | 95.03       | 107.99   |
| 1   | B     | 265 | LEU  | N-CA-C    | 7.33  | 119.34      | 111.36   |
| 1   | B     | 307 | ASP  | N-CA-C    | 7.32  | 121.01      | 110.10   |
| 1   | B     | 237 | ALA  | N-CA-C    | 7.32  | 119.18      | 108.86   |
| 1   | B     | 268 | MET  | CA-C-N    | -7.31 | 112.43      | 122.30   |
| 1   | B     | 268 | MET  | C-N-CA    | -7.31 | 112.43      | 122.30   |
| 1   | A     | 39  | LYS  | N-CA-C    | 7.31  | 126.36      | 110.80   |
| 1   | A     | 313 | GLY  | O-C-N     | 7.30  | 132.20      | 122.70   |
| 1   | B     | 99  | ALA  | CB-CA-C   | -7.30 | 98.26       | 110.68   |
| 1   | B     | 100 | LYS  | CB-CG-CD  | 7.30  | 128.09      | 111.30   |
| 1   | A     | 303 | LEU  | CA-C-O    | -7.30 | 113.17      | 121.19   |
| 1   | B     | 163 | THR  | CB-CA-C   | -7.29 | 95.91       | 110.42   |
| 1   | A     | 330 | VAL  | CA-C-N    | -7.29 | 110.99      | 122.73   |
| 1   | A     | 330 | VAL  | C-N-CA    | -7.29 | 110.99      | 122.73   |
| 1   | B     | 200 | TRP  | CB-CG-CD2 | 7.29  | 137.01      | 126.80   |
| 1   | A     | 135 | LYS  | CB-CG-CD  | 7.28  | 128.04      | 111.30   |
| 1   | B     | 43  | ARG  | CA-CB-CG  | 7.28  | 128.66      | 114.10   |
| 1   | A     | 174 | ASP  | CA-CB-CG  | -7.27 | 105.33      | 112.60   |
| 1   | A     | 50  | SER  | N-CA-C    | 7.27  | 119.28      | 111.36   |
| 1   | A     | 100 | LYS  | CA-C-N    | -7.27 | 110.50      | 120.46   |
| 1   | A     | 100 | LYS  | C-N-CA    | -7.27 | 110.50      | 120.46   |
| 1   | A     | 171 | GLU  | CA-C-N    | -7.27 | 113.27      | 122.43   |
| 1   | A     | 171 | GLU  | C-N-CA    | -7.27 | 113.27      | 122.43   |
| 1   | B     | 195 | ASN  | CA-CB-CG  | -7.27 | 105.33      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 176 | PHE  | CA-C-N     | -7.26 | 109.88      | 122.37   |
| 1   | B     | 176 | PHE  | C-N-CA     | -7.26 | 109.88      | 122.37   |
| 1   | B     | 306 | VAL  | CG1-CB-CG2 | -7.26 | 94.84       | 110.80   |
| 1   | B     | 258 | ILE  | CA-C-N     | -7.25 | 108.62      | 120.87   |
| 1   | B     | 258 | ILE  | C-N-CA     | -7.25 | 108.62      | 120.87   |
| 1   | B     | 263 | VAL  | CB-CA-C    | 7.24  | 121.35      | 110.63   |
| 1   | B     | 47  | ALA  | CA-C-N     | -7.23 | 109.03      | 120.60   |
| 1   | B     | 47  | ALA  | C-N-CA     | -7.23 | 109.03      | 120.60   |
| 1   | A     | 27  | GLU  | CA-C-N     | -7.22 | 109.31      | 122.38   |
| 1   | A     | 27  | GLU  | C-N-CA     | -7.22 | 109.31      | 122.38   |
| 1   | B     | 316 | SER  | CA-C-N     | -7.22 | 107.25      | 121.41   |
| 1   | B     | 316 | SER  | C-N-CA     | -7.22 | 107.25      | 121.41   |
| 1   | B     | 206 | THR  | N-CA-C     | 7.22  | 121.34      | 112.54   |
| 1   | B     | 273 | HIS  | ND1-CG-CD2 | 7.21  | 113.31      | 106.10   |
| 1   | B     | 291 | GLY  | O-C-N      | -7.20 | 116.60      | 123.87   |
| 1   | A     | 100 | LYS  | CA-C-O     | 7.19  | 127.69      | 119.27   |
| 1   | A     | 282 | LYS  | CB-CA-C    | 7.19  | 122.69      | 109.46   |
| 1   | A     | 223 | ALA  | CA-C-N     | 7.18  | 128.81      | 119.84   |
| 1   | A     | 223 | ALA  | C-N-CA     | 7.18  | 128.81      | 119.84   |
| 1   | B     | 33  | GLN  | N-CA-C     | 7.17  | 123.15      | 113.97   |
| 1   | B     | 168 | TYR  | N-CA-C     | 7.17  | 131.07      | 111.00   |
| 1   | B     | 254 | PRO  | CB-CA-C    | 7.16  | 123.38      | 111.56   |
| 1   | A     | 347 | ASN  | CA-C-N     | -7.16 | 111.88      | 122.41   |
| 1   | A     | 347 | ASN  | C-N-CA     | -7.16 | 111.88      | 122.41   |
| 1   | B     | 105 | ASP  | CA-CB-CG   | 7.16  | 119.76      | 112.60   |
| 1   | A     | 126 | LYS  | O-C-N      | -7.15 | 113.08      | 122.59   |
| 1   | B     | 89  | PRO  | N-CA-C     | 7.15  | 127.20      | 112.47   |
| 1   | B     | 207 | ASN  | CA-CB-CG   | -7.14 | 105.46      | 112.60   |
| 1   | B     | 26  | VAL  | CA-CB-CG2  | 7.14  | 122.53      | 110.40   |
| 1   | B     | 242 | LYS  | N-CA-CB    | 7.13  | 122.53      | 110.49   |
| 1   | B     | 346 | PHE  | CA-C-O     | 7.12  | 129.00      | 120.81   |
| 1   | B     | 106 | ASN  | CB-CA-C    | -7.12 | 96.25       | 110.42   |
| 1   | A     | 90  | LEU  | CB-CA-C    | 7.12  | 121.96      | 110.29   |
| 1   | A     | 219 | ALA  | CA-C-N     | -7.11 | 113.05      | 120.38   |
| 1   | A     | 219 | ALA  | C-N-CA     | -7.11 | 113.05      | 120.38   |
| 1   | B     | 90  | LEU  | N-CA-C     | 7.11  | 121.04      | 109.59   |
| 1   | B     | 99  | ALA  | N-CA-CB    | 7.11  | 120.73      | 110.06   |
| 1   | A     | 313 | GLY  | CA-C-O     | -7.11 | 108.20      | 120.57   |
| 1   | B     | 340 | TYR  | O-C-N      | -7.10 | 114.96      | 123.27   |
| 1   | B     | 214 | GLN  | N-CA-C     | 7.09  | 123.25      | 112.54   |
| 1   | A     | 297 | PRO  | N-CA-CB    | -7.08 | 95.81       | 103.25   |
| 1   | B     | 69  | LEU  | CA-C-N     | -7.05 | 108.55      | 121.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 69  | LEU  | C-N-CA      | -7.05 | 108.55      | 121.52   |
| 1   | A     | 194 | HIS  | CE1-NE2-CD2 | -7.04 | 101.95      | 109.00   |
| 1   | B     | 135 | LYS  | CA-C-N      | -7.04 | 108.09      | 121.54   |
| 1   | B     | 135 | LYS  | C-N-CA      | -7.04 | 108.09      | 121.54   |
| 1   | A     | 152 | ILE  | N-CA-CB     | 7.04  | 118.01      | 110.62   |
| 1   | A     | 336 | VAL  | N-CA-CB     | 7.03  | 122.97      | 111.44   |
| 1   | A     | 31  | ASP  | N-CA-CB     | -7.03 | 101.96      | 110.53   |
| 1   | A     | 67  | GLN  | CA-C-O      | 7.03  | 128.03      | 119.81   |
| 1   | A     | 141 | LYS  | CA-C-O      | -7.03 | 112.93      | 121.36   |
| 1   | B     | 67  | GLN  | CB-CG-CD    | 7.03  | 124.54      | 112.60   |
| 1   | B     | 232 | LYS  | CA-C-O      | 7.02  | 131.62      | 121.86   |
| 1   | A     | 238 | ASP  | CB-CA-C     | -7.02 | 97.76       | 109.55   |
| 1   | A     | 320 | ASP  | O-C-N       | -7.02 | 113.26      | 122.59   |
| 1   | A     | 326 | ASN  | OD1-CG-ND2  | -7.00 | 115.59      | 122.60   |
| 1   | B     | 338 | LEU  | CB-CA-C     | 7.00  | 122.36      | 110.81   |
| 1   | A     | 322 | SER  | N-CA-CB     | 7.00  | 121.13      | 110.70   |
| 1   | B     | 208 | PHE  | N-CA-C      | 6.99  | 125.69      | 110.80   |
| 1   | B     | 138 | THR  | CA-CB-CG2   | 6.99  | 122.38      | 110.50   |
| 1   | B     | 93  | ASN  | CB-CA-C     | 6.98  | 125.78      | 111.11   |
| 1   | A     | 179 | GLU  | CA-C-N      | -6.98 | 106.66      | 121.32   |
| 1   | A     | 179 | GLU  | C-N-CA      | -6.98 | 106.66      | 121.32   |
| 1   | A     | 255 | ILE  | CA-C-O      | -6.98 | 112.85      | 120.67   |
| 1   | A     | 145 | ARG  | N-CA-C      | 6.97  | 125.66      | 110.80   |
| 1   | A     | 153 | ILE  | N-CA-C      | 6.97  | 123.84      | 109.34   |
| 1   | B     | 63  | SER  | O-C-N       | -6.97 | 114.45      | 122.68   |
| 1   | A     | 134 | GLU  | CA-C-N      | 6.96  | 133.94      | 120.99   |
| 1   | A     | 134 | GLU  | C-N-CA      | 6.96  | 133.94      | 120.99   |
| 1   | A     | 248 | HIS  | CE1-NE2-CD2 | -6.96 | 102.04      | 109.00   |
| 1   | A     | 196 | ARG  | N-CA-C      | 6.96  | 121.65      | 109.96   |
| 1   | A     | 140 | ILE  | CB-CA-C     | 6.96  | 118.81      | 111.09   |
| 1   | A     | 304 | ASP  | CA-C-N      | -6.95 | 108.69      | 120.77   |
| 1   | A     | 304 | ASP  | C-N-CA      | -6.95 | 108.69      | 120.77   |
| 1   | A     | 349 | LYS  | CA-C-N      | 6.95  | 134.20      | 121.70   |
| 1   | A     | 349 | LYS  | C-N-CA      | 6.95  | 134.20      | 121.70   |
| 1   | A     | 240 | VAL  | CA-CB-CG2   | 6.94  | 122.20      | 110.40   |
| 1   | B     | 241 | SER  | N-CA-C      | 6.93  | 125.56      | 110.80   |
| 1   | B     | 165 | HIS  | N-CA-C      | 6.92  | 125.55      | 110.80   |
| 1   | B     | 279 | LYS  | CA-C-O      | 6.92  | 128.05      | 120.71   |
| 1   | A     | 338 | LEU  | N-CA-C      | 6.92  | 120.41      | 110.10   |
| 1   | B     | 46  | GLN  | N-CA-CB     | -6.91 | 99.90       | 110.20   |
| 1   | A     | 126 | LYS  | CB-CA-C     | 6.91  | 124.17      | 110.42   |
| 1   | A     | 118 | ARG  | NE-CZ-NH2   | -6.91 | 112.98      | 119.20   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 167 | ALA  | CA-C-N    | 6.90  | 134.12      | 121.70   |
| 1   | B     | 167 | ALA  | C-N-CA    | 6.90  | 134.12      | 121.70   |
| 1   | B     | 80  | PRO  | CA-C-O    | -6.90 | 114.03      | 121.27   |
| 1   | A     | 277 | ILE  | CA-CB-CG2 | -6.89 | 98.78       | 110.50   |
| 1   | B     | 45  | ILE  | N-CA-C    | 6.89  | 119.70      | 111.09   |
| 1   | A     | 300 | ASN  | N-CA-C    | 6.88  | 120.53      | 108.56   |
| 1   | A     | 259 | LEU  | CA-C-N    | -6.88 | 112.96      | 123.14   |
| 1   | A     | 259 | LEU  | C-N-CA    | -6.88 | 112.96      | 123.14   |
| 1   | A     | 124 | SER  | N-CA-CB   | 6.87  | 122.17      | 110.50   |
| 1   | A     | 229 | MET  | N-CA-C    | 6.86  | 119.64      | 111.33   |
| 1   | A     | 109 | ASP  | N-CA-CB   | -6.86 | 99.77       | 110.06   |
| 1   | A     | 111 | GLU  | CA-CB-CG  | 6.86  | 127.82      | 114.10   |
| 1   | B     | 184 | CYS  | N-CA-CB   | 6.86  | 122.08      | 110.49   |
| 1   | A     | 289 | GLY  | CA-C-O    | 6.86  | 132.50      | 120.57   |
| 1   | A     | 40  | LEU  | CB-CA-C   | -6.84 | 99.99       | 110.26   |
| 1   | A     | 172 | VAL  | CA-C-O    | 6.84  | 129.09      | 120.75   |
| 1   | A     | 287 | VAL  | CA-C-O    | -6.84 | 113.25      | 120.57   |
| 1   | A     | 39  | LYS  | CB-CA-C   | -6.83 | 96.83       | 110.42   |
| 1   | B     | 81  | HIS  | O-C-N     | -6.82 | 115.19      | 123.30   |
| 1   | A     | 103 | MET  | CA-CB-CG  | 6.82  | 127.73      | 114.10   |
| 1   | A     | 220 | PRO  | N-CA-C    | -6.81 | 102.39      | 110.70   |
| 1   | A     | 198 | LEU  | CA-C-N    | -6.81 | 111.90      | 122.59   |
| 1   | A     | 198 | LEU  | C-N-CA    | -6.81 | 111.90      | 122.59   |
| 1   | B     | 135 | LYS  | CA-C-O    | 6.80  | 127.74      | 119.31   |
| 1   | B     | 145 | ARG  | CB-CA-C   | -6.80 | 95.97       | 110.32   |
| 1   | A     | 28  | TYR  | CA-C-N    | 6.80  | 134.53      | 121.54   |
| 1   | A     | 28  | TYR  | C-N-CA    | 6.80  | 134.53      | 121.54   |
| 1   | A     | 239 | MET  | CA-C-N    | -6.80 | 108.60      | 120.29   |
| 1   | A     | 239 | MET  | C-N-CA    | -6.80 | 108.60      | 120.29   |
| 1   | A     | 268 | MET  | N-CA-C    | 6.80  | 119.58      | 109.59   |
| 1   | A     | 123 | ASP  | N-CA-C    | 6.79  | 120.36      | 108.75   |
| 1   | B     | 122 | ASP  | CA-CB-CG  | -6.79 | 105.81      | 112.60   |
| 1   | A     | 175 | ILE  | N-CA-C    | 6.78  | 118.68      | 106.61   |
| 1   | B     | 308 | VAL  | O-C-N     | 6.78  | 128.83      | 121.10   |
| 1   | A     | 57  | GLN  | CA-CB-CG  | 6.78  | 127.65      | 114.10   |
| 1   | A     | 110 | ILE  | CA-C-O    | -6.78 | 114.22      | 121.27   |
| 1   | A     | 118 | ARG  | CA-CB-CG  | -6.77 | 100.56      | 114.10   |
| 1   | A     | 180 | ARG  | CD-NE-CZ  | -6.77 | 114.92      | 124.40   |
| 1   | B     | 152 | ILE  | CA-C-N    | -6.76 | 112.25      | 120.70   |
| 1   | B     | 152 | ILE  | C-N-CA    | -6.76 | 112.25      | 120.70   |
| 1   | B     | 21  | MET  | N-CA-C    | 6.75  | 125.18      | 110.80   |
| 1   | A     | 122 | ASP  | CA-C-O    | 6.74  | 130.15      | 120.51   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 3   | LYS  | CA-CB-CG   | 6.74  | 127.57      | 114.10   |
| 1   | B     | 268 | MET  | CG-SD-CE   | 6.73  | 115.70      | 100.90   |
| 1   | A     | 240 | VAL  | O-C-N      | 6.72  | 131.03      | 121.82   |
| 1   | A     | 314 | ILE  | CB-CG1-CD1 | -6.72 | 99.70       | 113.80   |
| 1   | B     | 37  | LEU  | CA-C-N     | -6.71 | 111.67      | 120.13   |
| 1   | B     | 37  | LEU  | C-N-CA     | -6.71 | 111.67      | 120.13   |
| 1   | A     | 110 | ILE  | CB-CG1-CD1 | -6.71 | 99.71       | 113.80   |
| 1   | B     | 314 | ILE  | CA-C-O     | 6.71  | 128.19      | 120.67   |
| 1   | A     | 332 | ASP  | CA-C-N     | -6.71 | 108.75      | 120.29   |
| 1   | A     | 332 | ASP  | C-N-CA     | -6.71 | 108.75      | 120.29   |
| 1   | A     | 318 | VAL  | N-CA-CB    | -6.71 | 100.16      | 111.23   |
| 1   | A     | 346 | PHE  | CB-CA-C    | 6.71  | 120.85      | 109.72   |
| 1   | A     | 168 | TYR  | N-CA-C     | 6.70  | 129.75      | 111.00   |
| 1   | B     | 145 | ARG  | O-C-N      | 6.70  | 131.09      | 122.39   |
| 1   | A     | 197 | ARG  | N-CA-CB    | 6.69  | 123.25      | 111.13   |
| 1   | B     | 152 | ILE  | CB-CG1-CD1 | -6.69 | 99.74       | 113.80   |
| 1   | A     | 271 | LEU  | CA-C-N     | -6.68 | 111.85      | 122.08   |
| 1   | A     | 271 | LEU  | C-N-CA     | -6.68 | 111.85      | 122.08   |
| 1   | A     | 245 | ASN  | CA-CB-CG   | -6.68 | 105.92      | 112.60   |
| 1   | B     | 64  | SER  | N-CA-C     | 6.68  | 120.75      | 110.20   |
| 1   | A     | 292 | LYS  | CA-C-N     | -6.68 | 113.89      | 122.77   |
| 1   | A     | 292 | LYS  | C-N-CA     | -6.68 | 113.89      | 122.77   |
| 1   | B     | 255 | ILE  | CA-CB-CG1  | 6.67  | 121.74      | 110.40   |
| 1   | A     | 237 | ALA  | N-CA-C     | 6.67  | 119.85      | 109.52   |
| 1   | B     | 347 | ASN  | CB-CA-C    | 6.67  | 120.40      | 110.14   |
| 1   | A     | 175 | ILE  | CB-CG1-CD1 | -6.66 | 99.81       | 113.80   |
| 1   | B     | 38  | GLY  | CA-C-O     | 6.66  | 127.25      | 120.45   |
| 1   | A     | 43  | ARG  | NE-CZ-NH1  | 6.66  | 128.16      | 121.50   |
| 1   | B     | 50  | SER  | CA-CB-OG   | -6.66 | 97.79       | 111.10   |
| 1   | B     | 295 | PRO  | CA-N-CD    | -6.65 | 102.69      | 112.00   |
| 1   | A     | 55  | VAL  | CA-C-N     | -6.64 | 109.22      | 120.58   |
| 1   | A     | 55  | VAL  | C-N-CA     | -6.64 | 109.22      | 120.58   |
| 1   | B     | 242 | LYS  | CA-C-O     | 6.64  | 130.01      | 120.51   |
| 1   | B     | 97  | VAL  | CA-C-O     | -6.63 | 113.09      | 120.25   |
| 1   | B     | 4   | LEU  | N-CA-C     | 6.63  | 118.45      | 109.24   |
| 1   | B     | 63  | SER  | CA-C-N     | -6.62 | 111.95      | 121.42   |
| 1   | B     | 63  | SER  | C-N-CA     | -6.62 | 111.95      | 121.42   |
| 1   | B     | 1   | LYS  | CB-CG-CD   | 6.61  | 126.51      | 111.30   |
| 1   | A     | 273 | HIS  | N-CA-C     | -6.60 | 100.19      | 109.69   |
| 1   | B     | 117 | LEU  | N-CA-C     | 6.59  | 119.02      | 111.11   |
| 1   | B     | 333 | ILE  | N-CA-C     | 6.59  | 120.27      | 111.17   |
| 1   | A     | 335 | GLN  | N-CA-CB    | -6.59 | 96.96       | 110.67   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 96  | SER  | CA-C-N     | -6.59 | 108.95      | 120.29   |
| 1   | B     | 96  | SER  | C-N-CA     | -6.59 | 108.95      | 120.29   |
| 1   | B     | 302 | SER  | N-CA-C     | 6.59  | 124.83      | 110.80   |
| 1   | B     | 339 | LYS  | N-CA-C     | 6.59  | 121.64      | 111.56   |
| 1   | B     | 174 | ASP  | CA-C-N     | -6.58 | 110.12      | 121.97   |
| 1   | B     | 174 | ASP  | C-N-CA     | -6.58 | 110.12      | 121.97   |
| 1   | B     | 148 | GLU  | N-CA-CB    | 6.58  | 120.70      | 110.44   |
| 1   | B     | 158 | LYS  | CA-C-N     | -6.58 | 110.48      | 122.38   |
| 1   | B     | 158 | LYS  | C-N-CA     | -6.58 | 110.48      | 122.38   |
| 1   | A     | 124 | SER  | CA-C-O     | -6.57 | 109.63      | 120.80   |
| 1   | A     | 159 | ASN  | OD1-CG-ND2 | 6.57  | 129.17      | 122.60   |
| 1   | B     | 232 | LYS  | N-CA-C     | 6.57  | 118.44      | 109.11   |
| 1   | A     | 140 | ILE  | O-C-N      | -6.57 | 116.34      | 122.71   |
| 1   | A     | 18  | VAL  | N-CA-C     | 6.57  | 119.26      | 111.05   |
| 1   | A     | 110 | ILE  | CA-CB-CG1  | -6.57 | 99.24       | 110.40   |
| 1   | B     | 69  | LEU  | CD1-CG-CD2 | 6.56  | 125.23      | 110.80   |
| 1   | A     | 76  | TYR  | CB-CA-C    | 6.55  | 123.46      | 110.42   |
| 1   | A     | 85  | MET  | N-CA-C     | 6.55  | 124.76      | 110.80   |
| 1   | A     | 102 | GLU  | N-CA-C     | 6.55  | 118.08      | 111.07   |
| 1   | B     | 151 | GLU  | CB-CA-C    | 6.54  | 121.27      | 110.81   |
| 1   | A     | 283 | GLY  | CA-C-N     | -6.54 | 113.98      | 123.00   |
| 1   | A     | 283 | GLY  | C-N-CA     | -6.54 | 113.98      | 123.00   |
| 1   | B     | 287 | VAL  | CA-C-O     | 6.53  | 127.29      | 120.36   |
| 1   | A     | 1   | LYS  | CG-CD-CE   | 6.53  | 126.32      | 111.30   |
| 1   | B     | 174 | ASP  | N-CA-C     | 6.53  | 119.34      | 109.23   |
| 1   | B     | 300 | ASN  | CA-C-N     | -6.53 | 110.22      | 121.97   |
| 1   | B     | 300 | ASN  | C-N-CA     | -6.53 | 110.22      | 121.97   |
| 1   | B     | 228 | TYR  | CA-C-O     | -6.52 | 112.94      | 120.31   |
| 1   | B     | 309 | PRO  | N-CA-CB    | -6.52 | 96.40       | 103.25   |
| 1   | A     | 147 | SER  | CB-CA-C    | -6.52 | 98.36       | 109.51   |
| 1   | B     | 170 | LEU  | N-CA-C     | 6.52  | 120.48      | 111.55   |
| 1   | A     | 336 | VAL  | N-CA-C     | 6.51  | 118.17      | 108.46   |
| 1   | B     | 152 | ILE  | N-CA-C     | 6.51  | 117.26      | 110.62   |
| 1   | B     | 308 | VAL  | CA-C-O     | -6.50 | 111.23      | 119.95   |
| 1   | A     | 111 | GLU  | CA-C-N     | -6.50 | 109.64      | 120.30   |
| 1   | A     | 111 | GLU  | C-N-CA     | -6.50 | 109.64      | 120.30   |
| 1   | B     | 158 | LYS  | O-C-N      | -6.50 | 114.64      | 122.11   |
| 1   | B     | 336 | VAL  | CA-CB-CG2  | 6.50  | 121.44      | 110.40   |
| 1   | A     | 152 | ILE  | CA-CB-CG1  | 6.47  | 121.40      | 110.40   |
| 1   | B     | 280 | LEU  | CD1-CG-CD2 | 6.47  | 125.03      | 110.80   |
| 1   | B     | 112 | VAL  | CG1-CB-CG2 | -6.47 | 96.57       | 110.80   |
| 1   | B     | 161 | HIS  | CA-C-N     | -6.46 | 111.63      | 122.29   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 161 | HIS  | C-N-CA    | -6.46 | 111.63      | 122.29   |
| 1   | A     | 9   | GLN  | N-CA-C    | 6.45  | 119.14      | 111.33   |
| 1   | B     | 317 | GLY  | N-CA-C    | 6.45  | 128.46      | 113.18   |
| 1   | A     | 282 | LYS  | CB-CG-CD  | 6.44  | 126.12      | 111.30   |
| 1   | A     | 111 | GLU  | CB-CG-CD  | 6.44  | 123.55      | 112.60   |
| 1   | A     | 91  | LEU  | N-CA-CB   | -6.44 | 100.88      | 110.60   |
| 1   | B     | 58  | ALA  | CB-CA-C   | -6.43 | 100.69      | 110.92   |
| 1   | B     | 292 | LYS  | CA-CB-CG  | 6.43  | 126.96      | 114.10   |
| 1   | A     | 294 | THR  | CA-CB-CG2 | 6.41  | 121.40      | 110.50   |
| 1   | A     | 333 | ILE  | CA-C-O    | 6.41  | 127.17      | 120.25   |
| 1   | A     | 73  | ASN  | CA-CB-CG  | -6.41 | 106.19      | 112.60   |
| 1   | A     | 74  | ARG  | N-CA-C    | 6.41  | 118.34      | 111.36   |
| 1   | A     | 77  | THR  | CA-CB-CG2 | 6.40  | 121.39      | 110.50   |
| 1   | B     | 218 | ILE  | N-CA-C    | 6.40  | 118.70      | 108.85   |
| 1   | B     | 263 | VAL  | CA-CB-CG2 | 6.40  | 121.27      | 110.40   |
| 1   | A     | 336 | VAL  | CA-CB-CG2 | 6.39  | 121.27      | 110.40   |
| 1   | A     | 166 | ASN  | CA-C-N    | -6.39 | 110.20      | 121.70   |
| 1   | A     | 166 | ASN  | C-N-CA    | -6.39 | 110.20      | 121.70   |
| 1   | B     | 149 | GLU  | N-CA-CB   | 6.39  | 119.24      | 109.91   |
| 1   | A     | 201 | HIS  | CA-C-N    | -6.38 | 115.38      | 121.57   |
| 1   | A     | 201 | HIS  | C-N-CA    | -6.38 | 115.38      | 121.57   |
| 1   | A     | 60  | SER  | CA-C-N    | -6.38 | 113.42      | 123.12   |
| 1   | A     | 60  | SER  | C-N-CA    | -6.38 | 113.42      | 123.12   |
| 1   | B     | 24  | ALA  | CA-C-O    | 6.38  | 127.73      | 120.90   |
| 1   | B     | 35  | MET  | CA-C-O    | 6.38  | 128.78      | 120.74   |
| 1   | B     | 171 | GLU  | CA-C-N    | -6.38 | 114.73      | 122.90   |
| 1   | B     | 171 | GLU  | C-N-CA    | -6.38 | 114.73      | 122.90   |
| 1   | B     | 196 | ARG  | CD-NE-CZ  | -6.37 | 115.48      | 124.40   |
| 1   | A     | 268 | MET  | CA-C-O    | 6.37  | 127.97      | 120.58   |
| 1   | B     | 112 | VAL  | N-CA-CB   | 6.37  | 119.69      | 110.52   |
| 1   | A     | 126 | LYS  | N-CA-CB   | -6.36 | 99.74       | 110.49   |
| 1   | B     | 288 | LYS  | CA-C-O    | 6.36  | 127.32      | 120.32   |
| 1   | A     | 322 | SER  | CA-C-N    | -6.36 | 112.19      | 122.36   |
| 1   | A     | 322 | SER  | C-N-CA    | -6.36 | 112.19      | 122.36   |
| 1   | B     | 302 | SER  | CB-CA-C   | -6.36 | 97.77       | 110.42   |
| 1   | A     | 105 | ASP  | CA-C-O    | 6.35  | 127.49      | 120.82   |
| 1   | B     | 2   | SER  | CA-C-N    | 6.35  | 130.76      | 120.60   |
| 1   | B     | 2   | SER  | C-N-CA    | 6.35  | 130.76      | 120.60   |
| 1   | A     | 20  | SER  | N-CA-C    | 6.35  | 119.01      | 111.71   |
| 1   | B     | 193 | LEU  | N-CA-CB   | -6.35 | 101.03      | 110.17   |
| 1   | A     | 155 | LYS  | CB-CG-CD  | 6.34  | 125.89      | 111.30   |
| 1   | A     | 330 | VAL  | N-CA-C    | 6.34  | 117.25      | 108.12   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 56  | GLN  | CB-CA-C    | 6.34  | 122.41      | 109.55   |
| 1   | A     | 47  | ALA  | N-CA-CB    | 6.33  | 119.56      | 110.06   |
| 1   | B     | 253 | ASP  | N-CA-C     | 6.33  | 123.80      | 109.81   |
| 1   | A     | 59  | VAL  | N-CA-CB    | 6.32  | 118.67      | 110.57   |
| 1   | B     | 151 | GLU  | CA-CB-CG   | 6.32  | 126.74      | 114.10   |
| 1   | B     | 192 | GLN  | N-CA-C     | 6.32  | 118.98      | 111.71   |
| 1   | A     | 155 | LYS  | CA-C-O     | 6.31  | 127.45      | 120.82   |
| 1   | B     | 83  | PHE  | N-CA-C     | 6.31  | 120.84      | 113.20   |
| 1   | B     | 129 | ILE  | CA-C-N     | -6.31 | 111.19      | 120.28   |
| 1   | B     | 129 | ILE  | C-N-CA     | -6.31 | 111.19      | 120.28   |
| 1   | A     | 91  | LEU  | CB-CA-C    | 6.31  | 122.15      | 112.00   |
| 1   | A     | 163 | THR  | N-CA-CB    | -6.30 | 99.84       | 110.49   |
| 1   | A     | 305 | GLY  | CA-C-O     | 6.30  | 127.42      | 119.80   |
| 1   | B     | 329 | ILE  | CA-CB-CG2  | 6.30  | 121.20      | 110.50   |
| 1   | B     | 264 | ALA  | N-CA-C     | 6.29  | 120.03      | 108.58   |
| 1   | B     | 322 | SER  | O-C-N      | -6.29 | 112.30      | 122.42   |
| 1   | B     | 339 | LYS  | CA-C-O     | 6.29  | 128.17      | 120.56   |
| 1   | A     | 293 | THR  | CA-C-N     | -6.28 | 107.61      | 122.31   |
| 1   | A     | 293 | THR  | C-N-CA     | -6.28 | 107.61      | 122.31   |
| 1   | B     | 331 | TYR  | CA-C-O     | 6.28  | 126.91      | 119.56   |
| 1   | A     | 47  | ALA  | N-CA-C     | 6.28  | 118.93      | 111.33   |
| 1   | A     | 301 | ILE  | CA-C-O     | -6.28 | 112.93      | 120.78   |
| 1   | A     | 45  | ILE  | CA-CB-CG1  | 6.28  | 121.07      | 110.40   |
| 1   | B     | 39  | LYS  | N-CA-CB    | 6.26  | 119.95      | 110.30   |
| 1   | B     | 43  | ARG  | CA-C-N     | -6.26 | 110.26      | 120.72   |
| 1   | B     | 43  | ARG  | C-N-CA     | -6.26 | 110.26      | 120.72   |
| 1   | A     | 296 | ASP  | O-C-N      | 6.25  | 128.51      | 121.32   |
| 1   | A     | 46  | GLN  | CB-CA-C    | 6.25  | 120.70      | 110.88   |
| 1   | A     | 230 | PHE  | CA-C-N     | -6.25 | 109.17      | 121.41   |
| 1   | A     | 230 | PHE  | C-N-CA     | -6.25 | 109.17      | 121.41   |
| 1   | B     | 58  | ALA  | CA-C-N     | -6.25 | 110.43      | 120.86   |
| 1   | B     | 58  | ALA  | C-N-CA     | -6.25 | 110.43      | 120.86   |
| 1   | A     | 144 | ASP  | O-C-N      | -6.25 | 114.28      | 122.59   |
| 1   | B     | 260 | LEU  | CB-CA-C    | -6.25 | 97.44       | 109.37   |
| 1   | B     | 74  | ARG  | CD-NE-CZ   | -6.24 | 115.66      | 124.40   |
| 1   | A     | 149 | GLU  | N-CA-C     | 6.24  | 117.77      | 110.97   |
| 1   | A     | 314 | ILE  | CB-CA-C    | -6.23 | 102.28      | 111.19   |
| 1   | A     | 59  | VAL  | O-C-N      | 6.23  | 128.38      | 121.90   |
| 1   | B     | 74  | ARG  | O-C-N      | 6.22  | 130.99      | 122.46   |
| 1   | B     | 319 | ASN  | OD1-CG-ND2 | 6.22  | 128.82      | 122.60   |
| 1   | A     | 326 | ASN  | CA-C-N     | 6.21  | 133.78      | 122.92   |
| 1   | A     | 326 | ASN  | C-N-CA     | 6.21  | 133.78      | 122.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 334 | ALA  | CA-C-O      | 6.20  | 126.92      | 119.10   |
| 1   | A     | 345 | LYS  | O-C-N       | 6.20  | 130.94      | 123.13   |
| 1   | B     | 115 | SER  | CB-CA-C     | -6.20 | 99.16       | 110.63   |
| 1   | A     | 228 | TYR  | N-CA-C      | 6.20  | 119.66      | 108.69   |
| 1   | B     | 230 | PHE  | CA-CB-CG    | 6.20  | 120.00      | 113.80   |
| 1   | B     | 134 | GLU  | N-CA-C      | 6.19  | 118.54      | 111.11   |
| 1   | A     | 40  | LEU  | N-CA-CB     | 6.18  | 119.23      | 109.71   |
| 1   | A     | 127 | ASP  | N-CA-CB     | -6.18 | 99.36       | 110.37   |
| 1   | B     | 302 | SER  | N-CA-CB     | 6.18  | 120.93      | 110.49   |
| 1   | A     | 105 | ASP  | CA-CB-CG    | 6.18  | 118.78      | 112.60   |
| 1   | B     | 173 | ILE  | CA-C-O      | -6.17 | 113.53      | 120.32   |
| 1   | A     | 214 | GLN  | CA-CB-CG    | 6.17  | 126.43      | 114.10   |
| 1   | B     | 298 | SER  | CA-C-N      | -6.17 | 109.76      | 121.54   |
| 1   | B     | 298 | SER  | C-N-CA      | -6.17 | 109.76      | 121.54   |
| 1   | A     | 112 | VAL  | CA-C-N      | 6.16  | 129.36      | 120.79   |
| 1   | A     | 112 | VAL  | C-N-CA      | 6.16  | 129.36      | 120.79   |
| 1   | A     | 165 | HIS  | CB-CG-CD2   | -6.16 | 123.19      | 131.20   |
| 1   | A     | 243 | SER  | N-CA-C      | 6.16  | 119.26      | 111.69   |
| 1   | A     | 2   | SER  | N-CA-C      | 6.15  | 123.91      | 110.80   |
| 1   | A     | 211 | ILE  | CA-C-N      | -6.15 | 110.20      | 121.52   |
| 1   | A     | 211 | ILE  | C-N-CA      | -6.15 | 110.20      | 121.52   |
| 1   | A     | 6   | LYS  | N-CA-C      | 6.15  | 123.39      | 109.81   |
| 1   | B     | 254 | PRO  | N-CA-CB     | -6.14 | 96.80       | 103.25   |
| 1   | B     | 36  | PRO  | N-CA-CB     | -6.14 | 97.19       | 103.15   |
| 1   | B     | 349 | LYS  | CG-CD-CE    | 6.14  | 125.42      | 111.30   |
| 1   | A     | 42  | LYS  | CA-C-O      | 6.14  | 127.02      | 120.70   |
| 1   | B     | 276 | HIS  | CA-C-N      | -6.14 | 110.92      | 121.97   |
| 1   | B     | 276 | HIS  | C-N-CA      | -6.14 | 110.92      | 121.97   |
| 1   | A     | 234 | ILE  | N-CA-C      | 6.13  | 117.54      | 107.24   |
| 1   | A     | 23  | LYS  | N-CA-CB     | -6.13 | 100.87      | 110.06   |
| 1   | A     | 257 | LEU  | N-CA-C      | 6.12  | 119.14      | 110.50   |
| 1   | A     | 51  | ILE  | CA-C-N      | -6.12 | 111.44      | 120.38   |
| 1   | A     | 51  | ILE  | C-N-CA      | -6.12 | 111.44      | 120.38   |
| 1   | B     | 41  | SER  | N-CA-CB     | -6.12 | 101.05      | 111.69   |
| 1   | A     | 126 | LYS  | N-CA-C      | 6.11  | 123.82      | 110.80   |
| 1   | B     | 337 | ASN  | CA-C-O      | 6.11  | 127.66      | 120.20   |
| 1   | A     | 162 | ALA  | N-CA-C      | 6.11  | 118.68      | 108.96   |
| 1   | A     | 327 | GLU  | N-CA-C      | 6.11  | 120.56      | 107.67   |
| 1   | A     | 66  | SER  | N-CA-C      | 6.10  | 123.79      | 110.80   |
| 1   | B     | 175 | ILE  | CA-C-N      | -6.10 | 109.89      | 121.54   |
| 1   | B     | 175 | ILE  | C-N-CA      | -6.10 | 109.89      | 121.54   |
| 1   | A     | 194 | HIS  | ND1-CE1-NE2 | 6.10  | 114.50      | 108.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 143 | VAL  | CB-CA-C    | -6.09 | 102.25      | 111.33   |
| 1   | A     | 316 | SER  | CA-C-N     | -6.09 | 105.06      | 122.06   |
| 1   | A     | 316 | SER  | C-N-CA     | -6.09 | 105.06      | 122.06   |
| 1   | A     | 327 | GLU  | N-CA-CB    | -6.09 | 101.71      | 111.58   |
| 1   | B     | 143 | VAL  | O-C-N      | 6.08  | 130.17      | 122.57   |
| 1   | B     | 143 | VAL  | CA-CB-CG1  | 6.08  | 120.74      | 110.40   |
| 1   | A     | 18  | VAL  | CA-C-N     | -6.08 | 112.54      | 120.44   |
| 1   | A     | 18  | VAL  | C-N-CA     | -6.08 | 112.54      | 120.44   |
| 1   | B     | 265 | LEU  | N-CA-CB    | -6.08 | 101.17      | 110.16   |
| 1   | B     | 3   | LYS  | N-CA-C     | 6.07  | 119.78      | 112.38   |
| 1   | A     | 204 | ARG  | CD-NE-CZ   | -6.06 | 115.91      | 124.40   |
| 1   | B     | 280 | LEU  | O-C-N      | 6.06  | 128.40      | 121.31   |
| 1   | B     | 175 | ILE  | CB-CG1-CD1 | -6.06 | 101.08      | 113.80   |
| 1   | B     | 151 | GLU  | N-CA-CB    | -6.06 | 100.92      | 109.94   |
| 1   | A     | 118 | ARG  | N-CA-C     | 6.05  | 123.69      | 110.80   |
| 1   | B     | 280 | LEU  | N-CA-CB    | -6.05 | 102.00      | 110.04   |
| 1   | B     | 262 | GLU  | N-CA-C     | -6.05 | 99.34       | 108.96   |
| 1   | B     | 97  | VAL  | CA-CB-CG2  | -6.05 | 100.12      | 110.40   |
| 1   | A     | 69  | LEU  | N-CA-C     | 6.04  | 119.49      | 111.75   |
| 1   | A     | 241 | SER  | CA-C-O     | -6.04 | 111.87      | 120.51   |
| 1   | B     | 90  | LEU  | CA-C-O     | 6.04  | 127.12      | 120.71   |
| 1   | B     | 217 | ARG  | CB-CA-C    | -6.04 | 99.01       | 111.22   |
| 1   | A     | 82  | ASP  | CA-C-N     | 6.04  | 133.32      | 122.38   |
| 1   | A     | 82  | ASP  | C-N-CA     | 6.04  | 133.32      | 122.38   |
| 1   | A     | 143 | VAL  | CA-C-O     | -6.04 | 114.15      | 121.04   |
| 1   | A     | 283 | GLY  | CA-C-O     | 6.04  | 125.44      | 119.04   |
| 1   | B     | 29  | GLU  | CA-CB-CG   | -6.04 | 102.03      | 114.10   |
| 1   | A     | 292 | LYS  | O-C-N      | -6.04 | 114.40      | 122.43   |
| 1   | A     | 173 | ILE  | O-C-N      | 6.03  | 129.30      | 121.94   |
| 1   | B     | 117 | LEU  | CB-CA-C    | 6.03  | 120.46      | 110.81   |
| 1   | B     | 144 | ASP  | CA-C-N     | -6.02 | 110.97      | 120.60   |
| 1   | B     | 144 | ASP  | C-N-CA     | -6.02 | 110.97      | 120.60   |
| 1   | A     | 142 | VAL  | CA-C-N     | -6.02 | 112.79      | 120.98   |
| 1   | A     | 142 | VAL  | C-N-CA     | -6.02 | 112.79      | 120.98   |
| 1   | B     | 64  | SER  | N-CA-CB    | 6.01  | 119.14      | 110.06   |
| 1   | B     | 197 | ARG  | CD-NE-CZ   | 6.01  | 132.81      | 124.40   |
| 1   | B     | 253 | ASP  | CA-CB-CG   | 6.00  | 118.61      | 112.60   |
| 1   | A     | 120 | GLY  | CA-C-N     | -6.00 | 108.27      | 122.20   |
| 1   | A     | 120 | GLY  | C-N-CA     | -6.00 | 108.27      | 122.20   |
| 1   | B     | 35  | MET  | N-CA-CB    | 6.00  | 119.66      | 111.20   |
| 1   | B     | 67  | GLN  | N-CA-C     | 6.00  | 118.31      | 111.11   |
| 1   | B     | 88  | PRO  | N-CA-CB    | -6.00 | 97.26       | 103.08   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 186 | ARG  | N-CA-C     | 6.00  | 121.26      | 111.37   |
| 1   | B     | 223 | ALA  | CA-C-N     | -6.00 | 113.35      | 120.13   |
| 1   | B     | 223 | ALA  | C-N-CA     | -6.00 | 113.35      | 120.13   |
| 1   | B     | 269 | TYR  | CA-C-O     | 5.99  | 127.14      | 120.43   |
| 1   | A     | 97  | VAL  | CB-CA-C    | 5.99  | 119.86      | 112.02   |
| 1   | A     | 16  | PHE  | CA-CB-CG   | -5.98 | 107.82      | 113.80   |
| 1   | A     | 348 | PHE  | CA-C-O     | -5.98 | 114.70      | 120.92   |
| 1   | B     | 79  | ILE  | CA-C-N     | 5.98  | 126.91      | 119.98   |
| 1   | B     | 79  | ILE  | C-N-CA     | 5.98  | 126.91      | 119.98   |
| 1   | B     | 33  | GLN  | O-C-N      | 5.97  | 129.70      | 122.48   |
| 1   | A     | 98  | GLN  | CA-C-O     | 5.96  | 126.87      | 120.55   |
| 1   | A     | 343 | LYS  | N-CA-C     | 5.96  | 118.43      | 108.96   |
| 1   | A     | 19  | GLU  | CB-CG-CD   | 5.96  | 122.72      | 112.60   |
| 1   | A     | 100 | LYS  | CA-CB-CG   | 5.95  | 126.00      | 114.10   |
| 1   | B     | 99  | ALA  | N-CA-C     | 5.94  | 118.52      | 111.33   |
| 1   | B     | 118 | ARG  | CB-CA-C    | 5.94  | 120.28      | 110.90   |
| 1   | B     | 98  | GLN  | CA-C-N     | -5.93 | 112.25      | 120.38   |
| 1   | B     | 98  | GLN  | C-N-CA     | -5.93 | 112.25      | 120.38   |
| 1   | B     | 117 | LEU  | CD1-CG-CD2 | 5.93  | 123.85      | 110.80   |
| 1   | A     | 29  | GLU  | CA-C-O     | 5.93  | 128.99      | 120.51   |
| 1   | B     | 42  | LYS  | CA-C-O     | 5.93  | 127.04      | 120.82   |
| 1   | B     | 188 | LYS  | CA-CB-CG   | 5.92  | 125.95      | 114.10   |
| 1   | A     | 251 | GLN  | CA-C-O     | -5.92 | 112.05      | 120.51   |
| 1   | A     | 278 | SER  | N-CA-CB    | 5.91  | 120.48      | 110.49   |
| 1   | B     | 214 | GLN  | CB-CG-CD   | -5.91 | 102.56      | 112.60   |
| 1   | B     | 211 | ILE  | CA-CB-CG1  | 5.90  | 120.42      | 110.40   |
| 1   | B     | 111 | GLU  | N-CA-CB    | 5.90  | 121.05      | 110.32   |
| 1   | B     | 149 | GLU  | CA-C-O     | -5.89 | 114.81      | 121.00   |
| 1   | B     | 277 | ILE  | CA-C-O     | 5.89  | 128.14      | 120.78   |
| 1   | A     | 60  | SER  | CA-C-O     | 5.88  | 126.61      | 119.49   |
| 1   | A     | 213 | SER  | CA-C-N     | -5.88 | 112.44      | 122.56   |
| 1   | A     | 213 | SER  | C-N-CA     | -5.88 | 112.44      | 122.56   |
| 1   | A     | 185 | GLN  | N-CA-C     | 5.88  | 123.32      | 110.80   |
| 1   | B     | 98  | GLN  | O-C-N      | -5.87 | 115.98      | 122.09   |
| 1   | B     | 282 | LYS  | CG-CD-CE   | 5.87  | 124.81      | 111.30   |
| 1   | A     | 203 | SER  | CA-C-N     | -5.87 | 112.87      | 122.26   |
| 1   | A     | 203 | SER  | C-N-CA     | -5.87 | 112.87      | 122.26   |
| 1   | A     | 263 | VAL  | CA-C-N     | 5.87  | 131.27      | 122.23   |
| 1   | A     | 263 | VAL  | C-N-CA     | 5.87  | 131.27      | 122.23   |
| 1   | B     | 112 | VAL  | N-CA-C     | 5.87  | 116.52      | 110.82   |
| 1   | A     | 110 | ILE  | CB-CA-C    | -5.87 | 104.37      | 111.88   |
| 1   | A     | 242 | LYS  | CB-CG-CD   | 5.87  | 124.80      | 111.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 74  | ARG  | CD-NE-CZ   | 5.87  | 132.62      | 124.40   |
| 1   | B     | 322 | SER  | N-CA-CB    | 5.87  | 119.50      | 110.46   |
| 1   | A     | 168 | TYR  | N-CA-CB    | -5.87 | 100.53      | 110.50   |
| 1   | B     | 3   | LYS  | CG-CD-CE   | 5.87  | 124.79      | 111.30   |
| 1   | B     | 97  | VAL  | N-CA-C     | 5.87  | 119.30      | 111.44   |
| 1   | A     | 74  | ARG  | CA-C-O     | 5.86  | 126.64      | 120.42   |
| 1   | A     | 178 | ILE  | CA-CB-CG2  | -5.86 | 100.53      | 110.50   |
| 1   | B     | 217 | ARG  | NH1-CZ-NH2 | 5.86  | 126.92      | 119.30   |
| 1   | A     | 97  | VAL  | CA-C-N     | -5.85 | 112.45      | 120.28   |
| 1   | A     | 97  | VAL  | C-N-CA     | -5.85 | 112.45      | 120.28   |
| 1   | B     | 89  | PRO  | CA-C-N     | -5.85 | 114.45      | 122.93   |
| 1   | B     | 89  | PRO  | C-N-CA     | -5.85 | 114.45      | 122.93   |
| 1   | A     | 10  | ASP  | O-C-N      | 5.84  | 128.81      | 122.15   |
| 1   | B     | 44  | GLN  | N-CA-C     | 5.84  | 119.67      | 112.54   |
| 1   | B     | 295 | PRO  | O-C-N      | 5.84  | 130.53      | 122.64   |
| 1   | A     | 267 | ASN  | CB-CG-ND2  | -5.84 | 107.65      | 116.40   |
| 1   | B     | 344 | LEU  | CB-CA-C    | 5.83  | 120.54      | 110.45   |
| 1   | B     | 105 | ASP  | N-CA-CB    | -5.83 | 100.64      | 110.49   |
| 1   | A     | 159 | ASN  | CA-CB-CG   | -5.83 | 106.77      | 112.60   |
| 1   | B     | 255 | ILE  | CB-CA-C    | -5.82 | 104.27      | 111.08   |
| 1   | B     | 238 | ASP  | O-C-N      | 5.81  | 129.68      | 122.19   |
| 1   | A     | 344 | LEU  | N-CA-C     | 5.80  | 119.27      | 109.76   |
| 1   | B     | 93  | ASN  | CA-CB-CG   | -5.79 | 106.81      | 112.60   |
| 1   | B     | 267 | ASN  | CB-CA-C    | 5.79  | 119.56      | 110.19   |
| 1   | B     | 186 | ARG  | O-C-N      | 5.78  | 128.76      | 122.11   |
| 1   | B     | 109 | ASP  | CA-C-N     | -5.78 | 111.57      | 121.97   |
| 1   | B     | 109 | ASP  | C-N-CA     | -5.78 | 111.57      | 121.97   |
| 1   | A     | 304 | ASP  | CB-CA-C    | -5.78 | 98.92       | 110.42   |
| 1   | B     | 341 | LEU  | N-CA-CB    | -5.78 | 101.94      | 110.49   |
| 1   | A     | 136 | LEU  | CD1-CG-CD2 | -5.78 | 98.09       | 110.80   |
| 1   | B     | 303 | LEU  | CB-CA-C    | 5.78  | 118.92      | 110.26   |
| 1   | B     | 312 | THR  | N-CA-C     | 5.78  | 123.10      | 110.80   |
| 1   | A     | 263 | VAL  | CG1-CB-CG2 | -5.77 | 98.10       | 110.80   |
| 1   | B     | 223 | ALA  | N-CA-C     | 5.77  | 117.86      | 109.84   |
| 1   | B     | 319 | ASN  | CB-CA-C    | 5.77  | 120.55      | 111.72   |
| 1   | B     | 70  | ASP  | CA-CB-CG   | -5.77 | 106.83      | 112.60   |
| 1   | A     | 271 | LEU  | O-C-N      | -5.76 | 116.20      | 123.17   |
| 1   | B     | 168 | TYR  | CB-CA-C    | -5.76 | 99.16       | 110.10   |
| 1   | A     | 322 | SER  | CB-CA-C    | -5.75 | 101.45      | 110.94   |
| 1   | B     | 91  | LEU  | N-CA-C     | 5.75  | 118.24      | 109.62   |
| 1   | A     | 77  | THR  | N-CA-CB    | -5.74 | 100.79      | 110.49   |
| 1   | A     | 36  | PRO  | CB-CA-C    | -5.73 | 104.52      | 111.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 14  | MET  | N-CA-C      | 5.73  | 123.01      | 110.80   |
| 1   | A     | 201 | HIS  | O-C-N       | -5.72 | 115.65      | 122.63   |
| 1   | A     | 9   | GLN  | CA-C-N      | -5.71 | 112.18      | 120.29   |
| 1   | A     | 9   | GLN  | C-N-CA      | -5.71 | 112.18      | 120.29   |
| 1   | B     | 26  | VAL  | N-CA-CB     | 5.71  | 120.65      | 111.23   |
| 1   | B     | 262 | GLU  | OE1-CD-OE2  | -5.71 | 109.20      | 122.90   |
| 1   | B     | 267 | ASN  | N-CA-CB     | -5.71 | 101.11      | 110.42   |
| 1   | A     | 317 | GLY  | CA-C-N      | -5.70 | 111.71      | 121.97   |
| 1   | A     | 317 | GLY  | C-N-CA      | -5.70 | 111.71      | 121.97   |
| 1   | B     | 332 | ASP  | N-CA-C      | 5.70  | 118.16      | 108.02   |
| 1   | B     | 176 | PHE  | O-C-N       | -5.70 | 115.02      | 122.59   |
| 1   | A     | 103 | MET  | CA-C-O      | -5.69 | 114.81      | 120.90   |
| 1   | A     | 43  | ARG  | N-CA-C      | 5.69  | 122.92      | 110.80   |
| 1   | A     | 303 | LEU  | CB-CA-C     | 5.69  | 119.16      | 109.72   |
| 1   | B     | 246 | TYR  | O-C-N       | -5.68 | 115.03      | 122.59   |
| 1   | A     | 184 | CYS  | CA-CB-SG    | -5.68 | 101.34      | 114.40   |
| 1   | B     | 49  | TYR  | CA-C-N      | -5.68 | 111.67      | 121.66   |
| 1   | B     | 49  | TYR  | C-N-CA      | -5.68 | 111.67      | 121.66   |
| 1   | B     | 107 | LEU  | O-C-N       | 5.67  | 129.35      | 122.48   |
| 1   | B     | 171 | GLU  | N-CA-C      | 5.67  | 122.89      | 110.80   |
| 1   | A     | 104 | LEU  | N-CA-C      | 5.67  | 118.23      | 111.71   |
| 1   | A     | 229 | MET  | N-CA-CB     | 5.67  | 118.57      | 110.06   |
| 1   | B     | 7   | PRO  | CA-C-O      | 5.67  | 129.01      | 120.05   |
| 1   | A     | 31  | ASP  | CA-CB-CG    | 5.67  | 118.27      | 112.60   |
| 1   | A     | 29  | GLU  | N-CA-CB     | 5.66  | 120.06      | 110.49   |
| 1   | A     | 199 | LEU  | CA-C-N      | -5.66 | 113.03      | 120.95   |
| 1   | A     | 199 | LEU  | C-N-CA      | -5.66 | 113.03      | 120.95   |
| 1   | A     | 315 | SER  | N-CA-C      | 5.66  | 117.95      | 108.73   |
| 1   | A     | 33  | GLN  | CB-CG-CD    | 5.65  | 122.21      | 112.60   |
| 1   | A     | 99  | ALA  | CB-CA-C     | -5.65 | 99.17       | 110.42   |
| 1   | B     | 63  | SER  | N-CA-CB     | -5.64 | 102.61      | 110.29   |
| 1   | B     | 245 | ASN  | OD1-CG-ND2  | -5.64 | 116.95      | 122.60   |
| 1   | A     | 24  | ALA  | CA-C-N      | 5.64  | 128.63      | 120.79   |
| 1   | A     | 24  | ALA  | C-N-CA      | 5.64  | 128.63      | 120.79   |
| 1   | A     | 248 | HIS  | ND1-CE1-NE2 | 5.64  | 114.04      | 108.40   |
| 1   | B     | 334 | ALA  | CA-C-N      | -5.64 | 114.24      | 122.86   |
| 1   | B     | 334 | ALA  | C-N-CA      | -5.64 | 114.24      | 122.86   |
| 1   | A     | 293 | THR  | CA-C-O      | 5.63  | 126.39      | 120.36   |
| 1   | B     | 49  | TYR  | CA-C-O      | 5.63  | 126.43      | 119.79   |
| 1   | B     | 270 | GLU  | N-CA-C      | 5.63  | 118.06      | 109.62   |
| 1   | B     | 111 | GLU  | CA-C-N      | -5.63 | 112.69      | 120.74   |
| 1   | B     | 111 | GLU  | C-N-CA      | -5.63 | 112.69      | 120.74   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 143 | VAL  | O-C-N      | 5.62  | 128.80      | 122.67   |
| 1   | A     | 336 | VAL  | CA-C-O     | 5.62  | 126.97      | 120.67   |
| 1   | B     | 67  | GLN  | OE1-CD-NE2 | -5.62 | 116.98      | 122.60   |
| 1   | B     | 319 | ASN  | CB-CG-ND2  | -5.62 | 107.98      | 116.40   |
| 1   | A     | 66  | SER  | CB-CA-C    | -5.61 | 99.25       | 110.42   |
| 1   | A     | 96  | SER  | CA-C-N     | -5.61 | 113.38      | 120.56   |
| 1   | A     | 96  | SER  | C-N-CA     | -5.61 | 113.38      | 120.56   |
| 1   | A     | 133 | TYR  | CA-C-O     | -5.61 | 112.49      | 120.51   |
| 1   | B     | 109 | ASP  | CA-CB-CG   | 5.61  | 118.21      | 112.60   |
| 1   | A     | 57  | GLN  | OE1-CD-NE2 | -5.61 | 116.99      | 122.60   |
| 1   | B     | 68  | ILE  | CG1-CB-CG2 | -5.60 | 93.90       | 110.70   |
| 1   | A     | 110 | ILE  | O-C-N      | 5.59  | 127.53      | 121.94   |
| 1   | A     | 58  | ALA  | N-CA-C     | 5.59  | 118.14      | 111.71   |
| 1   | A     | 178 | ILE  | N-CA-CB    | 5.59  | 119.68      | 111.52   |
| 1   | A     | 252 | GLY  | CA-C-N     | 5.58  | 131.75      | 121.70   |
| 1   | A     | 252 | GLY  | C-N-CA     | 5.58  | 131.75      | 121.70   |
| 1   | B     | 104 | LEU  | CA-C-O     | 5.58  | 125.72      | 119.41   |
| 1   | B     | 187 | TYR  | CA-C-N     | -5.58 | 108.18      | 121.80   |
| 1   | B     | 187 | TYR  | C-N-CA     | -5.58 | 108.18      | 121.80   |
| 1   | B     | 203 | SER  | CA-CB-OG   | 5.58  | 122.26      | 111.10   |
| 1   | A     | 98  | GLN  | CA-CB-CG   | 5.58  | 125.26      | 114.10   |
| 1   | A     | 132 | ASN  | N-CA-C     | 5.57  | 122.67      | 110.80   |
| 1   | B     | 202 | GLY  | N-CA-C     | 5.57  | 118.83      | 111.03   |
| 1   | A     | 266 | GLY  | N-CA-C     | 5.57  | 126.38      | 113.18   |
| 1   | A     | 55  | VAL  | CA-CB-CG1  | 5.56  | 119.85      | 110.40   |
| 1   | A     | 332 | ASP  | CA-C-O     | 5.55  | 127.57      | 121.40   |
| 1   | B     | 302 | SER  | CA-C-N     | -5.55 | 113.24      | 121.24   |
| 1   | B     | 302 | SER  | C-N-CA     | -5.55 | 113.24      | 121.24   |
| 1   | A     | 298 | SER  | N-CA-C     | 5.55  | 122.63      | 110.80   |
| 1   | B     | 51  | ILE  | CA-C-O     | -5.55 | 115.28      | 121.17   |
| 1   | B     | 29  | GLU  | CB-CA-C    | 5.55  | 120.65      | 110.10   |
| 1   | B     | 171 | GLU  | CA-CB-CG   | 5.55  | 125.20      | 114.10   |
| 1   | B     | 197 | ARG  | CG-CD-NE   | 5.55  | 124.21      | 112.00   |
| 1   | B     | 242 | LYS  | CD-CE-NZ   | 5.55  | 129.65      | 111.90   |
| 1   | A     | 257 | LEU  | N-CA-CB    | -5.55 | 102.18      | 110.17   |
| 1   | A     | 19  | GLU  | O-C-N      | 5.54  | 127.78      | 122.07   |
| 1   | B     | 239 | MET  | CA-C-N     | -5.54 | 112.01      | 121.97   |
| 1   | B     | 239 | MET  | C-N-CA     | -5.54 | 112.01      | 121.97   |
| 1   | B     | 229 | MET  | CG-SD-CE   | -5.53 | 88.73       | 100.90   |
| 1   | A     | 131 | VAL  | CB-CA-C    | 5.53  | 120.36      | 111.29   |
| 1   | B     | 25  | MET  | O-C-N      | 5.53  | 129.94      | 122.59   |
| 1   | A     | 102 | GLU  | N-CA-CB    | 5.52  | 118.02      | 110.01   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 341 | LEU  | N-CA-C     | 5.52  | 118.36      | 107.98   |
| 1   | A     | 109 | ASP  | N-CA-C     | 5.51  | 118.00      | 111.33   |
| 1   | B     | 287 | VAL  | CA-CB-CG2  | 5.51  | 119.77      | 110.40   |
| 1   | A     | 122 | ASP  | CB-CA-C    | 5.51  | 121.38      | 110.42   |
| 1   | B     | 180 | ARG  | N-CA-CB    | 5.51  | 118.05      | 109.85   |
| 1   | A     | 24  | ALA  | CA-C-O     | 5.50  | 126.60      | 120.82   |
| 1   | B     | 217 | ARG  | CA-C-O     | -5.50 | 114.94      | 121.60   |
| 1   | B     | 214 | GLN  | OE1-CD-NE2 | 5.50  | 128.10      | 122.60   |
| 1   | A     | 103 | MET  | CG-SD-CE   | -5.50 | 88.80       | 100.90   |
| 1   | A     | 342 | LEU  | CA-C-N     | -5.50 | 114.88      | 122.30   |
| 1   | A     | 342 | LEU  | C-N-CA     | -5.50 | 114.88      | 122.30   |
| 1   | A     | 52  | LEU  | N-CA-C     | 5.49  | 118.78      | 111.75   |
| 1   | B     | 156 | TYR  | CB-CG-CD1  | 5.49  | 129.03      | 120.80   |
| 1   | A     | 134 | GLU  | O-C-N      | 5.48  | 129.35      | 122.23   |
| 1   | B     | 249 | THR  | CB-CA-C    | 5.48  | 118.84      | 109.80   |
| 1   | A     | 213 | SER  | CA-C-O     | 5.47  | 126.34      | 120.70   |
| 1   | B     | 121 | SER  | CA-C-N     | -5.47 | 113.70      | 122.62   |
| 1   | B     | 121 | SER  | C-N-CA     | -5.47 | 113.70      | 122.62   |
| 1   | A     | 132 | ASN  | CA-CB-CG   | -5.47 | 107.13      | 112.60   |
| 1   | B     | 74  | ARG  | CA-C-N     | 5.47  | 131.98      | 121.54   |
| 1   | B     | 74  | ARG  | C-N-CA     | 5.47  | 131.98      | 121.54   |
| 1   | B     | 184 | CYS  | CA-C-N     | -5.47 | 113.01      | 120.44   |
| 1   | B     | 184 | CYS  | C-N-CA     | -5.47 | 113.01      | 120.44   |
| 1   | B     | 300 | ASN  | N-CA-C     | 5.47  | 117.62      | 109.59   |
| 1   | B     | 341 | LEU  | CA-C-O     | -5.46 | 115.46      | 121.58   |
| 1   | B     | 134 | GLU  | CB-CG-CD   | 5.46  | 121.88      | 112.60   |
| 1   | B     | 204 | ARG  | CD-NE-CZ   | -5.46 | 116.76      | 124.40   |
| 1   | A     | 349 | LYS  | CB-CG-CD   | 5.46  | 123.85      | 111.30   |
| 1   | A     | 120 | GLY  | N-CA-C     | 5.45  | 126.11      | 113.18   |
| 1   | B     | 240 | VAL  | CG1-CB-CG2 | 5.45  | 122.80      | 110.80   |
| 1   | B     | 9   | GLN  | N-CA-CB    | 5.45  | 118.10      | 109.82   |
| 1   | A     | 194 | HIS  | CB-CG-ND1  | 5.45  | 130.87      | 122.70   |
| 1   | A     | 186 | ARG  | CA-CB-CG   | 5.45  | 124.99      | 114.10   |
| 1   | B     | 148 | GLU  | CA-C-N     | -5.44 | 113.47      | 120.65   |
| 1   | B     | 148 | GLU  | C-N-CA     | -5.44 | 113.47      | 120.65   |
| 1   | B     | 196 | ARG  | CA-C-N     | -5.44 | 112.84      | 122.74   |
| 1   | B     | 196 | ARG  | C-N-CA     | -5.44 | 112.84      | 122.74   |
| 1   | B     | 175 | ILE  | N-CA-C     | 5.43  | 120.63      | 109.34   |
| 1   | A     | 334 | ALA  | CA-C-O     | 5.42  | 126.22      | 120.10   |
| 1   | A     | 127 | ASP  | N-CA-C     | 5.41  | 121.78      | 109.81   |
| 1   | A     | 217 | ARG  | CD-NE-CZ   | -5.41 | 116.82      | 124.40   |
| 1   | B     | 44  | GLN  | O-C-N      | 5.41  | 129.68      | 122.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 322 | SER  | CA-C-N      | -5.41 | 113.24      | 122.33   |
| 1   | B     | 322 | SER  | C-N-CA      | -5.41 | 113.24      | 122.33   |
| 1   | B     | 176 | PHE  | CA-C-O      | 5.41  | 128.24      | 120.51   |
| 1   | B     | 129 | ILE  | CA-CB-CG1   | 5.40  | 119.58      | 110.40   |
| 1   | A     | 176 | PHE  | CB-CA-C     | -5.40 | 100.95      | 109.80   |
| 1   | A     | 200 | TRP  | NE1-CE2-CZ2 | -5.40 | 122.00      | 130.10   |
| 1   | A     | 73  | ASN  | N-CA-C      | 5.39  | 118.66      | 111.75   |
| 1   | B     | 200 | TRP  | CG-CD2-CE3  | -5.39 | 128.51      | 133.90   |
| 1   | B     | 38  | GLY  | CA-C-N      | -5.39 | 111.51      | 120.68   |
| 1   | B     | 38  | GLY  | C-N-CA      | -5.39 | 111.51      | 120.68   |
| 1   | A     | 334 | ALA  | N-CA-C      | 5.39  | 117.91      | 111.71   |
| 1   | B     | 152 | ILE  | CA-C-O      | 5.38  | 126.54      | 120.95   |
| 1   | B     | 266 | GLY  | N-CA-C      | 5.38  | 121.02      | 111.02   |
| 1   | A     | 291 | GLY  | CA-C-O      | -5.38 | 116.74      | 121.58   |
| 1   | B     | 325 | TYR  | N-CA-C      | 5.38  | 117.16      | 108.34   |
| 1   | A     | 281 | PRO  | CA-C-N      | -5.37 | 112.47      | 121.39   |
| 1   | A     | 281 | PRO  | C-N-CA      | -5.37 | 112.47      | 121.39   |
| 1   | B     | 109 | ASP  | O-C-N       | -5.37 | 114.38      | 122.28   |
| 1   | B     | 235 | TYR  | CB-CG-CD2   | -5.37 | 112.74      | 120.80   |
| 1   | A     | 178 | ILE  | CA-C-O      | -5.36 | 114.68      | 120.36   |
| 1   | A     | 272 | LYS  | CB-CG-CD    | -5.36 | 98.97       | 111.30   |
| 1   | B     | 247 | CYS  | CA-CB-SG    | 5.36  | 126.72      | 114.40   |
| 1   | A     | 114 | TYR  | CA-C-N      | -5.35 | 112.57      | 120.28   |
| 1   | A     | 114 | TYR  | C-N-CA      | -5.35 | 112.57      | 120.28   |
| 1   | A     | 229 | MET  | CA-CB-CG    | 5.35  | 124.81      | 114.10   |
| 1   | A     | 41  | SER  | CA-CB-OG    | -5.35 | 100.39      | 111.10   |
| 1   | A     | 137 | LYS  | CA-C-O      | 5.35  | 128.16      | 120.51   |
| 1   | A     | 267 | ASN  | N-CA-CB     | 5.35  | 118.71      | 110.21   |
| 1   | A     | 288 | LYS  | CB-CA-C     | 5.34  | 120.41      | 111.22   |
| 1   | B     | 247 | CYS  | N-CA-C      | -5.34 | 106.93      | 113.50   |
| 1   | B     | 324 | LEU  | N-CA-C      | 5.34  | 117.19      | 111.36   |
| 1   | A     | 146 | ASP  | CB-CA-C     | 5.34  | 120.88      | 110.57   |
| 1   | B     | 169 | ASP  | N-CA-C      | 5.34  | 118.26      | 109.72   |
| 1   | A     | 213 | SER  | O-C-N       | -5.34 | 116.33      | 122.09   |
| 1   | B     | 314 | ILE  | CA-CB-CG2   | 5.33  | 119.57      | 110.50   |
| 1   | B     | 336 | VAL  | CA-CB-CG1   | 5.33  | 119.47      | 110.40   |
| 1   | B     | 164 | THR  | CA-CB-CG2   | 5.33  | 119.56      | 110.50   |
| 1   | A     | 133 | TYR  | CB-CA-C     | -5.33 | 99.82       | 110.42   |
| 1   | B     | 118 | ARG  | CG-CD-NE    | 5.32  | 123.71      | 112.00   |
| 1   | A     | 204 | ARG  | N-CA-C      | 5.31  | 117.77      | 108.52   |
| 1   | B     | 22  | LYS  | CB-CG-CD    | 5.31  | 123.52      | 111.30   |
| 1   | B     | 125 | SER  | N-CA-C      | 5.31  | 120.08      | 111.37   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 137 | LYS  | N-CA-C     | 5.31  | 122.12      | 110.80   |
| 1   | A     | 14  | MET  | CA-C-O     | 5.31  | 126.23      | 120.55   |
| 1   | B     | 101 | VAL  | O-C-N      | 5.31  | 127.02      | 121.87   |
| 1   | B     | 327 | GLU  | N-CA-C     | 5.31  | 117.26      | 109.24   |
| 1   | A     | 313 | GLY  | CA-C-N     | 5.30  | 130.09      | 122.45   |
| 1   | A     | 313 | GLY  | C-N-CA     | 5.30  | 130.09      | 122.45   |
| 1   | A     | 49  | TYR  | CB-CG-CD2  | -5.30 | 112.85      | 120.80   |
| 1   | A     | 176 | PHE  | N-CA-CB    | 5.29  | 118.90      | 110.16   |
| 1   | A     | 128 | PRO  | CA-C-N     | -5.29 | 116.11      | 122.35   |
| 1   | A     | 128 | PRO  | C-N-CA     | -5.29 | 116.11      | 122.35   |
| 1   | A     | 112 | VAL  | CA-CB-CG2  | 5.28  | 119.38      | 110.40   |
| 1   | A     | 27  | GLU  | CA-C-O     | 5.28  | 125.92      | 119.05   |
| 1   | B     | 144 | ASP  | CA-CB-CG   | 5.28  | 117.88      | 112.60   |
| 1   | A     | 67  | GLN  | CB-CG-CD   | -5.27 | 103.64      | 112.60   |
| 1   | A     | 94  | ALA  | N-CA-CB    | 5.27  | 118.05      | 110.20   |
| 1   | A     | 164 | THR  | N-CA-C     | 5.27  | 118.49      | 111.75   |
| 1   | A     | 226 | THR  | N-CA-C     | 5.27  | 119.33      | 113.01   |
| 1   | B     | 16  | PHE  | CB-CA-C    | -5.27 | 99.93       | 110.42   |
| 1   | A     | 57  | GLN  | N-CA-CB    | 5.26  | 117.82      | 109.82   |
| 1   | A     | 197 | ARG  | NE-CZ-NH2  | 5.26  | 123.94      | 119.20   |
| 1   | A     | 148 | GLU  | CA-CB-CG   | 5.26  | 124.62      | 114.10   |
| 1   | B     | 143 | VAL  | CB-CA-C    | -5.26 | 102.67      | 111.29   |
| 1   | B     | 301 | ILE  | CA-C-O     | -5.26 | 114.21      | 120.78   |
| 1   | B     | 335 | GLN  | CA-CB-CG   | 5.26  | 124.61      | 114.10   |
| 1   | A     | 180 | ARG  | NE-CZ-NH2  | -5.25 | 114.47      | 119.20   |
| 1   | A     | 84  | GLY  | N-CA-C     | 5.25  | 125.63      | 113.18   |
| 1   | B     | 159 | ASN  | CA-C-N     | -5.25 | 114.25      | 122.49   |
| 1   | B     | 159 | ASN  | C-N-CA     | -5.25 | 114.25      | 122.49   |
| 1   | B     | 250 | SER  | N-CA-CB    | -5.24 | 103.44      | 111.56   |
| 1   | A     | 220 | PRO  | O-C-N      | 5.24  | 127.64      | 121.46   |
| 1   | A     | 136 | LEU  | CA-C-N     | 5.24  | 131.54      | 121.54   |
| 1   | A     | 136 | LEU  | C-N-CA     | 5.24  | 131.54      | 121.54   |
| 1   | B     | 227 | GLY  | CA-C-N     | 5.24  | 133.12      | 121.81   |
| 1   | B     | 227 | GLY  | C-N-CA     | 5.24  | 133.12      | 121.81   |
| 1   | B     | 332 | ASP  | CA-C-O     | 5.24  | 125.98      | 120.33   |
| 1   | A     | 224 | PRO  | CA-C-N     | -5.23 | 112.88      | 121.19   |
| 1   | A     | 224 | PRO  | C-N-CA     | -5.23 | 112.88      | 121.19   |
| 1   | A     | 250 | SER  | CA-C-O     | 5.22  | 127.99      | 121.46   |
| 1   | B     | 241 | SER  | N-CA-CB    | -5.22 | 101.66      | 110.49   |
| 1   | A     | 229 | MET  | CA-C-N     | -5.22 | 111.57      | 121.54   |
| 1   | A     | 229 | MET  | C-N-CA     | -5.22 | 111.57      | 121.54   |
| 1   | A     | 116 | LEU  | CD1-CG-CD2 | -5.22 | 99.32       | 110.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 91  | LEU  | CA-C-O     | -5.22 | 115.90      | 122.63   |
| 1   | A     | 25  | MET  | O-C-N      | 5.21  | 127.65      | 122.08   |
| 1   | A     | 292 | LYS  | CA-CB-CG   | 5.21  | 124.52      | 114.10   |
| 1   | A     | 64  | SER  | N-CA-CB    | -5.20 | 101.18      | 109.19   |
| 1   | A     | 258 | ILE  | CA-C-N     | -5.20 | 113.17      | 122.07   |
| 1   | A     | 258 | ILE  | C-N-CA     | -5.20 | 113.17      | 122.07   |
| 1   | B     | 74  | ARG  | CA-CB-CG   | 5.20  | 124.51      | 114.10   |
| 1   | B     | 340 | TYR  | N-CA-C     | 5.20  | 116.87      | 108.34   |
| 1   | A     | 175 | ILE  | CA-C-N     | -5.20 | 114.86      | 122.19   |
| 1   | A     | 175 | ILE  | C-N-CA     | -5.20 | 114.86      | 122.19   |
| 1   | B     | 96  | SER  | CA-C-O     | -5.20 | 113.08      | 120.51   |
| 1   | B     | 180 | ARG  | CA-CB-CG   | 5.20  | 124.50      | 114.10   |
| 1   | A     | 206 | THR  | N-CA-C     | 5.20  | 121.87      | 110.80   |
| 1   | B     | 56  | GLN  | CA-CB-CG   | -5.20 | 103.71      | 114.10   |
| 1   | B     | 185 | GLN  | CG-CD-OE1  | 5.20  | 131.19      | 120.80   |
| 1   | B     | 318 | VAL  | N-CA-C     | 5.20  | 120.14      | 109.34   |
| 1   | B     | 53  | SER  | N-CA-C     | 5.19  | 117.74      | 111.40   |
| 1   | A     | 270 | GLU  | O-C-N      | 5.19  | 129.14      | 123.27   |
| 1   | B     | 114 | TYR  | N-CA-C     | 5.19  | 121.86      | 110.80   |
| 1   | A     | 85  | MET  | CB-CA-C    | 5.19  | 120.75      | 110.42   |
| 1   | B     | 50  | SER  | CA-C-N     | -5.19 | 114.02      | 120.56   |
| 1   | B     | 50  | SER  | C-N-CA     | -5.19 | 114.02      | 120.56   |
| 1   | A     | 43  | ARG  | CA-CB-CG   | 5.18  | 124.47      | 114.10   |
| 1   | A     | 75  | PHE  | CA-C-O     | 5.18  | 126.04      | 120.55   |
| 1   | B     | 81  | HIS  | N-CA-C     | 5.18  | 117.34      | 108.90   |
| 1   | A     | 51  | ILE  | CB-CG1-CD1 | -5.18 | 102.92      | 113.80   |
| 1   | B     | 177 | LYS  | CA-C-N     | -5.17 | 116.22      | 123.10   |
| 1   | B     | 177 | LYS  | C-N-CA     | -5.17 | 116.22      | 123.10   |
| 1   | B     | 328 | TYR  | CB-CG-CD2  | -5.17 | 113.05      | 120.80   |
| 1   | A     | 241 | SER  | N-CA-C     | 5.17  | 121.81      | 110.80   |
| 1   | B     | 304 | ASP  | CA-C-N     | -5.16 | 112.77      | 121.85   |
| 1   | B     | 304 | ASP  | C-N-CA     | -5.16 | 112.77      | 121.85   |
| 1   | B     | 256 | GLY  | CA-C-N     | 5.16  | 131.24      | 122.37   |
| 1   | B     | 256 | GLY  | C-N-CA     | 5.16  | 131.24      | 122.37   |
| 1   | A     | 209 | ALA  | N-CA-C     | 5.15  | 119.86      | 111.37   |
| 1   | A     | 108 | LEU  | CD1-CG-CD2 | 5.14  | 122.12      | 110.80   |
| 1   | A     | 217 | ARG  | CA-C-O     | -5.14 | 115.91      | 121.36   |
| 1   | B     | 149 | GLU  | CB-CG-CD   | -5.14 | 103.86      | 112.60   |
| 1   | B     | 62  | GLY  | CA-C-N     | -5.14 | 111.80      | 120.95   |
| 1   | B     | 62  | GLY  | C-N-CA     | -5.14 | 111.80      | 120.95   |
| 1   | B     | 155 | LYS  | CA-CB-CG   | 5.14  | 124.38      | 114.10   |
| 1   | B     | 214 | GLN  | N-CA-CB    | 5.14  | 121.83      | 111.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 161 | HIS  | CB-CG-CD2  | -5.13 | 124.53      | 131.20   |
| 1   | A     | 208 | PHE  | N-CA-CB    | 5.13  | 118.12      | 110.22   |
| 1   | A     | 224 | PRO  | CB-CA-C    | -5.13 | 103.09      | 111.56   |
| 1   | A     | 130 | ASP  | N-CA-C     | 5.13  | 119.69      | 112.72   |
| 1   | B     | 127 | ASP  | O-C-N      | 5.13  | 127.03      | 121.60   |
| 1   | A     | 190 | PHE  | CA-CB-CG   | -5.12 | 108.67      | 113.80   |
| 1   | B     | 229 | MET  | N-CA-C     | 5.12  | 118.31      | 111.75   |
| 1   | B     | 328 | TYR  | CB-CA-C    | -5.12 | 99.53       | 109.68   |
| 1   | B     | 234 | ILE  | O-C-N      | 5.12  | 128.31      | 122.98   |
| 1   | A     | 115 | SER  | N-CA-C     | 5.12  | 117.60      | 111.71   |
| 1   | B     | 159 | ASN  | CB-CG-ND2  | -5.12 | 108.73      | 116.40   |
| 1   | A     | 79  | ILE  | N-CA-C     | 5.11  | 119.92      | 108.88   |
| 1   | A     | 327 | GLU  | CB-CA-C    | -5.11 | 104.54      | 111.95   |
| 1   | A     | 54  | GLU  | CA-CB-CG   | 5.11  | 124.32      | 114.10   |
| 1   | A     | 320 | ASP  | CA-C-N     | -5.10 | 114.31      | 122.53   |
| 1   | A     | 320 | ASP  | C-N-CA     | -5.10 | 114.31      | 122.53   |
| 1   | A     | 109 | ASP  | CA-C-O     | 5.10  | 126.14      | 120.63   |
| 1   | B     | 109 | ASP  | CB-CA-C    | -5.10 | 100.47      | 110.11   |
| 1   | A     | 30  | ILE  | CB-CG1-CD1 | -5.10 | 103.09      | 113.80   |
| 1   | A     | 316 | SER  | N-CA-CB    | 5.10  | 117.73      | 110.44   |
| 1   | A     | 230 | PHE  | CA-C-O     | 5.10  | 127.80      | 120.51   |
| 1   | B     | 2   | SER  | CA-CB-OG   | 5.10  | 121.29      | 111.10   |
| 1   | A     | 304 | ASP  | CA-C-O     | 5.09  | 127.79      | 120.51   |
| 1   | B     | 109 | ASP  | N-CA-C     | 5.09  | 119.53      | 112.45   |
| 1   | B     | 295 | PRO  | N-CD-CG    | 5.09  | 110.84      | 103.20   |
| 1   | B     | 329 | ILE  | CA-C-O     | -5.09 | 115.45      | 120.90   |
| 1   | B     | 301 | ILE  | CA-CB-CG2  | 5.09  | 119.15      | 110.50   |
| 1   | A     | 299 | ALA  | CA-C-N     | -5.08 | 114.53      | 122.16   |
| 1   | A     | 299 | ALA  | C-N-CA     | -5.08 | 114.53      | 122.16   |
| 1   | B     | 316 | SER  | CB-CA-C    | -5.08 | 100.95      | 111.22   |
| 1   | B     | 325 | TYR  | CB-CA-C    | -5.08 | 102.01      | 110.14   |
| 1   | A     | 263 | VAL  | O-C-N      | 5.08  | 128.69      | 123.20   |
| 1   | B     | 150 | ALA  | CB-CA-C    | -5.08 | 100.32      | 110.42   |
| 1   | B     | 39  | LYS  | CA-CB-CG   | 5.07  | 124.25      | 114.10   |
| 1   | A     | 249 | THR  | CA-CB-OG1  | 5.07  | 117.20      | 109.60   |
| 1   | A     | 304 | ASP  | CA-CB-CG   | 5.06  | 117.66      | 112.60   |
| 1   | B     | 170 | LEU  | N-CA-CB    | -5.06 | 103.48      | 110.42   |
| 1   | A     | 86  | LYS  | CA-CB-CG   | -5.06 | 103.98      | 114.10   |
| 1   | A     | 280 | LEU  | CA-C-O     | -5.06 | 113.95      | 119.61   |
| 1   | A     | 287 | VAL  | O-C-N      | 5.06  | 128.64      | 123.03   |
| 1   | A     | 316 | SER  | N-CA-C     | -5.06 | 104.01      | 110.53   |
| 1   | B     | 217 | ARG  | NE-CZ-NH2  | -5.05 | 114.65      | 119.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 203 | SER  | O-C-N      | -5.05 | 117.49      | 123.25   |
| 1   | B     | 196 | ARG  | CB-CA-C    | -5.05 | 103.00      | 110.67   |
| 1   | A     | 34  | LYS  | CA-C-N     | 5.05  | 134.12      | 121.80   |
| 1   | A     | 34  | LYS  | C-N-CA     | 5.05  | 134.12      | 121.80   |
| 1   | A     | 350 | THR  | CB-CA-C    | 5.05  | 120.21      | 109.10   |
| 1   | B     | 57  | GLN  | CA-C-N     | -5.05 | 113.78      | 120.79   |
| 1   | B     | 57  | GLN  | C-N-CA     | -5.05 | 113.78      | 120.79   |
| 1   | B     | 144 | ASP  | N-CA-C     | 5.05  | 117.53      | 109.96   |
| 1   | A     | 301 | ILE  | N-CA-CB    | -5.04 | 102.91      | 111.23   |
| 1   | B     | 345 | LYS  | CA-CB-CG   | 5.04  | 124.18      | 114.10   |
| 1   | B     | 34  | LYS  | CB-CA-C    | -5.04 | 100.42      | 109.24   |
| 1   | A     | 205 | THR  | CA-C-O     | -5.04 | 113.30      | 120.51   |
| 1   | B     | 345 | LYS  | CA-C-N     | -5.03 | 113.90      | 120.95   |
| 1   | B     | 345 | LYS  | C-N-CA     | -5.03 | 113.90      | 120.95   |
| 1   | B     | 245 | ASN  | O-C-N      | -5.03 | 115.90      | 122.59   |
| 1   | B     | 263 | VAL  | N-CA-C     | 5.03  | 115.15      | 108.11   |
| 1   | A     | 56  | GLN  | O-C-N      | 5.03  | 128.76      | 122.23   |
| 1   | A     | 296 | ASP  | CA-C-O     | -5.02 | 113.29      | 120.16   |
| 1   | A     | 92  | ASN  | CA-CB-CG   | 5.01  | 117.61      | 112.60   |
| 1   | A     | 147 | SER  | CA-C-N     | -5.01 | 111.97      | 121.54   |
| 1   | A     | 147 | SER  | C-N-CA     | -5.01 | 111.97      | 121.54   |
| 1   | B     | 330 | VAL  | N-CA-C     | 5.00  | 116.56      | 108.85   |
| 1   | A     | 122 | ASP  | N-CA-C     | 5.00  | 121.45      | 110.80   |
| 1   | B     | 346 | PHE  | CG-CD2-CE2 | -5.00 | 112.20      | 120.70   |

There are no chirality outliers.

All (86) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 119 | GLY  | Peptide   |
| 1   | A     | 120 | GLY  | Peptide   |
| 1   | A     | 121 | SER  | Peptide   |
| 1   | A     | 125 | SER  | Peptide   |
| 1   | A     | 131 | VAL  | Mainchain |
| 1   | A     | 132 | ASN  | Peptide   |
| 1   | A     | 133 | TYR  | Sidechain |
| 1   | A     | 144 | ASP  | Peptide   |
| 1   | A     | 145 | ARG  | Sidechain |
| 1   | A     | 154 | ARG  | Sidechain |
| 1   | A     | 16  | PHE  | Sidechain |
| 1   | A     | 160 | THR  | Peptide   |
| 1   | A     | 162 | ALA  | Peptide   |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 165 | HIS  | Peptide           |
| 1   | A     | 166 | ASN  | Peptide           |
| 1   | A     | 167 | ALA  | Peptide           |
| 1   | A     | 168 | TYR  | Sidechain         |
| 1   | A     | 169 | ASP  | Peptide           |
| 1   | A     | 184 | CYS  | Peptide           |
| 1   | A     | 2   | SER  | Peptide           |
| 1   | A     | 205 | THR  | Peptide           |
| 1   | A     | 217 | ARG  | Sidechain         |
| 1   | A     | 228 | TYR  | Sidechain         |
| 1   | A     | 230 | PHE  | Sidechain         |
| 1   | A     | 246 | TYR  | Sidechain         |
| 1   | A     | 251 | GLN  | Peptide           |
| 1   | A     | 269 | TYR  | Sidechain         |
| 1   | A     | 276 | HIS  | Sidechain         |
| 1   | A     | 28  | TYR  | Sidechain         |
| 1   | A     | 319 | ASN  | Peptide           |
| 1   | A     | 328 | TYR  | Sidechain         |
| 1   | A     | 331 | TYR  | Peptide           |
| 1   | A     | 340 | TYR  | Sidechain,Peptide |
| 1   | A     | 348 | PHE  | Sidechain         |
| 1   | A     | 37  | LEU  | Peptide           |
| 1   | A     | 39  | LYS  | Peptide,Mainchain |
| 1   | A     | 42  | LYS  | Peptide           |
| 1   | A     | 43  | ARG  | Sidechain         |
| 1   | A     | 49  | TYR  | Sidechain         |
| 1   | A     | 65  | ASP  | Peptide           |
| 1   | A     | 71  | LEU  | Peptide           |
| 1   | A     | 76  | TYR  | Sidechain         |
| 1   | A     | 83  | PHE  | Sidechain,Peptide |
| 1   | A     | 84  | GLY  | Peptide           |
| 1   | B     | 102 | GLU  | Peptide           |
| 1   | B     | 109 | ASP  | Peptide           |
| 1   | B     | 113 | ALA  | Peptide           |
| 1   | B     | 114 | TYR  | Sidechain         |
| 1   | B     | 146 | ASP  | Peptide           |
| 1   | B     | 156 | TYR  | Sidechain         |
| 1   | B     | 160 | THR  | Peptide           |
| 1   | B     | 162 | ALA  | Peptide           |
| 1   | B     | 169 | ASP  | Peptide           |
| 1   | B     | 175 | ILE  | Peptide           |
| 1   | B     | 176 | PHE  | Sidechain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | B     | 18  | VAL  | Peptide           |
| 1   | B     | 194 | HIS  | Peptide           |
| 1   | B     | 196 | ARG  | Sidechain         |
| 1   | B     | 20  | SER  | Peptide           |
| 1   | B     | 217 | ARG  | Sidechain         |
| 1   | B     | 240 | VAL  | Peptide           |
| 1   | B     | 246 | TYR  | Sidechain         |
| 1   | B     | 252 | GLY  | Peptide           |
| 1   | B     | 259 | LEU  | Peptide           |
| 1   | B     | 28  | TYR  | Sidechain,Peptide |
| 1   | B     | 294 | THR  | Peptide           |
| 1   | B     | 311 | GLY  | Peptide           |
| 1   | B     | 319 | ASN  | Peptide           |
| 1   | B     | 325 | TYR  | Peptide           |
| 1   | B     | 328 | TYR  | Sidechain         |
| 1   | B     | 331 | TYR  | Sidechain         |
| 1   | B     | 347 | ASN  | Peptide           |
| 1   | B     | 349 | LYS  | Peptide           |
| 1   | B     | 35  | MET  | Peptide           |
| 1   | B     | 46  | GLN  | Peptide           |
| 1   | B     | 49  | TYR  | Sidechain         |
| 1   | B     | 50  | SER  | Peptide           |
| 1   | B     | 76  | TYR  | Sidechain         |
| 1   | B     | 83  | PHE  | Peptide           |
| 1   | B     | 84  | GLY  | Peptide           |
| 1   | B     | 87  | LYS  | Peptide           |
| 1   | B     | 93  | ASN  | Sidechain         |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2754  | 0        | 2798     | 224     | 0            |
| 1   | B     | 2754  | 0        | 2798     | 319     | 0            |
| 2   | A     | 28    | 0        | 24       | 2       | 0            |
| 2   | B     | 28    | 0        | 24       | 0       | 0            |
| 3   | A     | 124   | 0        | 0        | 12      | 0            |
| 3   | B     | 129   | 0        | 0        | 27      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 5817  | 0        | 5644     | 543     | 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 48.

All (543) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:282:LYS:C    | 1:B:282:LYS:CA   | 1.76                     | 1.58              |
| 1:A:138:THR:HG23 | 1:A:180:ARG:HB3  | 1.49                     | 0.95              |
| 1:A:138:THR:HG21 | 1:A:212:LEU:HD23 | 1.52                     | 0.90              |
| 1:B:202:GLY:HA3  | 1:B:243:SER:O    | 1.74                     | 0.88              |
| 1:A:133:TYR:HE1  | 1:A:140:ILE:HG13 | 1.38                     | 0.88              |
| 1:A:59:VAL:HG21  | 1:A:92:ASN:HA    | 1.56                     | 0.87              |
| 1:A:296:ASP:HB2  | 1:A:314:ILE:HD13 | 1.57                     | 0.86              |
| 1:A:301:ILE:HD12 | 1:A:310:LEU:HD11 | 1.56                     | 0.85              |
| 1:B:25:MET:HE3   | 1:B:107:LEU:HD22 | 1.57                     | 0.84              |
| 1:A:123:ASP:HA   | 1:A:124:SER:HB3  | 1.59                     | 0.84              |
| 1:B:67:GLN:NE2   | 1:B:71:LEU:HG    | 1.93                     | 0.83              |
| 1:A:165:HIS:CD2  | 1:A:241:SER:HB3  | 2.14                     | 0.82              |
| 1:A:112:VAL:O    | 1:A:116:LEU:HB2  | 1.78                     | 0.82              |
| 1:B:230:PHE:HA   | 1:B:275:SER:O    | 1.79                     | 0.82              |
| 1:B:109:ASP:HB2  | 1:B:207:ASN:OD1  | 1.78                     | 0.81              |
| 1:B:170:LEU:HD21 | 1:B:344:LEU:HD21 | 1.60                     | 0.81              |
| 1:B:282:LYS:CA   | 1:B:283:GLY:N    | 2.44                     | 0.81              |
| 1:A:318:VAL:HG12 | 1:A:321:THR:CG2  | 2.12                     | 0.80              |
| 1:B:37:LEU:HD22  | 1:B:114:TYR:HD1  | 1.47                     | 0.80              |
| 1:A:90:LEU:HB3   | 1:A:92:ASN:OD1   | 1.82                     | 0.79              |
| 1:A:149:GLU:O    | 1:A:153:ILE:HG13 | 1.83                     | 0.78              |
| 1:A:318:VAL:HG12 | 1:A:321:THR:HG21 | 1.66                     | 0.77              |
| 1:A:280:LEU:HD12 | 1:A:281:PRO:HD2  | 1.67                     | 0.77              |
| 1:A:19:GLU:HG2   | 3:A:530:HOH:O    | 1.85                     | 0.76              |
| 1:B:84:GLY:H     | 1:B:85:MET:HA    | 1.52                     | 0.75              |
| 1:B:171:GLU:HG2  | 1:B:345:LYS:HZ2  | 1.51                     | 0.75              |
| 1:B:138:THR:HG22 | 1:B:140:ILE:HD13 | 1.69                     | 0.75              |
| 1:A:184:CYS:SG   | 1:A:191:LYS:NZ   | 2.60                     | 0.75              |
| 1:A:118:ARG:HD3  | 3:A:504:HOH:O    | 1.86                     | 0.74              |
| 1:B:43:ARG:H     | 1:B:43:ARG:HE    | 1.33                     | 0.74              |
| 1:B:156:TYR:OH   | 1:B:309:PRO:HD2  | 1.87                     | 0.74              |
| 1:B:198:LEU:HG   | 1:B:260:LEU:HD22 | 1.70                     | 0.74              |
| 1:A:315:SER:HB2  | 3:A:523:HOH:O    | 1.88                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:109:ASP:HB3  | 1:A:207:ASN:HA   | 1.69                     | 0.73              |
| 1:A:173:ILE:HB   | 1:A:343:LYS:HG2  | 1.68                     | 0.73              |
| 1:B:45:ILE:HG23  | 1:B:104:LEU:HD22 | 1.70                     | 0.73              |
| 1:B:37:LEU:HA    | 3:B:524:HOH:O    | 1.87                     | 0.73              |
| 1:B:269:TYR:HE2  | 3:B:613:HOH:O    | 1.72                     | 0.73              |
| 1:A:31:ASP:HB2   | 1:A:82:ASP:N     | 2.05                     | 0.72              |
| 1:A:133:TYR:CE1  | 1:A:140:ILE:HG13 | 2.25                     | 0.71              |
| 1:B:161:HIS:NE2  | 1:B:168:TYR:HE1  | 1.89                     | 0.71              |
| 1:A:45:ILE:HG23  | 1:A:104:LEU:HD22 | 1.71                     | 0.71              |
| 1:B:61:GLN:HB3   | 3:B:548:HOH:O    | 1.89                     | 0.71              |
| 1:B:154:ARG:HG2  | 1:B:172:VAL:HG21 | 1.72                     | 0.71              |
| 1:A:21:MET:O     | 1:A:25:MET:HG3   | 1.91                     | 0.71              |
| 1:A:144:ASP:HA   | 1:A:145:ARG:HD2  | 1.73                     | 0.70              |
| 1:A:93:ASN:HD21  | 1:A:96:SER:H     | 1.38                     | 0.70              |
| 1:B:208:PHE:O    | 1:B:212:LEU:HG   | 1.93                     | 0.69              |
| 1:A:11:LEU:HG    | 1:A:15:ILE:HD13  | 1.73                     | 0.69              |
| 1:A:28:TYR:CG    | 1:A:103:MET:HB2  | 2.27                     | 0.69              |
| 1:B:282:LYS:C    | 1:B:282:LYS:CB   | 2.65                     | 0.69              |
| 1:A:64:SER:HB3   | 1:A:67:GLN:HB2   | 1.73                     | 0.69              |
| 1:B:242:LYS:HD3  | 1:B:325:TYR:HD2  | 1.58                     | 0.69              |
| 1:B:97:VAL:O     | 1:B:101:VAL:HG23 | 1.93                     | 0.69              |
| 1:B:15:ILE:HG13  | 1:B:16:PHE:HD2   | 1.57                     | 0.68              |
| 1:B:96:SER:O     | 1:B:100:LYS:HG2  | 1.92                     | 0.68              |
| 1:B:210:GLY:HA2  | 1:B:213:SER:OG   | 1.94                     | 0.68              |
| 1:B:84:GLY:N     | 1:B:85:MET:HA    | 2.08                     | 0.68              |
| 1:B:86:LYS:HD3   | 1:B:87:LYS:N     | 2.07                     | 0.68              |
| 1:B:67:GLN:HE21  | 1:B:71:LEU:HG    | 1.58                     | 0.67              |
| 1:B:186:ARG:HB3  | 3:B:577:HOH:O    | 1.95                     | 0.67              |
| 1:B:28:TYR:C     | 1:B:29:GLU:HG3   | 2.19                     | 0.67              |
| 1:B:238:ASP:HA   | 3:B:612:HOH:O    | 1.95                     | 0.67              |
| 1:B:195:ASN:O    | 1:B:265:LEU:HB2  | 1.94                     | 0.67              |
| 1:B:349:LYS:HD3  | 1:B:350:THR:H    | 1.59                     | 0.67              |
| 1:B:165:HIS:CD2  | 1:B:245:ASN:HD21 | 2.13                     | 0.66              |
| 1:B:292:LYS:HE3  | 1:B:319:ASN:HB2  | 1.76                     | 0.66              |
| 1:A:93:ASN:HD21  | 1:A:96:SER:N     | 1.93                     | 0.66              |
| 1:B:301:ILE:HG22 | 1:B:303:LEU:HB3  | 1.77                     | 0.65              |
| 1:B:204:ARG:O    | 1:B:207:ASN:HB2  | 1.97                     | 0.65              |
| 1:A:168:TYR:HB3  | 1:A:348:PHE:CD2  | 2.32                     | 0.65              |
| 1:A:246:TYR:HD1  | 3:A:518:HOH:O    | 1.79                     | 0.65              |
| 1:A:68:ILE:HG21  | 1:A:92:ASN:HB3   | 1.78                     | 0.64              |
| 1:A:144:ASP:CG   | 1:A:145:ARG:HD2  | 2.21                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:167:ALA:HA   | 1:B:349:LYS:HB3  | 1.77                     | 0.64              |
| 1:B:260:LEU:HD11 | 3:B:590:HOH:O    | 1.96                     | 0.64              |
| 1:B:144:ASP:O    | 1:B:147:SER:HB3  | 1.98                     | 0.64              |
| 1:A:183:GLU:OE1  | 1:A:337:ASN:HA   | 1.96                     | 0.64              |
| 1:A:287:VAL:HG23 | 1:A:331:TYR:HE1  | 1.64                     | 0.63              |
| 1:A:15:ILE:CG2   | 1:A:257:LEU:HD11 | 2.27                     | 0.63              |
| 1:A:234:ILE:HG22 | 1:A:236:PHE:CE1  | 2.34                     | 0.63              |
| 1:A:234:ILE:HD11 | 1:A:333:ILE:HG22 | 1.81                     | 0.63              |
| 1:A:116:LEU:HD12 | 1:A:135:LYS:HZ2  | 1.64                     | 0.63              |
| 1:B:32:LEU:HB2   | 3:B:572:HOH:O    | 1.98                     | 0.63              |
| 1:B:75:PHE:CD2   | 1:B:91:LEU:HD11  | 2.34                     | 0.62              |
| 1:B:295:PRO:HA   | 1:B:311:GLY:O    | 1.99                     | 0.62              |
| 1:B:292:LYS:HE3  | 1:B:319:ASN:ND2  | 2.14                     | 0.62              |
| 1:A:324:LEU:HD22 | 1:A:325:TYR:CE2  | 2.35                     | 0.62              |
| 1:B:161:HIS:CE1  | 1:B:168:TYR:CE1  | 2.88                     | 0.62              |
| 1:B:153:ILE:HD13 | 3:B:563:HOH:O    | 1.99                     | 0.62              |
| 1:A:292:LYS:HB3  | 1:A:318:VAL:O    | 2.00                     | 0.61              |
| 1:A:35:MET:HG2   | 1:A:39:LYS:HG2   | 1.82                     | 0.61              |
| 1:B:246:TYR:N    | 1:B:246:TYR:CD2  | 2.68                     | 0.61              |
| 1:B:279:LYS:HA   | 3:B:536:HOH:O    | 2.00                     | 0.61              |
| 1:A:84:GLY:HA3   | 3:A:587:HOH:O    | 2.00                     | 0.61              |
| 1:B:110:ILE:HG12 | 1:B:206:THR:HB   | 1.82                     | 0.61              |
| 1:B:78:LEU:O     | 1:B:79:ILE:HD13  | 2.01                     | 0.61              |
| 1:A:138:THR:HG21 | 1:A:212:LEU:CD2  | 2.28                     | 0.61              |
| 1:B:339:LYS:HB3  | 1:B:340:TYR:CD2  | 2.36                     | 0.61              |
| 1:A:23:LYS:O     | 1:A:27:GLU:HG3   | 2.00                     | 0.61              |
| 1:B:194:HIS:HB2  | 3:B:625:HOH:O    | 2.01                     | 0.60              |
| 1:A:110:ILE:O    | 1:A:113:ALA:HB3  | 2.00                     | 0.60              |
| 1:B:161:HIS:NE2  | 1:B:168:TYR:CE1  | 2.68                     | 0.60              |
| 1:B:186:ARG:HE   | 1:B:334:ALA:HA   | 1.66                     | 0.60              |
| 1:A:43:ARG:HD3   | 1:A:43:ARG:N     | 2.17                     | 0.60              |
| 1:B:13:LYS:CG    | 1:B:129:ILE:HD11 | 2.32                     | 0.60              |
| 1:A:37:LEU:H     | 1:A:37:LEU:HD12  | 1.65                     | 0.60              |
| 1:B:62:GLY:HA3   | 3:B:603:HOH:O    | 2.02                     | 0.60              |
| 1:B:246:TYR:H    | 1:B:246:TYR:HD2  | 1.50                     | 0.59              |
| 1:B:247:CYS:SG   | 3:B:573:HOH:O    | 2.52                     | 0.59              |
| 1:A:155:LYS:O    | 1:A:158:LYS:HB3  | 2.03                     | 0.59              |
| 1:B:86:LYS:HD3   | 1:B:87:LYS:H     | 1.66                     | 0.59              |
| 1:A:144:ASP:HA   | 1:A:145:ARG:CD   | 2.33                     | 0.59              |
| 1:A:296:ASP:CG   | 1:A:298:SER:HG   | 2.10                     | 0.59              |
| 1:B:187:TYR:CD2  | 1:B:337:ASN:HB2  | 2.38                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:18:VAL:HG12  | 1:A:22:LYS:HE2   | 1.85                     | 0.58              |
| 1:B:20:SER:HA    | 1:B:23:LYS:HB3   | 1.85                     | 0.58              |
| 1:B:161:HIS:HD2  | 1:B:240:VAL:HG13 | 1.69                     | 0.58              |
| 1:A:55:VAL:HG22  | 1:A:68:ILE:HD12  | 1.85                     | 0.58              |
| 1:A:196:ARG:HG3  | 1:A:264:ALA:HA   | 1.85                     | 0.58              |
| 1:B:214:GLN:HG2  | 1:B:217:ARG:CZ   | 2.34                     | 0.58              |
| 1:A:68:ILE:HD13  | 1:A:71:LEU:HD12  | 1.84                     | 0.58              |
| 1:B:55:VAL:HG12  | 1:B:56:GLN:HG3   | 1.86                     | 0.58              |
| 1:B:180:ARG:HB2  | 1:B:183:GLU:HG3  | 1.85                     | 0.58              |
| 1:A:193:LEU:HD11 | 1:A:266:GLY:HA3  | 1.85                     | 0.58              |
| 1:B:141:LYS:O    | 1:B:176:PHE:HA   | 2.04                     | 0.58              |
| 1:B:152:ILE:HA   | 1:B:155:LYS:HE3  | 1.85                     | 0.58              |
| 1:B:293:THR:HB   | 1:B:325:TYR:HD1  | 1.68                     | 0.58              |
| 1:B:215:GLY:O    | 1:B:216:LEU:C    | 2.47                     | 0.57              |
| 1:A:20:SER:O     | 1:A:23:LYS:HB2   | 2.03                     | 0.57              |
| 1:B:234:ILE:O    | 1:B:329:ILE:HA   | 2.04                     | 0.57              |
| 1:A:280:LEU:HD22 | 1:A:331:TYR:CD1  | 2.39                     | 0.57              |
| 1:B:161:HIS:NE2  | 1:B:170:LEU:HB2  | 2.20                     | 0.57              |
| 1:B:242:LYS:HD3  | 1:B:325:TYR:CD2  | 2.40                     | 0.57              |
| 1:A:86:LYS:O     | 1:A:88:PRO:HD3   | 2.04                     | 0.57              |
| 1:A:104:LEU:HD23 | 1:A:107:LEU:HD12 | 1.86                     | 0.57              |
| 1:A:345:LYS:HZ1  | 1:A:347:ASN:CG   | 2.13                     | 0.57              |
| 1:B:42:LYS:HD2   | 1:B:43:ARG:CZ    | 2.34                     | 0.57              |
| 1:B:111:GLU:O    | 1:B:115:SER:HB2  | 2.05                     | 0.57              |
| 1:A:42:LYS:HG3   | 1:A:43:ARG:CD    | 2.35                     | 0.57              |
| 1:A:45:ILE:HD13  | 1:A:108:LEU:HD23 | 1.86                     | 0.57              |
| 1:B:117:LEU:C    | 1:B:117:LEU:HD12 | 2.30                     | 0.57              |
| 1:B:157:VAL:HG13 | 1:B:240:VAL:HG11 | 1.86                     | 0.57              |
| 1:B:214:GLN:HG2  | 1:B:217:ARG:NE   | 2.20                     | 0.57              |
| 1:B:5:PRO:O      | 1:B:6:LYS:C      | 2.48                     | 0.57              |
| 1:B:94:ALA:O     | 1:B:98:GLN:HG2   | 2.05                     | 0.57              |
| 1:A:15:ILE:HG22  | 1:A:257:LEU:HD11 | 1.86                     | 0.56              |
| 1:B:77:THR:C     | 3:B:631:HOH:O    | 2.48                     | 0.56              |
| 1:B:180:ARG:NH1  | 1:B:214:GLN:HA   | 2.20                     | 0.56              |
| 1:A:144:ASP:CA   | 1:A:145:ARG:HD2  | 2.35                     | 0.56              |
| 1:B:25:MET:HE3   | 1:B:107:LEU:CD2  | 2.31                     | 0.56              |
| 1:B:255:ILE:HD13 | 1:B:345:LYS:HG2  | 1.87                     | 0.56              |
| 1:A:94:ALA:O     | 1:A:97:VAL:HG12  | 2.05                     | 0.56              |
| 1:B:12:ILE:HD12  | 1:B:133:TYR:HB2  | 1.86                     | 0.56              |
| 1:A:262:GLU:HG3  | 1:A:306:VAL:HG11 | 1.88                     | 0.56              |
| 1:B:296:ASP:HB2  | 1:B:314:ILE:HD12 | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:218:ILE:HG22 | 1:A:234:ILE:HD11 | 1.87                     | 0.55              |
| 1:B:13:LYS:HG3   | 1:B:129:ILE:HD11 | 1.87                     | 0.55              |
| 1:B:321:THR:OG1  | 1:B:323:LEU:N    | 2.40                     | 0.55              |
| 1:A:224:PRO:O    | 1:A:228:TYR:CE1  | 2.60                     | 0.55              |
| 1:A:42:LYS:HG3   | 1:A:43:ARG:HD3   | 1.88                     | 0.55              |
| 1:B:271:LEU:HD13 | 1:B:275:SER:OG   | 2.06                     | 0.55              |
| 1:A:11:LEU:HG    | 1:A:15:ILE:CD1   | 2.37                     | 0.55              |
| 1:A:139:ASP:C    | 1:A:140:ILE:HG12 | 2.32                     | 0.55              |
| 1:A:242:LYS:O    | 1:A:246:TYR:CE2  | 2.60                     | 0.55              |
| 1:B:12:ILE:HD11  | 1:B:133:TYR:HD1  | 1.71                     | 0.55              |
| 1:B:230:PHE:O    | 1:B:231:GLY:C    | 2.50                     | 0.55              |
| 1:B:161:HIS:NE2  | 1:B:170:LEU:HD22 | 2.20                     | 0.55              |
| 1:B:109:ASP:O    | 1:B:112:VAL:N    | 2.40                     | 0.55              |
| 1:B:292:LYS:HE3  | 1:B:319:ASN:HD22 | 1.71                     | 0.55              |
| 1:B:234:ILE:HG22 | 1:B:235:TYR:H    | 1.72                     | 0.54              |
| 1:B:267:ASN:OD1  | 1:B:283:GLY:O    | 2.25                     | 0.54              |
| 1:B:43:ARG:H     | 1:B:43:ARG:NE    | 2.04                     | 0.54              |
| 1:B:187:TYR:OH   | 1:B:262:GLU:HG2  | 2.08                     | 0.54              |
| 1:A:22:LYS:HB3   | 1:A:32:LEU:HD11  | 1.90                     | 0.54              |
| 1:A:200:TRP:CE3  | 1:A:258:ILE:HD11 | 2.43                     | 0.54              |
| 1:A:58:ALA:HB1   | 1:A:63:SER:HB2   | 1.90                     | 0.54              |
| 1:A:205:THR:HA   | 1:A:208:PHE:CD1  | 2.43                     | 0.54              |
| 1:B:24:ALA:O     | 1:B:27:GLU:HG2   | 2.08                     | 0.54              |
| 1:B:311:GLY:O    | 1:B:312:THR:C    | 2.51                     | 0.54              |
| 1:B:12:ILE:CD1   | 1:B:133:TYR:HB2  | 2.37                     | 0.54              |
| 1:B:51:ILE:CD1   | 1:B:74:ARG:HG3   | 2.38                     | 0.54              |
| 1:B:85:MET:SD    | 1:B:85:MET:N     | 2.81                     | 0.54              |
| 1:B:165:HIS:HE1  | 1:B:325:TYR:HE2  | 1.55                     | 0.54              |
| 1:A:37:LEU:O     | 1:A:114:TYR:CE2  | 2.61                     | 0.54              |
| 1:B:55:VAL:O     | 1:B:59:VAL:HG23  | 2.08                     | 0.54              |
| 1:B:173:ILE:O    | 1:B:174:ASP:CG   | 2.52                     | 0.53              |
| 1:A:133:TYR:OH   | 1:A:139:ASP:HA   | 2.08                     | 0.53              |
| 1:B:35:MET:SD    | 1:B:80:PRO:HD2   | 2.48                     | 0.53              |
| 1:B:98:GLN:O     | 1:B:99:ALA:C     | 2.50                     | 0.53              |
| 1:A:198:LEU:HG   | 1:A:260:LEU:HD22 | 1.90                     | 0.53              |
| 1:A:218:ILE:HD12 | 1:A:233:GLY:HA2  | 1.90                     | 0.53              |
| 1:A:12:ILE:HG13  | 1:A:129:ILE:HG23 | 1.90                     | 0.53              |
| 1:B:24:ALA:HA    | 1:B:27:GLU:OE2   | 2.08                     | 0.53              |
| 1:B:36:PRO:O     | 1:B:39:LYS:N     | 2.42                     | 0.53              |
| 1:B:170:LEU:CD2  | 1:B:344:LEU:HD21 | 2.33                     | 0.53              |
| 1:A:134:GLU:HB3  | 3:A:531:HOH:O    | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:116:LEU:HD12 | 1:A:135:LYS:NZ   | 2.23                     | 0.53              |
| 1:A:210:GLY:HA2  | 1:A:213:SER:OG   | 2.09                     | 0.53              |
| 1:A:224:PRO:O    | 1:A:228:TYR:HE1  | 1.91                     | 0.53              |
| 1:A:10:ASP:HA    | 1:A:13:LYS:HE3   | 1.90                     | 0.53              |
| 1:A:31:ASP:CG    | 1:A:82:ASP:HB2   | 2.34                     | 0.53              |
| 1:B:112:VAL:O    | 1:B:113:ALA:C    | 2.52                     | 0.53              |
| 1:B:211:ILE:O    | 1:B:215:GLY:HA2  | 2.08                     | 0.53              |
| 1:A:124:SER:H    | 1:A:127:ASP:HA   | 1.74                     | 0.53              |
| 1:A:132:ASN:N    | 1:A:132:ASN:OD1  | 2.38                     | 0.52              |
| 1:B:10:ASP:O     | 1:B:11:LEU:C     | 2.51                     | 0.52              |
| 1:B:231:GLY:H    | 1:B:276:HIS:HA   | 1.74                     | 0.52              |
| 1:A:102:GLU:O    | 1:A:103:MET:C    | 2.48                     | 0.52              |
| 1:A:242:LYS:O    | 1:A:246:TYR:CD2  | 2.62                     | 0.52              |
| 1:B:28:TYR:CD1   | 1:B:103:MET:HG3  | 2.45                     | 0.52              |
| 1:B:259:LEU:HD22 | 1:B:338:LEU:HD22 | 1.92                     | 0.52              |
| 1:A:95:ASP:O     | 1:A:96:SER:C     | 2.50                     | 0.52              |
| 1:A:205:THR:HA   | 1:A:208:PHE:HD1  | 1.74                     | 0.52              |
| 1:B:349:LYS:HB2  | 3:B:619:HOH:O    | 2.09                     | 0.52              |
| 1:A:42:LYS:N     | 1:A:43:ARG:HD3   | 2.24                     | 0.52              |
| 1:A:36:PRO:O     | 1:A:39:LYS:N     | 2.43                     | 0.52              |
| 1:B:158:LYS:HG3  | 1:B:159:ASN:OD1  | 2.10                     | 0.52              |
| 1:A:153:ILE:HD12 | 1:A:175:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:207:ASN:O    | 1:A:211:ILE:HG13 | 2.10                     | 0.52              |
| 1:B:19:GLU:HA    | 1:B:22:LYS:HE2   | 1.91                     | 0.52              |
| 1:B:75:PHE:O     | 1:B:78:LEU:HB2   | 2.10                     | 0.52              |
| 1:B:123:ASP:HA   | 1:B:124:SER:OG   | 2.10                     | 0.52              |
| 1:B:161:HIS:CE1  | 1:B:168:TYR:CD1  | 2.97                     | 0.52              |
| 1:A:238:ASP:OD2  | 1:A:328:TYR:OH   | 2.25                     | 0.52              |
| 1:B:58:ALA:O     | 1:B:59:VAL:C     | 2.50                     | 0.52              |
| 1:A:37:LEU:HD12  | 1:A:37:LEU:N     | 2.24                     | 0.51              |
| 1:B:346:PHE:N    | 1:B:346:PHE:CD1  | 2.73                     | 0.51              |
| 1:A:83:PHE:CE2   | 1:A:89:PRO:HD2   | 2.45                     | 0.51              |
| 1:B:233:GLY:HA3  | 1:B:330:VAL:O    | 2.10                     | 0.51              |
| 1:A:291:GLY:HA3  | 1:A:325:TYR:C    | 2.35                     | 0.51              |
| 1:B:1:LYS:HG3    | 1:B:2:SER:H      | 1.76                     | 0.51              |
| 1:B:293:THR:HB   | 1:B:325:TYR:CD1  | 2.44                     | 0.51              |
| 1:B:72:SER:HB2   | 1:B:91:LEU:HB2   | 1.91                     | 0.51              |
| 1:B:262:GLU:OE1  | 1:B:306:VAL:CG2  | 2.58                     | 0.51              |
| 1:B:279:LYS:HD2  | 1:B:280:LEU:O    | 2.10                     | 0.51              |
| 1:B:301:ILE:CG2  | 1:B:303:LEU:HB3  | 2.40                     | 0.51              |
| 1:A:76:TYR:O     | 1:A:77:THR:C     | 2.54                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:138:THR:HG23 | 1:B:178:ILE:HG22 | 1.93                     | 0.51              |
| 1:B:4:LEU:CD2    | 1:B:8:VAL:HG12   | 2.40                     | 0.51              |
| 1:B:346:PHE:HB3  | 1:B:348:PHE:CZ   | 2.46                     | 0.51              |
| 1:A:165:HIS:NE2  | 1:A:241:SER:HB3  | 2.26                     | 0.51              |
| 1:B:249:THR:HG22 | 1:B:253:ASP:OD2  | 2.10                     | 0.51              |
| 1:B:121:SER:HB2  | 1:B:131:VAL:HG11 | 1.92                     | 0.50              |
| 1:A:104:LEU:HA   | 1:A:107:LEU:HB2  | 1.93                     | 0.50              |
| 1:A:123:ASP:HA   | 1:A:124:SER:CB   | 2.38                     | 0.50              |
| 1:B:112:VAL:O    | 1:B:113:ALA:O    | 2.29                     | 0.50              |
| 1:B:259:LEU:HD22 | 1:B:338:LEU:CD2  | 2.41                     | 0.50              |
| 1:B:259:LEU:HD13 | 1:B:338:LEU:HD21 | 1.94                     | 0.50              |
| 1:A:218:ILE:HG22 | 1:A:234:ILE:CD1  | 2.40                     | 0.50              |
| 1:B:133:TYR:HA   | 1:B:136:LEU:HD12 | 1.93                     | 0.50              |
| 1:B:87:LYS:N     | 1:B:87:LYS:HD2   | 2.26                     | 0.50              |
| 1:B:174:ASP:HB2  | 1:B:176:PHE:CE2  | 2.46                     | 0.50              |
| 1:B:199:LEU:HD12 | 1:B:263:VAL:HG13 | 1.93                     | 0.50              |
| 1:B:345:LYS:HZ3  | 1:B:347:ASN:HB2  | 1.77                     | 0.50              |
| 1:B:200:TRP:CD1  | 3:B:612:HOH:O    | 2.65                     | 0.50              |
| 1:B:273:HIS:HD2  | 3:B:558:HOH:O    | 1.94                     | 0.50              |
| 1:A:55:VAL:HG23  | 1:A:71:LEU:HD13  | 1.93                     | 0.50              |
| 1:A:200:TRP:CE2  | 1:A:240:VAL:HB   | 2.47                     | 0.50              |
| 1:B:4:LEU:O      | 1:B:5:PRO:C      | 2.53                     | 0.50              |
| 1:B:28:TYR:N     | 1:B:29:GLU:HA    | 2.26                     | 0.50              |
| 1:B:88:PRO:O     | 1:B:90:LEU:HD22  | 2.11                     | 0.50              |
| 1:B:207:ASN:O    | 1:B:210:GLY:N    | 2.45                     | 0.50              |
| 1:A:4:LEU:HD21   | 1:A:133:TYR:CD2  | 2.46                     | 0.50              |
| 1:A:270:GLU:O    | 1:A:271:LEU:HD23 | 2.12                     | 0.50              |
| 1:A:21:MET:SD    | 1:A:114:TYR:HB2  | 2.52                     | 0.49              |
| 1:B:142:VAL:O    | 1:B:143:VAL:C    | 2.48                     | 0.49              |
| 1:A:210:GLY:O    | 1:A:214:GLN:N    | 2.42                     | 0.49              |
| 1:B:41:SER:O     | 1:B:45:ILE:HG13  | 2.12                     | 0.49              |
| 1:B:250:SER:O    | 1:B:252:GLY:N    | 2.45                     | 0.49              |
| 1:A:157:VAL:HG22 | 1:A:200:TRP:CH2  | 2.47                     | 0.49              |
| 1:B:98:GLN:HB3   | 3:B:600:HOH:O    | 2.13                     | 0.49              |
| 1:B:46:GLN:HB3   | 1:B:222:GLU:OE1  | 2.12                     | 0.49              |
| 1:B:234:ILE:HG22 | 1:B:235:TYR:N    | 2.27                     | 0.49              |
| 1:B:281:PRO:O    | 1:B:282:LYS:C    | 2.55                     | 0.49              |
| 1:A:232:LYS:HB2  | 3:A:507:HOH:O    | 2.12                     | 0.49              |
| 1:B:188:LYS:O    | 1:B:189:PRO:C    | 2.53                     | 0.49              |
| 1:A:28:TYR:CD1   | 1:A:103:MET:HB2  | 2.47                     | 0.49              |
| 1:B:15:ILE:HG13  | 1:B:16:PHE:CD2   | 2.44                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:218:ILE:O    | 1:B:219:ALA:C    | 2.55                     | 0.49              |
| 1:A:55:VAL:O     | 1:A:59:VAL:HG23  | 2.12                     | 0.49              |
| 1:B:349:LYS:HD3  | 1:B:350:THR:N    | 2.26                     | 0.49              |
| 1:A:254:PRO:O    | 1:A:346:PHE:HB2  | 2.12                     | 0.48              |
| 1:A:296:ASP:CB   | 1:A:314:ILE:HD13 | 2.38                     | 0.48              |
| 1:A:1:LYS:HD2    | 1:A:127:ASP:OD1  | 2.14                     | 0.48              |
| 1:B:150:ALA:HB1  | 1:B:154:ARG:NH1  | 2.28                     | 0.48              |
| 1:A:287:VAL:HG23 | 1:A:331:TYR:CE1  | 2.47                     | 0.48              |
| 1:A:304:ASP:O    | 1:A:305:GLY:C    | 2.55                     | 0.48              |
| 1:B:49:TYR:OH    | 1:B:105:ASP:OD1  | 2.26                     | 0.48              |
| 1:B:168:TYR:CE1  | 1:B:170:LEU:HD22 | 2.49                     | 0.48              |
| 1:B:9:GLN:O      | 1:B:10:ASP:C     | 2.55                     | 0.48              |
| 1:B:37:LEU:HD22  | 1:B:114:TYR:CD1  | 2.36                     | 0.48              |
| 1:B:218:ILE:HG21 | 1:B:232:LYS:O    | 2.13                     | 0.48              |
| 1:B:241:SER:C    | 1:B:243:SER:N    | 2.70                     | 0.48              |
| 1:B:345:LYS:HZ2  | 1:B:345:LYS:HB3  | 1.77                     | 0.48              |
| 1:A:251:GLN:HA   | 1:A:251:GLN:HE21 | 1.78                     | 0.48              |
| 1:A:341:LEU:O    | 1:A:342:LEU:HD12 | 2.14                     | 0.48              |
| 1:B:64:SER:O     | 1:B:67:GLN:N     | 2.46                     | 0.48              |
| 1:B:123:ASP:HA   | 1:B:124:SER:HG   | 1.79                     | 0.48              |
| 1:B:345:LYS:HB3  | 1:B:345:LYS:NZ   | 2.29                     | 0.48              |
| 1:B:47:ALA:O     | 1:B:48:ALA:C     | 2.53                     | 0.48              |
| 1:B:135:LYS:O    | 1:B:136:LEU:C    | 2.49                     | 0.48              |
| 1:A:39:LYS:O     | 1:A:40:LEU:C     | 2.56                     | 0.47              |
| 1:A:283:GLY:C    | 3:A:580:HOH:O    | 2.57                     | 0.47              |
| 1:B:145:ARG:H    | 1:B:145:ARG:NE   | 2.12                     | 0.47              |
| 1:A:43:ARG:HD3   | 1:A:43:ARG:H     | 1.79                     | 0.47              |
| 1:B:30:ILE:HD11  | 1:B:107:LEU:HD11 | 1.95                     | 0.47              |
| 1:B:260:LEU:HD21 | 3:B:590:HOH:O    | 2.14                     | 0.47              |
| 1:A:204:ARG:NH2  | 1:A:248:HIS:ND1  | 2.62                     | 0.47              |
| 1:A:140:ILE:HG22 | 1:A:176:PHE:HD1  | 1.80                     | 0.47              |
| 1:B:153:ILE:O    | 1:B:156:TYR:N    | 2.47                     | 0.47              |
| 1:B:171:GLU:HG2  | 1:B:345:LYS:HB3  | 1.96                     | 0.47              |
| 1:B:312:THR:O    | 1:B:313:GLY:C    | 2.58                     | 0.47              |
| 1:A:267:ASN:ND2  | 1:A:285:HIS:CE1  | 2.82                     | 0.47              |
| 1:B:198:LEU:HA   | 1:B:261:GLY:O    | 2.13                     | 0.47              |
| 1:B:23:LYS:O     | 1:B:26:VAL:HG23  | 2.15                     | 0.47              |
| 1:B:99:ALA:O     | 1:B:103:MET:HB2  | 2.15                     | 0.47              |
| 1:B:170:LEU:O    | 1:B:171:GLU:C    | 2.58                     | 0.47              |
| 1:B:211:ILE:HD13 | 1:B:211:ILE:HG21 | 1.70                     | 0.47              |
| 1:B:295:PRO:O    | 1:B:297:PRO:HD3  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:31:ASP:O     | 1:A:33:GLN:N     | 2.48                     | 0.47              |
| 1:A:239:MET:HG3  | 1:A:325:TYR:CD1  | 2.50                     | 0.47              |
| 1:A:43:ARG:CD    | 1:A:43:ARG:H     | 2.27                     | 0.47              |
| 1:B:15:ILE:HG13  | 1:B:16:PHE:H     | 1.80                     | 0.47              |
| 1:B:170:LEU:HG   | 1:B:344:LEU:HD11 | 1.97                     | 0.47              |
| 1:B:83:PHE:HB3   | 1:B:88:PRO:HB3   | 1.97                     | 0.46              |
| 1:B:150:ALA:HB1  | 1:B:154:ARG:HH12 | 1.80                     | 0.46              |
| 1:B:170:LEU:HD11 | 1:B:346:PHE:CZ   | 2.50                     | 0.46              |
| 1:B:230:PHE:CD2  | 1:B:329:ILE:HD11 | 2.50                     | 0.46              |
| 1:A:162:ALA:O    | 1:A:163:THR:C    | 2.59                     | 0.46              |
| 1:A:208:PHE:HA   | 1:A:211:ILE:HB   | 1.98                     | 0.46              |
| 1:A:211:ILE:HG21 | 1:A:259:LEU:HD11 | 1.97                     | 0.46              |
| 1:A:236:PHE:CE1  | 1:A:263:VAL:HG11 | 2.50                     | 0.46              |
| 1:A:280:LEU:HG   | 1:A:284:LYS:O    | 2.16                     | 0.46              |
| 1:B:102:GLU:O    | 1:B:105:ASP:HB2  | 2.16                     | 0.46              |
| 1:B:165:HIS:CD2  | 1:B:241:SER:HB2  | 2.50                     | 0.46              |
| 1:B:332:ASP:OD1  | 1:B:332:ASP:C    | 2.58                     | 0.46              |
| 1:A:205:THR:OG1  | 1:A:206:THR:N    | 2.49                     | 0.46              |
| 1:B:200:TRP:NE1  | 3:B:612:HOH:O    | 2.49                     | 0.46              |
| 1:B:211:ILE:HG23 | 1:B:216:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:42:LYS:HG3   | 1:A:43:ARG:NE    | 2.30                     | 0.46              |
| 1:B:183:GLU:O    | 1:B:184:CYS:C    | 2.52                     | 0.46              |
| 1:B:268:MET:HE2  | 3:B:537:HOH:O    | 2.16                     | 0.46              |
| 1:A:201:HIS:HB3  | 1:A:259:LEU:HB2  | 1.97                     | 0.46              |
| 1:A:258:ILE:HG21 | 1:A:258:ILE:HD13 | 1.35                     | 0.46              |
| 1:A:262:GLU:HB2  | 1:A:339:LYS:HD3  | 1.98                     | 0.46              |
| 1:B:16:PHE:CD2   | 1:B:16:PHE:N     | 2.84                     | 0.45              |
| 1:B:36:PRO:O     | 1:B:37:LEU:C     | 2.60                     | 0.45              |
| 1:B:159:ASN:HB3  | 1:B:312:THR:H    | 1.81                     | 0.45              |
| 1:A:56:GLN:OE1   | 1:A:226:THR:HB   | 2.16                     | 0.45              |
| 1:B:199:LEU:HB3  | 1:B:237:ALA:O    | 2.16                     | 0.45              |
| 1:A:128:PRO:O    | 1:A:129:ILE:HD13 | 2.15                     | 0.45              |
| 1:B:21:MET:HE2   | 1:B:206:THR:HG22 | 1.98                     | 0.45              |
| 1:B:270:GLU:HA   | 1:B:288:LYS:O    | 2.15                     | 0.45              |
| 1:A:31:ASP:HB2   | 1:A:81:HIS:C     | 2.40                     | 0.45              |
| 1:A:65:ASP:N     | 1:A:65:ASP:OD1   | 2.49                     | 0.45              |
| 1:A:143:VAL:HG23 | 1:A:175:ILE:O    | 2.16                     | 0.45              |
| 1:B:149:GLU:O    | 1:B:150:ALA:C    | 2.59                     | 0.45              |
| 1:B:191:LYS:O    | 1:B:192:GLN:C    | 2.55                     | 0.45              |
| 1:B:19:GLU:OE2   | 1:B:20:SER:HA    | 2.16                     | 0.45              |
| 1:B:104:LEU:HD23 | 1:B:107:LEU:HD12 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:201:HIS:NE2  | 2:A:501:FRM:H202 | 2.31                     | 0.45              |
| 1:B:15:ILE:HG13  | 1:B:16:PHE:N     | 2.31                     | 0.45              |
| 1:B:16:PHE:HD2   | 1:B:16:PHE:N     | 2.14                     | 0.45              |
| 1:B:21:MET:HG3   | 1:B:206:THR:CG2  | 2.47                     | 0.45              |
| 1:B:129:ILE:O    | 1:B:132:ASN:N    | 2.49                     | 0.45              |
| 1:B:69:LEU:C     | 1:B:69:LEU:HD22  | 2.42                     | 0.45              |
| 1:B:109:ASP:HB2  | 1:B:207:ASN:HA   | 1.98                     | 0.45              |
| 1:A:31:ASP:O     | 1:A:32:LEU:C     | 2.60                     | 0.45              |
| 1:B:42:LYS:HE3   | 1:B:43:ARG:NH1   | 2.31                     | 0.45              |
| 1:B:51:ILE:HD13  | 1:B:74:ARG:HG3   | 1.99                     | 0.45              |
| 1:B:123:ASP:HA   | 1:B:124:SER:CB   | 2.46                     | 0.45              |
| 1:B:204:ARG:HD3  | 1:B:248:HIS:ND1  | 2.31                     | 0.45              |
| 1:B:51:ILE:HD13  | 1:B:51:ILE:HG21  | 1.73                     | 0.45              |
| 1:B:127:ASP:O    | 1:B:128:PRO:C    | 2.59                     | 0.45              |
| 1:B:288:LYS:HE2  | 1:B:326:ASN:HD21 | 1.82                     | 0.45              |
| 1:B:96:SER:N     | 3:B:581:HOH:O    | 2.50                     | 0.44              |
| 1:B:152:ILE:HG21 | 1:B:152:ILE:HD13 | 1.45                     | 0.44              |
| 1:B:168:TYR:HE1  | 1:B:170:LEU:HD22 | 1.82                     | 0.44              |
| 1:A:208:PHE:HB3  | 1:A:212:LEU:HD12 | 1.99                     | 0.44              |
| 1:B:42:LYS:H     | 1:B:42:LYS:HG3   | 1.56                     | 0.44              |
| 1:B:129:ILE:O    | 1:B:130:ASP:C    | 2.58                     | 0.44              |
| 1:B:162:ALA:C    | 1:B:163:THR:O    | 2.60                     | 0.44              |
| 1:A:249:THR:OG1  | 1:A:346:PHE:CG   | 2.64                     | 0.44              |
| 1:B:349:LYS:CD   | 1:B:350:THR:H    | 2.27                     | 0.44              |
| 1:A:145:ARG:H    | 1:A:145:ARG:HG3  | 1.69                     | 0.44              |
| 1:A:296:ASP:HA   | 1:A:297:PRO:HD2  | 1.76                     | 0.44              |
| 1:B:173:ILE:C    | 1:B:174:ASP:CG   | 2.86                     | 0.44              |
| 1:B:292:LYS:HG2  | 1:B:319:ASN:HB2  | 1.99                     | 0.44              |
| 1:B:301:ILE:CG2  | 1:B:303:LEU:HD13 | 2.48                     | 0.44              |
| 1:A:2:SER:HA     | 1:A:3:LYS:HD2    | 1.99                     | 0.44              |
| 1:B:37:LEU:HB3   | 1:B:114:TYR:CE1  | 2.53                     | 0.44              |
| 1:B:153:ILE:O    | 1:B:154:ARG:C    | 2.60                     | 0.44              |
| 1:A:267:ASN:ND2  | 1:A:285:HIS:NE2  | 2.66                     | 0.44              |
| 1:A:310:LEU:H    | 1:A:310:LEU:HG   | 1.58                     | 0.44              |
| 1:B:4:LEU:HG     | 1:B:8:VAL:CG1    | 2.48                     | 0.44              |
| 1:B:31:ASP:HB2   | 1:B:80:PRO:C     | 2.43                     | 0.44              |
| 1:A:205:THR:HG22 | 1:A:257:LEU:H    | 1.82                     | 0.44              |
| 1:A:281:PRO:HG2  | 1:A:284:LYS:HG3  | 1.99                     | 0.44              |
| 1:A:289:GLY:N    | 3:A:529:HOH:O    | 2.51                     | 0.44              |
| 1:B:70:ASP:O     | 1:B:73:ASN:N     | 2.50                     | 0.44              |
| 1:A:106:ASN:O    | 1:A:107:LEU:C    | 2.60                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:202:GLY:N    | 2:A:501:FRM:O14  | 2.50                     | 0.43              |
| 1:B:49:TYR:HB3   | 1:B:223:ALA:HA   | 2.00                     | 0.43              |
| 1:B:112:VAL:O    | 1:B:116:LEU:HB2  | 2.18                     | 0.43              |
| 1:B:208:PHE:CE1  | 1:B:257:LEU:HB2  | 2.53                     | 0.43              |
| 1:B:52:LEU:HA    | 1:B:52:LEU:HD23  | 1.77                     | 0.43              |
| 1:A:13:LYS:O     | 1:A:17:ASP:HB3   | 2.19                     | 0.43              |
| 1:A:206:THR:HG22 | 3:A:615:HOH:O    | 2.18                     | 0.43              |
| 1:B:3:LYS:HE2    | 1:B:130:ASP:OD2  | 2.18                     | 0.43              |
| 1:B:22:LYS:H     | 1:B:22:LYS:HG2   | 1.47                     | 0.43              |
| 1:B:33:GLN:HE21  | 1:B:33:GLN:HB3   | 1.52                     | 0.43              |
| 1:B:84:GLY:O     | 1:B:85:MET:SD    | 2.76                     | 0.43              |
| 1:B:112:VAL:CG1  | 1:B:116:LEU:HG   | 2.48                     | 0.43              |
| 1:B:112:VAL:HG12 | 1:B:116:LEU:HG   | 1.99                     | 0.43              |
| 1:B:230:PHE:O    | 1:B:231:GLY:O    | 2.36                     | 0.43              |
| 1:A:93:ASN:ND2   | 1:A:96:SER:N     | 2.64                     | 0.43              |
| 1:B:40:LEU:HD23  | 1:B:40:LEU:HA    | 1.64                     | 0.43              |
| 1:A:126:LYS:HE2  | 1:A:134:GLU:OE1  | 2.18                     | 0.43              |
| 1:B:71:LEU:HD23  | 1:B:74:ARG:NH1   | 2.34                     | 0.43              |
| 1:A:43:ARG:N     | 1:A:43:ARG:CD    | 2.82                     | 0.43              |
| 1:A:270:GLU:HG2  | 1:A:288:LYS:HB3  | 2.01                     | 0.43              |
| 1:B:11:LEU:O     | 1:B:12:ILE:C     | 2.61                     | 0.43              |
| 1:A:93:ASN:ND2   | 1:A:96:SER:H     | 2.11                     | 0.43              |
| 1:A:107:LEU:HD23 | 1:A:107:LEU:HA   | 1.85                     | 0.43              |
| 1:A:140:ILE:HG22 | 1:A:176:PHE:CD1  | 2.54                     | 0.43              |
| 1:B:239:MET:HE2  | 1:B:295:PRO:HD3  | 2.01                     | 0.43              |
| 1:B:241:SER:O    | 1:B:244:ALA:N    | 2.40                     | 0.43              |
| 1:A:18:VAL:O     | 1:A:19:GLU:C     | 2.59                     | 0.43              |
| 1:A:327:GLU:C    | 3:A:529:HOH:O    | 2.62                     | 0.43              |
| 1:B:135:LYS:HE2  | 1:B:135:LYS:HB2  | 1.79                     | 0.43              |
| 1:B:153:ILE:HG21 | 1:B:342:LEU:HD11 | 2.00                     | 0.43              |
| 1:B:159:ASN:HB2  | 1:B:310:LEU:O    | 2.18                     | 0.43              |
| 1:B:288:LYS:HD3  | 1:B:290:LEU:CD2  | 2.48                     | 0.43              |
| 1:A:161:HIS:NE2  | 1:A:170:LEU:HB2  | 2.34                     | 0.42              |
| 1:A:166:ASN:HA   | 1:A:167:ALA:HA   | 1.27                     | 0.42              |
| 1:B:21:MET:HG3   | 1:B:206:THR:HG21 | 2.00                     | 0.42              |
| 1:B:51:ILE:O     | 1:B:52:LEU:C     | 2.60                     | 0.42              |
| 1:B:205:THR:HG23 | 3:B:512:HOH:O    | 2.18                     | 0.42              |
| 1:B:287:VAL:HG23 | 1:B:331:TYR:HE1  | 1.83                     | 0.42              |
| 1:A:15:ILE:HG21  | 1:A:257:LEU:HD11 | 2.01                     | 0.42              |
| 1:A:37:LEU:O     | 1:A:114:TYR:CD2  | 2.72                     | 0.42              |
| 1:A:95:ASP:O     | 1:A:97:VAL:N     | 2.51                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:105:ASP:O    | 1:A:108:LEU:HB2  | 2.19                     | 0.42              |
| 1:A:139:ASP:C    | 1:A:140:ILE:CG1  | 2.92                     | 0.42              |
| 1:B:22:LYS:O     | 1:B:23:LYS:C     | 2.62                     | 0.42              |
| 1:B:281:PRO:C    | 1:B:282:LYS:C    | 2.87                     | 0.42              |
| 1:A:218:ILE:HD13 | 1:A:218:ILE:HG21 | 1.54                     | 0.42              |
| 1:B:78:LEU:O     | 1:B:80:PRO:HD3   | 2.19                     | 0.42              |
| 1:B:216:LEU:HB3  | 1:B:234:ILE:HG21 | 2.00                     | 0.42              |
| 1:B:239:MET:CE   | 1:B:295:PRO:HD3  | 2.50                     | 0.42              |
| 1:B:277:ILE:HB   | 1:B:278:SER:H    | 1.58                     | 0.42              |
| 1:B:320:ASP:OD2  | 1:B:320:ASP:C    | 2.61                     | 0.42              |
| 1:A:324:LEU:CD2  | 1:A:325:TYR:CE2  | 3.01                     | 0.42              |
| 1:B:108:LEU:HD23 | 1:B:108:LEU:HA   | 1.60                     | 0.42              |
| 1:B:157:VAL:HG22 | 1:B:200:TRP:CH2  | 2.54                     | 0.42              |
| 1:B:67:GLN:O     | 1:B:68:ILE:C     | 2.62                     | 0.42              |
| 1:B:153:ILE:HG21 | 3:B:563:HOH:O    | 2.18                     | 0.42              |
| 1:A:204:ARG:HH22 | 1:A:248:HIS:CG   | 2.38                     | 0.42              |
| 1:A:218:ILE:HD12 | 1:A:232:LYS:O    | 2.19                     | 0.42              |
| 1:B:29:GLU:O     | 1:B:30:ILE:C     | 2.61                     | 0.42              |
| 1:A:100:LYS:NZ   | 1:A:103:MET:SD   | 2.92                     | 0.42              |
| 1:A:267:ASN:ND2  | 1:A:283:GLY:O    | 2.53                     | 0.42              |
| 1:A:309:PRO:C    | 1:A:311:GLY:H    | 2.26                     | 0.42              |
| 1:B:114:TYR:CD2  | 1:B:114:TYR:C    | 2.98                     | 0.42              |
| 1:B:26:VAL:HA    | 1:B:32:LEU:HD12  | 2.01                     | 0.42              |
| 1:B:161:HIS:NE2  | 1:B:170:LEU:CD2  | 2.83                     | 0.42              |
| 1:A:272:LYS:HG2  | 1:A:321:THR:HB   | 2.02                     | 0.42              |
| 1:B:167:ALA:CA   | 1:B:349:LYS:HB3  | 2.47                     | 0.42              |
| 1:B:269:TYR:O    | 1:B:288:LYS:N    | 2.53                     | 0.42              |
| 1:B:333:ILE:C    | 1:B:335:GLN:H    | 2.27                     | 0.42              |
| 1:B:149:GLU:O    | 1:B:152:ILE:N    | 2.52                     | 0.42              |
| 1:B:152:ILE:O    | 1:B:153:ILE:C    | 2.61                     | 0.42              |
| 1:B:256:GLY:HA3  | 1:B:346:PHE:HE1  | 1.84                     | 0.41              |
| 1:B:349:LYS:HG2  | 1:B:350:THR:HG23 | 2.01                     | 0.41              |
| 1:A:270:GLU:HB3  | 1:A:290:LEU:HD11 | 2.02                     | 0.41              |
| 1:B:110:ILE:CG1  | 1:B:206:THR:HB   | 2.49                     | 0.41              |
| 1:B:249:THR:HB   | 1:B:254:PRO:HA   | 2.02                     | 0.41              |
| 1:B:291:GLY:O    | 1:B:318:VAL:HB   | 2.19                     | 0.41              |
| 1:A:76:TYR:O     | 1:A:78:LEU:N     | 2.53                     | 0.41              |
| 1:A:257:LEU:O    | 1:A:258:ILE:HG22 | 2.20                     | 0.41              |
| 1:A:284:LYS:HG2  | 3:A:580:HOH:O    | 2.20                     | 0.41              |
| 1:B:186:ARG:NE   | 1:B:334:ALA:HA   | 2.34                     | 0.41              |
| 1:A:108:LEU:O    | 1:A:112:VAL:HG23 | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:38:GLY:HA3   | 3:B:556:HOH:O    | 2.21                     | 0.41              |
| 1:B:78:LEU:C     | 1:B:80:PRO:HD3   | 2.44                     | 0.41              |
| 1:A:88:PRO:HA    | 1:A:89:PRO:HD3   | 1.61                     | 0.41              |
| 1:A:144:ASP:O    | 1:A:145:ARG:C    | 2.61                     | 0.41              |
| 1:A:285:HIS:CD2  | 1:A:285:HIS:N    | 2.88                     | 0.41              |
| 1:A:5:PRO:O      | 1:A:9:GLN:HG3    | 2.20                     | 0.41              |
| 1:A:84:GLY:HA2   | 1:A:85:MET:HA    | 1.38                     | 0.41              |
| 1:B:292:LYS:HE3  | 1:B:319:ASN:CB   | 2.48                     | 0.41              |
| 1:A:83:PHE:CE2   | 1:A:89:PRO:CD    | 3.04                     | 0.41              |
| 1:A:128:PRO:C    | 1:A:129:ILE:HD13 | 2.45                     | 0.41              |
| 1:A:216:LEU:HD23 | 1:A:216:LEU:HA   | 1.76                     | 0.41              |
| 1:A:233:GLY:C    | 1:A:234:ILE:HG13 | 2.45                     | 0.41              |
| 1:B:54:GLU:O     | 1:B:55:VAL:C     | 2.61                     | 0.41              |
| 1:B:116:LEU:HD22 | 1:B:135:LYS:HB3  | 2.02                     | 0.41              |
| 1:B:196:ARG:HA   | 1:B:263:VAL:O    | 2.20                     | 0.41              |
| 1:A:175:ILE:HG21 | 1:A:175:ILE:HD13 | 1.16                     | 0.41              |
| 1:A:193:LEU:O    | 1:A:196:ARG:HD3  | 2.20                     | 0.41              |
| 1:A:304:ASP:OD2  | 1:A:304:ASP:N    | 2.53                     | 0.41              |
| 1:B:238:ASP:C    | 3:B:612:HOH:O    | 2.64                     | 0.41              |
| 1:B:256:GLY:O    | 1:B:257:LEU:HD23 | 2.20                     | 0.41              |
| 1:A:204:ARG:HH21 | 1:A:204:ARG:HD2  | 1.70                     | 0.41              |
| 1:A:231:GLY:HA3  | 1:A:277:ILE:O    | 2.20                     | 0.41              |
| 1:B:12:ILE:HA    | 1:B:12:ILE:HD13  | 1.90                     | 0.41              |
| 1:B:18:VAL:HA    | 1:B:21:MET:HB2   | 2.03                     | 0.41              |
| 1:B:21:MET:HB3   | 1:B:37:LEU:HD11  | 2.03                     | 0.41              |
| 1:B:138:THR:CG2  | 1:B:178:ILE:HG22 | 2.50                     | 0.41              |
| 1:B:187:TYR:CE2  | 1:B:191:LYS:HG2  | 2.56                     | 0.41              |
| 1:B:251:GLN:HA   | 1:B:254:PRO:HB3  | 2.02                     | 0.41              |
| 1:B:287:VAL:HG21 | 1:B:331:TYR:OH   | 2.21                     | 0.41              |
| 1:A:147:SER:O    | 1:A:148:GLU:C    | 2.62                     | 0.41              |
| 1:B:25:MET:O     | 1:B:26:VAL:C     | 2.63                     | 0.41              |
| 1:B:341:LEU:O    | 1:B:341:LEU:CD2  | 2.69                     | 0.41              |
| 1:A:296:ASP:OD1  | 1:A:298:SER:OG   | 2.34                     | 0.40              |
| 1:B:36:PRO:HD2   | 1:B:39:LYS:HB2   | 2.03                     | 0.40              |
| 1:B:130:ASP:O    | 1:B:134:GLU:HB2  | 2.21                     | 0.40              |
| 1:B:161:HIS:HE1  | 1:B:168:TYR:CD1  | 2.36                     | 0.40              |
| 1:B:228:TYR:HD1  | 1:B:232:LYS:HG2  | 1.86                     | 0.40              |
| 1:A:7:PRO:HB3    | 1:A:174:ASP:OD1  | 2.20                     | 0.40              |
| 1:A:98:GLN:O     | 1:A:101:VAL:N    | 2.54                     | 0.40              |
| 1:A:102:GLU:H    | 1:A:102:GLU:HG2  | 1.53                     | 0.40              |
| 1:A:251:GLN:HA   | 1:A:251:GLN:NE2  | 2.36                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:288:LYS:HE3  | 1:A:328:TYR:CE2  | 2.57                     | 0.40              |
| 1:A:346:PHE:HB3  | 1:A:348:PHE:CE1  | 2.56                     | 0.40              |
| 1:B:83:PHE:CB    | 1:B:88:PRO:HB3   | 2.51                     | 0.40              |
| 1:B:104:LEU:HD23 | 1:B:104:LEU:HA   | 1.92                     | 0.40              |
| 1:B:164:THR:O    | 1:B:166:ASN:N    | 2.55                     | 0.40              |
| 1:B:212:LEU:HA   | 1:B:212:LEU:HD23 | 1.79                     | 0.40              |
| 1:B:230:PHE:C    | 3:B:623:HOH:O    | 2.64                     | 0.40              |
| 1:A:38:GLY:O     | 1:A:39:LYS:C     | 2.63                     | 0.40              |
| 1:A:180:ARG:HH11 | 1:A:180:ARG:HD2  | 1.68                     | 0.40              |
| 1:A:204:ARG:O    | 1:A:206:THR:N    | 2.55                     | 0.40              |
| 1:A:208:PHE:O    | 1:A:209:ALA:C    | 2.63                     | 0.40              |
| 1:A:245:ASN:O    | 1:A:247:CYS:N    | 2.54                     | 0.40              |
| 1:A:254:PRO:HG2  | 1:A:255:ILE:HG13 | 2.03                     | 0.40              |
| 1:B:63:SER:CB    | 3:B:548:HOH:O    | 2.70                     | 0.40              |
| 1:B:82:ASP:O     | 1:B:82:ASP:CG    | 2.62                     | 0.40              |
| 1:A:308:VAL:HA   | 1:A:309:PRO:HD3  | 1.96                     | 0.40              |
| 1:B:191:LYS:HB3  | 1:B:196:ARG:NH2  | 2.36                     | 0.40              |
| 1:A:30:ILE:HD11  | 1:A:103:MET:CG   | 2.52                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed   | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|-----------|----------|-------------|---|
| 1   | A     | 348/350 (99%) | 241 (69%) | 61 (18%)  | 46 (13%) | 0           | 1 |
| 1   | B     | 348/350 (99%) | 235 (68%) | 61 (18%)  | 52 (15%) | 0           | 0 |
| All | All   | 696/700 (99%) | 476 (68%) | 122 (18%) | 98 (14%) | 0           | 1 |

All (98) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | SER  |
| 1   | A     | 12  | ILE  |
| 1   | A     | 39  | LYS  |
| 1   | A     | 43  | ARG  |
| 1   | A     | 66  | SER  |
| 1   | A     | 95  | ASP  |
| 1   | A     | 117 | LEU  |
| 1   | A     | 118 | ARG  |
| 1   | A     | 124 | SER  |
| 1   | A     | 133 | TYR  |
| 1   | A     | 144 | ASP  |
| 1   | A     | 145 | ARG  |
| 1   | A     | 168 | TYR  |
| 1   | A     | 185 | GLN  |
| 1   | A     | 205 | THR  |
| 1   | A     | 278 | SER  |
| 1   | A     | 297 | PRO  |
| 1   | A     | 313 | GLY  |
| 1   | A     | 320 | ASP  |
| 1   | A     | 349 | LYS  |
| 1   | B     | 10  | ASP  |
| 1   | B     | 21  | MET  |
| 1   | B     | 40  | LEU  |
| 1   | B     | 76  | TYR  |
| 1   | B     | 95  | ASP  |
| 1   | B     | 96  | SER  |
| 1   | B     | 114 | TYR  |
| 1   | B     | 137 | LYS  |
| 1   | B     | 161 | HIS  |
| 1   | B     | 163 | THR  |
| 1   | B     | 165 | HIS  |
| 1   | B     | 167 | ALA  |
| 1   | B     | 176 | PHE  |
| 1   | B     | 231 | GLY  |
| 1   | B     | 241 | SER  |
| 1   | B     | 251 | GLN  |
| 1   | B     | 312 | THR  |
| 1   | B     | 320 | ASP  |
| 1   | B     | 326 | ASN  |
| 1   | A     | 3   | LYS  |
| 1   | A     | 13  | LYS  |
| 1   | A     | 29  | GLU  |
| 1   | A     | 62  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 163 | THR  |
| 1   | A     | 166 | ASN  |
| 1   | A     | 215 | GLY  |
| 1   | A     | 301 | ILE  |
| 1   | B     | 26  | VAL  |
| 1   | B     | 30  | ILE  |
| 1   | B     | 68  | ILE  |
| 1   | B     | 75  | PHE  |
| 1   | B     | 103 | MET  |
| 1   | B     | 113 | ALA  |
| 1   | B     | 182 | GLY  |
| 1   | B     | 208 | PHE  |
| 1   | B     | 215 | GLY  |
| 1   | B     | 302 | SER  |
| 1   | B     | 349 | LYS  |
| 1   | A     | 32  | LEU  |
| 1   | A     | 116 | LEU  |
| 1   | A     | 119 | GLY  |
| 1   | A     | 132 | ASN  |
| 1   | A     | 241 | SER  |
| 1   | B     | 66  | SER  |
| 1   | B     | 128 | PRO  |
| 1   | B     | 254 | PRO  |
| 1   | B     | 282 | LYS  |
| 1   | B     | 290 | LEU  |
| 1   | B     | 313 | GLY  |
| 1   | A     | 77  | THR  |
| 1   | A     | 86  | LYS  |
| 1   | A     | 96  | SER  |
| 1   | A     | 242 | LYS  |
| 1   | B     | 105 | ASP  |
| 1   | B     | 110 | ILE  |
| 1   | B     | 124 | SER  |
| 1   | B     | 216 | LEU  |
| 1   | B     | 295 | PRO  |
| 1   | A     | 295 | PRO  |
| 1   | A     | 298 | SER  |
| 1   | A     | 304 | ASP  |
| 1   | B     | 32  | LEU  |
| 1   | B     | 120 | GLY  |
| 1   | B     | 157 | VAL  |
| 1   | B     | 195 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 276 | HIS  |
| 1   | B     | 37  | LEU  |
| 1   | B     | 47  | ALA  |
| 1   | B     | 65  | ASP  |
| 1   | A     | 153 | ILE  |
| 1   | B     | 89  | PRO  |
| 1   | A     | 127 | ASP  |
| 1   | A     | 266 | GLY  |
| 1   | B     | 301 | ILE  |
| 1   | A     | 5   | PRO  |
| 1   | B     | 55  | VAL  |
| 1   | B     | 253 | ASP  |
| 1   | A     | 296 | ASP  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |   |
|-----|-------|----------------|-----------|-----------|-------------|---|
| 1   | A     | 308/308 (100%) | 212 (69%) | 96 (31%)  | 0           | 1 |
| 1   | B     | 308/308 (100%) | 207 (67%) | 101 (33%) | 0           | 1 |
| All | All   | 616/616 (100%) | 419 (68%) | 197 (32%) | 0           | 1 |

All (197) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | LYS  |
| 1   | A     | 4   | LEU  |
| 1   | A     | 6   | LYS  |
| 1   | A     | 12  | ILE  |
| 1   | A     | 13  | LYS  |
| 1   | A     | 14  | MET  |
| 1   | A     | 15  | ILE  |
| 1   | A     | 19  | GLU  |
| 1   | A     | 20  | SER  |
| 1   | A     | 25  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 26  | VAL  |
| 1   | A     | 27  | GLU  |
| 1   | A     | 29  | GLU  |
| 1   | A     | 33  | GLN  |
| 1   | A     | 37  | LEU  |
| 1   | A     | 39  | LYS  |
| 1   | A     | 42  | LYS  |
| 1   | A     | 43  | ARG  |
| 1   | A     | 44  | GLN  |
| 1   | A     | 46  | GLN  |
| 1   | A     | 50  | SER  |
| 1   | A     | 55  | VAL  |
| 1   | A     | 56  | GLN  |
| 1   | A     | 57  | GLN  |
| 1   | A     | 61  | GLN  |
| 1   | A     | 69  | LEU  |
| 1   | A     | 79  | ILE  |
| 1   | A     | 83  | PHE  |
| 1   | A     | 85  | MET  |
| 1   | A     | 86  | LYS  |
| 1   | A     | 90  | LEU  |
| 1   | A     | 92  | ASN  |
| 1   | A     | 93  | ASN  |
| 1   | A     | 97  | VAL  |
| 1   | A     | 100 | LYS  |
| 1   | A     | 101 | VAL  |
| 1   | A     | 102 | GLU  |
| 1   | A     | 116 | LEU  |
| 1   | A     | 117 | LEU  |
| 1   | A     | 121 | SER  |
| 1   | A     | 125 | SER  |
| 1   | A     | 130 | ASP  |
| 1   | A     | 135 | LYS  |
| 1   | A     | 138 | THR  |
| 1   | A     | 139 | ASP  |
| 1   | A     | 140 | ILE  |
| 1   | A     | 141 | LYS  |
| 1   | A     | 145 | ARG  |
| 1   | A     | 146 | ASP  |
| 1   | A     | 148 | GLU  |
| 1   | A     | 149 | GLU  |
| 1   | A     | 151 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 165 | HIS  |
| 1   | A     | 171 | GLU  |
| 1   | A     | 175 | ILE  |
| 1   | A     | 176 | PHE  |
| 1   | A     | 178 | ILE  |
| 1   | A     | 179 | GLU  |
| 1   | A     | 180 | ARG  |
| 1   | A     | 184 | CYS  |
| 1   | A     | 204 | ARG  |
| 1   | A     | 212 | LEU  |
| 1   | A     | 218 | ILE  |
| 1   | A     | 226 | THR  |
| 1   | A     | 232 | LYS  |
| 1   | A     | 238 | ASP  |
| 1   | A     | 242 | LYS  |
| 1   | A     | 245 | ASN  |
| 1   | A     | 247 | CYS  |
| 1   | A     | 250 | SER  |
| 1   | A     | 253 | ASP  |
| 1   | A     | 254 | PRO  |
| 1   | A     | 255 | ILE  |
| 1   | A     | 258 | ILE  |
| 1   | A     | 271 | LEU  |
| 1   | A     | 277 | ILE  |
| 1   | A     | 279 | LYS  |
| 1   | A     | 280 | LEU  |
| 1   | A     | 282 | LYS  |
| 1   | A     | 285 | HIS  |
| 1   | A     | 288 | LYS  |
| 1   | A     | 298 | SER  |
| 1   | A     | 300 | ASN  |
| 1   | A     | 302 | SER  |
| 1   | A     | 303 | LEU  |
| 1   | A     | 306 | VAL  |
| 1   | A     | 309 | PRO  |
| 1   | A     | 310 | LEU  |
| 1   | A     | 314 | ILE  |
| 1   | A     | 321 | THR  |
| 1   | A     | 324 | LEU  |
| 1   | A     | 331 | TYR  |
| 1   | A     | 336 | VAL  |
| 1   | A     | 342 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 343 | LYS  |
| 1   | A     | 345 | LYS  |
| 1   | B     | 3   | LYS  |
| 1   | B     | 4   | LEU  |
| 1   | B     | 14  | MET  |
| 1   | B     | 16  | PHE  |
| 1   | B     | 18  | VAL  |
| 1   | B     | 19  | GLU  |
| 1   | B     | 20  | SER  |
| 1   | B     | 22  | LYS  |
| 1   | B     | 26  | VAL  |
| 1   | B     | 27  | GLU  |
| 1   | B     | 31  | ASP  |
| 1   | B     | 33  | GLN  |
| 1   | B     | 34  | LYS  |
| 1   | B     | 35  | MET  |
| 1   | B     | 42  | LYS  |
| 1   | B     | 43  | ARG  |
| 1   | B     | 53  | SER  |
| 1   | B     | 57  | GLN  |
| 1   | B     | 61  | GLN  |
| 1   | B     | 63  | SER  |
| 1   | B     | 66  | SER  |
| 1   | B     | 69  | LEU  |
| 1   | B     | 70  | ASP  |
| 1   | B     | 74  | ARG  |
| 1   | B     | 78  | LEU  |
| 1   | B     | 83  | PHE  |
| 1   | B     | 85  | MET  |
| 1   | B     | 87  | LYS  |
| 1   | B     | 89  | PRO  |
| 1   | B     | 90  | LEU  |
| 1   | B     | 95  | ASP  |
| 1   | B     | 96  | SER  |
| 1   | B     | 98  | GLN  |
| 1   | B     | 103 | MET  |
| 1   | B     | 111 | GLU  |
| 1   | B     | 112 | VAL  |
| 1   | B     | 115 | SER  |
| 1   | B     | 117 | LEU  |
| 1   | B     | 118 | ARG  |
| 1   | B     | 126 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 127 | ASP  |
| 1   | B     | 129 | ILE  |
| 1   | B     | 131 | VAL  |
| 1   | B     | 134 | GLU  |
| 1   | B     | 135 | LYS  |
| 1   | B     | 137 | LYS  |
| 1   | B     | 138 | THR  |
| 1   | B     | 140 | ILE  |
| 1   | B     | 145 | ARG  |
| 1   | B     | 152 | ILE  |
| 1   | B     | 158 | LYS  |
| 1   | B     | 159 | ASN  |
| 1   | B     | 161 | HIS  |
| 1   | B     | 164 | THR  |
| 1   | B     | 166 | ASN  |
| 1   | B     | 171 | GLU  |
| 1   | B     | 173 | ILE  |
| 1   | B     | 175 | ILE  |
| 1   | B     | 177 | LYS  |
| 1   | B     | 178 | ILE  |
| 1   | B     | 179 | GLU  |
| 1   | B     | 181 | GLU  |
| 1   | B     | 183 | GLU  |
| 1   | B     | 184 | CYS  |
| 1   | B     | 192 | GLN  |
| 1   | B     | 193 | LEU  |
| 1   | B     | 195 | ASN  |
| 1   | B     | 196 | ARG  |
| 1   | B     | 197 | ARG  |
| 1   | B     | 198 | LEU  |
| 1   | B     | 200 | TRP  |
| 1   | B     | 205 | THR  |
| 1   | B     | 206 | THR  |
| 1   | B     | 217 | ARG  |
| 1   | B     | 218 | ILE  |
| 1   | B     | 226 | THR  |
| 1   | B     | 232 | LYS  |
| 1   | B     | 234 | ILE  |
| 1   | B     | 245 | ASN  |
| 1   | B     | 251 | GLN  |
| 1   | B     | 260 | LEU  |
| 1   | B     | 263 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 268 | MET  |
| 1   | B     | 277 | ILE  |
| 1   | B     | 278 | SER  |
| 1   | B     | 279 | LYS  |
| 1   | B     | 280 | LEU  |
| 1   | B     | 281 | PRO  |
| 1   | B     | 282 | LYS  |
| 1   | B     | 294 | THR  |
| 1   | B     | 295 | PRO  |
| 1   | B     | 298 | SER  |
| 1   | B     | 300 | ASN  |
| 1   | B     | 302 | SER  |
| 1   | B     | 303 | LEU  |
| 1   | B     | 310 | LEU  |
| 1   | B     | 319 | ASN  |
| 1   | B     | 321 | THR  |
| 1   | B     | 336 | VAL  |
| 1   | B     | 338 | LEU  |
| 1   | B     | 345 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 46  | GLN  |
| 1   | A     | 93  | ASN  |
| 1   | A     | 159 | ASN  |
| 1   | A     | 245 | ASN  |
| 1   | A     | 251 | GLN  |
| 1   | A     | 267 | ASN  |
| 1   | A     | 300 | ASN  |
| 1   | A     | 326 | ASN  |
| 1   | A     | 337 | ASN  |
| 1   | A     | 347 | ASN  |
| 1   | B     | 33  | GLN  |
| 1   | B     | 46  | GLN  |
| 1   | B     | 67  | GLN  |
| 1   | B     | 106 | ASN  |
| 1   | B     | 165 | HIS  |
| 1   | B     | 214 | GLN  |
| 1   | B     | 267 | ASN  |
| 1   | B     | 273 | HIS  |
| 1   | B     | 300 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 319 | ASN  |
| 1   | B     | 326 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 2   | FRM  | B     | 502 | -    | 29,31,31     | 1.68 | 7 (24%)     | 39,43,43    | 2.70 | 12 (30%)    |
| 2   | FRM  | A     | 501 | -    | 29,31,31     | 1.57 | 6 (20%)     | 39,43,43    | 2.79 | 20 (51%)    |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | FRM  | B     | 502 | -    | -       | 1/10/20/20 | 0/4/4/4 |
| 2   | FRM  | A     | 501 | -    | -       | 5/10/20/20 | 0/4/4/4 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 502 | FRM  | C29-N26 | -4.16 | 1.42        | 1.46     |
| 2   | A     | 501 | FRM  | C13-N12 | -3.91 | 1.31        | 1.37     |
| 2   | B     | 502 | FRM  | C3-C2   | -3.68 | 1.35        | 1.40     |
| 2   | B     | 502 | FRM  | C40-C31 | -3.39 | 1.43        | 1.48     |
| 2   | A     | 501 | FRM  | C4-C13  | -3.10 | 1.42        | 1.47     |
| 2   | B     | 502 | FRM  | C7-C2   | -2.85 | 1.45        | 1.51     |
| 2   | A     | 501 | FRM  | C4-C3   | -2.78 | 1.37        | 1.41     |
| 2   | B     | 502 | FRM  | C46-C40 | -2.59 | 1.35        | 1.39     |
| 2   | A     | 501 | FRM  | C3-C2   | -2.55 | 1.37        | 1.40     |
| 2   | A     | 501 | FRM  | C3-N10  | -2.32 | 1.34        | 1.38     |
| 2   | B     | 502 | FRM  | C13-N12 | -2.10 | 1.34        | 1.37     |
| 2   | A     | 501 | FRM  | C46-C45 | -2.08 | 1.35        | 1.38     |
| 2   | B     | 502 | FRM  | C33-N26 | -2.06 | 1.41        | 1.46     |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 502 | FRM  | C32-C33-N26 | 10.52 | 120.58      | 111.19   |
| 2   | A     | 501 | FRM  | C46-C40-C31 | -5.88 | 114.18      | 121.22   |
| 2   | A     | 501 | FRM  | C30-C29-N26 | -5.70 | 108.39      | 112.89   |
| 2   | A     | 501 | FRM  | C4-C13-N12  | 5.13  | 120.34      | 114.93   |
| 2   | B     | 502 | FRM  | C29-N26-C33 | 5.01  | 114.75      | 109.78   |
| 2   | A     | 501 | FRM  | C3-C4-C13   | -4.96 | 114.65      | 119.42   |
| 2   | B     | 502 | FRM  | C3-C4-C13   | -4.89 | 114.72      | 119.42   |
| 2   | B     | 502 | FRM  | C32-C31-C30 | -4.52 | 116.87      | 120.63   |
| 2   | A     | 501 | FRM  | N12-C11-N10 | -4.34 | 117.57      | 123.08   |
| 2   | A     | 501 | FRM  | C43-C42-C40 | -4.33 | 116.18      | 120.80   |
| 2   | A     | 501 | FRM  | C46-C45-C44 | -4.05 | 114.21      | 118.38   |
| 2   | B     | 502 | FRM  | N12-C11-N10 | -3.97 | 118.05      | 123.08   |
| 2   | A     | 501 | FRM  | C13-N12-C11 | -3.75 | 121.73      | 123.90   |
| 2   | B     | 502 | FRM  | C23-N26-C33 | 3.22  | 119.82      | 111.24   |
| 2   | A     | 501 | FRM  | C45-C46-C40 | 3.22  | 124.23      | 120.80   |
| 2   | A     | 501 | FRM  | C6-C5-C4    | -3.20 | 114.01      | 119.80   |
| 2   | B     | 502 | FRM  | C20-C23-N26 | 3.20  | 122.92      | 113.93   |
| 2   | A     | 501 | FRM  | C4-C3-N10   | -3.19 | 119.18      | 122.33   |
| 2   | A     | 501 | FRM  | C32-C31-C30 | -3.17 | 118.00      | 120.63   |
| 2   | A     | 501 | FRM  | C20-C23-N26 | -3.16 | 105.05      | 113.93   |
| 2   | A     | 501 | FRM  | C42-C40-C31 | 3.14  | 124.97      | 121.22   |
| 2   | A     | 501 | FRM  | C32-C33-N26 | -3.13 | 108.39      | 111.19   |
| 2   | B     | 502 | FRM  | C5-C4-C13   | 3.04  | 124.59      | 120.13   |
| 2   | B     | 502 | FRM  | C4-C3-C2    | -2.85 | 118.17      | 120.56   |
| 2   | B     | 502 | FRM  | C30-C29-N26 | 2.61  | 114.95      | 112.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 502 | FRM  | C1-C2-C3    | 2.58  | 121.37      | 118.11   |
| 2   | A     | 501 | FRM  | F1-C44-C45  | -2.57 | 114.43      | 118.55   |
| 2   | A     | 501 | FRM  | C5-C6-C1    | 2.52  | 123.49      | 120.24   |
| 2   | A     | 501 | FRM  | C42-C43-C44 | 2.51  | 120.96      | 118.38   |
| 2   | A     | 501 | FRM  | C4-C3-C2    | 2.34  | 122.53      | 120.56   |
| 2   | A     | 501 | FRM  | C5-C4-C3    | 2.30  | 123.23      | 118.51   |
| 2   | B     | 502 | FRM  | F1-C44-C43  | 2.05  | 121.84      | 118.55   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

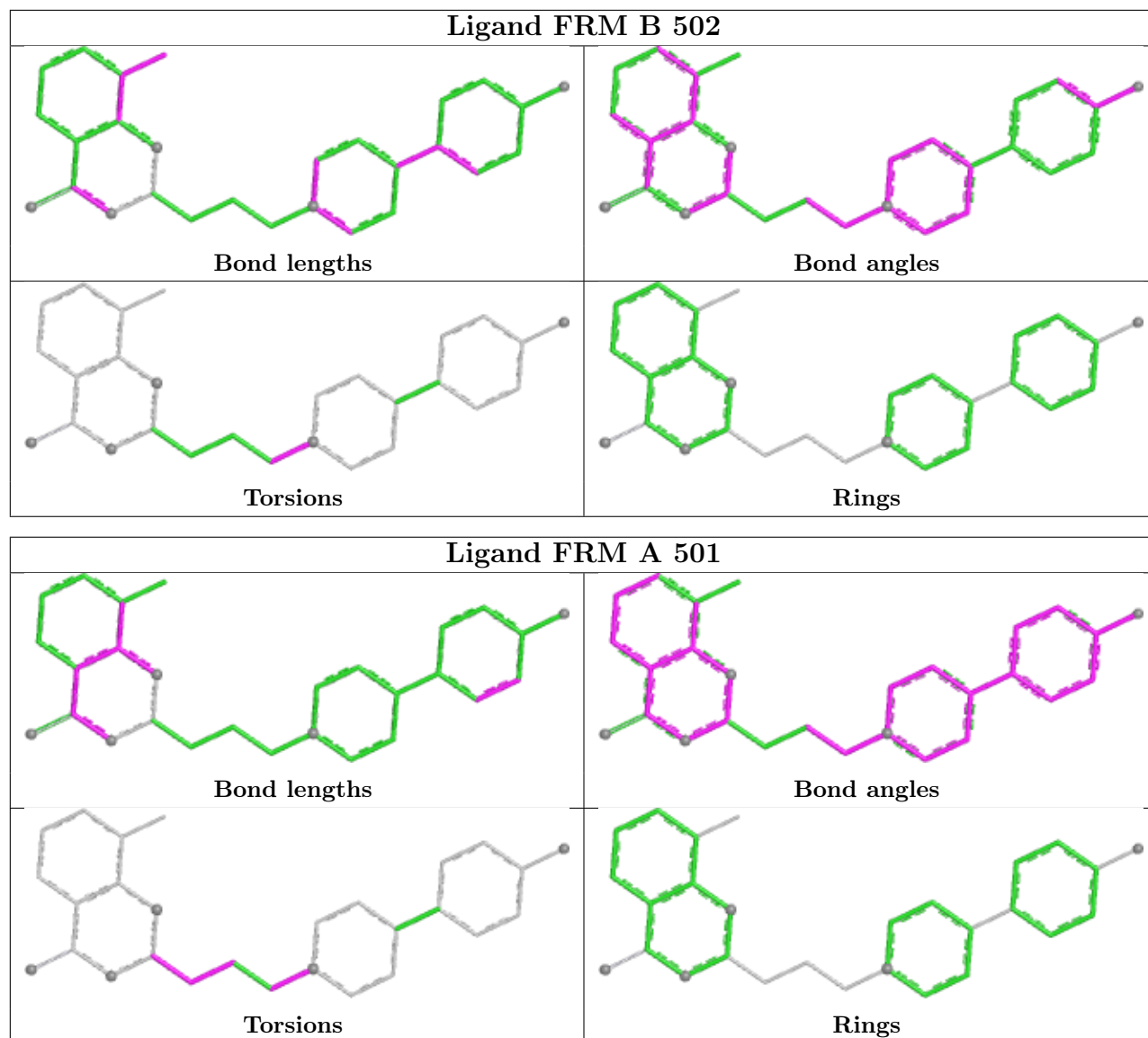
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 501 | FRM  | N10-C11-C17-C20 |
| 2   | A     | 501 | FRM  | C11-C17-C20-C23 |
| 2   | A     | 501 | FRM  | C20-C23-N26-C29 |
| 2   | A     | 501 | FRM  | C20-C23-N26-C33 |
| 2   | B     | 502 | FRM  | C20-C23-N26-C29 |
| 2   | A     | 501 | FRM  | N12-C11-C17-C20 |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 501 | FRM  | 2       | 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 350/350 (100%) | -0.27  | 2 (0%) 85 69 | 2, 10, 26, 38         | 0     |
| 1   | B     | 350/350 (100%) | -0.15  | 3 (0%) 81 61 | 2, 12, 28, 43         | 0     |
| All | All   | 700/700 (100%) | -0.21  | 5 (0%) 84 66 | 2, 11, 27, 43         | 0     |

All (5) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 124 | SER  | 3.2  |
| 1   | B     | 123 | ASP  | 2.7  |
| 1   | B     | 122 | ASP  | 2.3  |
| 1   | A     | 126 | LYS  | 2.2  |
| 1   | A     | 124 | SER  | 2.1  |

### 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](#)

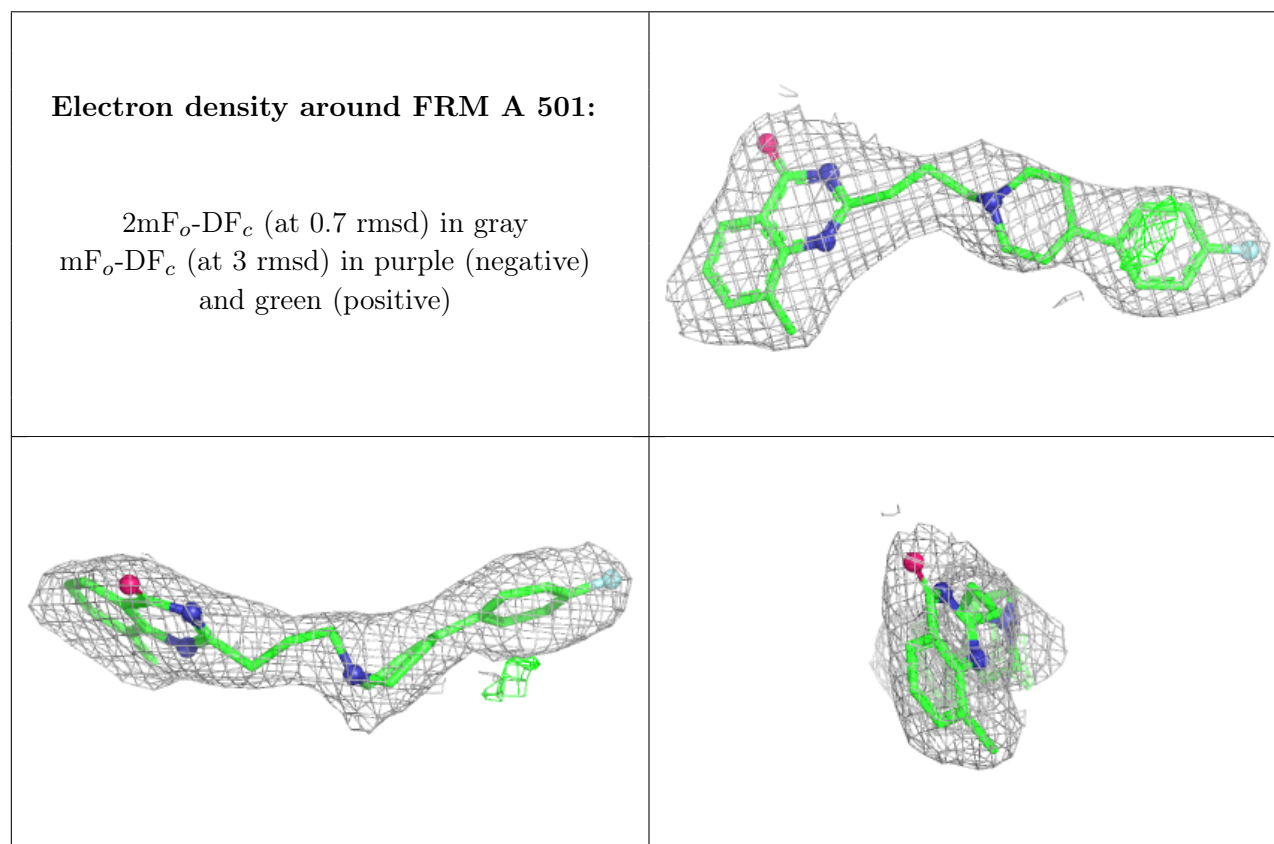
There are no oligosaccharides in this entry.

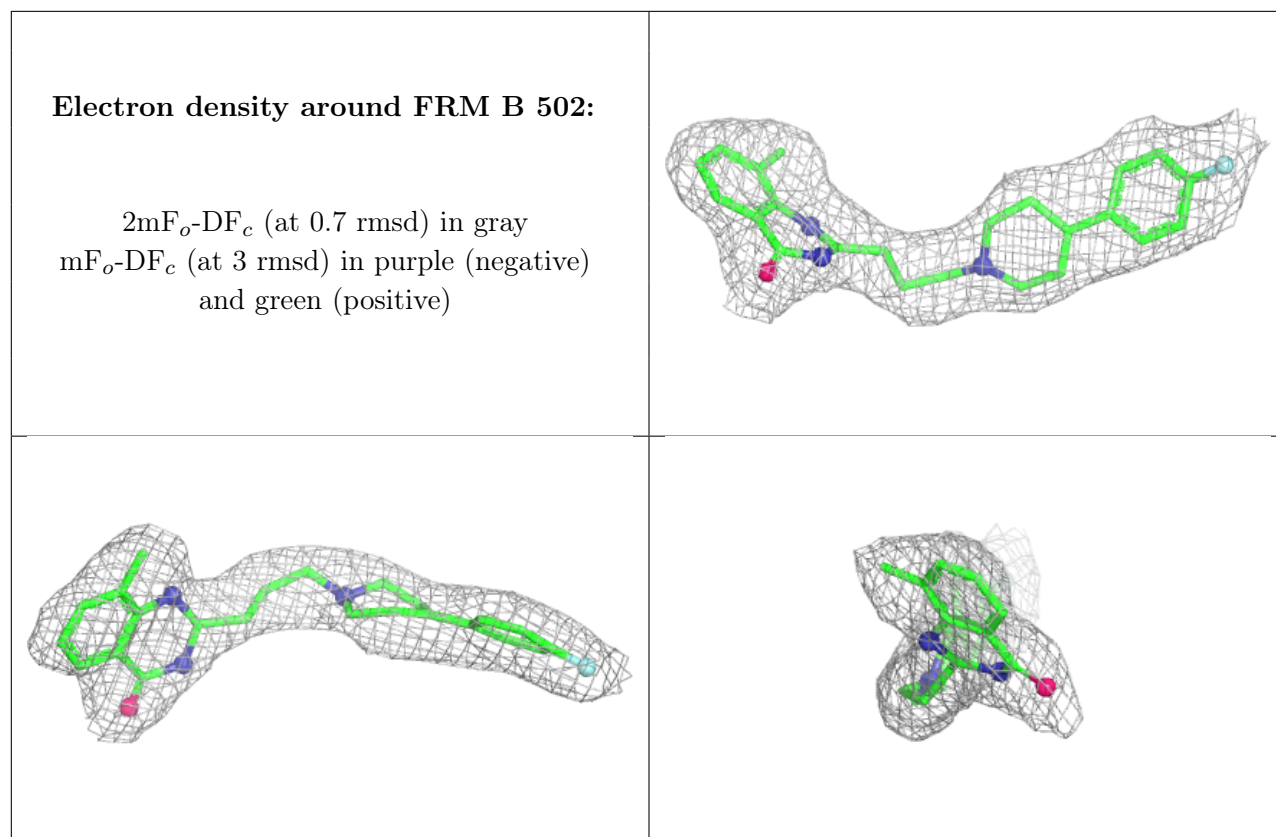
### 6.4 Ligands [i](#)

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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | FRM  | A     | 501 | 28/28 | 0.95 | 0.09 | 2,7,16,17                   | 0     |
| 2   | FRM  | B     | 502 | 28/28 | 0.96 | 0.08 | 2,2,6,9                     | 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.