



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:33 PM UTC

PDB ID : 1PYG / pdb\_00001pyg  
Title : STRUCTURAL BASIS FOR THE ACTIVATION OF GLYCOGEN PHOSPHORYLASE B BY ADENOSINE MONOPHOSPHATE  
Authors : Sprang, S.  
Deposited on : 1992-07-07  
Resolution : 2.87 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

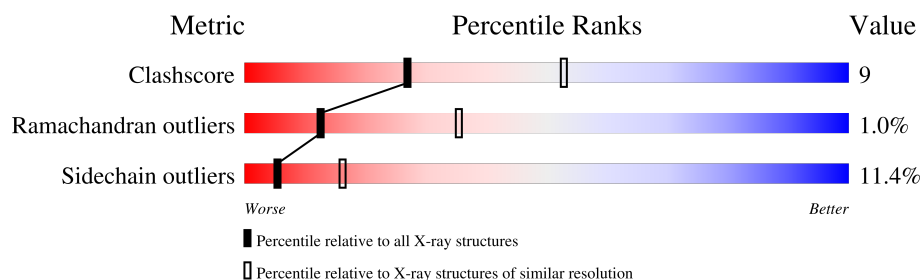
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.87 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                      | 3801 (2.90-2.86)                                      |
| Ramachandran outliers | 187476                      | 3699 (2.90-2.86)                                      |
| Sidechain outliers    | 187428                      | 3702 (2.90-2.86)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 842    |                  |
| 1   | B     | 842    |                  |
| 1   | C     | 842    |                  |
| 1   | D     | 842    |                  |

## 2 Entry composition [i](#)

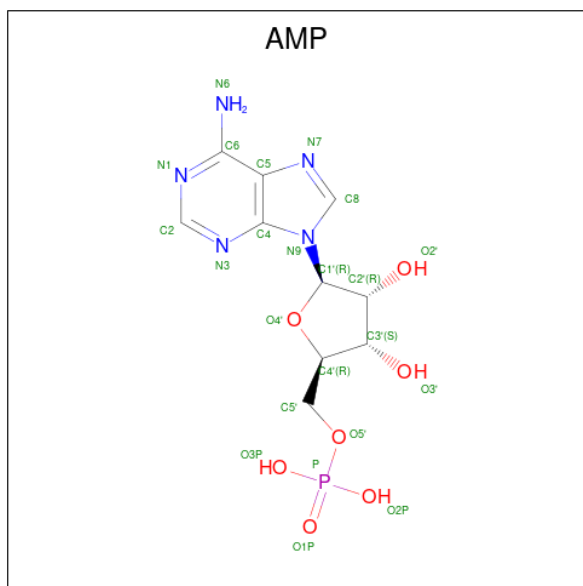
There are 3 unique types of molecules in this entry. The entry contains 26214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLYCOGEN PHOSPHORYLASE B.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 801      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6512  | 4147 | 1155 | 1180 | 30 |         |         |       |
| 1   | B     | 791      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6434  | 4099 | 1137 | 1168 | 30 |         |         |       |
| 1   | C     | 801      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6512  | 4147 | 1155 | 1180 | 30 |         |         |       |
| 1   | D     | 801      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6512  | 4147 | 1155 | 1180 | 30 |         |         |       |

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



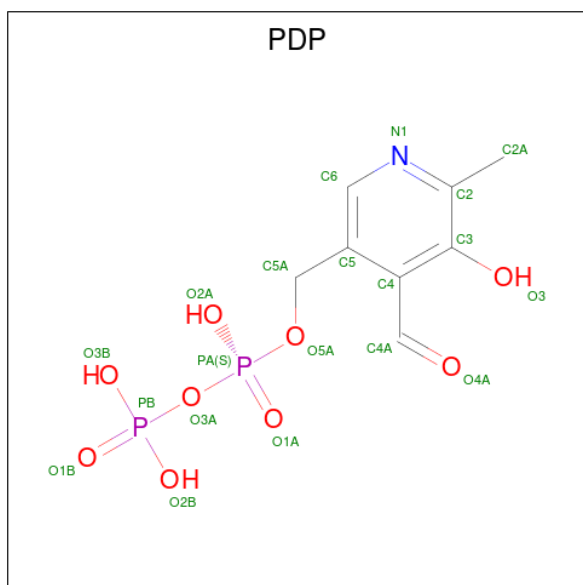
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 23    | 10 | 5 | 7 | 1 |         |         |
| 2   | B     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 23    | 10 | 5 | 7 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 2   | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 23    | 10 | 5 | 7 | 1 |         |         |
| 2   | D     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 23    | 10 | 5 | 7 | 1 |         |         |

- Molecule 3 is PYRIDOXAL-5'-DIPHOSPHATE (CCD ID: PDP) (formula:  $C_8H_{11}NO_9P_2$ ).



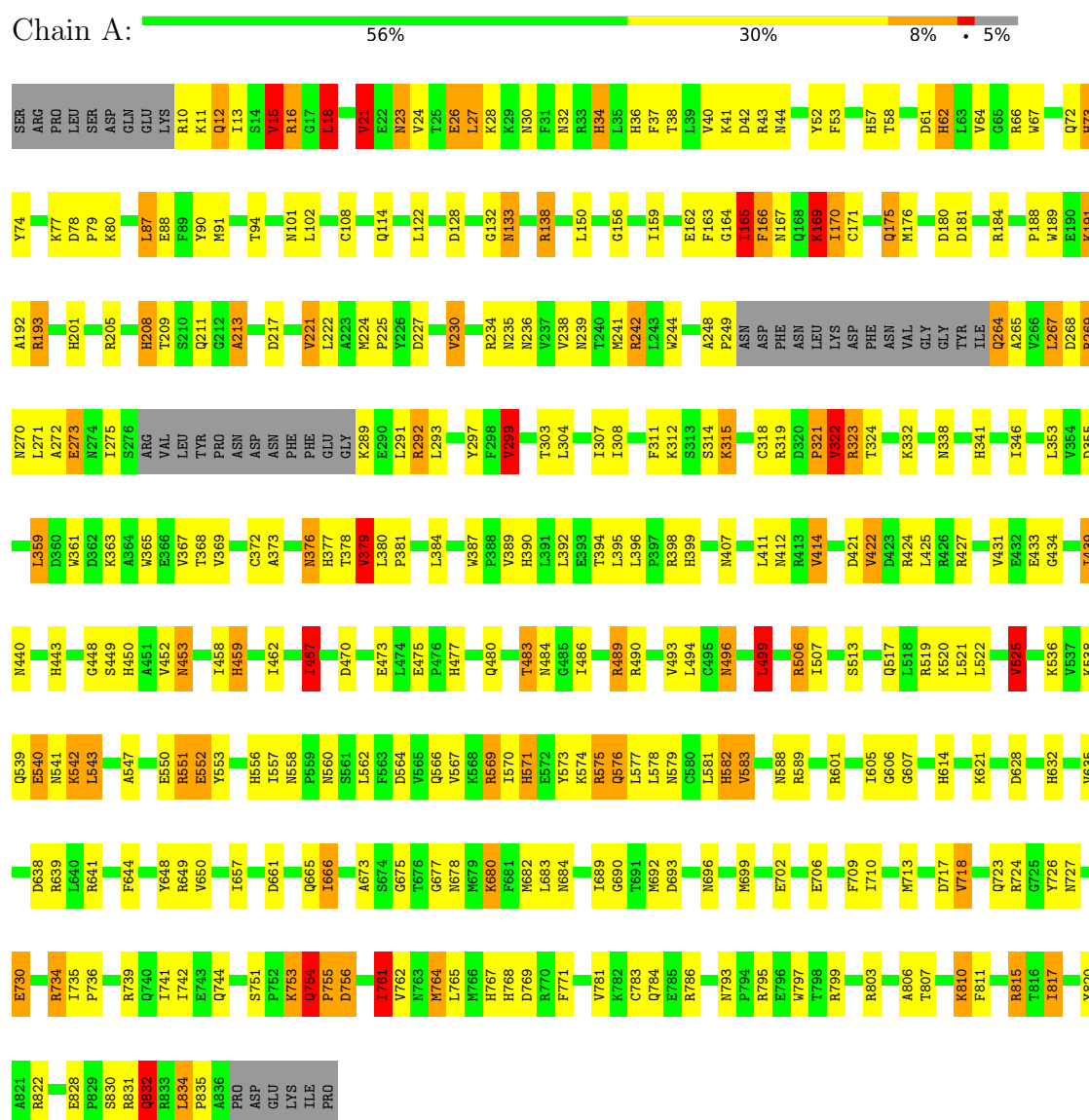
| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O  | P | 0       | 1       |
|     |       |          | 38    | 16 | 2 | 16 | 4 |         |         |
| 3   | B     | 1        | Total | C  | N | O  | P | 0       | 1       |
|     |       |          | 38    | 16 | 2 | 16 | 4 |         |         |
| 3   | C     | 1        | Total | C  | N | O  | P | 0       | 1       |
|     |       |          | 38    | 16 | 2 | 16 | 4 |         |         |
| 3   | D     | 1        | Total | C  | N | O  | P | 0       | 1       |
|     |       |          | 38    | 16 | 2 | 16 | 4 |         |         |

### 3 Residue-property plots

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

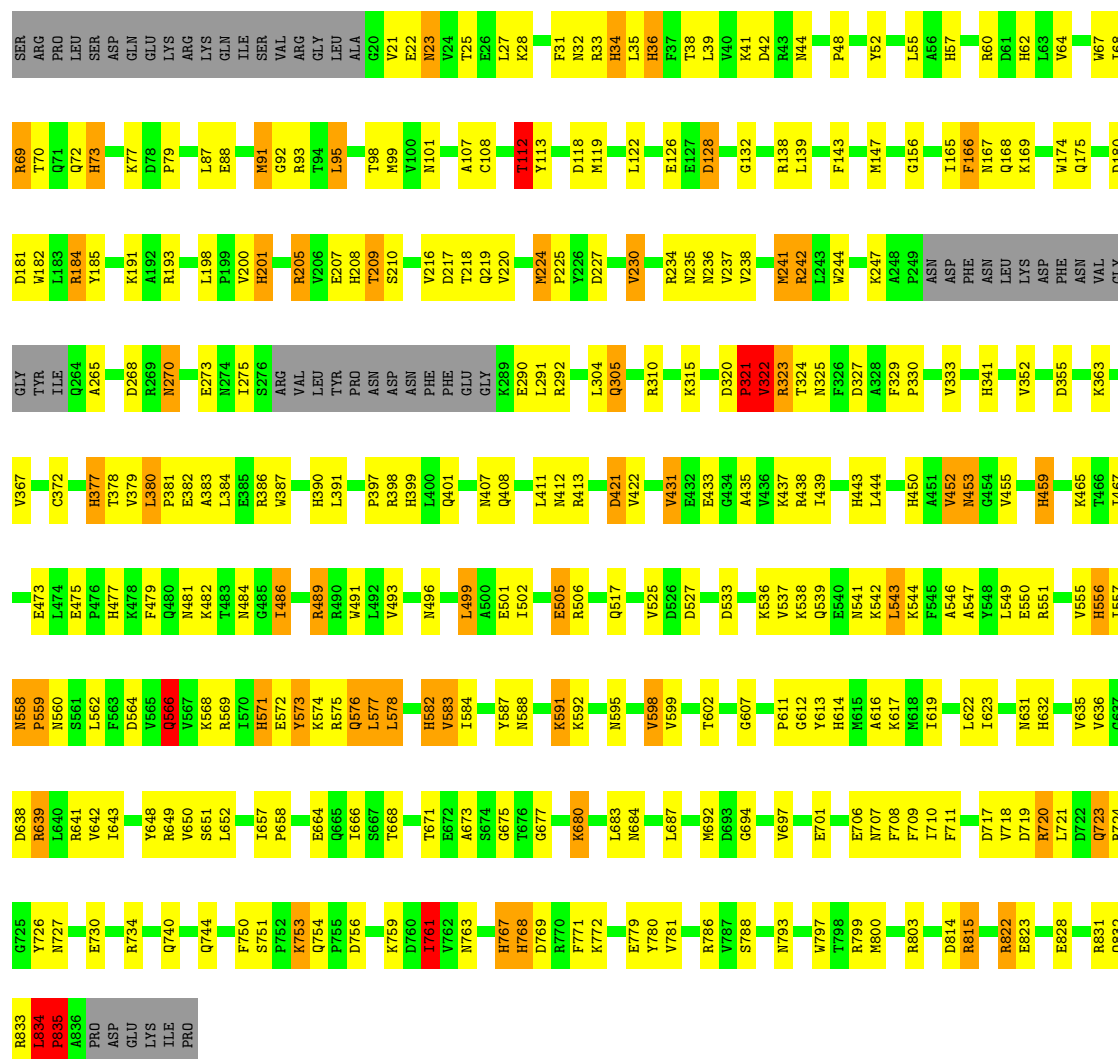
Note EDS was not executed.

#### • Molecule 1: GLYCOGEN PHOSPHORYLASE B



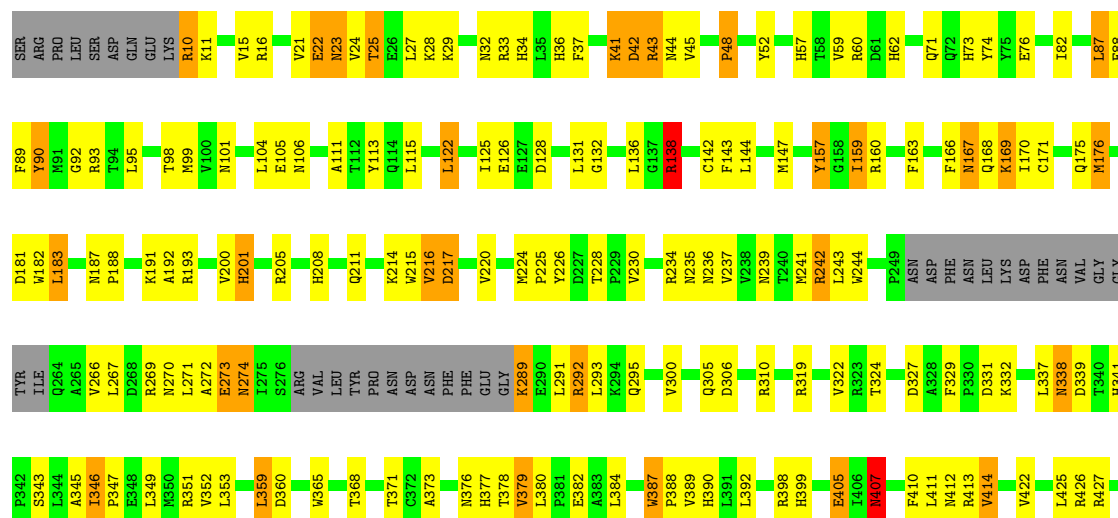
#### • Molecule 1: GLYCOGEN PHOSPHORYLASE B

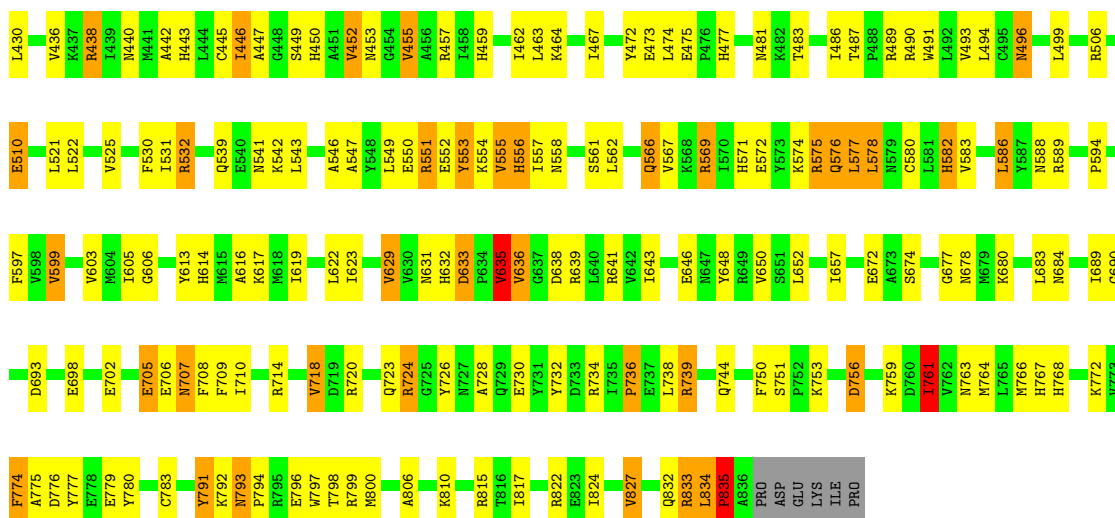




● Molecule 1: GLYCOGEN PHOSPHORYLASE B

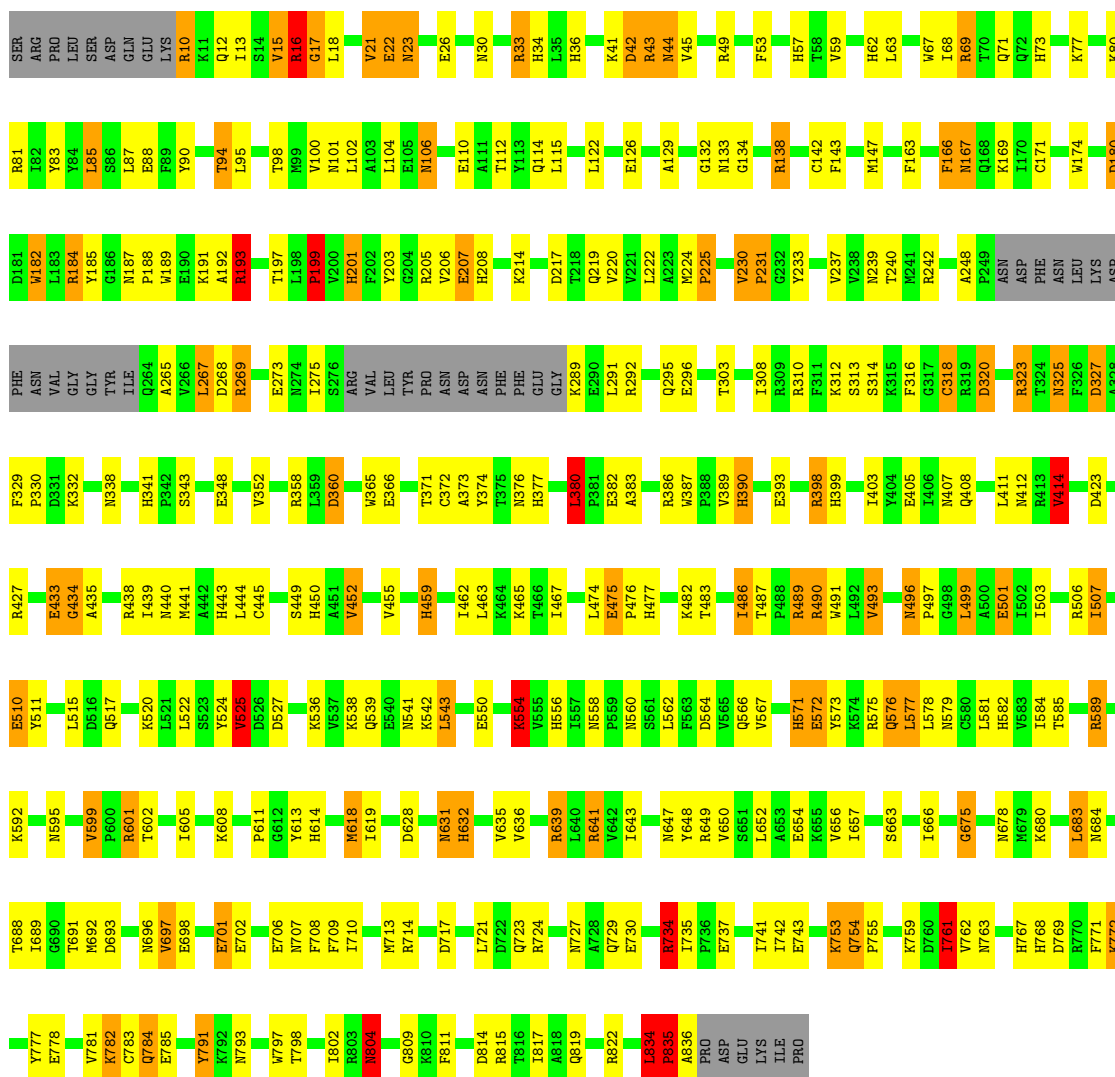
Chain C: 54% 33% 8% 5%





### ● Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain D: 55% 30% 9% 5%



## 4 Data and refinement statistics

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

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | P 21 21 2                                       | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 169.90Å 209.90Å 123.40Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 8.00 – 2.87                                     | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (8.00-2.87)                     | Depositor |
| $R_{merge}$                                              | (Not available)                                 | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | X-PLOR                                          | Depositor |
| R, $R_{free}$                                            | 0.185 , (Not available)                         | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 26214                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 15.0                                            | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$      | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 1.09         | 33/6655 (0.5%)   | 1.94        | 188/9001 (2.1%)  |
| 1   | B     | 1.10         | 34/6577 (0.5%)   | 1.89        | 167/8898 (1.9%)  |
| 1   | C     | 1.05         | 28/6655 (0.4%)   | 1.87        | 161/9001 (1.8%)  |
| 1   | D     | 1.10         | 31/6655 (0.5%)   | 1.90        | 174/9001 (1.9%)  |
| All | All   | 1.08         | 126/26542 (0.5%) | 1.90        | 690/35901 (1.9%) |

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                   | 2                   |
| 1   | B     | 0                   | 2                   |
| 1   | C     | 0                   | 2                   |
| 1   | D     | 0                   | 2                   |
| All | All   | 0                   | 8                   |

All (126) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 230 | VAL  | CA-CB   | 9.13  | 1.62        | 1.54     |
| 1   | B     | 230 | VAL  | CA-CB   | 8.78  | 1.61        | 1.54     |
| 1   | D     | 36  | HIS  | CD2-NE2 | -7.89 | 1.29        | 1.37     |
| 1   | A     | 459 | HIS  | CD2-NE2 | -7.66 | 1.29        | 1.37     |
| 1   | C     | 341 | HIS  | CD2-NE2 | -7.62 | 1.29        | 1.37     |
| 1   | A     | 377 | HIS  | CD2-NE2 | -7.51 | 1.29        | 1.37     |
| 1   | D     | 657 | ILE  | CA-CB   | 7.51  | 1.59        | 1.53     |
| 1   | B     | 583 | VAL  | CA-CB   | 7.51  | 1.64        | 1.54     |
| 1   | D     | 571 | HIS  | CD2-NE2 | -7.50 | 1.29        | 1.37     |
| 1   | A     | 34  | HIS  | CD2-NE2 | -7.47 | 1.29        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 761 | ILE  | CA-CB   | 7.44  | 1.64        | 1.54     |
| 1   | B     | 36  | HIS  | CD2-NE2 | -7.34 | 1.29        | 1.37     |
| 1   | A     | 201 | HIS  | CD2-NE2 | -7.30 | 1.29        | 1.37     |
| 1   | D     | 34  | HIS  | CD2-NE2 | -7.29 | 1.29        | 1.37     |
| 1   | B     | 459 | HIS  | CD2-NE2 | -7.25 | 1.29        | 1.37     |
| 1   | B     | 341 | HIS  | CD2-NE2 | -7.11 | 1.30        | 1.37     |
| 1   | D     | 201 | HIS  | CD2-NE2 | -7.10 | 1.30        | 1.37     |
| 1   | C     | 377 | HIS  | CD2-NE2 | -7.07 | 1.30        | 1.37     |
| 1   | A     | 571 | HIS  | CD2-NE2 | -7.06 | 1.30        | 1.37     |
| 1   | D     | 632 | HIS  | CD2-NE2 | -6.93 | 1.30        | 1.37     |
| 1   | B     | 571 | HIS  | CD2-NE2 | -6.93 | 1.30        | 1.37     |
| 1   | B     | 201 | HIS  | CD2-NE2 | -6.92 | 1.30        | 1.37     |
| 1   | A     | 399 | HIS  | CD2-NE2 | -6.91 | 1.30        | 1.37     |
| 1   | D     | 582 | HIS  | CD2-NE2 | -6.91 | 1.30        | 1.37     |
| 1   | B     | 377 | HIS  | CD2-NE2 | -6.90 | 1.30        | 1.37     |
| 1   | D     | 493 | VAL  | CA-CB   | 6.90  | 1.64        | 1.54     |
| 1   | A     | 583 | VAL  | CA-CB   | 6.89  | 1.63        | 1.54     |
| 1   | C     | 443 | HIS  | CD2-NE2 | -6.87 | 1.30        | 1.37     |
| 1   | B     | 399 | HIS  | CD2-NE2 | -6.84 | 1.30        | 1.37     |
| 1   | B     | 767 | HIS  | CD2-NE2 | -6.81 | 1.30        | 1.37     |
| 1   | C     | 34  | HIS  | CD2-NE2 | -6.79 | 1.30        | 1.37     |
| 1   | B     | 73  | HIS  | CD2-NE2 | -6.76 | 1.30        | 1.37     |
| 1   | D     | 377 | HIS  | CD2-NE2 | -6.76 | 1.30        | 1.37     |
| 1   | B     | 632 | HIS  | CD2-NE2 | -6.75 | 1.30        | 1.37     |
| 1   | D     | 73  | HIS  | CD2-NE2 | -6.74 | 1.30        | 1.37     |
| 1   | A     | 62  | HIS  | CD2-NE2 | -6.72 | 1.30        | 1.37     |
| 1   | A     | 36  | HIS  | CD2-NE2 | -6.70 | 1.30        | 1.37     |
| 1   | A     | 443 | HIS  | CD2-NE2 | -6.68 | 1.30        | 1.37     |
| 1   | D     | 230 | VAL  | CA-CB   | 6.66  | 1.62        | 1.54     |
| 1   | C     | 459 | HIS  | CD2-NE2 | -6.65 | 1.30        | 1.37     |
| 1   | C     | 556 | HIS  | CD2-NE2 | -6.62 | 1.30        | 1.37     |
| 1   | B     | 34  | HIS  | CD2-NE2 | -6.60 | 1.30        | 1.37     |
| 1   | A     | 165 | ILE  | CA-CB   | 6.59  | 1.63        | 1.54     |
| 1   | C     | 632 | HIS  | CD2-NE2 | -6.59 | 1.30        | 1.37     |
| 1   | C     | 571 | HIS  | CD2-NE2 | -6.52 | 1.30        | 1.37     |
| 1   | D     | 341 | HIS  | CD2-NE2 | -6.52 | 1.30        | 1.37     |
| 1   | D     | 459 | HIS  | CD2-NE2 | -6.51 | 1.30        | 1.37     |
| 1   | A     | 582 | HIS  | CD2-NE2 | -6.50 | 1.30        | 1.37     |
| 1   | C     | 635 | VAL  | CA-CB   | 6.48  | 1.63        | 1.54     |
| 1   | B     | 443 | HIS  | CD2-NE2 | -6.47 | 1.30        | 1.37     |
| 1   | A     | 73  | HIS  | CD2-NE2 | -6.46 | 1.30        | 1.37     |
| 1   | C     | 477 | HIS  | CD2-NE2 | -6.45 | 1.30        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 443 | HIS  | CD2-NE2 | -6.44 | 1.30        | 1.37     |
| 1   | C     | 768 | HIS  | CD2-NE2 | -6.41 | 1.30        | 1.37     |
| 1   | A     | 450 | HIS  | CD2-NE2 | -6.41 | 1.30        | 1.37     |
| 1   | D     | 399 | HIS  | CD2-NE2 | -6.36 | 1.30        | 1.37     |
| 1   | C     | 399 | HIS  | CD2-NE2 | -6.35 | 1.30        | 1.37     |
| 1   | D     | 556 | HIS  | CD2-NE2 | -6.33 | 1.30        | 1.37     |
| 1   | C     | 36  | HIS  | CD2-NE2 | -6.30 | 1.30        | 1.37     |
| 1   | B     | 57  | HIS  | CD2-NE2 | -6.30 | 1.30        | 1.37     |
| 1   | D     | 57  | HIS  | CD2-NE2 | -6.26 | 1.30        | 1.37     |
| 1   | D     | 390 | HIS  | CD2-NE2 | -6.25 | 1.30        | 1.37     |
| 1   | A     | 341 | HIS  | CD2-NE2 | -6.24 | 1.30        | 1.37     |
| 1   | C     | 452 | VAL  | CA-CB   | 6.18  | 1.62        | 1.54     |
| 1   | B     | 477 | HIS  | CD2-NE2 | -6.18 | 1.31        | 1.37     |
| 1   | A     | 477 | HIS  | CD2-NE2 | -6.17 | 1.31        | 1.37     |
| 1   | C     | 57  | HIS  | CD2-NE2 | -6.14 | 1.31        | 1.37     |
| 1   | B     | 208 | HIS  | CD2-NE2 | -6.11 | 1.31        | 1.37     |
| 1   | D     | 450 | HIS  | CD2-NE2 | -6.10 | 1.31        | 1.37     |
| 1   | A     | 614 | HIS  | CD2-NE2 | -6.09 | 1.31        | 1.37     |
| 1   | C     | 582 | HIS  | CD2-NE2 | -6.07 | 1.31        | 1.37     |
| 1   | B     | 450 | HIS  | CD2-NE2 | -6.06 | 1.31        | 1.37     |
| 1   | D     | 768 | HIS  | CD2-NE2 | -6.03 | 1.31        | 1.37     |
| 1   | B     | 450 | HIS  | CG-ND1  | -6.02 | 1.31        | 1.38     |
| 1   | B     | 62  | HIS  | CD2-NE2 | -5.97 | 1.31        | 1.37     |
| 1   | D     | 571 | HIS  | CG-ND1  | -5.93 | 1.31        | 1.38     |
| 1   | C     | 450 | HIS  | CD2-NE2 | -5.92 | 1.31        | 1.37     |
| 1   | C     | 767 | HIS  | CD2-NE2 | -5.89 | 1.31        | 1.37     |
| 1   | B     | 582 | HIS  | CD2-NE2 | -5.84 | 1.31        | 1.37     |
| 1   | D     | 767 | HIS  | CD2-NE2 | -5.84 | 1.31        | 1.37     |
| 1   | C     | 614 | HIS  | CD2-NE2 | -5.83 | 1.31        | 1.37     |
| 1   | B     | 209 | THR  | CA-CB   | 5.83  | 1.61        | 1.53     |
| 1   | A     | 767 | HIS  | CD2-NE2 | -5.82 | 1.31        | 1.37     |
| 1   | D     | 614 | HIS  | CD2-NE2 | -5.78 | 1.31        | 1.37     |
| 1   | A     | 556 | HIS  | CD2-NE2 | -5.76 | 1.31        | 1.37     |
| 1   | A     | 57  | HIS  | CD2-NE2 | -5.75 | 1.31        | 1.37     |
| 1   | A     | 768 | HIS  | CD2-NE2 | -5.71 | 1.31        | 1.37     |
| 1   | C     | 62  | HIS  | CD2-NE2 | -5.70 | 1.31        | 1.37     |
| 1   | C     | 443 | HIS  | CG-ND1  | -5.67 | 1.32        | 1.38     |
| 1   | C     | 718 | VAL  | CA-CB   | 5.64  | 1.62        | 1.54     |
| 1   | B     | 390 | HIS  | CD2-NE2 | -5.63 | 1.31        | 1.37     |
| 1   | C     | 761 | ILE  | CA-CB   | 5.62  | 1.61        | 1.54     |
| 1   | C     | 208 | HIS  | CD2-NE2 | -5.61 | 1.31        | 1.37     |
| 1   | B     | 556 | HIS  | CD2-NE2 | -5.58 | 1.31        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 57  | HIS  | CG-ND1  | -5.57 | 1.32        | 1.38     |
| 1   | C     | 201 | HIS  | CD2-NE2 | -5.57 | 1.31        | 1.37     |
| 1   | B     | 201 | HIS  | CG-ND1  | -5.57 | 1.32        | 1.38     |
| 1   | D     | 62  | HIS  | CD2-NE2 | -5.57 | 1.31        | 1.37     |
| 1   | B     | 761 | ILE  | CA-CB   | 5.54  | 1.61        | 1.54     |
| 1   | A     | 761 | ILE  | CA-CB   | 5.49  | 1.61        | 1.54     |
| 1   | C     | 170 | ILE  | CA-CB   | 5.44  | 1.59        | 1.53     |
| 1   | A     | 208 | HIS  | CD2-NE2 | -5.43 | 1.31        | 1.37     |
| 1   | C     | 73  | HIS  | CD2-NE2 | -5.41 | 1.31        | 1.37     |
| 1   | A     | 390 | HIS  | CD2-NE2 | -5.40 | 1.31        | 1.37     |
| 1   | B     | 768 | HIS  | CD2-NE2 | -5.39 | 1.31        | 1.37     |
| 1   | D     | 689 | ILE  | CA-CB   | 5.38  | 1.60        | 1.54     |
| 1   | D     | 477 | HIS  | CD2-NE2 | -5.37 | 1.31        | 1.37     |
| 1   | A     | 36  | HIS  | CG-ND1  | -5.36 | 1.32        | 1.38     |
| 1   | A     | 718 | VAL  | CA-CB   | 5.36  | 1.61        | 1.54     |
| 1   | B     | 36  | HIS  | CG-ND1  | -5.36 | 1.32        | 1.38     |
| 1   | A     | 632 | HIS  | CD2-NE2 | -5.33 | 1.31        | 1.37     |
| 1   | B     | 614 | HIS  | CD2-NE2 | -5.33 | 1.31        | 1.37     |
| 1   | B     | 443 | HIS  | CG-ND1  | -5.26 | 1.32        | 1.38     |
| 1   | A     | 34  | HIS  | CG-ND1  | -5.26 | 1.32        | 1.38     |
| 1   | A     | 767 | HIS  | CG-ND1  | -5.24 | 1.32        | 1.38     |
| 1   | D     | 414 | VAL  | CA-CB   | 5.22  | 1.61        | 1.54     |
| 1   | B     | 571 | HIS  | CG-ND1  | -5.18 | 1.32        | 1.38     |
| 1   | B     | 582 | HIS  | CG-ND1  | -5.18 | 1.32        | 1.38     |
| 1   | A     | 209 | THR  | CA-CB   | 5.13  | 1.61        | 1.53     |
| 1   | D     | 208 | HIS  | CD2-NE2 | -5.11 | 1.32        | 1.37     |
| 1   | A     | 459 | HIS  | CG-ND1  | -5.10 | 1.32        | 1.38     |
| 1   | B     | 767 | HIS  | CG-ND1  | -5.10 | 1.32        | 1.38     |
| 1   | A     | 377 | HIS  | CG-ND1  | -5.08 | 1.32        | 1.38     |
| 1   | D     | 73  | HIS  | CG-ND1  | -5.08 | 1.32        | 1.38     |
| 1   | C     | 230 | VAL  | CA-CB   | 5.07  | 1.60        | 1.54     |
| 1   | D     | 36  | HIS  | CG-ND1  | -5.03 | 1.32        | 1.38     |

All (690) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | C     | 556 | HIS  | CA-CB-CG | -13.23 | 100.57      | 113.80   |
| 1   | B     | 556 | HIS  | CA-CB-CG | -12.58 | 101.22      | 113.80   |
| 1   | A     | 42  | ASP  | CA-CB-CG | 12.48  | 125.08      | 112.60   |
| 1   | B     | 42  | ASP  | CA-CB-CG | 11.69  | 124.29      | 112.60   |
| 1   | B     | 166 | PHE  | CA-CB-CG | 10.55  | 124.35      | 113.80   |
| 1   | A     | 268 | ASP  | CA-CB-CG | 10.46  | 123.06      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | C     | 427 | ARG  | N-CA-C     | 10.33  | 122.54      | 111.28   |
| 1   | B     | 101 | ASN  | OD1-CG-ND2 | -10.13 | 112.47      | 122.60   |
| 1   | A     | 440 | ASN  | OD1-CG-ND2 | -9.98  | 112.62      | 122.60   |
| 1   | C     | 793 | ASN  | OD1-CG-ND2 | -9.88  | 112.72      | 122.60   |
| 1   | A     | 541 | ASN  | OD1-CG-ND2 | -9.84  | 112.76      | 122.60   |
| 1   | D     | 575 | ARG  | CB-CG-CD   | -9.77  | 88.84       | 111.30   |
| 1   | D     | 180 | ASP  | CA-CB-CG   | 9.71   | 122.31      | 112.60   |
| 1   | D     | 314 | SER  | N-CA-C     | 9.63   | 124.29      | 112.54   |
| 1   | C     | 407 | ASN  | OD1-CG-ND2 | -9.54  | 113.06      | 122.60   |
| 1   | C     | 576 | GLN  | OE1-CD-NE2 | -9.17  | 113.43      | 122.60   |
| 1   | A     | 735 | ILE  | N-CA-C     | 9.13   | 117.19      | 108.15   |
| 1   | C     | 390 | HIS  | CA-CB-CG   | 9.11   | 122.91      | 113.80   |
| 1   | C     | 772 | LYS  | N-CA-C     | 9.10   | 123.68      | 111.30   |
| 1   | C     | 455 | VAL  | N-CA-C     | 9.05   | 119.97      | 111.91   |
| 1   | B     | 270 | ASN  | OD1-CG-ND2 | -9.03  | 113.57      | 122.60   |
| 1   | C     | 217 | ASP  | CA-CB-CG   | 9.03   | 121.63      | 112.60   |
| 1   | D     | 793 | ASN  | OD1-CG-ND2 | -8.99  | 113.61      | 122.60   |
| 1   | A     | 314 | SER  | N-CA-C     | 8.90   | 124.27      | 113.23   |
| 1   | A     | 380 | LEU  | N-CA-C     | 8.86   | 122.52      | 109.50   |
| 1   | D     | 632 | HIS  | CA-CB-CG   | -8.85  | 104.95      | 113.80   |
| 1   | D     | 455 | VAL  | N-CA-C     | 8.77   | 120.53      | 112.29   |
| 1   | D     | 338 | ASN  | OD1-CG-ND2 | -8.70  | 113.90      | 122.60   |
| 1   | D     | 187 | ASN  | CA-CB-CG   | 8.63   | 121.23      | 112.60   |
| 1   | C     | 167 | ASN  | CA-CB-CG   | -8.62  | 103.98      | 112.60   |
| 1   | A     | 835 | PRO  | N-CA-C     | 8.55   | 130.08      | 112.47   |
| 1   | D     | 239 | ASN  | OD1-CG-ND2 | -8.53  | 114.07      | 122.60   |
| 1   | D     | 595 | ASN  | OD1-CG-ND2 | -8.51  | 114.09      | 122.60   |
| 1   | C     | 292 | ARG  | CA-CB-CG   | -8.44  | 97.22       | 114.10   |
| 1   | A     | 72  | GLN  | OE1-CD-NE2 | -8.39  | 114.21      | 122.60   |
| 1   | A     | 239 | ASN  | OD1-CG-ND2 | -8.39  | 114.21      | 122.60   |
| 1   | B     | 575 | ARG  | N-CA-C     | 8.30   | 122.94      | 111.74   |
| 1   | A     | 552 | GLU  | CB-CG-CD   | 8.28   | 126.68      | 112.60   |
| 1   | D     | 106 | ASN  | CA-CB-CG   | -8.25  | 104.35      | 112.60   |
| 1   | B     | 390 | HIS  | CA-CB-CG   | 8.18   | 121.98      | 113.80   |
| 1   | A     | 693 | ASP  | CA-CB-CG   | 8.17   | 120.77      | 112.60   |
| 1   | C     | 453 | ASN  | CA-CB-CG   | 8.17   | 120.77      | 112.60   |
| 1   | D     | 663 | SER  | CA-CB-OG   | 8.15   | 127.41      | 111.10   |
| 1   | C     | 399 | HIS  | CA-CB-CG   | -8.05  | 105.75      | 113.80   |
| 1   | A     | 517 | GLN  | OE1-CD-NE2 | -8.04  | 114.56      | 122.60   |
| 1   | D     | 507 | ILE  | N-CA-C     | 8.04   | 119.07      | 111.91   |
| 1   | B     | 763 | ASN  | CA-CB-CG   | -8.01  | 104.59      | 112.60   |
| 1   | B     | 236 | ASN  | OD1-CG-ND2 | -7.98  | 114.62      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 481 | ASN  | OD1-CG-ND2 | -7.97 | 114.63      | 122.60   |
| 1   | C     | 167 | ASN  | OD1-CG-ND2 | -7.90 | 114.70      | 122.60   |
| 1   | C     | 768 | HIS  | CB-CG-CD2  | -7.86 | 120.98      | 131.20   |
| 1   | A     | 769 | ASP  | CA-CB-CG   | 7.86  | 120.46      | 112.60   |
| 1   | B     | 91  | MET  | N-CA-C     | 7.83  | 120.90      | 111.82   |
| 1   | A     | 506 | ARG  | CA-CB-CG   | -7.81 | 98.48       | 114.10   |
| 1   | B     | 101 | ASN  | CB-CG-ND2  | 7.81  | 128.11      | 116.40   |
| 1   | B     | 412 | ASN  | OD1-CG-ND2 | -7.81 | 114.79      | 122.60   |
| 1   | C     | 106 | ASN  | OD1-CG-ND2 | -7.72 | 114.88      | 122.60   |
| 1   | C     | 576 | GLN  | N-CA-C     | -7.62 | 102.98      | 111.82   |
| 1   | A     | 13  | ILE  | N-CA-C     | -7.62 | 96.16       | 107.51   |
| 1   | B     | 832 | GLN  | OE1-CD-NE2 | -7.62 | 114.98      | 122.60   |
| 1   | B     | 769 | ASP  | CA-CB-CG   | 7.59  | 120.19      | 112.60   |
| 1   | B     | 128 | ASP  | CA-CB-CG   | 7.58  | 120.18      | 112.60   |
| 1   | B     | 525 | VAL  | CB-CA-C    | -7.58 | 102.11      | 112.04   |
| 1   | A     | 558 | ASN  | CA-CB-CG   | 7.57  | 120.17      | 112.60   |
| 1   | B     | 305 | GLN  | N-CA-C     | -7.56 | 103.12      | 111.36   |
| 1   | D     | 797 | TRP  | N-CA-C     | -7.55 | 102.65      | 111.03   |
| 1   | D     | 541 | ASN  | OD1-CG-ND2 | -7.54 | 115.06      | 122.60   |
| 1   | A     | 412 | ASN  | OD1-CG-ND2 | -7.51 | 115.09      | 122.60   |
| 1   | A     | 632 | HIS  | CA-CB-CG   | -7.48 | 106.32      | 113.80   |
| 1   | D     | 793 | ASN  | CB-CG-ND2  | 7.46  | 127.59      | 116.40   |
| 1   | B     | 595 | ASN  | CA-CB-CG   | -7.43 | 105.17      | 112.60   |
| 1   | D     | 771 | PHE  | CA-CB-CG   | -7.43 | 106.37      | 113.80   |
| 1   | D     | 383 | ALA  | N-CA-C     | 7.42  | 121.77      | 112.87   |
| 1   | A     | 376 | ASN  | OD1-CG-ND2 | -7.41 | 115.19      | 122.60   |
| 1   | A     | 665 | GLN  | N-CA-CB    | -7.40 | 101.84      | 110.35   |
| 1   | D     | 576 | GLN  | OE1-CD-NE2 | -7.38 | 115.22      | 122.60   |
| 1   | A     | 517 | GLN  | CG-CD-NE2  | 7.37  | 127.45      | 116.40   |
| 1   | A     | 201 | HIS  | CB-CG-CD2  | -7.37 | 121.62      | 131.20   |
| 1   | A     | 268 | ASP  | CB-CA-C    | -7.32 | 99.29       | 110.92   |
| 1   | C     | 23  | ASN  | CA-CB-CG   | 7.31  | 119.91      | 112.60   |
| 1   | B     | 455 | VAL  | N-CA-C     | 7.30  | 118.40      | 111.91   |
| 1   | B     | 455 | VAL  | N-CA-CB    | -7.28 | 103.88      | 112.39   |
| 1   | A     | 234 | ARG  | N-CA-C     | 7.27  | 121.49      | 112.47   |
| 1   | A     | 723 | GLN  | OE1-CD-NE2 | -7.26 | 115.34      | 122.60   |
| 1   | D     | 768 | HIS  | CB-CG-CD2  | -7.24 | 121.79      | 131.20   |
| 1   | A     | 540 | GLU  | CA-CB-CG   | 7.20  | 128.50      | 114.10   |
| 1   | B     | 496 | ASN  | OD1-CG-ND2 | -7.20 | 115.40      | 122.60   |
| 1   | C     | 566 | GLN  | OE1-CD-NE2 | -7.20 | 115.41      | 122.60   |
| 1   | B     | 372 | CYS  | N-CA-C     | 7.19  | 121.75      | 110.32   |
| 1   | A     | 407 | ASN  | OD1-CG-ND2 | -7.18 | 115.42      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 22  | GLU  | N-CA-C     | -7.18 | 95.25       | 108.24   |
| 1   | D     | 166 | PHE  | N-CA-C     | 7.16  | 126.06      | 110.80   |
| 1   | B     | 184 | ARG  | CA-CB-CG   | 7.16  | 128.42      | 114.10   |
| 1   | D     | 784 | GLN  | OE1-CD-NE2 | -7.15 | 115.45      | 122.60   |
| 1   | B     | 834 | LEU  | CA-C-N     | 7.13  | 128.75      | 119.84   |
| 1   | B     | 834 | LEU  | C-N-CA     | 7.13  | 128.75      | 119.84   |
| 1   | D     | 769 | ASP  | CA-CB-CG   | 7.13  | 119.73      | 112.60   |
| 1   | A     | 324 | THR  | N-CA-C     | -7.12 | 104.46      | 113.72   |
| 1   | C     | 588 | ASN  | OD1-CG-ND2 | -7.12 | 115.48      | 122.60   |
| 1   | C     | 211 | GLN  | OE1-CD-NE2 | -7.10 | 115.50      | 122.60   |
| 1   | D     | 217 | ASP  | CA-CB-CG   | 7.10  | 119.70      | 112.60   |
| 1   | C     | 530 | PHE  | N-CA-C     | -7.09 | 102.09      | 111.24   |
| 1   | D     | 239 | ASN  | CB-CG-ND2  | 7.06  | 126.99      | 116.40   |
| 1   | A     | 467 | ILE  | CB-CA-C    | -7.05 | 102.85      | 111.88   |
| 1   | C     | 407 | ASN  | CB-CG-ND2  | 7.05  | 126.98      | 116.40   |
| 1   | C     | 638 | ASP  | CA-CB-CG   | 7.04  | 119.64      | 112.60   |
| 1   | A     | 453 | ASN  | OD1-CG-ND2 | -7.04 | 115.56      | 122.60   |
| 1   | C     | 576 | GLN  | CG-CD-NE2  | 7.02  | 126.94      | 116.40   |
| 1   | D     | 611 | PRO  | N-CA-C     | -7.02 | 100.22      | 111.03   |
| 1   | B     | 541 | ASN  | OD1-CG-ND2 | -7.00 | 115.60      | 122.60   |
| 1   | C     | 541 | ASN  | OD1-CG-ND2 | -7.00 | 115.60      | 122.60   |
| 1   | C     | 101 | ASN  | OD1-CG-ND2 | -7.00 | 115.60      | 122.60   |
| 1   | A     | 341 | HIS  | CB-CG-CD2  | -6.98 | 122.13      | 131.20   |
| 1   | D     | 482 | LYS  | N-CA-C     | -6.97 | 95.60       | 108.02   |
| 1   | C     | 36  | HIS  | CA-CB-CG   | -6.97 | 106.83      | 113.80   |
| 1   | A     | 588 | ASN  | OD1-CG-ND2 | -6.97 | 115.63      | 122.60   |
| 1   | D     | 22  | GLU  | CB-CG-CD   | 6.96  | 124.44      | 112.60   |
| 1   | D     | 201 | HIS  | CB-CG-CD2  | -6.94 | 122.18      | 131.20   |
| 1   | A     | 793 | ASN  | OD1-CG-ND2 | -6.93 | 115.67      | 122.60   |
| 1   | B     | 270 | ASN  | CB-CG-ND2  | 6.93  | 126.80      | 116.40   |
| 1   | D     | 207 | GLU  | CA-CB-CG   | 6.93  | 127.96      | 114.10   |
| 1   | A     | 607 | GLY  | CA-C-O     | -6.92 | 114.81      | 121.87   |
| 1   | D     | 691 | THR  | O-C-N      | -6.89 | 115.34      | 123.06   |
| 1   | D     | 248 | ALA  | CA-C-O     | -6.89 | 112.81      | 120.25   |
| 1   | D     | 112 | THR  | CA-C-O     | -6.89 | 113.59      | 120.82   |
| 1   | A     | 754 | GLN  | CA-C-N     | 6.88  | 126.49      | 119.19   |
| 1   | A     | 754 | GLN  | C-N-CA     | 6.88  | 126.49      | 119.19   |
| 1   | C     | 239 | ASN  | OD1-CG-ND2 | -6.87 | 115.73      | 122.60   |
| 1   | C     | 310 | ARG  | NE-CZ-NH2  | -6.87 | 113.02      | 119.20   |
| 1   | C     | 106 | ASN  | CB-CG-ND2  | 6.85  | 126.67      | 116.40   |
| 1   | B     | 527 | ASP  | CA-CB-CG   | 6.84  | 119.44      | 112.60   |
| 1   | C     | 272 | ALA  | N-CA-C     | -6.82 | 103.08      | 111.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 560 | ASN  | OD1-CG-ND2 | -6.78 | 115.82      | 122.60   |
| 1   | B     | 219 | GLN  | N-CA-C     | -6.78 | 99.54       | 110.32   |
| 1   | A     | 273 | GLU  | CB-CG-CD   | 6.78  | 124.12      | 112.60   |
| 1   | A     | 440 | ASN  | CB-CG-ND2  | 6.77  | 126.56      | 116.40   |
| 1   | C     | 159 | ILE  | O-C-N      | -6.77 | 115.72      | 122.76   |
| 1   | B     | 632 | HIS  | CA-CB-CG   | -6.76 | 107.04      | 113.80   |
| 1   | D     | 579 | ASN  | OD1-CG-ND2 | -6.75 | 115.84      | 122.60   |
| 1   | D     | 44  | ASN  | OD1-CG-ND2 | -6.75 | 115.85      | 122.60   |
| 1   | A     | 832 | GLN  | CA-CB-CG   | 6.75  | 127.60      | 114.10   |
| 1   | B     | 467 | ILE  | N-CA-C     | 6.74  | 116.89      | 110.42   |
| 1   | B     | 797 | TRP  | N-CA-C     | -6.73 | 103.56      | 111.03   |
| 1   | C     | 43  | ARG  | N-CA-C     | -6.73 | 103.95      | 111.28   |
| 1   | A     | 576 | GLN  | OE1-CD-NE2 | -6.72 | 115.88      | 122.60   |
| 1   | A     | 156 | GLY  | CA-C-O     | -6.72 | 115.06      | 120.91   |
| 1   | A     | 666 | ILE  | N-CA-C     | 6.72  | 123.31      | 109.34   |
| 1   | B     | 95  | LEU  | N-CA-C     | 6.72  | 119.17      | 111.11   |
| 1   | B     | 379 | VAL  | N-CA-C     | -6.72 | 106.69      | 113.47   |
| 1   | A     | 379 | VAL  | N-CA-C     | -6.71 | 95.37       | 109.34   |
| 1   | D     | 475 | GLU  | N-CA-C     | 6.71  | 118.43      | 108.76   |
| 1   | B     | 496 | ASN  | CB-CG-ND2  | 6.71  | 126.46      | 116.40   |
| 1   | B     | 107 | ALA  | N-CA-C     | -6.71 | 104.05      | 111.36   |
| 1   | B     | 479 | PHE  | CA-CB-CG   | -6.69 | 107.11      | 113.80   |
| 1   | B     | 321 | PRO  | N-CA-C     | 6.69  | 126.26      | 112.47   |
| 1   | C     | 822 | ARG  | CA-CB-CG   | 6.69  | 127.48      | 114.10   |
| 1   | A     | 730 | GLU  | CA-CB-CG   | -6.68 | 100.74      | 114.10   |
| 1   | B     | 486 | ILE  | O-C-N      | -6.68 | 116.02      | 123.03   |
| 1   | A     | 101 | ASN  | OD1-CG-ND2 | -6.67 | 115.93      | 122.60   |
| 1   | A     | 62  | HIS  | CA-CB-CG   | -6.67 | 107.13      | 113.80   |
| 1   | B     | 584 | ILE  | N-CA-C     | -6.66 | 103.83      | 110.62   |
| 1   | A     | 525 | VAL  | CB-CA-C    | -6.64 | 101.50      | 112.26   |
| 1   | D     | 729 | GLN  | OE1-CD-NE2 | -6.64 | 115.96      | 122.60   |
| 1   | A     | 227 | ASP  | CA-CB-CG   | 6.64  | 119.24      | 112.60   |
| 1   | C     | 475 | GLU  | CA-C-N     | 6.64  | 126.42      | 119.05   |
| 1   | C     | 475 | GLU  | C-N-CA     | 6.64  | 126.42      | 119.05   |
| 1   | B     | 23  | ASN  | N-CA-C     | -6.63 | 96.68       | 110.80   |
| 1   | B     | 167 | ASN  | N-CA-C     | -6.63 | 97.55       | 108.76   |
| 1   | A     | 114 | GLN  | OE1-CD-NE2 | -6.61 | 115.99      | 122.60   |
| 1   | C     | 399 | HIS  | CB-CG-CD2  | -6.60 | 122.62      | 131.20   |
| 1   | D     | 318 | CYS  | N-CA-C     | 6.60  | 118.66      | 109.15   |
| 1   | A     | 365 | TRP  | CG-CD2-CE3 | 6.58  | 140.48      | 133.90   |
| 1   | A     | 552 | GLU  | CA-CB-CG   | 6.57  | 127.24      | 114.10   |
| 1   | B     | 481 | ASN  | OD1-CG-ND2 | -6.55 | 116.05      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 684 | ASN  | CA-CB-CG   | -6.55 | 106.05      | 112.60   |
| 1   | D     | 506 | ARG  | CA-CB-CG   | -6.54 | 101.01      | 114.10   |
| 1   | D     | 483 | THR  | CA-CB-OG1  | -6.54 | 99.79       | 109.60   |
| 1   | C     | 723 | GLN  | OE1-CD-NE2 | -6.53 | 116.07      | 122.60   |
| 1   | D     | 101 | ASN  | CA-CB-CG   | -6.52 | 106.08      | 112.60   |
| 1   | B     | 27  | LEU  | CB-CA-C    | -6.51 | 100.62      | 110.90   |
| 1   | A     | 477 | HIS  | CA-CB-CG   | -6.50 | 107.30      | 113.80   |
| 1   | D     | 602 | THR  | N-CA-C     | -6.50 | 97.69       | 108.34   |
| 1   | C     | 324 | THR  | N-CA-CB    | -6.49 | 101.13      | 110.80   |
| 1   | C     | 510 | GLU  | N-CA-C     | 6.48  | 119.17      | 111.71   |
| 1   | C     | 834 | LEU  | N-CA-C     | -6.48 | 101.67      | 110.36   |
| 1   | A     | 399 | HIS  | CB-CG-CD2  | -6.45 | 122.81      | 131.20   |
| 1   | B     | 421 | ASP  | N-CA-C     | 6.45  | 124.53      | 110.80   |
| 1   | D     | 434 | GLY  | CA-C-O     | -6.45 | 117.07      | 122.29   |
| 1   | A     | 90  | TYR  | CA-CB-CG   | 6.44  | 125.49      | 113.90   |
| 1   | D     | 16  | ARG  | N-CA-C     | 6.44  | 124.52      | 110.80   |
| 1   | D     | 834 | LEU  | N-CA-C     | -6.43 | 101.44      | 110.31   |
| 1   | A     | 768 | HIS  | CB-CG-CD2  | -6.42 | 122.85      | 131.20   |
| 1   | D     | 564 | ASP  | CA-CB-CG   | 6.42  | 119.02      | 112.60   |
| 1   | A     | 268 | ASP  | N-CA-CB    | 6.41  | 119.56      | 109.82   |
| 1   | A     | 771 | PHE  | CA-CB-CG   | -6.40 | 107.40      | 113.80   |
| 1   | B     | 793 | ASN  | OD1-CG-ND2 | -6.40 | 116.20      | 122.60   |
| 1   | D     | 727 | ASN  | OD1-CG-ND2 | -6.40 | 116.20      | 122.60   |
| 1   | A     | 552 | GLU  | N-CA-C     | -6.40 | 97.17       | 110.80   |
| 1   | B     | 377 | HIS  | CA-CB-CG   | 6.39  | 120.19      | 113.80   |
| 1   | C     | 556 | HIS  | CB-CG-CD2  | -6.38 | 122.90      | 131.20   |
| 1   | D     | 835 | PRO  | N-CA-C     | 6.38  | 125.62      | 112.47   |
| 1   | A     | 73  | HIS  | CB-CG-CD2  | -6.38 | 122.91      | 131.20   |
| 1   | A     | 638 | ASP  | CA-CB-CG   | 6.37  | 118.97      | 112.60   |
| 1   | B     | 793 | ASN  | CB-CG-ND2  | 6.37  | 125.95      | 116.40   |
| 1   | D     | 59  | VAL  | N-CA-C     | -6.36 | 104.65      | 110.82   |
| 1   | D     | 316 | PHE  | CA-CB-CG   | -6.36 | 107.44      | 113.80   |
| 1   | A     | 78  | ASP  | CA-CB-CG   | 6.35  | 118.95      | 112.60   |
| 1   | A     | 422 | VAL  | CB-CA-C    | -6.34 | 101.82      | 112.16   |
| 1   | B     | 234 | ARG  | N-CA-C     | 6.34  | 120.33      | 112.47   |
| 1   | A     | 793 | ASN  | CB-CG-ND2  | 6.33  | 125.89      | 116.40   |
| 1   | B     | 723 | GLN  | OE1-CD-NE2 | -6.32 | 116.28      | 122.60   |
| 1   | D     | 85  | LEU  | N-CA-CB    | -6.32 | 100.63      | 110.55   |
| 1   | B     | 407 | ASN  | OD1-CG-ND2 | -6.31 | 116.29      | 122.60   |
| 1   | A     | 275 | ILE  | CA-C-N     | 6.31  | 133.06      | 121.70   |
| 1   | A     | 275 | ILE  | C-N-CA     | 6.31  | 133.06      | 121.70   |
| 1   | D     | 772 | LYS  | N-CA-C     | 6.31  | 120.26      | 111.74   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 94  | THR  | N-CA-C     | 6.31  | 119.14      | 111.82   |
| 1   | D     | 376 | ASN  | OD1-CG-ND2 | -6.30 | 116.30      | 122.60   |
| 1   | B     | 459 | HIS  | CA-CB-CG   | 6.30  | 120.10      | 113.80   |
| 1   | A     | 665 | GLN  | OE1-CD-NE2 | -6.29 | 116.31      | 122.60   |
| 1   | D     | 556 | HIS  | CB-CG-CD2  | -6.29 | 123.03      | 131.20   |
| 1   | B     | 323 | ARG  | CA-CB-CG   | -6.27 | 101.56      | 114.10   |
| 1   | B     | 42  | ASP  | N-CA-CB    | -6.26 | 101.85      | 111.56   |
| 1   | D     | 182 | TRP  | CG-CD2-CE3 | 6.26  | 140.16      | 133.90   |
| 1   | D     | 433 | GLU  | N-CA-C     | 6.26  | 118.69      | 109.24   |
| 1   | A     | 21  | VAL  | CB-CA-C    | -6.25 | 102.01      | 111.33   |
| 1   | C     | 797 | TRP  | CG-CD2-CE3 | 6.25  | 140.15      | 133.90   |
| 1   | A     | 303 | THR  | CA-CB-OG1  | -6.24 | 100.23      | 109.60   |
| 1   | D     | 166 | PHE  | CA-CB-CG   | 6.24  | 120.04      | 113.80   |
| 1   | C     | 306 | ASP  | CA-CB-CG   | 6.24  | 118.83      | 112.60   |
| 1   | C     | 73  | HIS  | CA-CB-CG   | -6.23 | 107.57      | 113.80   |
| 1   | A     | 365 | TRP  | CB-CG-CD1  | -6.22 | 117.56      | 126.90   |
| 1   | D     | 490 | ARG  | CA-C-O     | -6.21 | 114.30      | 120.82   |
| 1   | A     | 21  | VAL  | N-CA-CB    | 6.20  | 117.94      | 110.31   |
| 1   | C     | 678 | ASN  | OD1-CG-ND2 | -6.20 | 116.40      | 122.60   |
| 1   | A     | 380 | LEU  | CA-C-N     | 6.19  | 126.38      | 119.32   |
| 1   | A     | 380 | LEU  | C-N-CA     | 6.19  | 126.38      | 119.32   |
| 1   | D     | 613 | TYR  | N-CA-C     | -6.19 | 97.03       | 107.99   |
| 1   | C     | 266 | VAL  | N-CA-C     | -6.19 | 96.47       | 109.34   |
| 1   | D     | 36  | HIS  | CB-CG-CD2  | -6.17 | 123.18      | 131.20   |
| 1   | B     | 201 | HIS  | CB-CG-CD2  | -6.17 | 123.19      | 131.20   |
| 1   | C     | 793 | ASN  | CA-CB-CG   | -6.17 | 106.43      | 112.60   |
| 1   | D     | 240 | THR  | N-CA-C     | 6.17  | 118.95      | 108.90   |
| 1   | A     | 797 | TRP  | CG-CD2-CE3 | 6.15  | 140.05      | 133.90   |
| 1   | A     | 244 | TRP  | CG-CD2-CE3 | 6.15  | 140.05      | 133.90   |
| 1   | D     | 163 | PHE  | N-CA-C     | -6.12 | 95.39       | 107.69   |
| 1   | A     | 15  | VAL  | CB-CA-C    | -6.12 | 102.35      | 112.26   |
| 1   | A     | 755 | PRO  | N-CA-C     | 6.12  | 121.58      | 113.57   |
| 1   | A     | 80  | LYS  | N-CA-C     | -6.11 | 99.32       | 109.46   |
| 1   | B     | 275 | ILE  | CA-C-N     | 6.11  | 132.69      | 121.70   |
| 1   | B     | 275 | ILE  | C-N-CA     | 6.11  | 132.69      | 121.70   |
| 1   | B     | 167 | ASN  | OD1-CG-ND2 | -6.11 | 116.50      | 122.60   |
| 1   | A     | 23  | ASN  | CA-CB-CG   | 6.10  | 118.70      | 112.60   |
| 1   | A     | 30  | ASN  | CA-CB-CG   | -6.09 | 106.51      | 112.60   |
| 1   | C     | 693 | ASP  | CA-CB-CG   | 6.09  | 118.69      | 112.60   |
| 1   | C     | 200 | VAL  | N-CA-C     | -6.09 | 99.28       | 108.17   |
| 1   | D     | 578 | LEU  | N-CA-C     | -6.08 | 104.57      | 111.14   |
| 1   | B     | 525 | VAL  | N-CA-CB    | 6.08  | 118.06      | 110.47   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 635 | VAL  | CB-CA-C    | -6.07 | 103.95      | 112.14   |
| 1   | C     | 360 | ASP  | CA-CB-CG   | 6.07  | 118.67      | 112.60   |
| 1   | C     | 793 | ASN  | CB-CG-ND2  | 6.07  | 125.50      | 116.40   |
| 1   | B     | 835 | PRO  | N-CA-C     | 6.06  | 124.95      | 112.47   |
| 1   | B     | 650 | VAL  | N-CA-C     | 6.06  | 116.80      | 110.62   |
| 1   | C     | 187 | ASN  | CA-CB-CG   | 6.06  | 118.66      | 112.60   |
| 1   | D     | 804 | ASN  | OD1-CG-ND2 | -6.06 | 116.54      | 122.60   |
| 1   | D     | 268 | ASP  | CA-CB-CG   | 6.05  | 118.65      | 112.60   |
| 1   | A     | 169 | LYS  | N-CA-C     | -6.05 | 99.54       | 109.40   |
| 1   | D     | 727 | ASN  | N-CA-C     | -6.04 | 97.26       | 108.02   |
| 1   | D     | 43  | ARG  | N-CA-C     | -6.04 | 104.62      | 112.23   |
| 1   | D     | 133 | ASN  | O-C-N      | -6.04 | 114.89      | 122.19   |
| 1   | B     | 649 | ARG  | CG-CD-NE   | -6.03 | 98.73       | 112.00   |
| 1   | B     | 236 | ASN  | CB-CG-ND2  | 6.03  | 125.44      | 116.40   |
| 1   | A     | 37  | PHE  | CA-CB-CG   | -6.03 | 107.78      | 113.80   |
| 1   | A     | 239 | ASN  | CA-CB-CG   | 6.02  | 118.62      | 112.60   |
| 1   | C     | 555 | VAL  | CA-C-N     | -6.02 | 114.29      | 123.07   |
| 1   | C     | 555 | VAL  | C-N-CA     | -6.02 | 114.29      | 123.07   |
| 1   | C     | 201 | HIS  | CB-CG-CD2  | -6.01 | 123.38      | 131.20   |
| 1   | B     | 355 | ASP  | CA-CB-CG   | 6.01  | 118.61      | 112.60   |
| 1   | D     | 366 | GLU  | N-CA-C     | -6.00 | 104.64      | 111.07   |
| 1   | D     | 558 | ASN  | CA-CB-CG   | 6.00  | 118.59      | 112.60   |
| 1   | A     | 834 | LEU  | N-CA-C     | -5.99 | 102.33      | 110.36   |
| 1   | D     | 295 | GLN  | OE1-CD-NE2 | -5.99 | 116.61      | 122.60   |
| 1   | A     | 628 | ASP  | CA-CB-CG   | 5.99  | 118.58      | 112.60   |
| 1   | A     | 421 | ASP  | CA-CB-CG   | 5.98  | 118.58      | 112.60   |
| 1   | B     | 408 | GLN  | CA-CB-CG   | 5.98  | 126.06      | 114.10   |
| 1   | D     | 341 | HIS  | CB-CG-CD2  | -5.97 | 123.43      | 131.20   |
| 1   | B     | 453 | ASN  | OD1-CG-ND2 | -5.97 | 116.63      | 122.60   |
| 1   | B     | 750 | PHE  | CA-CB-CG   | -5.97 | 107.83      | 113.80   |
| 1   | C     | 215 | TRP  | N-CA-C     | -5.96 | 97.43       | 107.99   |
| 1   | D     | 656 | VAL  | N-CA-C     | 5.96  | 116.74      | 110.72   |
| 1   | A     | 765 | LEU  | O-C-N      | 5.96  | 128.29      | 122.09   |
| 1   | A     | 811 | PHE  | CA-CB-CG   | -5.96 | 107.84      | 113.80   |
| 1   | A     | 30  | ASN  | CA-C-O     | -5.95 | 114.11      | 120.42   |
| 1   | A     | 696 | ASN  | OD1-CG-ND2 | -5.95 | 116.65      | 122.60   |
| 1   | D     | 763 | ASN  | OD1-CG-ND2 | -5.95 | 116.65      | 122.60   |
| 1   | B     | 759 | LYS  | CA-CB-CG   | -5.95 | 102.20      | 114.10   |
| 1   | C     | 496 | ASN  | OD1-CG-ND2 | -5.95 | 116.65      | 122.60   |
| 1   | D     | 95  | LEU  | N-CA-C     | 5.95  | 117.45      | 110.97   |
| 1   | B     | 588 | ASN  | OD1-CG-ND2 | -5.94 | 116.66      | 122.60   |
| 1   | D     | 608 | LYS  | CG-CD-CE   | -5.94 | 97.64       | 111.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 823 | GLU  | N-CA-C     | 5.93  | 118.98      | 111.69   |
| 1   | D     | 614 | HIS  | CB-CG-CD2  | -5.93 | 123.49      | 131.20   |
| 1   | A     | 18  | LEU  | N-CA-C     | 5.92  | 123.41      | 110.80   |
| 1   | D     | 735 | ILE  | CA-C-N     | 5.92  | 125.12      | 118.97   |
| 1   | D     | 735 | ILE  | C-N-CA     | 5.92  | 125.12      | 118.97   |
| 1   | B     | 27  | LEU  | N-CA-CB    | 5.92  | 118.65      | 110.07   |
| 1   | B     | 697 | VAL  | CB-CA-C    | -5.91 | 104.42      | 111.81   |
| 1   | D     | 134 | GLY  | CA-C-N     | 5.91  | 126.50      | 119.94   |
| 1   | D     | 134 | GLY  | C-N-CA     | 5.91  | 126.50      | 119.94   |
| 1   | D     | 387 | TRP  | CA-C-N     | 5.91  | 125.84      | 119.76   |
| 1   | D     | 387 | TRP  | C-N-CA     | 5.91  | 125.84      | 119.76   |
| 1   | D     | 723 | GLN  | OE1-CD-NE2 | -5.90 | 116.70      | 122.60   |
| 1   | A     | 267 | LEU  | CA-C-O     | -5.90 | 114.62      | 120.82   |
| 1   | B     | 835 | PRO  | N-CA-CB    | -5.90 | 97.06       | 103.25   |
| 1   | D     | 193 | ARG  | CA-C-N     | 5.89  | 125.59      | 119.05   |
| 1   | D     | 193 | ARG  | C-N-CA     | 5.89  | 125.59      | 119.05   |
| 1   | C     | 138 | ARG  | N-CA-C     | -5.89 | 104.94      | 111.36   |
| 1   | C     | 552 | GLU  | N-CA-C     | -5.89 | 105.69      | 114.64   |
| 1   | A     | 412 | ASN  | CB-CG-ND2  | 5.89  | 125.23      | 116.40   |
| 1   | C     | 633 | ASP  | O-C-N      | -5.89 | 116.46      | 121.23   |
| 1   | B     | 517 | GLN  | OE1-CD-NE2 | -5.88 | 116.72      | 122.60   |
| 1   | D     | 30  | ASN  | CA-CB-CG   | -5.88 | 106.72      | 112.60   |
| 1   | A     | 639 | ARG  | NE-CZ-NH2  | -5.88 | 113.91      | 119.20   |
| 1   | D     | 834 | LEU  | CA-C-N     | 5.88  | 127.19      | 119.84   |
| 1   | D     | 834 | LEU  | C-N-CA     | 5.88  | 127.19      | 119.84   |
| 1   | D     | 576 | GLN  | CG-CD-NE2  | 5.88  | 125.21      | 116.40   |
| 1   | C     | 216 | VAL  | N-CA-C     | 5.87  | 118.15      | 108.99   |
| 1   | C     | 98  | THR  | CA-CB-OG1  | -5.87 | 100.80      | 109.60   |
| 1   | C     | 822 | ARG  | N-CA-CB    | -5.87 | 101.45      | 110.20   |
| 1   | A     | 761 | ILE  | N-CA-C     | -5.86 | 104.62      | 111.00   |
| 1   | C     | 29  | LYS  | N-CA-C     | -5.86 | 104.80      | 111.07   |
| 1   | D     | 393 | GLU  | CA-CB-CG   | 5.86  | 125.81      | 114.10   |
| 1   | A     | 483 | THR  | CA-CB-OG1  | -5.84 | 100.84      | 109.60   |
| 1   | B     | 768 | HIS  | CB-CG-CD2  | -5.83 | 123.62      | 131.20   |
| 1   | D     | 34  | HIS  | CB-CG-CD2  | -5.83 | 123.62      | 131.20   |
| 1   | D     | 399 | HIS  | CB-CG-CD2  | -5.83 | 123.63      | 131.20   |
| 1   | D     | 184 | ARG  | CG-CD-NE   | 5.82  | 124.80      | 112.00   |
| 1   | C     | 483 | THR  | CA-CB-OG1  | -5.81 | 100.88      | 109.60   |
| 1   | D     | 601 | ARG  | NE-CZ-NH1  | 5.81  | 127.31      | 121.50   |
| 1   | B     | 34  | HIS  | CB-CG-CD2  | -5.81 | 123.65      | 131.20   |
| 1   | B     | 241 | MET  | N-CA-C     | -5.80 | 99.78       | 109.24   |
| 1   | A     | 377 | HIS  | CB-CG-CD2  | -5.80 | 123.66      | 131.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 452 | VAL  | N-CA-C     | -5.80 | 100.13      | 108.48   |
| 1   | D     | 33  | ARG  | N-CA-C     | -5.79 | 104.87      | 111.07   |
| 1   | B     | 684 | ASN  | N-CA-C     | 5.79  | 119.97      | 113.02   |
| 1   | D     | 171 | CYS  | CA-CB-SG   | -5.79 | 101.08      | 114.40   |
| 1   | A     | 387 | TRP  | CG-CD2-CE3 | 5.79  | 139.69      | 133.90   |
| 1   | C     | 707 | ASN  | OD1-CG-ND2 | -5.78 | 116.82      | 122.60   |
| 1   | C     | 689 | ILE  | N-CA-C     | -5.77 | 99.56       | 107.99   |
| 1   | D     | 791 | TYR  | CA-C-O     | -5.77 | 114.44      | 120.55   |
| 1   | C     | 208 | HIS  | CA-CB-CG   | -5.76 | 108.04      | 113.80   |
| 1   | A     | 34  | HIS  | CB-CG-CD2  | -5.75 | 123.72      | 131.20   |
| 1   | C     | 447 | ALA  | O-C-N      | 5.75  | 128.07      | 122.09   |
| 1   | B     | 377 | HIS  | CB-CG-CD2  | -5.75 | 123.72      | 131.20   |
| 1   | D     | 710 | ILE  | O-C-N      | -5.74 | 116.44      | 122.81   |
| 1   | D     | 325 | ASN  | OD1-CG-ND2 | -5.73 | 116.87      | 122.60   |
| 1   | B     | 224 | MET  | CA-C-N     | 5.73  | 125.49      | 119.76   |
| 1   | B     | 224 | MET  | C-N-CA     | 5.73  | 125.49      | 119.76   |
| 1   | C     | 365 | TRP  | CG-CD2-CE3 | 5.73  | 139.63      | 133.90   |
| 1   | D     | 62  | HIS  | CB-CG-CD2  | -5.72 | 123.76      | 131.20   |
| 1   | B     | 36  | HIS  | CB-CG-CD2  | -5.71 | 123.77      | 131.20   |
| 1   | C     | 720 | ARG  | N-CA-C     | -5.71 | 104.96      | 111.07   |
| 1   | C     | 599 | VAL  | N-CA-C     | -5.71 | 103.72      | 108.63   |
| 1   | C     | 739 | ARG  | CA-CB-CG   | -5.71 | 102.69      | 114.10   |
| 1   | B     | 573 | TYR  | CA-CB-CG   | 5.71  | 124.17      | 113.90   |
| 1   | C     | 90  | TYR  | CA-CB-CG   | 5.71  | 124.17      | 113.90   |
| 1   | D     | 365 | TRP  | CG-CD2-CE3 | 5.70  | 139.60      | 133.90   |
| 1   | A     | 499 | LEU  | N-CA-C     | -5.70 | 105.15      | 111.36   |
| 1   | C     | 322 | VAL  | N-CA-C     | -5.69 | 106.16      | 111.45   |
| 1   | A     | 170 | ILE  | N-CA-C     | -5.68 | 100.15      | 108.11   |
| 1   | B     | 575 | ARG  | CB-CG-CD   | -5.68 | 98.23       | 111.30   |
| 1   | C     | 657 | ILE  | CA-C-O     | -5.68 | 114.88      | 118.69   |
| 1   | B     | 383 | ALA  | N-CA-C     | 5.68  | 120.08      | 113.20   |
| 1   | C     | 377 | HIS  | CB-CG-CD2  | -5.68 | 123.81      | 131.20   |
| 1   | D     | 657 | ILE  | O-C-N      | -5.68 | 116.04      | 120.07   |
| 1   | A     | 784 | GLN  | OE1-CD-NE2 | -5.68 | 116.92      | 122.60   |
| 1   | C     | 455 | VAL  | N-CA-CB    | -5.68 | 105.75      | 112.39   |
| 1   | D     | 138 | ARG  | NE-CZ-NH2  | -5.68 | 114.09      | 119.20   |
| 1   | A     | 167 | ASN  | CA-CB-CG   | -5.67 | 106.93      | 112.60   |
| 1   | C     | 380 | LEU  | N-CA-C     | 5.66  | 116.79      | 109.65   |
| 1   | C     | 614 | HIS  | CB-CG-CD2  | -5.66 | 123.85      | 131.20   |
| 1   | D     | 491 | TRP  | N-CA-C     | 5.65  | 119.88      | 113.15   |
| 1   | B     | 399 | HIS  | CA-C-O     | -5.65 | 114.43      | 120.42   |
| 1   | D     | 201 | HIS  | CB-CG-ND1  | 5.65  | 131.17      | 122.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 193 | ARG  | NE-CZ-NH2  | -5.64 | 114.12      | 119.20   |
| 1   | B     | 814 | ASP  | CA-CB-CG   | 5.64  | 118.24      | 112.60   |
| 1   | C     | 390 | HIS  | CB-CG-CD2  | -5.64 | 123.87      | 131.20   |
| 1   | B     | 31  | PHE  | N-CA-C     | -5.63 | 105.04      | 111.07   |
| 1   | C     | 331 | ASP  | N-CA-C     | -5.63 | 106.41      | 113.28   |
| 1   | C     | 554 | LYS  | N-CA-C     | 5.63  | 122.80      | 110.80   |
| 1   | A     | 569 | ARG  | CA-C-O     | -5.62 | 114.86      | 121.16   |
| 1   | A     | 684 | ASN  | N-CA-C     | 5.62  | 118.92      | 112.57   |
| 1   | C     | 25  | THR  | CA-CB-OG1  | -5.62 | 101.17      | 109.60   |
| 1   | A     | 365 | TRP  | CE2-CD2-CG | -5.62 | 100.46      | 107.20   |
| 1   | C     | 101 | ASN  | CB-CG-ND2  | 5.62  | 124.82      | 116.40   |
| 1   | B     | 751 | SER  | CA-C-N     | 5.61  | 125.45      | 119.28   |
| 1   | B     | 751 | SER  | C-N-CA     | 5.61  | 125.45      | 119.28   |
| 1   | C     | 181 | ASP  | CA-CB-CG   | 5.61  | 118.21      | 112.60   |
| 1   | A     | 550 | GLU  | CA-CB-CG   | 5.60  | 125.31      | 114.10   |
| 1   | B     | 588 | ASN  | CB-CG-ND2  | 5.60  | 124.81      | 116.40   |
| 1   | B     | 832 | GLN  | CB-CG-CD   | 5.60  | 122.13      | 112.60   |
| 1   | D     | 412 | ASN  | OD1-CG-ND2 | -5.60 | 117.00      | 122.60   |
| 1   | C     | 338 | ASN  | OD1-CG-ND2 | -5.60 | 117.00      | 122.60   |
| 1   | A     | 346 | ILE  | CA-C-O     | -5.60 | 112.45      | 119.95   |
| 1   | C     | 684 | ASN  | N-CA-C     | 5.60  | 119.10      | 112.72   |
| 1   | C     | 327 | ASP  | CA-CB-CG   | 5.59  | 118.19      | 112.60   |
| 1   | C     | 756 | ASP  | CA-CB-CG   | 5.59  | 118.19      | 112.60   |
| 1   | B     | 638 | ASP  | CA-CB-CG   | 5.59  | 118.19      | 112.60   |
| 1   | B     | 60  | ARG  | CB-CG-CD   | -5.58 | 98.46       | 111.30   |
| 1   | B     | 558 | ASN  | OD1-CG-ND2 | -5.58 | 117.02      | 122.60   |
| 1   | C     | 22  | GLU  | N-CA-C     | -5.58 | 101.84      | 109.71   |
| 1   | D     | 380 | LEU  | CA-C-N     | 5.58  | 125.24      | 119.05   |
| 1   | D     | 380 | LEU  | C-N-CA     | 5.58  | 125.24      | 119.05   |
| 1   | D     | 793 | ASN  | CA-CB-CG   | 5.57  | 118.17      | 112.60   |
| 1   | B     | 156 | GLY  | CA-C-O     | -5.57 | 116.07      | 120.91   |
| 1   | B     | 62  | HIS  | CB-CG-CD2  | -5.56 | 123.97      | 131.20   |
| 1   | C     | 772 | LYS  | N-CA-CB    | -5.56 | 103.67      | 111.62   |
| 1   | B     | 599 | VAL  | CA-C-N     | 5.55  | 125.48      | 119.76   |
| 1   | B     | 599 | VAL  | C-N-CA     | 5.55  | 125.48      | 119.76   |
| 1   | B     | 320 | ASP  | CA-CB-CG   | 5.54  | 118.14      | 112.60   |
| 1   | A     | 551 | ARG  | N-CA-C     | 5.54  | 122.61      | 110.80   |
| 1   | A     | 355 | ASP  | CA-CB-CG   | 5.54  | 118.14      | 112.60   |
| 1   | D     | 814 | ASP  | CA-CB-CG   | 5.54  | 118.14      | 112.60   |
| 1   | B     | 491 | TRP  | N-CA-C     | 5.53  | 119.66      | 113.02   |
| 1   | C     | 774 | PHE  | CA-CB-CG   | 5.53  | 119.33      | 113.80   |
| 1   | A     | 614 | HIS  | CB-CG-CD2  | -5.52 | 124.02      | 131.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 387 | TRP  | CG-CD2-CE3 | 5.52  | 139.42      | 133.90   |
| 1   | B     | 399 | HIS  | CB-CG-CD2  | -5.52 | 124.02      | 131.20   |
| 1   | C     | 359 | LEU  | O-C-N      | -5.52 | 116.23      | 122.68   |
| 1   | D     | 684 | ASN  | N-CA-C     | 5.52  | 119.70      | 112.92   |
| 1   | D     | 313 | SER  | N-CA-CB    | -5.51 | 104.18      | 110.35   |
| 1   | D     | 486 | ILE  | O-C-N      | -5.51 | 116.93      | 123.04   |
| 1   | B     | 128 | ASP  | N-CA-C     | -5.50 | 102.74      | 110.50   |
| 1   | C     | 707 | ASN  | CB-CG-ND2  | 5.50  | 124.66      | 116.40   |
| 1   | B     | 718 | VAL  | N-CA-C     | -5.50 | 105.17      | 110.72   |
| 1   | C     | 763 | ASN  | CA-CB-CG   | 5.50  | 118.10      | 112.60   |
| 1   | A     | 372 | CYS  | N-CA-C     | 5.49  | 118.61      | 110.48   |
| 1   | B     | 320 | ASP  | CA-C-N     | 5.49  | 126.70      | 119.84   |
| 1   | B     | 320 | ASP  | C-N-CA     | 5.49  | 126.70      | 119.84   |
| 1   | A     | 91  | MET  | N-CA-C     | 5.49  | 117.34      | 111.36   |
| 1   | A     | 556 | HIS  | CB-CG-CD2  | -5.48 | 124.07      | 131.20   |
| 1   | B     | 444 | LEU  | N-CA-C     | -5.48 | 105.22      | 111.14   |
| 1   | C     | 835 | PRO  | N-CA-C     | 5.48  | 123.77      | 112.47   |
| 1   | B     | 181 | ASP  | N-CA-CB    | 5.48  | 119.63      | 110.53   |
| 1   | D     | 797 | TRP  | CG-CD2-CE3 | 5.48  | 139.38      | 133.90   |
| 1   | D     | 541 | ASN  | CB-CG-ND2  | 5.48  | 124.62      | 116.40   |
| 1   | A     | 64  | VAL  | CA-C-O     | -5.48 | 115.36      | 121.17   |
| 1   | B     | 576 | GLN  | OE1-CD-NE2 | -5.47 | 117.13      | 122.60   |
| 1   | B     | 22  | GLU  | N-CA-C     | -5.47 | 96.36       | 107.41   |
| 1   | C     | 575 | ARG  | N-CA-C     | 5.47  | 118.79      | 111.24   |
| 1   | D     | 275 | ILE  | CA-C-N     | 5.47  | 131.55      | 121.70   |
| 1   | D     | 275 | ILE  | C-N-CA     | 5.47  | 131.55      | 121.70   |
| 1   | A     | 489 | ARG  | CB-CG-CD   | -5.46 | 98.74       | 111.30   |
| 1   | C     | 42  | ASP  | CA-CB-CG   | 5.46  | 118.06      | 112.60   |
| 1   | C     | 34  | HIS  | CB-CG-CD2  | -5.46 | 124.11      | 131.20   |
| 1   | C     | 440 | ASN  | OD1-CG-ND2 | -5.46 | 117.14      | 122.60   |
| 1   | C     | 74  | TYR  | CA-C-O     | -5.45 | 114.64      | 120.42   |
| 1   | A     | 810 | LYS  | N-CA-C     | -5.45 | 105.90      | 112.54   |
| 1   | B     | 815 | ARG  | NE-CZ-NH2  | -5.45 | 114.30      | 119.20   |
| 1   | A     | 201 | HIS  | CB-CG-ND1  | 5.44  | 130.86      | 122.70   |
| 1   | A     | 43  | ARG  | CA-CB-CG   | -5.43 | 103.23      | 114.10   |
| 1   | D     | 558 | ASN  | N-CA-CB    | -5.43 | 103.28      | 110.17   |
| 1   | A     | 265 | ALA  | N-CA-C     | -5.42 | 106.36      | 112.87   |
| 1   | A     | 486 | ILE  | O-C-N      | -5.42 | 117.28      | 122.97   |
| 1   | B     | 564 | ASP  | O-C-N      | -5.42 | 116.90      | 123.13   |
| 1   | C     | 23  | ASN  | OD1-CG-ND2 | -5.42 | 117.18      | 122.60   |
| 1   | B     | 44  | ASN  | OD1-CG-ND2 | -5.42 | 117.19      | 122.60   |
| 1   | C     | 714 | ARG  | N-CA-C     | -5.41 | 102.18      | 110.14   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 579 | ASN  | OD1-CG-ND2 | -5.41 | 117.19      | 122.60   |
| 1   | A     | 72  | GLN  | CG-CD-NE2  | 5.40  | 124.50      | 116.40   |
| 1   | A     | 399 | HIS  | CA-CB-CG   | -5.40 | 108.40      | 113.80   |
| 1   | D     | 585 | THR  | CA-CB-OG1  | -5.40 | 101.50      | 109.60   |
| 1   | B     | 25  | THR  | CA-CB-OG1  | -5.40 | 101.51      | 109.60   |
| 1   | A     | 735 | ILE  | CA-C-N     | 5.39  | 125.04      | 119.05   |
| 1   | A     | 735 | ILE  | C-N-CA     | 5.39  | 125.04      | 119.05   |
| 1   | B     | 566 | GLN  | OE1-CD-NE2 | -5.39 | 117.21      | 122.60   |
| 1   | A     | 820 | TYR  | CB-CA-C    | -5.39 | 102.18      | 110.81   |
| 1   | C     | 553 | TYR  | CA-CB-CG   | 5.39  | 123.60      | 113.90   |
| 1   | D     | 584 | ILE  | N-CA-C     | -5.39 | 105.28      | 110.72   |
| 1   | D     | 231 | PRO  | N-CA-C     | 5.39  | 118.94      | 110.80   |
| 1   | C     | 496 | ASN  | CB-CG-ND2  | 5.39  | 124.48      | 116.40   |
| 1   | C     | 352 | VAL  | CA-C-O     | -5.38 | 115.46      | 121.17   |
| 1   | D     | 589 | ARG  | CA-CB-CG   | -5.38 | 103.33      | 114.10   |
| 1   | B     | 292 | ARG  | CA-CB-CG   | -5.37 | 103.36      | 114.10   |
| 1   | C     | 71  | GLN  | OE1-CD-NE2 | -5.37 | 117.23      | 122.60   |
| 1   | B     | 182 | TRP  | CG-CD2-CE3 | 5.37  | 139.27      | 133.90   |
| 1   | D     | 496 | ASN  | OD1-CG-ND2 | -5.37 | 117.23      | 122.60   |
| 1   | B     | 657 | ILE  | O-C-N      | -5.36 | 116.99      | 120.42   |
| 1   | D     | 582 | HIS  | CB-CG-CD2  | -5.36 | 124.23      | 131.20   |
| 1   | D     | 365 | TRP  | CB-CG-CD1  | -5.36 | 118.87      | 126.90   |
| 1   | B     | 390 | HIS  | CB-CG-CD2  | -5.35 | 124.24      | 131.20   |
| 1   | A     | 12  | GLN  | OE1-CD-NE2 | -5.35 | 117.25      | 122.60   |
| 1   | A     | 166 | PHE  | CA-CB-CG   | 5.35  | 119.15      | 113.80   |
| 1   | A     | 828 | GLU  | CA-C-O     | -5.35 | 115.28      | 119.66   |
| 1   | A     | 62  | HIS  | CB-CG-CD2  | -5.34 | 124.25      | 131.20   |
| 1   | A     | 756 | ASP  | CA-CB-CG   | 5.34  | 117.94      | 112.60   |
| 1   | A     | 797 | TRP  | N-CA-C     | -5.34 | 105.37      | 111.14   |
| 1   | D     | 225 | PRO  | N-CA-C     | 5.34  | 120.46      | 111.32   |
| 1   | D     | 755 | PRO  | N-CA-C     | 5.34  | 121.71      | 113.75   |
| 1   | C     | 405 | GLU  | CB-CG-CD   | 5.34  | 121.68      | 112.60   |
| 1   | C     | 728 | ALA  | O-C-N      | 5.34  | 128.29      | 122.20   |
| 1   | B     | 352 | VAL  | N-CA-C     | -5.34 | 105.40      | 110.42   |
| 1   | B     | 380 | LEU  | CA-C-N     | 5.33  | 126.51      | 119.84   |
| 1   | B     | 380 | LEU  | C-N-CA     | 5.33  | 126.51      | 119.84   |
| 1   | D     | 811 | PHE  | CA-CB-CG   | -5.33 | 108.47      | 113.80   |
| 1   | C     | 62  | HIS  | CB-CG-CD2  | -5.33 | 124.28      | 131.20   |
| 1   | A     | 484 | ASN  | CB-CG-ND2  | 5.32  | 124.38      | 116.40   |
| 1   | D     | 80  | LYS  | N-CA-C     | -5.32 | 101.98      | 109.96   |
| 1   | B     | 69  | ARG  | CB-CG-CD   | 5.31  | 123.52      | 111.30   |
| 1   | C     | 387 | TRP  | CB-CG-CD1  | -5.31 | 118.93      | 126.90   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 556 | HIS  | O-C-N      | 5.31  | 130.13      | 123.12   |
| 1   | C     | 566 | GLN  | CG-CD-NE2  | 5.31  | 124.36      | 116.40   |
| 1   | A     | 832 | GLN  | CB-CG-CD   | 5.31  | 121.62      | 112.60   |
| 1   | A     | 213 | ALA  | CA-C-O     | -5.30 | 115.37      | 121.47   |
| 1   | B     | 797 | TRP  | CG-CD2-CE3 | 5.30  | 139.20      | 133.90   |
| 1   | C     | 477 | HIS  | CB-CG-CD2  | -5.30 | 124.31      | 131.20   |
| 1   | B     | 564 | ASP  | CA-CB-CG   | 5.29  | 117.89      | 112.60   |
| 1   | C     | 215 | TRP  | CG-CD2-CE3 | 5.29  | 139.19      | 133.90   |
| 1   | A     | 338 | ASN  | N-CA-CB    | -5.29 | 102.66      | 110.49   |
| 1   | B     | 98  | THR  | CA-CB-OG1  | -5.29 | 101.67      | 109.60   |
| 1   | C     | 341 | HIS  | CB-CG-CD2  | -5.29 | 124.32      | 131.20   |
| 1   | A     | 786 | ARG  | CD-NE-CZ   | -5.29 | 117.00      | 124.40   |
| 1   | D     | 114 | GLN  | OE1-CD-NE2 | -5.29 | 117.31      | 122.60   |
| 1   | D     | 126 | GLU  | CB-CG-CD   | 5.29  | 121.59      | 112.60   |
| 1   | A     | 32  | ASN  | OD1-CG-ND2 | -5.28 | 117.32      | 122.60   |
| 1   | C     | 105 | GLU  | N-CA-C     | 5.28  | 120.09      | 111.37   |
| 1   | B     | 112 | THR  | N-CA-CB    | -5.28 | 102.34      | 110.16   |
| 1   | D     | 734 | ARG  | CD-NE-CZ   | 5.28  | 131.79      | 124.40   |
| 1   | D     | 296 | GLU  | CA-CB-CG   | -5.28 | 103.54      | 114.10   |
| 1   | D     | 584 | ILE  | CA-C-O     | -5.28 | 115.25      | 120.85   |
| 1   | C     | 446 | ILE  | N-CA-C     | -5.28 | 105.46      | 110.42   |
| 1   | C     | 217 | ASP  | CB-CA-C    | -5.27 | 103.98      | 112.09   |
| 1   | A     | 477 | HIS  | CB-CG-CD2  | -5.27 | 124.35      | 131.20   |
| 1   | D     | 265 | ALA  | N-CA-C     | -5.26 | 105.71      | 111.82   |
| 1   | D     | 666 | ILE  | O-C-N      | -5.26 | 115.99      | 122.57   |
| 1   | A     | 422 | VAL  | CA-CB-CG1  | -5.26 | 101.46      | 110.40   |
| 1   | B     | 322 | VAL  | N-CA-CB    | 5.26  | 119.91      | 111.23   |
| 1   | C     | 346 | ILE  | CA-C-N     | 5.26  | 125.06      | 119.28   |
| 1   | C     | 346 | ILE  | C-N-CA     | 5.26  | 125.06      | 119.28   |
| 1   | C     | 475 | GLU  | N-CA-C     | 5.26  | 118.19      | 108.94   |
| 1   | D     | 360 | ASP  | CA-CB-CG   | 5.26  | 117.86      | 112.60   |
| 1   | C     | 412 | ASN  | OD1-CG-ND2 | -5.25 | 117.35      | 122.60   |
| 1   | B     | 701 | GLU  | CA-CB-CG   | 5.25  | 124.60      | 114.10   |
| 1   | D     | 688 | THR  | N-CA-C     | 5.25  | 118.37      | 109.76   |
| 1   | D     | 599 | VAL  | N-CA-C     | -5.25 | 103.81      | 108.95   |
| 1   | A     | 128 | ASP  | CA-CB-CG   | 5.25  | 117.84      | 112.60   |
| 1   | C     | 36  | HIS  | CB-CG-CD2  | -5.25 | 124.38      | 131.20   |
| 1   | D     | 585 | THR  | CA-CB-CG2  | 5.24  | 119.41      | 110.50   |
| 1   | B     | 180 | ASP  | N-CA-C     | 5.24  | 118.62      | 107.67   |
| 1   | A     | 832 | GLN  | OE1-CD-NE2 | -5.24 | 117.36      | 122.60   |
| 1   | C     | 761 | ILE  | N-CA-C     | -5.23 | 104.43      | 111.44   |
| 1   | A     | 390 | HIS  | CA-CB-CG   | 5.23  | 119.03      | 113.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 94  | THR  | N-CA-C     | 5.23  | 119.75      | 112.90   |
| 1   | D     | 527 | ASP  | CA-CB-CG   | 5.22  | 117.83      | 112.60   |
| 1   | A     | 368 | THR  | CA-CB-OG1  | -5.22 | 101.77      | 109.60   |
| 1   | B     | 614 | HIS  | CB-CG-CD2  | -5.22 | 124.41      | 131.20   |
| 1   | A     | 575 | ARG  | N-CA-C     | 5.22  | 118.82      | 111.52   |
| 1   | D     | 475 | GLU  | CA-C-N     | 5.21  | 125.26      | 119.32   |
| 1   | D     | 475 | GLU  | C-N-CA     | 5.21  | 125.26      | 119.32   |
| 1   | A     | 108 | CYS  | CA-C-O     | -5.21 | 115.03      | 120.55   |
| 1   | D     | 697 | VAL  | CA-C-O     | -5.20 | 115.66      | 121.17   |
| 1   | A     | 396 | LEU  | CA-C-N     | 5.19  | 124.81      | 119.05   |
| 1   | A     | 396 | LEU  | C-N-CA     | 5.19  | 124.81      | 119.05   |
| 1   | A     | 399 | HIS  | CA-C-O     | -5.19 | 114.48      | 120.24   |
| 1   | C     | 234 | ARG  | CA-CB-CG   | -5.19 | 103.71      | 114.10   |
| 1   | C     | 241 | MET  | N-CA-C     | -5.19 | 99.94       | 108.41   |
| 1   | B     | 200 | VAL  | O-C-N      | -5.19 | 117.65      | 123.26   |
| 1   | A     | 564 | ASP  | CA-CB-CG   | 5.19  | 117.79      | 112.60   |
| 1   | B     | 182 | TRP  | CE2-CD2-CG | -5.19 | 100.97      | 107.20   |
| 1   | A     | 734 | ARG  | CB-CG-CD   | 5.18  | 123.22      | 111.30   |
| 1   | A     | 90  | TYR  | N-CA-C     | -5.18 | 98.41       | 107.73   |
| 1   | C     | 768 | HIS  | CB-CG-ND1  | 5.18  | 130.47      | 122.70   |
| 1   | D     | 560 | ASN  | OD1-CG-ND2 | -5.17 | 117.42      | 122.60   |
| 1   | B     | 831 | ARG  | N-CA-C     | -5.17 | 107.49      | 112.97   |
| 1   | D     | 525 | VAL  | CB-CA-C    | -5.17 | 100.46      | 111.32   |
| 1   | B     | 555 | VAL  | CA-C-N     | -5.17 | 115.81      | 123.05   |
| 1   | B     | 555 | VAL  | C-N-CA     | -5.17 | 115.81      | 123.05   |
| 1   | B     | 23  | ASN  | CA-CB-CG   | 5.17  | 117.77      | 112.60   |
| 1   | A     | 61  | ASP  | CA-CB-CG   | 5.16  | 117.76      | 112.60   |
| 1   | C     | 157 | TYR  | CA-C-O     | -5.16 | 114.78      | 120.36   |
| 1   | B     | 118 | ASP  | CA-CB-CG   | 5.16  | 117.76      | 112.60   |
| 1   | D     | 510 | GLU  | CB-CG-CD   | 5.16  | 121.37      | 112.60   |
| 1   | A     | 657 | ILE  | N-CA-CB    | -5.15 | 107.26      | 110.50   |
| 1   | C     | 306 | ASP  | CB-CA-C    | -5.15 | 102.25      | 110.79   |
| 1   | D     | 248 | ALA  | N-CA-C     | -5.15 | 103.29      | 109.83   |
| 1   | A     | 815 | ARG  | NE-CZ-NH2  | -5.15 | 114.57      | 119.20   |
| 1   | C     | 426 | ARG  | N-CA-C     | -5.14 | 105.37      | 110.97   |
| 1   | D     | 572 | GLU  | CA-C-O     | -5.14 | 115.40      | 120.90   |
| 1   | C     | 723 | GLN  | CA-CB-CG   | 5.14  | 124.37      | 114.10   |
| 1   | D     | 407 | ASN  | CB-CG-ND2  | 5.14  | 124.11      | 116.40   |
| 1   | D     | 575 | ARG  | N-CA-C     | 5.14  | 118.71      | 111.52   |
| 1   | C     | 329 | PHE  | CA-C-O     | -5.13 | 113.70      | 118.73   |
| 1   | C     | 491 | TRP  | CE2-CD2-CG | -5.13 | 101.04      | 107.20   |
| 1   | A     | 439 | ILE  | N-CA-C     | -5.13 | 101.03      | 108.36   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 767 | HIS  | CB-CG-CD2  | -5.13 | 124.53      | 131.20   |
| 1   | D     | 554 | LYS  | CA-CB-CG   | -5.13 | 103.84      | 114.10   |
| 1   | C     | 34  | HIS  | CA-C-O     | -5.13 | 115.42      | 120.70   |
| 1   | D     | 631 | ASN  | OD1-CG-ND2 | -5.12 | 117.48      | 122.60   |
| 1   | A     | 387 | TRP  | CE2-CD2-CG | -5.12 | 101.06      | 107.20   |
| 1   | A     | 601 | ARG  | CB-CG-CD   | -5.12 | 99.53       | 111.30   |
| 1   | A     | 61  | ASP  | O-C-N      | -5.11 | 116.70      | 122.12   |
| 1   | B     | 408 | GLN  | OE1-CD-NE2 | -5.11 | 117.49      | 122.60   |
| 1   | B     | 422 | VAL  | N-CA-C     | 5.11  | 119.97      | 109.34   |
| 1   | A     | 67  | TRP  | CG-CD2-CE3 | 5.11  | 139.01      | 133.90   |
| 1   | B     | 431 | VAL  | N-CA-C     | -5.11 | 101.22      | 108.58   |
| 1   | B     | 602 | THR  | N-CA-C     | -5.11 | 100.19      | 108.52   |
| 1   | C     | 228 | THR  | CA-C-N     | 5.11  | 125.02      | 119.76   |
| 1   | C     | 228 | THR  | C-N-CA     | 5.11  | 125.02      | 119.76   |
| 1   | A     | 412 | ASN  | CA-CB-CG   | 5.11  | 117.71      | 112.60   |
| 1   | D     | 100 | VAL  | N-CA-C     | -5.10 | 105.73      | 110.53   |
| 1   | D     | 571 | HIS  | CA-CB-CG   | -5.10 | 108.70      | 113.80   |
| 1   | A     | 21  | VAL  | CA-C-O     | -5.09 | 115.23      | 121.04   |
| 1   | A     | 221 | VAL  | N-CA-C     | -5.09 | 100.88      | 108.46   |
| 1   | A     | 387 | TRP  | CB-CG-CD1  | -5.09 | 119.27      | 126.90   |
| 1   | B     | 489 | ARG  | NE-CZ-NH1  | 5.09  | 126.59      | 121.50   |
| 1   | D     | 167 | ASN  | N-CA-C     | -5.09 | 101.40      | 109.59   |
| 1   | D     | 372 | CYS  | N-CA-C     | 5.09  | 118.01      | 110.48   |
| 1   | A     | 208 | HIS  | CB-CG-CD2  | -5.08 | 124.59      | 131.20   |
| 1   | A     | 58  | THR  | CA-CB-OG1  | -5.08 | 101.98      | 109.60   |
| 1   | B     | 576 | GLN  | CG-CD-NE2  | 5.08  | 124.02      | 116.40   |
| 1   | A     | 11  | LYS  | CA-CB-CG   | 5.08  | 124.26      | 114.10   |
| 1   | B     | 207 | GLU  | CA-CB-CG   | 5.08  | 124.26      | 114.10   |
| 1   | D     | 371 | THR  | O-C-N      | -5.08 | 115.44      | 122.30   |
| 1   | B     | 756 | ASP  | CA-CB-CG   | 5.08  | 117.68      | 112.60   |
| 1   | A     | 175 | GLN  | OE1-CD-NE2 | -5.08 | 117.52      | 122.60   |
| 1   | A     | 525 | VAL  | N-CA-CB    | 5.08  | 119.96      | 110.77   |
| 1   | A     | 575 | ARG  | CB-CG-CD   | -5.08 | 99.62       | 111.30   |
| 1   | A     | 815 | ARG  | N-CA-C     | -5.08 | 104.69      | 111.24   |
| 1   | B     | 666 | ILE  | O-C-N      | -5.08 | 116.22      | 122.57   |
| 1   | C     | 457 | ARG  | N-CA-C     | 5.08  | 117.20      | 111.11   |
| 1   | D     | 567 | VAL  | O-C-N      | -5.08 | 117.56      | 122.99   |
| 1   | C     | 588 | ASN  | CB-CG-ND2  | 5.07  | 124.00      | 116.40   |
| 1   | D     | 163 | PHE  | CA-C-O     | -5.07 | 114.18      | 120.57   |
| 1   | C     | 572 | GLU  | O-C-N      | -5.07 | 116.76      | 122.03   |
| 1   | C     | 632 | HIS  | CB-CG-CD2  | -5.07 | 124.61      | 131.20   |
| 1   | A     | 496 | ASN  | CA-C-N     | 5.07  | 124.67      | 119.05   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 496 | ASN  | C-N-CA     | 5.07  | 124.67      | 119.05   |
| 1   | B     | 73  | HIS  | CB-CG-CD2  | -5.07 | 124.61      | 131.20   |
| 1   | B     | 182 | TRP  | CG-CD1-NE1 | -5.07 | 103.62      | 110.20   |
| 1   | C     | 76  | GLU  | N-CA-CB    | -5.07 | 102.66      | 110.16   |
| 1   | C     | 387 | TRP  | CE2-CD2-CG | -5.06 | 101.12      | 107.20   |
| 1   | A     | 767 | HIS  | CB-CA-C    | -5.06 | 102.63      | 109.16   |
| 1   | A     | 299 | VAL  | CA-CB-CG1  | 5.06  | 119.00      | 110.40   |
| 1   | D     | 777 | TYR  | N-CA-C     | 5.06  | 116.65      | 111.03   |
| 1   | B     | 174 | TRP  | CG-CD2-CE3 | 5.06  | 138.96      | 133.90   |
| 1   | C     | 183 | LEU  | N-CA-C     | 5.05  | 121.57      | 110.80   |
| 1   | D     | 34  | HIS  | CA-CB-CG   | -5.05 | 108.75      | 113.80   |
| 1   | C     | 491 | TRP  | CG-CD2-CE3 | 5.05  | 138.95      | 133.90   |
| 1   | B     | 341 | HIS  | CB-CG-CD2  | -5.05 | 124.64      | 131.20   |
| 1   | C     | 496 | ASN  | CA-C-N     | 5.05  | 125.33      | 119.47   |
| 1   | C     | 496 | ASN  | C-N-CA     | 5.05  | 125.33      | 119.47   |
| 1   | C     | 650 | VAL  | CA-C-O     | -5.05 | 116.02      | 121.27   |
| 1   | C     | 824 | ILE  | CA-C-O     | -5.05 | 116.31      | 120.80   |
| 1   | C     | 834 | LEU  | CA-C-N     | 5.05  | 126.15      | 119.84   |
| 1   | C     | 834 | LEU  | C-N-CA     | 5.05  | 126.15      | 119.84   |
| 1   | C     | 234 | ARG  | N-CA-C     | 5.05  | 118.73      | 112.47   |
| 1   | A     | 768 | HIS  | CB-CG-ND1  | 5.04  | 130.27      | 122.70   |
| 1   | D     | 566 | GLN  | OE1-CD-NE2 | -5.04 | 117.56      | 122.60   |
| 1   | D     | 666 | ILE  | N-CA-C     | 5.04  | 119.83      | 109.34   |
| 1   | B     | 793 | ASN  | CA-C-N     | 5.04  | 126.14      | 119.84   |
| 1   | B     | 793 | ASN  | C-N-CA     | 5.04  | 126.14      | 119.84   |
| 1   | D     | 605 | ILE  | O-C-N      | -5.04 | 118.00      | 123.14   |
| 1   | A     | 307 | ILE  | CA-C-O     | -5.04 | 115.83      | 121.17   |
| 1   | A     | 322 | VAL  | N-CA-CB    | 5.04  | 119.54      | 111.23   |
| 1   | B     | 174 | TRP  | CB-CG-CD1  | -5.04 | 119.35      | 126.90   |
| 1   | C     | 273 | GLU  | CB-CG-CD   | 5.04  | 121.16      | 112.60   |
| 1   | C     | 446 | ILE  | CB-CA-C    | -5.04 | 105.38      | 111.87   |
| 1   | B     | 182 | TRP  | N-CA-C     | -5.03 | 105.98      | 111.82   |
| 1   | B     | 680 | LYS  | CB-CG-CD   | 5.03  | 122.88      | 111.30   |
| 1   | D     | 85  | LEU  | O-C-N      | -5.03 | 117.33      | 123.27   |
| 1   | B     | 387 | TRP  | CE2-CD2-CG | -5.03 | 101.16      | 107.20   |
| 1   | B     | 598 | VAL  | N-CA-C     | -5.03 | 101.00      | 108.45   |
| 1   | A     | 189 | TRP  | CE2-CD2-CG | -5.03 | 101.16      | 107.20   |
| 1   | A     | 467 | ILE  | N-CA-CB    | 5.03  | 116.09      | 110.51   |
| 1   | B     | 217 | ASP  | CA-CB-CG   | 5.03  | 117.63      | 112.60   |
| 1   | D     | 817 | ILE  | CA-C-O     | -5.03 | 115.52      | 120.85   |
| 1   | D     | 295 | GLN  | CG-CD-NE2  | 5.03  | 123.94      | 116.40   |
| 1   | C     | 744 | GLN  | OE1-CD-NE2 | -5.02 | 117.58      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 365 | TRP  | CE2-CD2-CG | -5.02 | 101.17      | 107.20   |
| 1   | A     | 553 | TYR  | CA-CB-CG   | 5.02  | 122.94      | 113.90   |
| 1   | A     | 312 | LYS  | N-CA-C     | 5.02  | 116.75      | 111.28   |
| 1   | B     | 499 | LEU  | N-CA-C     | -5.02 | 105.72      | 111.14   |
| 1   | B     | 421 | ASP  | O-C-N      | -5.01 | 115.93      | 122.59   |
| 1   | B     | 671 | THR  | CA-CB-OG1  | -5.01 | 102.09      | 109.60   |
| 1   | A     | 552 | GLU  | O-C-N      | -5.00 | 115.93      | 122.59   |
| 1   | A     | 394 | THR  | CA-CB-OG1  | -5.00 | 102.10      | 109.60   |
| 1   | B     | 380 | LEU  | CA-C-O     | -5.00 | 115.16      | 119.36   |
| 1   | B     | 481 | ASN  | CB-CG-ND2  | 5.00  | 123.91      | 116.40   |
| 1   | A     | 241 | MET  | N-CA-C     | -5.00 | 100.26      | 108.41   |
| 1   | D     | 782 | LYS  | CA-CB-CG   | 5.00  | 124.11      | 114.10   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 297 | TYR  | Sidechain |
| 1   | A     | 52  | TYR  | Sidechain |
| 1   | B     | 52  | TYR  | Sidechain |
| 1   | B     | 834 | LEU  | Peptide   |
| 1   | C     | 52  | TYR  | Sidechain |
| 1   | C     | 791 | TYR  | Sidechain |
| 1   | D     | 511 | TYR  | Sidechain |
| 1   | D     | 524 | TYR  | Sidechain |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 6512  | 0        | 6484     | 118     | 0            |
| 1   | B     | 6434  | 0        | 6393     | 124     | 0            |
| 1   | C     | 6512  | 0        | 6484     | 135     | 0            |
| 1   | D     | 6512  | 0        | 6484     | 117     | 0            |
| 2   | A     | 23    | 0        | 12       | 0       | 0            |
| 2   | B     | 23    | 0        | 12       | 1       | 0            |
| 2   | C     | 23    | 0        | 12       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | D     | 23    | 0        | 12       | 0       | 0            |
| 3   | A     | 38    | 0        | 14       | 0       | 0            |
| 3   | B     | 38    | 0        | 14       | 1       | 0            |
| 3   | C     | 38    | 0        | 13       | 0       | 0            |
| 3   | D     | 38    | 0        | 14       | 0       | 0            |
| All | All   | 26214 | 0        | 25948    | 481     | 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 9.

All (481) 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:D:193:ARG:HB2  | 1:D:225:PRO:HG2  | 1.63                     | 0.81              |
| 1:C:225:PRO:HB2  | 1:C:242:ARG:HD2  | 1.61                     | 0.79              |
| 1:C:549:LEU:HD12 | 1:C:557:ILE:HD13 | 1.65                     | 0.79              |
| 1:B:95:LEU:HG    | 1:B:99:MET:HE2   | 1.66                     | 0.78              |
| 1:B:325:ASN:HD21 | 1:B:327:ASP:HB2  | 1.52                     | 0.75              |
| 1:C:88:GLU:HB2   | 1:C:132:GLY:HA2  | 1.68                     | 0.75              |
| 1:A:225:PRO:HB2  | 1:A:242:ARG:HD2  | 1.67                     | 0.74              |
| 1:B:201:HIS:CD2  | 1:B:220:VAL:HG22 | 2.23                     | 0.74              |
| 1:A:496:ASN:OD1  | 1:A:499:LEU:HB2  | 1.89                     | 0.73              |
| 1:B:235:ASN:HA   | 1:B:833:ARG:HG2  | 1.69                     | 0.72              |
| 1:B:753:LYS:HG2  | 1:B:754:GLN:HG3  | 1.72                     | 0.70              |
| 1:C:707:ASN:HA   | 1:C:800:MET:HE2  | 1.73                     | 0.70              |
| 1:A:582:HIS:HD2  | 1:A:781:VAL:HG22 | 1.56                     | 0.70              |
| 1:C:122:LEU:HA   | 1:C:125:ILE:HD12 | 1.72                     | 0.70              |
| 1:D:237:VAL:HG22 | 1:D:834:LEU:HD22 | 1.75                     | 0.68              |
| 1:C:578:LEU:HD22 | 1:C:780:TYR:CD2  | 2.28                     | 0.68              |
| 1:C:532:ARG:HH11 | 1:C:532:ARG:HB3  | 1.56                     | 0.68              |
| 1:B:290:GLU:HG3  | 1:B:391:LEU:HD11 | 1.75                     | 0.68              |
| 1:C:709:PHE:HB3  | 1:C:783:CYS:SG   | 2.34                     | 0.68              |
| 1:D:459:HIS:HA   | 1:D:462:ILE:HD12 | 1.75                     | 0.67              |
| 1:B:380:LEU:HB3  | 1:B:382:GLU:HB2  | 1.77                     | 0.67              |
| 1:C:539:GLN:NE2  | 1:C:543:LEU:HD22 | 2.09                     | 0.67              |
| 1:A:754:GLN:HE22 | 1:D:434:GLY:HA3  | 1.60                     | 0.66              |
| 1:A:379:VAL:HG22 | 1:A:673:ALA:HB2  | 1.78                     | 0.66              |
| 1:A:222:LEU:HG   | 1:A:249:PRO:HB3  | 1.78                     | 0.66              |
| 1:C:21:VAL:HG21  | 1:C:23:ASN:ND2   | 2.11                     | 0.66              |
| 1:C:82:ILE:HD11  | 1:C:827:VAL:HG21 | 1.78                     | 0.66              |
| 1:C:175:GLN:NE2  | 1:C:617:LYS:HE2  | 2.12                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:577:LEU:HD11 | 1:C:761:ILE:HD12 | 1.77                     | 0.65              |
| 1:B:33:ARG:HG2   | 1:B:33:ARG:HH11  | 1.61                     | 0.65              |
| 1:C:95:LEU:HG    | 1:C:99:MET:HE2   | 1.77                     | 0.65              |
| 1:D:730:GLU:O    | 1:D:734:ARG:HG2  | 1.97                     | 0.64              |
| 1:B:227:ASP:OD1  | 1:B:242:ARG:HD3  | 1.98                     | 0.64              |
| 1:D:269:ARG:HH11 | 1:D:269:ARG:HB2  | 1.63                     | 0.64              |
| 1:B:225:PRO:HG3  | 1:B:244:TRP:CZ3  | 2.33                     | 0.63              |
| 1:C:93:ARG:HD2   | 1:C:126:GLU:HB3  | 1.79                     | 0.63              |
| 1:A:753:LYS:HG2  | 1:A:754:GLN:HG2  | 1.81                     | 0.63              |
| 1:D:539:GLN:HE21 | 1:D:543:LEU:HD22 | 1.64                     | 0.63              |
| 1:C:629:VAL:HG21 | 1:C:750:PHE:HD1  | 1.64                     | 0.62              |
| 1:C:546:ALA:HA   | 1:C:557:ILE:HD11 | 1.81                     | 0.62              |
| 1:D:33:ARG:HG2   | 1:D:33:ARG:HH11  | 1.65                     | 0.62              |
| 1:A:677:GLY:HA2  | 1:A:680:LYS:HE2  | 1.82                     | 0.61              |
| 1:C:547:ALA:O    | 1:C:551:ARG:HG2  | 2.00                     | 0.61              |
| 1:B:35:LEU:HD12  | 1:B:39:LEU:HD12  | 1.82                     | 0.61              |
| 1:C:599:VAL:HG11 | 1:C:791:TYR:HD2  | 1.65                     | 0.61              |
| 1:B:613:TYR:CD2  | 1:B:616:ALA:HB2  | 2.36                     | 0.61              |
| 1:A:539:GLN:O    | 1:A:543:LEU:HD22 | 2.01                     | 0.61              |
| 1:B:201:HIS:HD2  | 1:B:220:VAL:HG22 | 1.64                     | 0.60              |
| 1:A:724:ARG:NH1  | 1:A:726:TYR:HA   | 2.16                     | 0.60              |
| 1:B:225:PRO:HB3  | 1:B:242:ARG:HD2  | 1.82                     | 0.60              |
| 1:C:648:TYR:HA   | 1:C:652:LEU:HD23 | 1.83                     | 0.60              |
| 1:A:795:ARG:O    | 1:A:799:ARG:HG3  | 2.02                     | 0.60              |
| 1:C:24:VAL:HG13  | 1:C:111:ALA:HA   | 1.84                     | 0.60              |
| 1:B:168:GLN:HG3  | 1:B:175:GLN:HG3  | 1.83                     | 0.59              |
| 1:C:810:LYS:O    | 1:C:815:ARG:HD3  | 2.02                     | 0.59              |
| 1:B:707:ASN:HA   | 1:B:800:MET:HE2  | 1.85                     | 0.59              |
| 1:A:566:GLN:HE22 | 1:A:576:GLN:HA   | 1.66                     | 0.59              |
| 1:C:10:ARG:N     | 1:D:115:LEU:O    | 2.36                     | 0.59              |
| 1:D:323:ARG:HH12 | 1:D:332:LYS:HE3  | 1.66                     | 0.59              |
| 1:D:753:LYS:HG2  | 1:D:754:GLN:HG3  | 1.85                     | 0.58              |
| 1:A:181:ASP:HB3  | 1:A:184:ARG:NH2  | 2.18                     | 0.58              |
| 1:D:692:MET:SD   | 1:D:697:VAL:HG22 | 2.43                     | 0.58              |
| 1:D:538:LYS:O    | 1:D:542:LYS:HG3  | 2.03                     | 0.58              |
| 1:C:343:SER:HB3  | 1:C:445:CYS:SG   | 2.43                     | 0.58              |
| 1:A:724:ARG:HH22 | 1:A:727:ASN:H    | 1.51                     | 0.58              |
| 1:C:235:ASN:HA   | 1:C:833:ARG:HG3  | 1.85                     | 0.58              |
| 1:D:192:ALA:HB1  | 1:D:224:MET:HE1  | 1.85                     | 0.58              |
| 1:B:384:LEU:HB2  | 1:B:386:ARG:NH1  | 2.19                     | 0.58              |
| 1:C:690:GLY:O    | 1:C:710:ILE:HA   | 2.04                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:112:THR:HG22 | 1:B:113:TYR:HD1  | 1.69                     | 0.57              |
| 1:A:414:VAL:HG22 | 1:A:425:LEU:HD23 | 1.86                     | 0.57              |
| 1:B:719:ASP:O    | 1:B:723:GLN:HG3  | 2.04                     | 0.57              |
| 1:D:21:VAL:HB    | 1:D:23:ASN:HB3   | 1.85                     | 0.57              |
| 1:A:248:ALA:HB2  | 1:A:269:ARG:HA   | 1.85                     | 0.57              |
| 1:D:325:ASN:HD21 | 1:D:327:ASP:HB2  | 1.69                     | 0.57              |
| 1:A:692:MET:HE2  | 1:A:710:ILE:HG21 | 1.87                     | 0.57              |
| 1:D:88:GLU:HB2   | 1:D:132:GLY:HA2  | 1.86                     | 0.57              |
| 1:B:224:MET:HB2  | 1:B:247:LYS:HE2  | 1.86                     | 0.57              |
| 1:B:612:GLY:H    | 1:B:617:LYS:HZ2  | 1.53                     | 0.57              |
| 1:D:510:GLU:HB2  | 1:D:517:GLN:HE22 | 1.70                     | 0.57              |
| 1:C:792:LYS:O    | 1:C:794:PRO:HD3  | 2.05                     | 0.57              |
| 1:B:184:ARG:HD2  | 1:B:185:TYR:CE2  | 2.40                     | 0.56              |
| 1:B:205:ARG:HG3  | 1:B:216:VAL:HG23 | 1.87                     | 0.56              |
| 1:C:613:TYR:CD2  | 1:C:616:ALA:HB2  | 2.40                     | 0.56              |
| 1:A:73:HIS:NE2   | 1:A:77:LYS:HD3   | 2.20                     | 0.56              |
| 1:B:668:THR:OG1  | 1:B:771:PHE:HB3  | 2.05                     | 0.56              |
| 1:C:293:LEU:HD21 | 1:C:392:LEU:HD23 | 1.86                     | 0.56              |
| 1:D:53:PHE:HE1   | 1:D:188:PRO:HD3  | 1.69                     | 0.56              |
| 1:B:384:LEU:HB2  | 1:B:386:ARG:HH12 | 1.71                     | 0.56              |
| 1:A:323:ARG:NH1  | 1:A:332:LYS:HE3  | 2.20                     | 0.56              |
| 1:C:463:LEU:HD23 | 1:C:467:ILE:HD12 | 1.88                     | 0.56              |
| 1:A:424:ARG:HG3  | 1:A:427:ARG:HH21 | 1.71                     | 0.56              |
| 1:D:462:ILE:HG22 | 1:D:467:ILE:HG13 | 1.87                     | 0.56              |
| 1:C:578:LEU:HD21 | 1:C:777:TYR:HA   | 1.87                     | 0.55              |
| 1:B:636:VAL:O    | 1:B:639:ARG:HD3  | 2.07                     | 0.55              |
| 1:C:455:VAL:HG23 | 1:C:674:SER:HB2  | 1.88                     | 0.55              |
| 1:B:453:ASN:ND2  | 1:B:482:LYS:HB2  | 2.21                     | 0.55              |
| 1:B:321:PRO:O    | 1:B:322:VAL:HG12 | 2.07                     | 0.55              |
| 1:D:318:CYS:SG   | 1:D:320:ASP:HB2  | 2.47                     | 0.55              |
| 1:D:636:VAL:O    | 1:D:639:ARG:HD3  | 2.06                     | 0.55              |
| 1:C:636:VAL:O    | 1:C:639:ARG:HD3  | 2.07                     | 0.55              |
| 1:C:269:ARG:HB2  | 1:C:269:ARG:HH11 | 1.72                     | 0.55              |
| 1:D:781:VAL:O    | 1:D:785:GLU:HG3  | 2.06                     | 0.55              |
| 1:C:726:TYR:HE1  | 1:C:775:ALA:HB2  | 1.72                     | 0.55              |
| 1:D:380:LEU:HD13 | 1:D:382:GLU:HB2  | 1.88                     | 0.55              |
| 1:D:486:ILE:HD13 | 1:D:680:LYS:HG3  | 1.87                     | 0.55              |
| 1:D:753:LYS:HD2  | 1:D:753:LYS:H    | 1.71                     | 0.55              |
| 1:A:571:HIS:HD2  | 1:A:573:TYR:H    | 1.53                     | 0.55              |
| 1:C:677:GLY:HA2  | 1:C:680:LYS:HD3  | 1.89                     | 0.55              |
| 1:B:734:ARG:HD2  | 1:B:734:ARG:N    | 2.22                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:343:SER:HB3  | 1:D:445:CYS:SG   | 2.46                     | 0.54              |
| 1:B:502:ILE:HA   | 1:B:505:GLU:HG2  | 1.89                     | 0.54              |
| 1:C:37:PHE:HE2   | 1:D:18:LEU:HB3   | 1.73                     | 0.54              |
| 1:D:203:TYR:HD2  | 1:D:219:GLN:HG2  | 1.72                     | 0.54              |
| 1:A:353:LEU:O    | 1:A:359:LEU:HB2  | 2.07                     | 0.54              |
| 1:B:622:LEU:HD22 | 1:B:761:ILE:HD13 | 1.89                     | 0.54              |
| 1:A:458:ILE:HG22 | 1:A:462:ILE:HD11 | 1.89                     | 0.54              |
| 1:B:32:ASN:O     | 1:B:36:HIS:HD2   | 1.90                     | 0.54              |
| 1:B:143:PHE:O    | 1:B:147:MET:HG3  | 2.08                     | 0.54              |
| 1:B:237:VAL:HG22 | 1:B:834:LEU:HD22 | 1.89                     | 0.54              |
| 1:D:42:ASP:HB2   | 1:D:45:VAL:HG22  | 1.89                     | 0.54              |
| 1:A:74:TYR:O     | 1:A:79:PRO:HD2   | 2.08                     | 0.54              |
| 1:A:88:GLU:HB2   | 1:A:132:GLY:HA2  | 1.90                     | 0.54              |
| 1:C:436:VAL:HG12 | 1:C:438:ARG:HG3  | 1.90                     | 0.54              |
| 1:C:575:ARG:HH22 | 1:C:776:ASP:HB2  | 1.72                     | 0.54              |
| 1:D:325:ASN:ND2  | 1:D:327:ASP:HB2  | 2.22                     | 0.54              |
| 1:B:93:ARG:HD3   | 1:B:126:GLU:O    | 2.08                     | 0.54              |
| 1:D:102:LEU:HD23 | 1:D:104:LEU:HD12 | 1.90                     | 0.54              |
| 1:B:108:CYS:O    | 1:B:112:THR:HB   | 2.08                     | 0.53              |
| 1:C:115:LEU:HD23 | 1:D:12:GLN:HE21  | 1.73                     | 0.53              |
| 1:D:650:VAL:O    | 1:D:654:GLU:HG3  | 2.07                     | 0.53              |
| 1:C:24:VAL:O     | 1:C:28:LYS:HG3   | 2.08                     | 0.53              |
| 1:A:133:ASN:OD1  | 1:A:165:ILE:HG12 | 2.09                     | 0.53              |
| 1:C:169:LYS:HB2  | 1:C:169:LYS:NZ   | 2.24                     | 0.53              |
| 1:D:174:TRP:CH2  | 1:D:618:MET:HE1  | 2.43                     | 0.53              |
| 1:B:721:LEU:HD23 | 1:B:772:LYS:HD3  | 1.90                     | 0.53              |
| 1:C:41:LYS:HG3   | 1:C:45:VAL:HG23  | 1.90                     | 0.53              |
| 1:A:170:ILE:HD13 | 1:A:175:GLN:HA   | 1.91                     | 0.53              |
| 1:C:413:ARG:NH1  | 1:C:474:LEU:HD21 | 2.24                     | 0.53              |
| 1:C:422:VAL:HA   | 1:C:425:LEU:HD12 | 1.90                     | 0.53              |
| 1:C:271:LEU:HA   | 1:C:274:ASN:HB2  | 1.91                     | 0.53              |
| 1:C:378:THR:HG21 | 1:C:384:LEU:HD21 | 1.90                     | 0.53              |
| 1:A:293:LEU:HD23 | 1:A:395:LEU:HD23 | 1.91                     | 0.53              |
| 1:D:380:LEU:CD1  | 1:D:382:GLU:HB2  | 2.38                     | 0.53              |
| 1:B:619:ILE:O    | 1:B:623:ILE:HG13 | 2.08                     | 0.52              |
| 1:C:142:CYS:SG   | 1:C:487:THR:HG22 | 2.49                     | 0.52              |
| 1:D:184:ARG:HD2  | 1:D:185:TYR:CE2  | 2.44                     | 0.52              |
| 1:A:567:VAL:HA   | 1:A:606:GLY:O    | 2.09                     | 0.52              |
| 1:C:205:ARG:HG3  | 1:C:216:VAL:HG23 | 1.91                     | 0.52              |
| 1:A:293:LEU:HD21 | 1:A:392:LEU:HD23 | 1.92                     | 0.52              |
| 1:D:63:LEU:HD11  | 1:D:231:PRO:HD3  | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:70:THR:O     | 1:B:73:HIS:HB3   | 2.09                     | 0.52              |
| 1:C:89:PHE:O     | 1:C:131:LEU:HB2  | 2.10                     | 0.52              |
| 1:D:713:MET:HB3  | 1:D:717:ASP:HB2  | 1.92                     | 0.52              |
| 1:C:32:ASN:OD1   | 1:D:13:ILE:HA    | 2.09                     | 0.52              |
| 1:C:532:ARG:HB3  | 1:C:532:ARG:NH1  | 2.24                     | 0.52              |
| 1:A:181:ASP:HB3  | 1:A:184:ARG:HH21 | 1.74                     | 0.52              |
| 1:A:159:ILE:HG13 | 1:A:299:VAL:HG23 | 1.92                     | 0.51              |
| 1:A:323:ARG:HH12 | 1:A:332:LYS:HE3  | 1.75                     | 0.51              |
| 1:B:225:PRO:HG3  | 1:B:244:TRP:HZ3  | 1.72                     | 0.51              |
| 1:D:289:LYS:HD2  | 1:D:291:LEU:HD13 | 1.92                     | 0.51              |
| 1:B:577:LEU:HD11 | 1:B:761:ILE:HD12 | 1.91                     | 0.51              |
| 1:D:486:ILE:HD11 | 1:D:683:LEU:HD12 | 1.93                     | 0.51              |
| 1:C:736:PRO:HG3  | 1:C:739:ARG:HH22 | 1.76                     | 0.51              |
| 1:D:737:GLU:O    | 1:D:741:ILE:HG13 | 2.11                     | 0.51              |
| 1:B:112:THR:HG22 | 1:B:113:TYR:CD1  | 2.46                     | 0.51              |
| 1:C:583:VAL:HG11 | 1:C:603:VAL:HG11 | 1.92                     | 0.51              |
| 1:D:577:LEU:HD13 | 1:D:619:ILE:HG12 | 1.93                     | 0.51              |
| 1:A:736:PRO:HG3  | 1:A:739:ARG:NH2  | 2.26                     | 0.51              |
| 1:C:522:LEU:O    | 1:C:525:VAL:HG23 | 2.10                     | 0.51              |
| 1:C:10:ARG:N     | 1:C:10:ARG:HD2   | 2.26                     | 0.51              |
| 1:D:499:LEU:HD22 | 1:D:503:ILE:HD11 | 1.93                     | 0.51              |
| 1:A:742:ILE:HG23 | 1:A:762:VAL:HG13 | 1.92                     | 0.50              |
| 1:C:442:ALA:O    | 1:C:446:ILE:HG12 | 2.11                     | 0.50              |
| 1:D:815:ARG:O    | 1:D:819:GLN:HG3  | 2.11                     | 0.50              |
| 1:B:578:LEU:HD22 | 1:B:780:TYR:CD2  | 2.47                     | 0.50              |
| 1:D:386:ARG:HA   | 1:D:439:ILE:O    | 2.11                     | 0.50              |
| 1:C:631:ASN:OD1  | 1:C:641:ARG:HA   | 2.11                     | 0.50              |
| 1:B:612:GLY:H    | 1:B:617:LYS:NZ   | 2.09                     | 0.50              |
| 1:C:157:TYR:CE2  | 1:C:242:ARG:HG2  | 2.45                     | 0.50              |
| 1:C:580:CYS:HA   | 1:C:583:VAL:HG22 | 1.93                     | 0.50              |
| 1:A:53:PHE:CE1   | 1:A:188:PRO:HG3  | 2.47                     | 0.50              |
| 1:A:235:ASN:O    | 1:A:236:ASN:HB2  | 2.10                     | 0.50              |
| 1:A:730:GLU:O    | 1:A:734:ARG:HG2  | 2.11                     | 0.50              |
| 1:B:34:HIS:O     | 1:B:38:THR:HB    | 2.12                     | 0.50              |
| 1:B:631:ASN:OD1  | 1:B:641:ARG:HA   | 2.12                     | 0.50              |
| 1:B:636:VAL:O    | 1:B:639:ARG:HB2  | 2.12                     | 0.50              |
| 1:A:605:ILE:O    | 1:A:644:PHE:HA   | 2.11                     | 0.50              |
| 1:A:689:ILE:HA   | 1:A:709:PHE:HB2  | 1.93                     | 0.50              |
| 1:C:182:TRP:CE2  | 1:C:183:LEU:HG   | 2.47                     | 0.50              |
| 1:C:622:LEU:HD22 | 1:C:761:ILE:HD11 | 1.94                     | 0.50              |
| 1:D:42:ASP:HB3   | 1:D:44:ASN:H     | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:713:MET:HB3  | 1:A:717:ASP:HB2  | 1.92                     | 0.50              |
| 1:B:465:LYS:HD2  | 1:B:465:LYS:N    | 2.27                     | 0.50              |
| 1:C:42:ASP:HB3   | 1:C:44:ASN:H     | 1.77                     | 0.50              |
| 1:C:289:LYS:HD3  | 1:C:291:LEU:H    | 1.76                     | 0.50              |
| 1:C:413:ARG:HH12 | 1:C:474:LEU:HD21 | 1.77                     | 0.50              |
| 1:C:192:ALA:HB1  | 1:C:224:MET:HE2  | 1.93                     | 0.50              |
| 1:B:587:TYR:O    | 1:B:591:LYS:HG2  | 2.12                     | 0.49              |
| 1:C:734:ARG:HH11 | 1:C:734:ARG:HB3  | 1.77                     | 0.49              |
| 1:A:536:LYS:O    | 1:A:540:GLU:HG3  | 2.12                     | 0.49              |
| 1:D:386:ARG:HG2  | 1:D:440:ASN:HD22 | 1.77                     | 0.49              |
| 1:B:822:ARG:HD2  | 1:B:828:GLU:OE1  | 2.12                     | 0.49              |
| 1:C:730:GLU:HB3  | 1:C:734:ARG:NH2  | 2.28                     | 0.49              |
| 1:D:522:LEU:O    | 1:D:525:VAL:HG22 | 2.11                     | 0.49              |
| 1:A:690:GLY:O    | 1:A:710:ILE:HA   | 2.12                     | 0.49              |
| 1:C:730:GLU:HB3  | 1:C:734:ARG:HH21 | 1.76                     | 0.49              |
| 1:B:68:ILE:O     | 1:B:72:GLN:HG3   | 2.13                     | 0.49              |
| 1:A:62:HIS:HB3   | 1:A:66:ARG:HH21  | 1.78                     | 0.49              |
| 1:C:269:ARG:HB2  | 1:C:269:ARG:NH1  | 2.28                     | 0.49              |
| 1:D:197:THR:CG2  | 1:D:222:LEU:HB3  | 2.42                     | 0.49              |
| 1:D:308:ILE:HG22 | 1:D:312:LYS:HE2  | 1.94                     | 0.49              |
| 1:D:323:ARG:NH1  | 1:D:332:LYS:HE3  | 2.28                     | 0.49              |
| 1:A:830:SER:OG   | 1:A:832:GLN:HG3  | 2.12                     | 0.49              |
| 1:C:171:CYS:SG   | 1:C:176:MET:SD   | 3.11                     | 0.49              |
| 1:D:174:TRP:HH2  | 1:D:618:MET:HE1  | 1.78                     | 0.48              |
| 1:A:318:CYS:SG   | 1:A:319:ARG:N    | 2.87                     | 0.48              |
| 1:A:21:VAL:HG23  | 1:A:26:GLU:HG2   | 1.94                     | 0.48              |
| 1:A:44:ASN:HD21  | 1:B:72:GLN:NE2   | 2.12                     | 0.48              |
| 1:C:486:ILE:HD13 | 1:C:680:LYS:HG3  | 1.95                     | 0.48              |
| 1:D:129:ALA:HA   | 1:D:182:TRP:CE3  | 2.48                     | 0.48              |
| 1:D:647:ASN:HB3  | 1:D:649:ARG:HH21 | 1.79                     | 0.48              |
| 1:A:24:VAL:HG12  | 1:A:28:LYS:HE2   | 1.94                     | 0.48              |
| 1:D:709:PHE:HB3  | 1:D:783:CYS:SG   | 2.53                     | 0.48              |
| 1:A:12:GLN:HE22  | 1:B:28:LYS:NZ    | 2.10                     | 0.48              |
| 1:B:767:HIS:O    | 1:B:768:HIS:ND1  | 2.47                     | 0.48              |
| 1:D:373:ALA:HA   | 1:D:449:SER:HB3  | 1.94                     | 0.48              |
| 1:D:423:ASP:O    | 1:D:427:ARG:HG3  | 2.13                     | 0.48              |
| 1:A:311:PHE:CZ   | 1:A:323:ARG:HD2  | 2.49                     | 0.48              |
| 1:A:832:GLN:HE22 | 1:A:834:LEU:HD13 | 1.79                     | 0.48              |
| 1:A:163:PHE:HA   | 1:A:180:ASP:O    | 2.13                     | 0.48              |
| 1:C:726:TYR:OH   | 1:C:774:PHE:HB2  | 2.14                     | 0.48              |
| 1:C:235:ASN:O    | 1:C:236:ASN:HB2  | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:597:PHE:HE2  | 1:C:792:LYS:HD3  | 1.79                     | 0.48              |
| 1:D:10:ARG:HA    | 1:D:13:ILE:HD12  | 1.96                     | 0.47              |
| 1:D:49:ARG:HG2   | 1:D:53:PHE:CE2   | 2.49                     | 0.47              |
| 1:D:85:LEU:HD13  | 1:D:303:THR:HG21 | 1.96                     | 0.47              |
| 1:B:538:LYS:HG3  | 1:B:542:LYS:HD3  | 1.96                     | 0.47              |
| 1:B:201:HIS:HB3  | 1:B:218:THR:HB   | 1.97                     | 0.47              |
| 1:B:753:LYS:H    | 1:B:753:LYS:HZ3  | 1.62                     | 0.47              |
| 1:C:732:TYR:HA   | 1:C:738:LEU:HD23 | 1.95                     | 0.47              |
| 1:B:325:ASN:ND2  | 1:B:327:ASP:HB2  | 2.24                     | 0.47              |
| 1:C:175:GLN:HE21 | 1:C:617:LYS:HE2  | 1.78                     | 0.47              |
| 1:C:237:VAL:HG22 | 1:C:834:LEU:HD22 | 1.97                     | 0.47              |
| 1:C:594:PRO:HB3  | 1:C:635:VAL:HG23 | 1.96                     | 0.47              |
| 1:B:67:TRP:HD1   | 1:B:238:VAL:HG12 | 1.80                     | 0.47              |
| 1:B:378:THR:O    | 1:B:459:HIS:NE2  | 2.48                     | 0.47              |
| 1:B:93:ARG:HD2   | 1:B:126:GLU:HB3  | 1.96                     | 0.47              |
| 1:B:486:ILE:HD13 | 1:B:680:LYS:HG3  | 1.97                     | 0.47              |
| 1:B:799:ARG:O    | 1:B:803:ARG:HG3  | 2.14                     | 0.47              |
| 1:B:800:MET:HA   | 1:B:803:ARG:NH1  | 2.30                     | 0.47              |
| 1:C:59:VAL:HG13  | 1:C:104:LEU:HD12 | 1.96                     | 0.47              |
| 1:C:90:TYR:HD2   | 1:C:138:ARG:HG2  | 1.79                     | 0.47              |
| 1:C:633:ASP:OD2  | 1:C:635:VAL:HG13 | 2.15                     | 0.47              |
| 1:D:94:THR:HG22  | 1:D:98:THR:OG1   | 2.15                     | 0.47              |
| 1:D:675:GLY:O    | 1:D:678:ASN:HB2  | 2.15                     | 0.47              |
| 1:A:373:ALA:HA   | 1:A:449:SER:HB3  | 1.97                     | 0.47              |
| 1:A:378:THR:O    | 1:A:459:HIS:NE2  | 2.48                     | 0.47              |
| 1:B:533:ASP:O    | 1:B:537:VAL:HG23 | 2.14                     | 0.47              |
| 1:C:756:ASP:HB3  | 1:C:759:LYS:HZ3  | 1.80                     | 0.47              |
| 1:A:810:LYS:O    | 1:A:815:ARG:HD3  | 2.13                     | 0.47              |
| 1:B:566:GLN:NE2  | 1:B:576:GLN:HA   | 2.30                     | 0.47              |
| 1:B:566:GLN:HB2  | 1:B:664:GLU:HB2  | 1.97                     | 0.47              |
| 1:B:692:MET:HE2  | 1:B:710:ILE:HG21 | 1.96                     | 0.47              |
| 1:A:569:ARG:O    | 1:A:574:LYS:HG3  | 2.15                     | 0.47              |
| 1:C:337:LEU:HD21 | 1:C:345:ALA:HB3  | 1.97                     | 0.47              |
| 1:D:83:TYR:HE2   | 1:D:310:ARG:HH21 | 1.63                     | 0.47              |
| 1:D:329:PHE:HB3  | 1:D:330:PRO:HD3  | 1.96                     | 0.47              |
| 1:B:413:ARG:HH22 | 1:B:475:GLU:CD   | 2.23                     | 0.46              |
| 1:C:793:ASN:OD1  | 1:C:796:GLU:HG2  | 2.15                     | 0.46              |
| 1:D:507:ILE:HG21 | 1:D:520:LYS:HB3  | 1.95                     | 0.46              |
| 1:C:143:PHE:O    | 1:C:147:MET:HG3  | 2.15                     | 0.46              |
| 1:C:525:VAL:HG12 | 1:C:799:ARG:NH1  | 2.30                     | 0.46              |
| 1:B:397:PRO:O    | 1:B:401:GLN:HG3  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:407:ASN:ND2  | 1:C:411:LEU:HD22 | 2.30                     | 0.46              |
| 1:D:206:VAL:HA   | 1:D:214:LYS:O    | 2.15                     | 0.46              |
| 1:B:717:ASP:HA   | 1:B:720:ARG:HH11 | 1.81                     | 0.46              |
| 1:B:721:LEU:HD21 | 1:B:726:TYR:HD1  | 1.80                     | 0.46              |
| 1:D:15:VAL:O     | 1:D:17:GLY:N     | 2.47                     | 0.46              |
| 1:D:507:ILE:HG21 | 1:D:520:LYS:CB   | 2.46                     | 0.46              |
| 1:A:761:ILE:HG13 | 1:A:762:VAL:N    | 2.28                     | 0.46              |
| 1:B:330:PRO:HD3  | 1:B:367:VAL:HG13 | 1.96                     | 0.46              |
| 1:B:721:LEU:HD21 | 1:B:726:TYR:CD1  | 2.49                     | 0.46              |
| 1:C:622:LEU:HD22 | 1:C:761:ILE:CD1  | 2.46                     | 0.46              |
| 1:B:677:GLY:HA2  | 1:B:680:LYS:HD3  | 1.96                     | 0.46              |
| 1:A:44:ASN:HD21  | 1:B:72:GLN:HE21  | 1.63                     | 0.46              |
| 1:B:386:ARG:HA   | 1:B:439:ILE:O    | 2.15                     | 0.46              |
| 1:A:434:GLY:HA2  | 1:D:754:GLN:HE22 | 1.81                     | 0.46              |
| 1:B:113:TYR:HE1  | 1:B:119:MET:H    | 1.62                     | 0.46              |
| 1:B:543:LEU:HD12 | 1:B:559:PRO:HB2  | 1.98                     | 0.46              |
| 1:B:431:VAL:HG11 | 1:B:437:LYS:HE3  | 1.98                     | 0.46              |
| 1:C:160:ARG:HG3  | 1:C:243:LEU:HD12 | 1.97                     | 0.46              |
| 1:D:693:ASP:O    | 1:D:696:ASN:HB2  | 2.16                     | 0.46              |
| 1:A:538:LYS:O    | 1:A:542:LYS:HG3  | 2.16                     | 0.46              |
| 1:B:165:ILE:HD12 | 1:B:165:ILE:HA   | 1.74                     | 0.46              |
| 1:C:531:ILE:O    | 1:C:798:THR:HG21 | 2.15                     | 0.45              |
| 1:C:629:VAL:HG21 | 1:C:750:PHE:CD1  | 2.47                     | 0.45              |
| 1:A:208:HIS:HA   | 1:A:213:ALA:HA   | 1.99                     | 0.45              |
| 1:D:192:ALA:HB1  | 1:D:224:MET:CE   | 2.46                     | 0.45              |
| 1:A:66:ARG:HB3   | 1:A:238:VAL:HG21 | 1.98                     | 0.45              |
| 1:A:221:VAL:HG13 | 1:A:272:ALA:HB1  | 1.98                     | 0.45              |
| 1:A:575:ARG:HD3  | 1:A:666:ILE:O    | 2.16                     | 0.45              |
| 1:C:349:LEU:HD23 | 1:C:368:THR:HG23 | 1.99                     | 0.45              |
| 1:D:648:TYR:HA   | 1:D:652:LEU:HD23 | 1.99                     | 0.45              |
| 1:A:73:HIS:CE1   | 1:A:77:LYS:HD3   | 2.51                     | 0.45              |
| 1:A:264:GLN:HG3  | 1:A:267:LEU:HG   | 1.97                     | 0.45              |
| 1:C:11:LYS:HA    | 1:D:43:ARG:CZ    | 2.47                     | 0.45              |
| 1:C:168:GLN:HG3  | 1:C:175:GLN:HG3  | 1.98                     | 0.45              |
| 1:C:225:PRO:HB3  | 1:C:244:TRP:CZ3  | 2.51                     | 0.45              |
| 1:D:515:LEU:HG   | 1:D:809:GLY:HA2  | 1.98                     | 0.45              |
| 1:C:464:LYS:HD3  | 1:C:472:TYR:CE1  | 2.51                     | 0.45              |
| 1:A:389:VAL:HG12 | 1:A:439:ILE:HG12 | 1.99                     | 0.45              |
| 1:A:567:VAL:HB   | 1:A:648:TYR:CZ   | 2.51                     | 0.45              |
| 1:B:69:ARG:HG2   | 1:B:69:ARG:HH11  | 1.81                     | 0.45              |
| 1:B:571:HIS:HD2  | 1:B:573:TYR:H    | 1.64                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:293:LEU:HD21 | 1:C:392:LEU:CD2  | 2.47                     | 0.45              |
| 1:C:566:GLN:O    | 1:C:605:ILE:HA   | 2.17                     | 0.45              |
| 1:D:98:THR:O     | 1:D:102:LEU:HB2  | 2.16                     | 0.45              |
| 1:B:648:TYR:HA   | 1:B:652:LEU:HD23 | 1.98                     | 0.45              |
| 1:D:721:LEU:HD23 | 1:D:772:LYS:HD3  | 1.99                     | 0.45              |
| 1:A:164:GLY:N    | 1:A:180:ASP:HB3  | 2.32                     | 0.45              |
| 1:A:525:VAL:O    | 1:A:799:ARG:HD2  | 2.16                     | 0.45              |
| 1:B:91:MET:HE3   | 1:B:241:MET:SD   | 2.56                     | 0.45              |
| 1:B:786:ARG:HG3  | 1:B:786:ARG:HH11 | 1.82                     | 0.45              |
| 1:C:192:ALA:HB2  | 1:C:226:TYR:CE2  | 2.52                     | 0.45              |
| 1:B:546:ALA:HA   | 1:B:557:ILE:HD11 | 1.98                     | 0.45              |
| 1:B:720:ARG:HA   | 1:B:723:GLN:OE1  | 2.17                     | 0.45              |
| 1:C:566:GLN:HE22 | 1:C:576:GLN:HA   | 1.82                     | 0.45              |
| 1:D:67:TRP:HE3   | 1:D:68:ILE:HG13  | 1.82                     | 0.45              |
| 1:D:463:LEU:HD23 | 1:D:467:ILE:HD12 | 1.98                     | 0.45              |
| 1:A:23:ASN:O     | 1:A:27:LEU:HD22  | 2.17                     | 0.44              |
| 1:A:289:LYS:HG3  | 1:A:291:LEU:H    | 1.82                     | 0.44              |
| 1:D:601:ARG:NH2  | 1:D:784:GLN:OE1  | 2.50                     | 0.44              |
| 1:A:192:ALA:HB1  | 1:A:224:MET:CE   | 2.47                     | 0.44              |
| 1:A:267:LEU:O    | 1:A:271:LEU:HG   | 2.17                     | 0.44              |
| 1:B:573:TYR:CZ   | 1:B:574:LYS:HE2  | 2.52                     | 0.44              |
| 1:C:550:GLU:HB2  | 1:C:556:HIS:NE2  | 2.33                     | 0.44              |
| 1:A:315:LYS:HB3  | 1:A:318:CYS:HB3  | 1.99                     | 0.44              |
| 1:A:507:ILE:HG21 | 1:A:520:LYS:HB2  | 1.99                     | 0.44              |
| 1:B:571:HIS:CD2  | 1:B:572:GLU:N    | 2.85                     | 0.44              |
| 1:B:611:PRO:HA   | 1:B:617:LYS:HZ1  | 1.82                     | 0.44              |
| 1:C:376:ASN:OD1  | 1:C:378:THR:HG22 | 2.16                     | 0.44              |
| 1:A:169:LYS:HG3  | 1:A:171:CYS:SG   | 2.56                     | 0.44              |
| 1:C:353:LEU:HD13 | 1:C:359:LEU:HD12 | 1.98                     | 0.44              |
| 1:C:616:ALA:HA   | 1:C:619:ILE:HD12 | 1.99                     | 0.44              |
| 1:A:736:PRO:HG3  | 1:A:739:ARG:HH22 | 1.80                     | 0.44              |
| 1:D:599:VAL:HG11 | 1:D:791:TYR:HD2  | 1.81                     | 0.44              |
| 1:D:707:ASN:HB3  | 1:D:804:ASN:HD21 | 1.82                     | 0.44              |
| 1:A:621:LYS:HA   | 1:A:621:LYS:HD2  | 1.86                     | 0.44              |
| 1:A:817:ILE:HD13 | 1:A:817:ILE:HA   | 1.79                     | 0.44              |
| 1:B:568:LYS:O    | 1:B:607:GLY:HA3  | 2.17                     | 0.44              |
| 1:C:48:PRO:HB3   | 1:C:125:ILE:HD11 | 2.00                     | 0.44              |
| 1:C:817:ILE:HD13 | 1:C:817:ILE:HA   | 1.74                     | 0.44              |
| 1:D:698:GLU:HA   | 1:D:701:GLU:HG3  | 2.00                     | 0.44              |
| 1:A:53:PHE:CD1   | 1:A:188:PRO:HG3  | 2.53                     | 0.44              |
| 1:A:379:VAL:O    | 1:A:467:ILE:HD11 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:741:ILE:HA   | 1:A:744:GLN:HE21 | 1.83                     | 0.44              |
| 1:B:92:GLY:O     | 1:B:128:ASP:HA   | 2.18                     | 0.44              |
| 1:C:567:VAL:HA   | 1:C:606:GLY:O    | 2.18                     | 0.44              |
| 1:A:205:ARG:HD3  | 1:A:217:ASP:OD2  | 2.17                     | 0.43              |
| 1:B:93:ARG:HD3   | 1:B:93:ARG:HH11  | 1.68                     | 0.43              |
| 1:D:199:PRO:HB2  | 1:D:220:VAL:HG13 | 1.99                     | 0.43              |
| 1:D:201:HIS:CD2  | 1:D:220:VAL:HG22 | 2.53                     | 0.43              |
| 1:D:414:VAL:HG12 | 1:D:474:LEU:HD22 | 1.99                     | 0.43              |
| 1:A:513:SER:HB2  | 1:A:831:ARG:HD3  | 2.00                     | 0.43              |
| 1:C:410:PHE:O    | 1:C:414:VAL:HG12 | 2.19                     | 0.43              |
| 1:C:201:HIS:ND1  | 1:C:220:VAL:HG22 | 2.33                     | 0.43              |
| 1:C:597:PHE:CE2  | 1:C:792:LYS:HD3  | 2.54                     | 0.43              |
| 1:D:143:PHE:HB3  | 1:D:147:MET:HE2  | 2.01                     | 0.43              |
| 1:A:682:MET:HB2  | 1:A:699:MET:HE3  | 2.01                     | 0.43              |
| 1:B:310:ARG:HH11 | 2:B:843:AMP:P    | 2.41                     | 0.43              |
| 1:C:11:LYS:HE3   | 1:C:11:LYS:HB2   | 1.87                     | 0.43              |
| 1:A:363:LYS:HE3  | 1:A:367:VAL:HG23 | 2.00                     | 0.43              |
| 1:C:387:TRP:HA   | 1:C:388:PRO:HD2  | 1.77                     | 0.43              |
| 1:D:628:ASP:O    | 1:D:632:HIS:HD2  | 2.01                     | 0.43              |
| 1:B:707:ASN:HA   | 1:B:800:MET:CE   | 2.47                     | 0.43              |
| 1:D:778:GLU:O    | 1:D:782:LYS:HG3  | 2.19                     | 0.43              |
| 1:A:754:GLN:HA   | 1:A:755:PRO:HD2  | 1.85                     | 0.43              |
| 1:B:329:PHE:CE1  | 1:B:333:VAL:HG21 | 2.54                     | 0.43              |
| 1:B:547:ALA:HB1  | 1:B:551:ARG:HH22 | 1.83                     | 0.43              |
| 1:B:687:LEU:HD13 | 1:B:709:PHE:HE2  | 1.82                     | 0.43              |
| 1:A:304:LEU:O    | 1:A:308:ILE:HG12 | 2.19                     | 0.43              |
| 1:A:547:ALA:O    | 1:A:551:ARG:HG2  | 2.18                     | 0.43              |
| 1:B:198:LEU:HD22 | 1:B:305:GLN:OE1  | 2.18                     | 0.43              |
| 1:B:33:ARG:HG2   | 1:B:33:ARG:NH1   | 2.31                     | 0.43              |
| 1:D:374:TYR:O    | 1:D:452:VAL:HA   | 2.18                     | 0.43              |
| 1:A:15:VAL:HA    | 1:A:18:LEU:HD12  | 2.00                     | 0.43              |
| 1:A:44:ASN:ND2   | 1:B:72:GLN:HE21  | 2.17                     | 0.43              |
| 1:A:724:ARG:HH12 | 1:A:726:TYR:HA   | 1.82                     | 0.43              |
| 1:A:34:HIS:O     | 1:A:38:THR:HB    | 2.20                     | 0.42              |
| 1:A:577:LEU:HD11 | 1:A:761:ILE:HD13 | 2.01                     | 0.42              |
| 1:C:159:ILE:CD1  | 1:C:295:GLN:HG2  | 2.48                     | 0.42              |
| 1:C:569:ARG:HG3  | 1:C:574:LYS:HE3  | 2.00                     | 0.42              |
| 1:D:233:TYR:HB2  | 1:D:489:ARG:HD3  | 2.01                     | 0.42              |
| 1:B:198:LEU:HD13 | 1:B:305:GLN:HB2  | 2.01                     | 0.42              |
| 1:C:169:LYS:O    | 1:C:176:MET:N    | 2.51                     | 0.42              |
| 1:C:619:ILE:O    | 1:C:623:ILE:HG13 | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:441:MET:HE3  | 1:D:444:LEU:HD23 | 2.01                     | 0.42              |
| 1:D:550:GLU:O    | 1:D:554:LYS:HA   | 2.19                     | 0.42              |
| 1:A:458:ILE:HG22 | 1:A:462:ILE:CD1  | 2.49                     | 0.42              |
| 1:B:642:VAL:O    | 1:B:643:ILE:HG13 | 2.19                     | 0.42              |
| 1:D:85:LEU:CD1   | 1:D:303:THR:HG21 | 2.50                     | 0.42              |
| 1:A:87:LEU:HD23  | 1:A:292:ARG:NH2  | 2.34                     | 0.42              |
| 1:A:369:VAL:HA   | 1:A:448:GLY:O    | 2.20                     | 0.42              |
| 1:B:727:ASN:ND2  | 1:C:724:ARG:HH21 | 2.18                     | 0.42              |
| 1:D:167:ASN:HD22 | 1:D:180:ASP:HA   | 1.84                     | 0.42              |
| 1:A:311:PHE:CE1  | 1:A:323:ARG:HD2  | 2.54                     | 0.42              |
| 1:A:458:ILE:O    | 1:A:462:ILE:HG13 | 2.20                     | 0.42              |
| 1:B:549:LEU:HD12 | 1:B:557:ILE:HD13 | 2.02                     | 0.42              |
| 1:A:191:LYS:HG2  | 1:A:193:ARG:NH2  | 2.34                     | 0.42              |
| 1:B:247:LYS:HE3  | 1:B:247:LYS:HB2  | 1.74                     | 0.42              |
| 1:B:616:ALA:HA   | 1:B:619:ILE:HD12 | 2.00                     | 0.42              |
| 1:C:764:MET:HE3  | 1:C:764:MET:HB3  | 1.91                     | 0.42              |
| 1:D:289:LYS:HG3  | 1:D:291:LEU:H    | 1.85                     | 0.42              |
| 1:D:761:ILE:HG13 | 1:D:762:VAL:N    | 2.32                     | 0.42              |
| 1:B:539:GLN:HE21 | 1:B:543:LEU:HD13 | 1.84                     | 0.42              |
| 1:C:411:LEU:HA   | 1:C:414:VAL:CG1  | 2.50                     | 0.42              |
| 1:A:248:ALA:CB   | 1:A:269:ARG:HA   | 2.50                     | 0.42              |
| 1:A:490:ARG:HA   | 1:A:494:LEU:HB3  | 2.02                     | 0.42              |
| 1:C:532:ARG:HD2  | 1:C:532:ARG:C    | 2.45                     | 0.42              |
| 1:D:439:ILE:HD13 | 1:D:439:ILE:HA   | 1.87                     | 0.42              |
| 1:D:69:ARG:HH21  | 1:D:836:ALA:HB3  | 1.85                     | 0.42              |
| 1:A:381:PRO:HA   | 1:A:384:LEU:HG   | 2.00                     | 0.41              |
| 1:A:519:ARG:NH1  | 1:A:807:THR:HG22 | 2.35                     | 0.41              |
| 1:B:582:HIS:HD2  | 1:B:781:VAL:HG22 | 1.84                     | 0.41              |
| 1:D:94:THR:HB    | 1:D:189:TRP:CE2  | 2.55                     | 0.41              |
| 1:A:138:ARG:HH21 | 1:A:650:VAL:HG11 | 1.86                     | 0.41              |
| 1:C:159:ILE:HG22 | 1:C:160:ARG:N    | 2.36                     | 0.41              |
| 1:B:571:HIS:H    | 1:B:576:GLN:HE22 | 1.68                     | 0.41              |
| 1:B:740:GLN:O    | 1:B:744:GLN:HG3  | 2.20                     | 0.41              |
| 1:C:92:GLY:O     | 1:C:128:ASP:HA   | 2.20                     | 0.41              |
| 1:C:373:ALA:HA   | 1:C:449:SER:HB3  | 2.02                     | 0.41              |
| 1:C:582:HIS:O    | 1:C:586:LEU:HD22 | 2.19                     | 0.41              |
| 1:D:42:ASP:HB3   | 1:D:44:ASN:N     | 2.34                     | 0.41              |
| 1:D:206:VAL:CG2  | 1:D:398:ARG:HG2  | 2.50                     | 0.41              |
| 1:B:673:ALA:O    | 1:B:694:GLY:HA2  | 2.21                     | 0.41              |
| 1:C:490:ARG:HA   | 1:C:494:LEU:HB3  | 2.02                     | 0.41              |
| 1:D:53:PHE:CE1   | 1:D:188:PRO:HD3  | 2.51                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:D:571:HIS:CD2     | 1:D:572:GLU:N      | 2.89                     | 0.41              |
| 1:A:709:PHE:HB3     | 1:A:783:CYS:SG     | 2.59                     | 0.41              |
| 1:D:142:CYS:SG      | 1:D:487:THR:HG22   | 2.61                     | 0.41              |
| 1:A:12:GLN:HE22     | 1:B:28:LYS:HZ1     | 1.68                     | 0.41              |
| 1:D:475:GLU:HA      | 1:D:476:PRO:HD2    | 1.91                     | 0.41              |
| 1:B:88:GLU:HB2      | 1:B:132:GLY:HA2    | 2.01                     | 0.41              |
| 1:B:536:LYS:HE2     | 1:B:536:LYS:HB3    | 1.83                     | 0.41              |
| 1:C:521:LEU:HB2     | 1:C:806:ALA:HB2    | 2.02                     | 0.41              |
| 1:D:496:ASN:ND2     | 1:D:499:LEU:HB2    | 2.36                     | 0.41              |
| 1:A:521:LEU:HB2     | 1:A:806:ALA:HB2    | 2.01                     | 0.41              |
| 1:C:136:LEU:HD21    | 1:C:338:ASN:HD22   | 1.86                     | 0.41              |
| 1:D:631:ASN:OD1     | 1:D:641:ARG:HA     | 2.21                     | 0.41              |
| 1:A:557:ILE:HD13    | 1:A:557:ILE:HG21   | 1.90                     | 0.41              |
| 3:B:860[B]:PDP:H5A2 | 3:B:860[B]:PDP:O2B | 2.21                     | 0.41              |
| 1:C:87:LEU:HD22     | 1:C:292:ARG:NH2    | 2.36                     | 0.41              |
| 1:D:102:LEU:HD23    | 1:D:104:LEU:CD1    | 2.51                     | 0.41              |
| 1:D:267:LEU:HA      | 1:D:267:LEU:HD22   | 1.87                     | 0.41              |
| 1:D:348:GLU:O       | 1:D:352:VAL:HG23   | 2.21                     | 0.41              |
| 1:D:571:HIS:CD2     | 1:D:573:TYR:HD1    | 2.38                     | 0.41              |
| 1:A:453:ASN:HA      | 1:A:480:GLN:O      | 2.21                     | 0.41              |
| 1:B:139:LEU:CD2     | 1:B:377:HIS:HE1    | 2.34                     | 0.41              |
| 1:B:560:ASN:HD22    | 1:B:560:ASN:HA     | 1.76                     | 0.41              |
| 1:B:711:PHE:CD1     | 1:B:711:PHE:C      | 2.98                     | 0.41              |
| 1:C:60:ARG:HD2      | 1:C:188:PRO:O      | 2.21                     | 0.41              |
| 1:C:346:ILE:HB      | 1:C:347:PRO:HD3    | 2.03                     | 0.41              |
| 1:A:205:ARG:HD3     | 1:A:205:ARG:HH11   | 1.75                     | 0.40              |
| 1:A:562:LEU:HD12    | 1:A:661:ASP:HB2    | 2.03                     | 0.40              |
| 1:B:265:ALA:HA      | 1:B:268:ASP:HB2    | 2.03                     | 0.40              |
| 1:C:33:ARG:HG2      | 1:C:33:ARG:HH11    | 1.86                     | 0.40              |
| 1:D:465:LYS:HA      | 1:D:465:LYS:HD3    | 1.91                     | 0.40              |
| 1:D:497:PRO:O       | 1:D:501:GLU:HB2    | 2.20                     | 0.40              |
| 1:A:522:LEU:O       | 1:A:525:VAL:HG22   | 2.21                     | 0.40              |
| 1:A:764:MET:HE3     | 1:A:764:MET:HB3    | 1.85                     | 0.40              |
| 1:A:40:VAL:HG13     | 1:B:64:VAL:HG13    | 2.04                     | 0.40              |
| 1:B:323:ARG:HH11    | 1:B:323:ARG:HD3    | 1.75                     | 0.40              |
| 1:C:291:LEU:O       | 1:C:295:GLN:HB2    | 2.21                     | 0.40              |
| 1:D:67:TRP:O        | 1:D:71:GLN:HG2     | 2.22                     | 0.40              |
| 1:C:332:LYS:HA      | 1:C:332:LYS:HD3    | 1.99                     | 0.40              |
| 1:C:726:TYR:CE1     | 1:C:775:ALA:HB2    | 2.54                     | 0.40              |
| 1:A:799:ARG:O       | 1:A:803:ARG:HG3    | 2.21                     | 0.40              |
| 1:B:55:LEU:HD23     | 1:B:95:LEU:HD21    | 2.02                     | 0.40              |

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| Atom-1        | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------|--------------------------|-------------------|
| 1:B:165:ILE:O | 1:B:165:ILE:HG23 | 2.21                     | 0.40              |
| 1:D:798:THR:O | 1:D:802:ILE:HG13 | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 795/842 (94%)   | 733 (92%)  | 51 (6%)  | 11 (1%)  | 9           | 28 |
| 1   | B     | 785/842 (93%)   | 725 (92%)  | 52 (7%)  | 8 (1%)   | 12          | 35 |
| 1   | C     | 795/842 (94%)   | 727 (91%)  | 61 (8%)  | 7 (1%)   | 14          | 38 |
| 1   | D     | 795/842 (94%)   | 746 (94%)  | 42 (5%)  | 7 (1%)   | 14          | 38 |
| All | All   | 3170/3368 (94%) | 2931 (92%) | 206 (6%) | 33 (1%)  | 12          | 35 |

All (33) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | LEU  |
| 1   | A     | 166 | PHE  |
| 1   | A     | 322 | VAL  |
| 1   | B     | 166 | PHE  |
| 1   | B     | 321 | PRO  |
| 1   | B     | 322 | VAL  |
| 1   | B     | 421 | ASP  |
| 1   | B     | 835 | PRO  |
| 1   | C     | 16  | ARG  |
| 1   | C     | 166 | PHE  |
| 1   | C     | 835 | PRO  |
| 1   | D     | 16  | ARG  |
| 1   | D     | 166 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 835 | PRO  |
| 1   | A     | 552 | GLU  |
| 1   | B     | 675 | GLY  |
| 1   | D     | 17  | GLY  |
| 1   | D     | 199 | PRO  |
| 1   | D     | 435 | ALA  |
| 1   | D     | 675 | GLY  |
| 1   | A     | 16  | ARG  |
| 1   | A     | 361 | TRP  |
| 1   | B     | 435 | ALA  |
| 1   | C     | 551 | ARG  |
| 1   | C     | 705 | GLU  |
| 1   | A     | 133 | ASN  |
| 1   | A     | 321 | PRO  |
| 1   | A     | 475 | GLU  |
| 1   | A     | 675 | GLY  |
| 1   | B     | 484 | ASN  |
| 1   | A     | 165 | ILE  |
| 1   | C     | 629 | VAL  |
| 1   | C     | 379 | VAL  |

### 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     | 693/731 (95%)   | 619 (89%)  | 74 (11%)  | 6           | 19 |
| 1   | B     | 685/731 (94%)   | 614 (90%)  | 71 (10%)  | 7           | 20 |
| 1   | C     | 693/731 (95%)   | 607 (88%)  | 86 (12%)  | 4           | 13 |
| 1   | D     | 693/731 (95%)   | 608 (88%)  | 85 (12%)  | 4           | 13 |
| All | All   | 2764/2924 (94%) | 2448 (89%) | 316 (11%) | 5           | 16 |

All (316) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 15  | VAL  |
| 1   | A     | 16  | ARG  |
| 1   | A     | 21  | VAL  |
| 1   | A     | 26  | GLU  |
| 1   | A     | 27  | LEU  |
| 1   | A     | 41  | LYS  |
| 1   | A     | 87  | LEU  |
| 1   | A     | 102 | LEU  |
| 1   | A     | 122 | LEU  |
| 1   | A     | 138 | ARG  |
| 1   | A     | 150 | LEU  |
| 1   | A     | 162 | GLU  |
| 1   | A     | 169 | LYS  |
| 1   | A     | 176 | MET  |
| 1   | A     | 191 | LYS  |
| 1   | A     | 193 | ARG  |
| 1   | A     | 211 | GLN  |
| 1   | A     | 230 | VAL  |
| 1   | A     | 242 | ARG  |
| 1   | A     | 264 | GLN  |
| 1   | A     | 269 | ARG  |
| 1   | A     | 270 | ASN  |
| 1   | A     | 273 | GLU  |
| 1   | A     | 292 | ARG  |
| 1   | A     | 299 | VAL  |
| 1   | A     | 315 | LYS  |
| 1   | A     | 321 | PRO  |
| 1   | A     | 322 | VAL  |
| 1   | A     | 323 | ARG  |
| 1   | A     | 359 | LEU  |
| 1   | A     | 376 | ASN  |
| 1   | A     | 379 | VAL  |
| 1   | A     | 398 | ARG  |
| 1   | A     | 411 | LEU  |
| 1   | A     | 414 | VAL  |
| 1   | A     | 422 | VAL  |
| 1   | A     | 431 | VAL  |
| 1   | A     | 433 | GLU  |
| 1   | A     | 452 | VAL  |
| 1   | A     | 467 | ILE  |
| 1   | A     | 470 | ASP  |
| 1   | A     | 473 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 483 | THR  |
| 1   | A     | 489 | ARG  |
| 1   | A     | 493 | VAL  |
| 1   | A     | 499 | LEU  |
| 1   | A     | 506 | ARG  |
| 1   | A     | 525 | VAL  |
| 1   | A     | 542 | LYS  |
| 1   | A     | 543 | LEU  |
| 1   | A     | 570 | ILE  |
| 1   | A     | 578 | LEU  |
| 1   | A     | 581 | LEU  |
| 1   | A     | 583 | VAL  |
| 1   | A     | 589 | ARG  |
| 1   | A     | 635 | VAL  |
| 1   | A     | 641 | ARG  |
| 1   | A     | 649 | ARG  |
| 1   | A     | 678 | ASN  |
| 1   | A     | 680 | LYS  |
| 1   | A     | 683 | LEU  |
| 1   | A     | 702 | GLU  |
| 1   | A     | 706 | GLU  |
| 1   | A     | 718 | VAL  |
| 1   | A     | 751 | SER  |
| 1   | A     | 753 | LYS  |
| 1   | A     | 754 | GLN  |
| 1   | A     | 756 | ASP  |
| 1   | A     | 761 | ILE  |
| 1   | A     | 764 | MET  |
| 1   | A     | 817 | ILE  |
| 1   | A     | 822 | ARG  |
| 1   | A     | 832 | GLN  |
| 1   | B     | 21  | VAL  |
| 1   | B     | 23  | ASN  |
| 1   | B     | 41  | LYS  |
| 1   | B     | 48  | PRO  |
| 1   | B     | 77  | LYS  |
| 1   | B     | 79  | PRO  |
| 1   | B     | 87  | LEU  |
| 1   | B     | 112 | THR  |
| 1   | B     | 122 | LEU  |
| 1   | B     | 138 | ARG  |
| 1   | B     | 169 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 191 | LYS  |
| 1   | B     | 193 | ARG  |
| 1   | B     | 205 | ARG  |
| 1   | B     | 209 | THR  |
| 1   | B     | 210 | SER  |
| 1   | B     | 230 | VAL  |
| 1   | B     | 242 | ARG  |
| 1   | B     | 270 | ASN  |
| 1   | B     | 273 | GLU  |
| 1   | B     | 291 | LEU  |
| 1   | B     | 304 | LEU  |
| 1   | B     | 315 | LYS  |
| 1   | B     | 321 | PRO  |
| 1   | B     | 324 | THR  |
| 1   | B     | 363 | LYS  |
| 1   | B     | 381 | PRO  |
| 1   | B     | 398 | ARG  |
| 1   | B     | 411 | LEU  |
| 1   | B     | 433 | GLU  |
| 1   | B     | 438 | ARG  |
| 1   | B     | 452 | VAL  |
| 1   | B     | 473 | GLU  |
| 1   | B     | 489 | ARG  |
| 1   | B     | 493 | VAL  |
| 1   | B     | 499 | LEU  |
| 1   | B     | 501 | GLU  |
| 1   | B     | 505 | GLU  |
| 1   | B     | 506 | ARG  |
| 1   | B     | 543 | LEU  |
| 1   | B     | 544 | LYS  |
| 1   | B     | 550 | GLU  |
| 1   | B     | 556 | HIS  |
| 1   | B     | 558 | ASN  |
| 1   | B     | 559 | PRO  |
| 1   | B     | 562 | LEU  |
| 1   | B     | 566 | GLN  |
| 1   | B     | 569 | ARG  |
| 1   | B     | 577 | LEU  |
| 1   | B     | 578 | LEU  |
| 1   | B     | 583 | VAL  |
| 1   | B     | 591 | LYS  |
| 1   | B     | 592 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 598 | VAL  |
| 1   | B     | 639 | ARG  |
| 1   | B     | 651 | SER  |
| 1   | B     | 658 | PRO  |
| 1   | B     | 683 | LEU  |
| 1   | B     | 706 | GLU  |
| 1   | B     | 708 | PHE  |
| 1   | B     | 720 | ARG  |
| 1   | B     | 724 | ARG  |
| 1   | B     | 730 | GLU  |
| 1   | B     | 753 | LYS  |
| 1   | B     | 761 | ILE  |
| 1   | B     | 779 | GLU  |
| 1   | B     | 788 | SER  |
| 1   | B     | 815 | ARG  |
| 1   | B     | 822 | ARG  |
| 1   | B     | 834 | LEU  |
| 1   | B     | 835 | PRO  |
| 1   | C     | 10  | ARG  |
| 1   | C     | 15  | VAL  |
| 1   | C     | 22  | GLU  |
| 1   | C     | 25  | THR  |
| 1   | C     | 27  | LEU  |
| 1   | C     | 41  | LYS  |
| 1   | C     | 43  | ARG  |
| 1   | C     | 48  | PRO  |
| 1   | C     | 87  | LEU  |
| 1   | C     | 113 | TYR  |
| 1   | C     | 122 | LEU  |
| 1   | C     | 138 | ARG  |
| 1   | C     | 144 | LEU  |
| 1   | C     | 163 | PHE  |
| 1   | C     | 167 | ASN  |
| 1   | C     | 169 | LYS  |
| 1   | C     | 176 | MET  |
| 1   | C     | 191 | LYS  |
| 1   | C     | 193 | ARG  |
| 1   | C     | 214 | LYS  |
| 1   | C     | 217 | ASP  |
| 1   | C     | 242 | ARG  |
| 1   | C     | 267 | LEU  |
| 1   | C     | 270 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 273 | GLU  |
| 1   | C     | 274 | ASN  |
| 1   | C     | 289 | LYS  |
| 1   | C     | 300 | VAL  |
| 1   | C     | 305 | GLN  |
| 1   | C     | 319 | ARG  |
| 1   | C     | 339 | ASP  |
| 1   | C     | 351 | ARG  |
| 1   | C     | 371 | THR  |
| 1   | C     | 379 | VAL  |
| 1   | C     | 382 | GLU  |
| 1   | C     | 389 | VAL  |
| 1   | C     | 398 | ARG  |
| 1   | C     | 405 | GLU  |
| 1   | C     | 407 | ASN  |
| 1   | C     | 414 | VAL  |
| 1   | C     | 430 | LEU  |
| 1   | C     | 438 | ARG  |
| 1   | C     | 452 | VAL  |
| 1   | C     | 462 | ILE  |
| 1   | C     | 473 | GLU  |
| 1   | C     | 489 | ARG  |
| 1   | C     | 493 | VAL  |
| 1   | C     | 496 | ASN  |
| 1   | C     | 499 | LEU  |
| 1   | C     | 506 | ARG  |
| 1   | C     | 510 | GLU  |
| 1   | C     | 532 | ARG  |
| 1   | C     | 542 | LYS  |
| 1   | C     | 553 | TYR  |
| 1   | C     | 555 | VAL  |
| 1   | C     | 558 | ASN  |
| 1   | C     | 561 | SER  |
| 1   | C     | 562 | LEU  |
| 1   | C     | 569 | ARG  |
| 1   | C     | 577 | LEU  |
| 1   | C     | 578 | LEU  |
| 1   | C     | 586 | LEU  |
| 1   | C     | 589 | ARG  |
| 1   | C     | 635 | VAL  |
| 1   | C     | 636 | VAL  |
| 1   | C     | 643 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 646 | GLU  |
| 1   | C     | 672 | GLU  |
| 1   | C     | 683 | LEU  |
| 1   | C     | 698 | GLU  |
| 1   | C     | 702 | GLU  |
| 1   | C     | 705 | GLU  |
| 1   | C     | 706 | GLU  |
| 1   | C     | 708 | PHE  |
| 1   | C     | 718 | VAL  |
| 1   | C     | 724 | ARG  |
| 1   | C     | 736 | PRO  |
| 1   | C     | 751 | SER  |
| 1   | C     | 753 | LYS  |
| 1   | C     | 761 | ILE  |
| 1   | C     | 766 | MET  |
| 1   | C     | 779 | GLU  |
| 1   | C     | 827 | VAL  |
| 1   | C     | 832 | GLN  |
| 1   | C     | 833 | ARG  |
| 1   | C     | 835 | PRO  |
| 1   | D     | 10  | ARG  |
| 1   | D     | 15  | VAL  |
| 1   | D     | 16  | ARG  |
| 1   | D     | 21  | VAL  |
| 1   | D     | 22  | GLU  |
| 1   | D     | 23  | ASN  |
| 1   | D     | 26  | GLU  |
| 1   | D     | 41  | LYS  |
| 1   | D     | 42  | ASP  |
| 1   | D     | 69  | ARG  |
| 1   | D     | 77  | LYS  |
| 1   | D     | 81  | ARG  |
| 1   | D     | 87  | LEU  |
| 1   | D     | 90  | TYR  |
| 1   | D     | 106 | ASN  |
| 1   | D     | 110 | GLU  |
| 1   | D     | 122 | LEU  |
| 1   | D     | 138 | ARG  |
| 1   | D     | 169 | LYS  |
| 1   | D     | 191 | LYS  |
| 1   | D     | 193 | ARG  |
| 1   | D     | 199 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 205 | ARG  |
| 1   | D     | 207 | GLU  |
| 1   | D     | 230 | VAL  |
| 1   | D     | 242 | ARG  |
| 1   | D     | 267 | LEU  |
| 1   | D     | 269 | ARG  |
| 1   | D     | 273 | GLU  |
| 1   | D     | 292 | ARG  |
| 1   | D     | 320 | ASP  |
| 1   | D     | 323 | ARG  |
| 1   | D     | 327 | ASP  |
| 1   | D     | 358 | ARG  |
| 1   | D     | 360 | ASP  |
| 1   | D     | 380 | LEU  |
| 1   | D     | 389 | VAL  |
| 1   | D     | 390 | HIS  |
| 1   | D     | 398 | ARG  |
| 1   | D     | 403 | ILE  |
| 1   | D     | 405 | GLU  |
| 1   | D     | 408 | GLN  |
| 1   | D     | 411 | LEU  |
| 1   | D     | 414 | VAL  |
| 1   | D     | 433 | GLU  |
| 1   | D     | 438 | ARG  |
| 1   | D     | 452 | VAL  |
| 1   | D     | 489 | ARG  |
| 1   | D     | 490 | ARG  |
| 1   | D     | 493 | VAL  |
| 1   | D     | 499 | LEU  |
| 1   | D     | 501 | GLU  |
| 1   | D     | 525 | VAL  |
| 1   | D     | 536 | LYS  |
| 1   | D     | 543 | LEU  |
| 1   | D     | 554 | LYS  |
| 1   | D     | 562 | LEU  |
| 1   | D     | 576 | GLN  |
| 1   | D     | 577 | LEU  |
| 1   | D     | 581 | LEU  |
| 1   | D     | 589 | ARG  |
| 1   | D     | 592 | LYS  |
| 1   | D     | 618 | MET  |
| 1   | D     | 635 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 639 | ARG  |
| 1   | D     | 641 | ARG  |
| 1   | D     | 643 | ILE  |
| 1   | D     | 683 | LEU  |
| 1   | D     | 701 | GLU  |
| 1   | D     | 702 | GLU  |
| 1   | D     | 706 | GLU  |
| 1   | D     | 708 | PHE  |
| 1   | D     | 714 | ARG  |
| 1   | D     | 724 | ARG  |
| 1   | D     | 734 | ARG  |
| 1   | D     | 742 | ILE  |
| 1   | D     | 743 | GLU  |
| 1   | D     | 753 | LYS  |
| 1   | D     | 754 | GLN  |
| 1   | D     | 759 | LYS  |
| 1   | D     | 761 | ILE  |
| 1   | D     | 804 | ASN  |
| 1   | D     | 822 | ARG  |
| 1   | D     | 834 | LEU  |
| 1   | D     | 835 | PRO  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | GLN  |
| 1   | A     | 36  | HIS  |
| 1   | A     | 44  | ASN  |
| 1   | A     | 62  | HIS  |
| 1   | A     | 201 | HIS  |
| 1   | A     | 295 | GLN  |
| 1   | A     | 376 | ASN  |
| 1   | A     | 412 | ASN  |
| 1   | A     | 453 | ASN  |
| 1   | A     | 484 | ASN  |
| 1   | A     | 496 | ASN  |
| 1   | A     | 566 | GLN  |
| 1   | A     | 571 | HIS  |
| 1   | A     | 582 | HIS  |
| 1   | A     | 588 | ASN  |
| 1   | A     | 684 | ASN  |
| 1   | A     | 744 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 754 | GLN  |
| 1   | A     | 832 | GLN  |
| 1   | B     | 36  | HIS  |
| 1   | B     | 62  | HIS  |
| 1   | B     | 71  | GLN  |
| 1   | B     | 72  | GLN  |
| 1   | B     | 201 | HIS  |
| 1   | B     | 211 | GLN  |
| 1   | B     | 219 | GLN  |
| 1   | B     | 274 | ASN  |
| 1   | B     | 295 | GLN  |
| 1   | B     | 407 | ASN  |
| 1   | B     | 453 | ASN  |
| 1   | B     | 517 | GLN  |
| 1   | B     | 539 | GLN  |
| 1   | B     | 556 | HIS  |
| 1   | B     | 560 | ASN  |
| 1   | B     | 566 | GLN  |
| 1   | B     | 571 | HIS  |
| 1   | B     | 576 | GLN  |
| 1   | B     | 588 | ASN  |
| 1   | B     | 614 | HIS  |
| 1   | B     | 632 | HIS  |
| 1   | B     | 740 | GLN  |
| 1   | B     | 744 | GLN  |
| 1   | B     | 763 | ASN  |
| 1   | C     | 12  | GLN  |
| 1   | C     | 30  | ASN  |
| 1   | C     | 57  | HIS  |
| 1   | C     | 133 | ASN  |
| 1   | C     | 208 | HIS  |
| 1   | C     | 341 | HIS  |
| 1   | C     | 390 | HIS  |
| 1   | C     | 453 | ASN  |
| 1   | C     | 477 | HIS  |
| 1   | C     | 496 | ASN  |
| 1   | C     | 517 | GLN  |
| 1   | C     | 539 | GLN  |
| 1   | C     | 541 | ASN  |
| 1   | C     | 566 | GLN  |
| 1   | C     | 571 | HIS  |
| 1   | C     | 576 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 579 | ASN  |
| 1   | C     | 582 | HIS  |
| 1   | C     | 588 | ASN  |
| 1   | C     | 632 | HIS  |
| 1   | C     | 684 | ASN  |
| 1   | C     | 744 | GLN  |
| 1   | D     | 12  | GLN  |
| 1   | D     | 30  | ASN  |
| 1   | D     | 57  | HIS  |
| 1   | D     | 62  | HIS  |
| 1   | D     | 101 | ASN  |
| 1   | D     | 167 | ASN  |
| 1   | D     | 201 | HIS  |
| 1   | D     | 264 | GLN  |
| 1   | D     | 274 | ASN  |
| 1   | D     | 305 | GLN  |
| 1   | D     | 341 | HIS  |
| 1   | D     | 399 | HIS  |
| 1   | D     | 412 | ASN  |
| 1   | D     | 453 | ASN  |
| 1   | D     | 496 | ASN  |
| 1   | D     | 517 | GLN  |
| 1   | D     | 539 | GLN  |
| 1   | D     | 541 | ASN  |
| 1   | D     | 556 | HIS  |
| 1   | D     | 566 | GLN  |
| 1   | D     | 571 | HIS  |
| 1   | D     | 576 | GLN  |
| 1   | D     | 579 | ASN  |
| 1   | D     | 588 | ASN  |
| 1   | D     | 632 | HIS  |
| 1   | D     | 647 | ASN  |
| 1   | D     | 684 | ASN  |
| 1   | D     | 744 | GLN  |
| 1   | D     | 754 | GLN  |
| 1   | D     | 804 | ASN  |
| 1   | D     | 819 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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 |
| 3   | PDP  | D     | 860[B] | 1    | 18,19,20     | 3.32 | 6 (33%)  | 26,29,30    | 1.81 | 8 (30%)  |
| 2   | AMP  | B     | 843    | -    | 25,25,25     | 0.97 | 0        | 37,38,38    | 0.85 | 1 (2%)   |
| 3   | PDP  | B     | 860[A] | 1    | 18,19,20     | 3.29 | 6 (33%)  | 26,29,30    | 1.57 | 6 (23%)  |
| 2   | AMP  | C     | 843    | -    | 25,25,25     | 1.04 | 2 (8%)   | 37,38,38    | 0.89 | 2 (5%)   |
| 3   | PDP  | C     | 860[B] | 1    | 18,19,20     | 3.36 | 6 (33%)  | 26,29,30    | 1.53 | 6 (23%)  |
| 2   | AMP  | A     | 843    | -    | 25,25,25     | 0.72 | 0        | 37,38,38    | 0.71 | 0        |
| 2   | AMP  | D     | 843    | -    | 25,25,25     | 0.86 | 0        | 37,38,38    | 1.06 | 2 (5%)   |
| 3   | PDP  | A     | 860[A] | 1    | 18,19,20     | 2.99 | 7 (38%)  | 26,29,30    | 1.63 | 8 (30%)  |
| 3   | PDP  | D     | 860[A] | 1    | 18,19,20     | 3.26 | 6 (33%)  | 26,29,30    | 1.70 | 7 (26%)  |
| 3   | PDP  | C     | 860[A] | 1    | 18,19,20     | 3.63 | 7 (38%)  | 26,29,30    | 1.51 | 5 (19%)  |
| 3   | PDP  | B     | 860[B] | 1    | 18,19,20     | 3.57 | 6 (33%)  | 26,29,30    | 2.24 | 7 (26%)  |
| 3   | PDP  | A     | 860[B] | 1    | 18,19,20     | 3.37 | 7 (38%)  | 26,29,30    | 1.60 | 7 (26%)  |

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   |
|-----|------|-------|--------|------|---------|------------|---------|
| 3   | PDP  | D     | 860[B] | 1    | -       | 3/12/12/14 | 0/1/1/1 |
| 2   | AMP  | B     | 843    | -    | -       | 0/10/26/26 | 0/3/3/3 |
| 3   | PDP  | B     | 860[A] | 1    | -       | 5/12/12/14 | 0/1/1/1 |
| 2   | AMP  | C     | 843    | -    | -       | 0/10/26/26 | 0/3/3/3 |
| 3   | PDP  | C     | 860[B] | 1    | -       | 4/12/12/14 | 0/1/1/1 |
| 2   | AMP  | A     | 843    | -    | -       | 2/10/26/26 | 0/3/3/3 |
| 2   | AMP  | D     | 843    | -    | -       | 1/10/26/26 | 0/3/3/3 |
| 3   | PDP  | A     | 860[A] | 1    | -       | 2/12/12/14 | 0/1/1/1 |
| 3   | PDP  | D     | 860[A] | 1    | -       | 2/12/12/14 | 0/1/1/1 |
| 3   | PDP  | C     | 860[A] | 1    | -       | 1/12/12/14 | 0/1/1/1 |
| 3   | PDP  | B     | 860[B] | 1    | -       | 1/12/12/14 | 0/1/1/1 |
| 3   | PDP  | A     | 860[B] | 1    | -       | 2/12/12/14 | 0/1/1/1 |

All (53) bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|--------|-------------|----------|
| 3   | B     | 860[B] | PDP  | PA-O3A | -11.96 | 1.46        | 1.59     |
| 3   | C     | 860[A] | PDP  | PA-O3A | -10.72 | 1.47        | 1.59     |
| 3   | D     | 860[B] | PDP  | PA-O3A | -10.07 | 1.48        | 1.59     |
| 3   | A     | 860[B] | PDP  | PA-O3A | -10.01 | 1.48        | 1.59     |
| 3   | B     | 860[A] | PDP  | PA-O3A | -9.98  | 1.48        | 1.59     |
| 3   | D     | 860[A] | PDP  | PA-O3A | -9.68  | 1.49        | 1.59     |
| 3   | C     | 860[B] | PDP  | PA-O3A | -9.66  | 1.49        | 1.59     |
| 3   | A     | 860[A] | PDP  | PA-O3A | -9.01  | 1.49        | 1.59     |
| 3   | C     | 860[B] | PDP  | C4A-C4 | -6.91  | 1.37        | 1.51     |
| 3   | D     | 860[B] | PDP  | C4A-C4 | -6.29  | 1.39        | 1.51     |
| 3   | D     | 860[A] | PDP  | C4A-C4 | -6.28  | 1.39        | 1.51     |
| 3   | B     | 860[A] | PDP  | C4A-C4 | -6.20  | 1.39        | 1.51     |
| 3   | C     | 860[A] | PDP  | C4A-C4 | -6.11  | 1.39        | 1.51     |
| 3   | B     | 860[B] | PDP  | C4A-C4 | -5.77  | 1.40        | 1.51     |
| 3   | C     | 860[A] | PDP  | C3-C2  | -5.43  | 1.35        | 1.41     |
| 3   | A     | 860[B] | PDP  | C4A-C4 | -5.35  | 1.40        | 1.51     |
| 3   | A     | 860[B] | PDP  | C3-C2  | -5.34  | 1.35        | 1.41     |
| 3   | A     | 860[A] | PDP  | C4A-C4 | -4.68  | 1.42        | 1.51     |
| 3   | C     | 860[B] | PDP  | C3-C2  | -4.49  | 1.36        | 1.41     |
| 3   | C     | 860[A] | PDP  | PB-O1B | 4.26   | 1.63        | 1.50     |
| 3   | B     | 860[A] | PDP  | PB-O1B | 4.03   | 1.63        | 1.50     |
| 3   | D     | 860[B] | PDP  | C3-C2  | -4.01  | 1.36        | 1.41     |
| 3   | D     | 860[A] | PDP  | C3-C2  | -3.98  | 1.36        | 1.41     |
| 3   | B     | 860[B] | PDP  | PB-O1B | 3.97   | 1.62        | 1.50     |
| 3   | A     | 860[A] | PDP  | PB-O1B | 3.88   | 1.62        | 1.50     |
| 3   | A     | 860[B] | PDP  | PB-O1B | 3.77   | 1.62        | 1.50     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 3   | B     | 860[A] | PDP  | C3-C2   | -3.61 | 1.37        | 1.41     |
| 3   | D     | 860[A] | PDP  | PB-O1B  | 3.36  | 1.60        | 1.50     |
| 3   | A     | 860[A] | PDP  | C3-C2   | -3.26 | 1.37        | 1.41     |
| 3   | C     | 860[A] | PDP  | PA-O5A  | -3.07 | 1.47        | 1.59     |
| 3   | C     | 860[B] | PDP  | PB-O1B  | 3.02  | 1.59        | 1.50     |
| 3   | B     | 860[B] | PDP  | C3-C2   | -3.00 | 1.37        | 1.41     |
| 3   | B     | 860[B] | PDP  | PA-O1A  | 2.94  | 1.61        | 1.50     |
| 3   | B     | 860[A] | PDP  | PA-O5A  | -2.92 | 1.48        | 1.59     |
| 3   | D     | 860[A] | PDP  | PA-O1A  | 2.91  | 1.60        | 1.50     |
| 3   | A     | 860[A] | PDP  | PA-O1A  | 2.85  | 1.60        | 1.50     |
| 3   | C     | 860[B] | PDP  | PA-O5A  | -2.85 | 1.48        | 1.59     |
| 3   | D     | 860[B] | PDP  | PB-O1B  | 2.84  | 1.59        | 1.50     |
| 3   | D     | 860[A] | PDP  | PA-O5A  | -2.79 | 1.48        | 1.59     |
| 3   | A     | 860[B] | PDP  | PA-O5A  | -2.78 | 1.48        | 1.59     |
| 3   | D     | 860[B] | PDP  | PA-O5A  | -2.76 | 1.48        | 1.59     |
| 3   | C     | 860[A] | PDP  | C5-C4   | -2.70 | 1.37        | 1.40     |
| 3   | B     | 860[B] | PDP  | PA-O5A  | -2.67 | 1.48        | 1.59     |
| 3   | A     | 860[A] | PDP  | PA-O5A  | -2.66 | 1.49        | 1.59     |
| 3   | A     | 860[B] | PDP  | PA-O1A  | 2.59  | 1.59        | 1.50     |
| 3   | C     | 860[B] | PDP  | PA-O1A  | 2.52  | 1.59        | 1.50     |
| 3   | D     | 860[B] | PDP  | PA-O1A  | 2.52  | 1.59        | 1.50     |
| 3   | B     | 860[A] | PDP  | PA-O1A  | 2.50  | 1.59        | 1.50     |
| 3   | C     | 860[A] | PDP  | PA-O1A  | 2.34  | 1.58        | 1.50     |
| 3   | A     | 860[B] | PDP  | C2A-C2  | 2.32  | 1.54        | 1.50     |
| 3   | A     | 860[A] | PDP  | C5A-C5  | 2.07  | 1.56        | 1.50     |
| 2   | C     | 843    | AMP  | C2'-C3' | -2.03 | 1.47        | 1.53     |
| 2   | C     | 843    | AMP  | C2-N3   | -2.03 | 1.30        | 1.33     |

All (59) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 3   | B     | 860[B] | PDP  | O5A-C5A-C5 | 7.64  | 123.67      | 109.36   |
| 3   | B     | 860[B] | PDP  | O3B-PB-O3A | 4.17  | 118.63      | 104.64   |
| 3   | C     | 860[B] | PDP  | O2B-PB-O3A | 3.99  | 118.01      | 104.64   |
| 3   | B     | 860[B] | PDP  | O2B-PB-O3A | 3.96  | 117.91      | 104.64   |
| 3   | D     | 860[A] | PDP  | O2B-PB-O3A | 3.85  | 117.55      | 104.64   |
| 3   | D     | 860[B] | PDP  | O3B-PB-O3A | 3.64  | 116.83      | 104.64   |
| 3   | D     | 860[B] | PDP  | O5A-C5A-C5 | 3.62  | 116.14      | 109.36   |
| 3   | C     | 860[A] | PDP  | O2B-PB-O3A | 3.55  | 116.53      | 104.64   |
| 3   | A     | 860[B] | PDP  | O3B-PB-O3A | 3.50  | 116.38      | 104.64   |
| 3   | A     | 860[A] | PDP  | O3B-PB-O3A | 3.29  | 115.68      | 104.64   |
| 3   | D     | 860[B] | PDP  | O2A-PA-O1A | -3.28 | 97.17       | 112.44   |

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| Mol | Chain | Res    | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 3   | D     | 860[A] | PDP  | O3B-PB-O3A | 3.26  | 115.58      | 104.64   |
| 3   | B     | 860[A] | PDP  | O2B-PB-O3A | 3.26  | 115.57      | 104.64   |
| 3   | A     | 860[A] | PDP  | O2B-PB-O3A | 3.23  | 115.47      | 104.64   |
| 3   | D     | 860[B] | PDP  | O2B-PB-O3A | 3.10  | 115.02      | 104.64   |
| 3   | A     | 860[A] | PDP  | O2A-PA-O1A | -3.07 | 98.16       | 112.44   |
| 3   | D     | 860[A] | PDP  | O5A-C5A-C5 | 3.00  | 114.98      | 109.36   |
| 3   | C     | 860[A] | PDP  | O2A-PA-O1A | -2.90 | 98.98       | 112.44   |
| 3   | B     | 860[A] | PDP  | O2A-PA-O3A | 2.84  | 114.95      | 107.27   |
| 3   | B     | 860[A] | PDP  | O3B-PB-O1B | -2.82 | 99.87       | 110.83   |
| 3   | D     | 860[B] | PDP  | O2A-PA-O3A | 2.78  | 114.80      | 107.27   |
| 3   | B     | 860[A] | PDP  | O2A-PA-O1A | -2.77 | 99.56       | 112.44   |
| 3   | B     | 860[A] | PDP  | O3B-PB-O3A | 2.70  | 113.68      | 104.64   |
| 3   | D     | 860[A] | PDP  | O2A-PA-O1A | -2.70 | 99.91       | 112.44   |
| 3   | B     | 860[B] | PDP  | O3B-PB-O1B | -2.67 | 100.42      | 110.83   |
| 3   | A     | 860[B] | PDP  | C5-C6-N1   | -2.67 | 119.49      | 123.83   |
| 2   | D     | 843    | AMP  | O2P-P-O5'  | -2.67 | 99.72       | 106.67   |
| 3   | D     | 860[B] | PDP  | O2B-PB-O1B | -2.65 | 100.53      | 110.83   |
| 3   | A     | 860[B] | PDP  | O2B-PB-O1B | -2.57 | 100.81      | 110.83   |
| 3   | B     | 860[B] | PDP  | O2B-PB-O1B | -2.57 | 100.83      | 110.83   |
| 2   | B     | 843    | AMP  | O4'-C1'-N9 | 2.57  | 113.02      | 108.09   |
| 3   | A     | 860[B] | PDP  | O2A-PA-O1A | -2.55 | 100.58      | 112.44   |
| 2   | D     | 843    | AMP  | O4'-C1'-N9 | 2.53  | 112.95      | 108.09   |
| 3   | C     | 860[B] | PDP  | C5-C6-N1   | -2.48 | 119.80      | 123.83   |
| 3   | A     | 860[B] | PDP  | O2B-PB-O3A | 2.41  | 112.73      | 104.64   |
| 3   | C     | 860[B] | PDP  | O3B-PB-O1B | -2.41 | 101.46      | 110.83   |
| 3   | C     | 860[B] | PDP  | O3B-PB-O3A | 2.39  | 112.65      | 104.64   |
| 3   | C     | 860[B] | PDP  | O2A-PA-O1A | -2.26 | 101.91      | 112.44   |
| 3   | D     | 860[A] | PDP  | O3A-PB-O1B | -2.25 | 99.20       | 111.04   |
| 3   | A     | 860[B] | PDP  | O3B-PB-O1B | -2.25 | 102.08      | 110.83   |
| 3   | B     | 860[B] | PDP  | C6-C5-C4   | 2.24  | 119.94      | 118.10   |
| 3   | C     | 860[A] | PDP  | O3B-PB-O3A | 2.23  | 112.11      | 104.64   |
| 3   | B     | 860[A] | PDP  | C6-C5-C4   | 2.22  | 119.91      | 118.10   |
| 3   | A     | 860[A] | PDP  | O3B-PB-O2B | 2.21  | 116.07      | 107.80   |
| 3   | A     | 860[A] | PDP  | O2A-PA-O3A | 2.19  | 113.19      | 107.27   |
| 3   | C     | 860[A] | PDP  | C5-C6-N1   | -2.18 | 120.29      | 123.83   |
| 2   | C     | 843    | AMP  | O4'-C1'-N9 | 2.18  | 112.27      | 108.09   |
| 3   | A     | 860[B] | PDP  | C6-C5-C4   | 2.14  | 119.85      | 118.10   |
| 3   | C     | 860[B] | PDP  | O2B-PB-O1B | -2.12 | 102.56      | 110.83   |
| 3   | D     | 860[A] | PDP  | O3B-PB-O1B | -2.12 | 102.58      | 110.83   |
| 3   | D     | 860[B] | PDP  | O3B-PB-O1B | -2.12 | 102.59      | 110.83   |
| 3   | D     | 860[A] | PDP  | C6-C5-C4   | 2.11  | 119.82      | 118.10   |
| 3   | B     | 860[B] | PDP  | O2A-PA-O1A | -2.09 | 102.72      | 112.44   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 3   | A     | 860[A] | PDP  | O3A-PB-O1B  | -2.06 | 100.21      | 111.04   |
| 3   | C     | 860[A] | PDP  | O5A-C5A-C5  | 2.04  | 113.18      | 109.36   |
| 3   | D     | 860[B] | PDP  | C5-C6-N1    | -2.04 | 120.51      | 123.83   |
| 3   | A     | 860[A] | PDP  | O3B-PB-O1B  | -2.02 | 102.98      | 110.83   |
| 3   | A     | 860[A] | PDP  | O2B-PB-O1B  | -2.00 | 103.03      | 110.83   |
| 2   | C     | 843    | AMP  | O3'-C3'-C2' | -2.00 | 105.39      | 111.82   |

There are no chirality outliers.

All (23) torsion outliers are listed below:

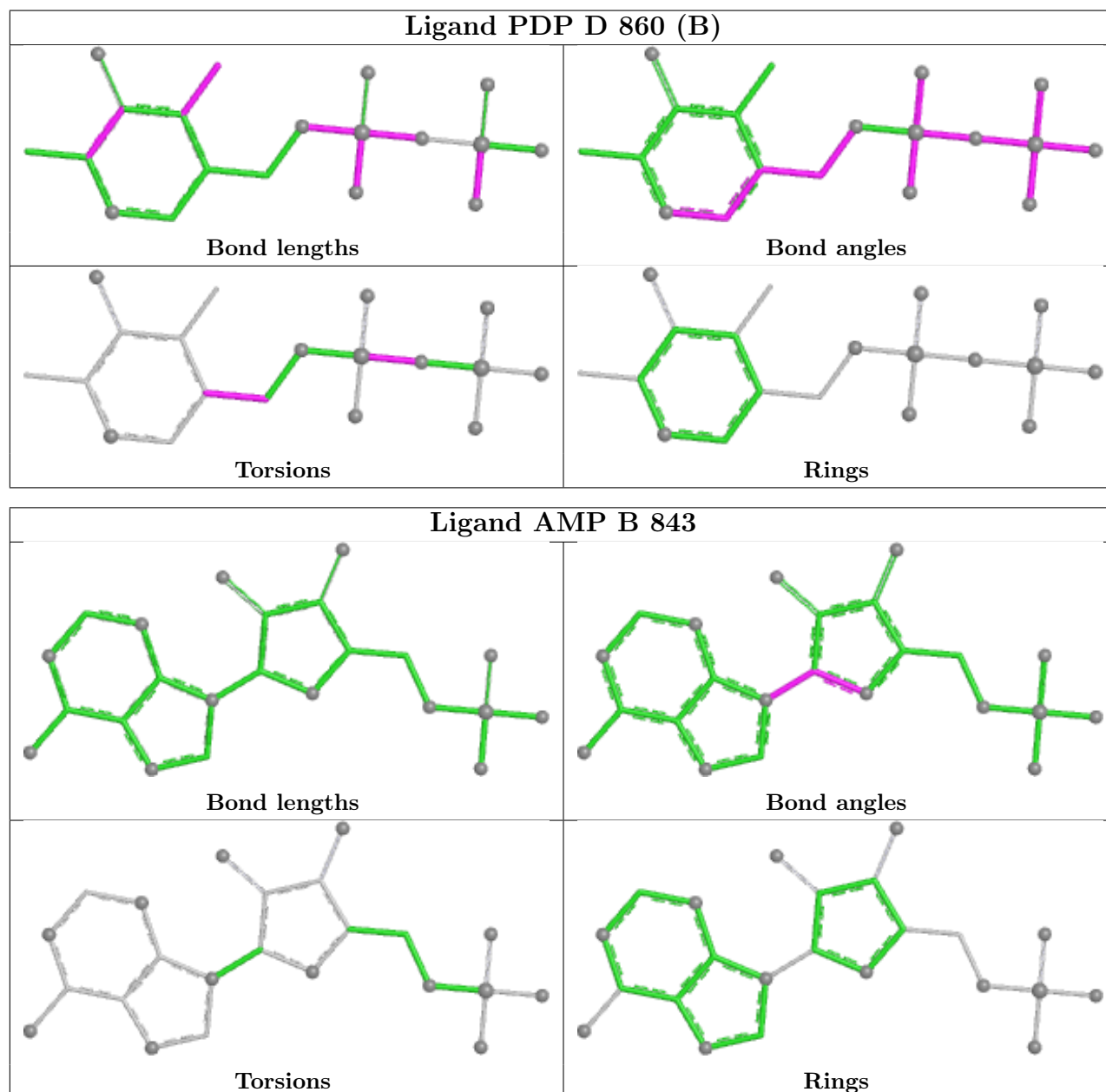
| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 2   | A     | 843    | AMP  | C5'-O5'-P-O2P   |
| 2   | A     | 843    | AMP  | C5'-O5'-P-O3P   |
| 3   | B     | 860[A] | PDP  | C5A-O5A-PA-O1A  |
| 3   | B     | 860[A] | PDP  | C5A-O5A-PA-O3A  |
| 3   | D     | 860[A] | PDP  | C5A-O5A-PA-O1A  |
| 3   | B     | 860[B] | PDP  | C5-C5A-O5A-PA   |
| 3   | C     | 860[B] | PDP  | C6-C5-C5A-O5A   |
| 3   | A     | 860[B] | PDP  | PA-O3A-PB-O2B   |
| 3   | A     | 860[A] | PDP  | C4-C5-C5A-O5A   |
| 3   | A     | 860[B] | PDP  | C4-C5-C5A-O5A   |
| 3   | C     | 860[B] | PDP  | C4-C5-C5A-O5A   |
| 3   | C     | 860[B] | PDP  | PB-O3A-PA-O1A   |
| 3   | D     | 860[B] | PDP  | C4-C5-C5A-O5A   |
| 3   | B     | 860[A] | PDP  | C5A-O5A-PA-O2A  |
| 3   | D     | 860[B] | PDP  | PB-O3A-PA-O2A   |
| 2   | D     | 843    | AMP  | O4'-C4'-C5'-O5' |
| 3   | D     | 860[B] | PDP  | C6-C5-C5A-O5A   |
| 3   | A     | 860[A] | PDP  | PB-O3A-PA-O2A   |
| 3   | B     | 860[A] | PDP  | PB-O3A-PA-O1A   |
| 3   | C     | 860[A] | PDP  | C4-C5-C5A-O5A   |
| 3   | C     | 860[B] | PDP  | PB-O3A-PA-O2A   |
| 3   | B     | 860[A] | PDP  | PB-O3A-PA-O2A   |
| 3   | D     | 860[A] | PDP  | PB-O3A-PA-O2A   |

There are no ring outliers.

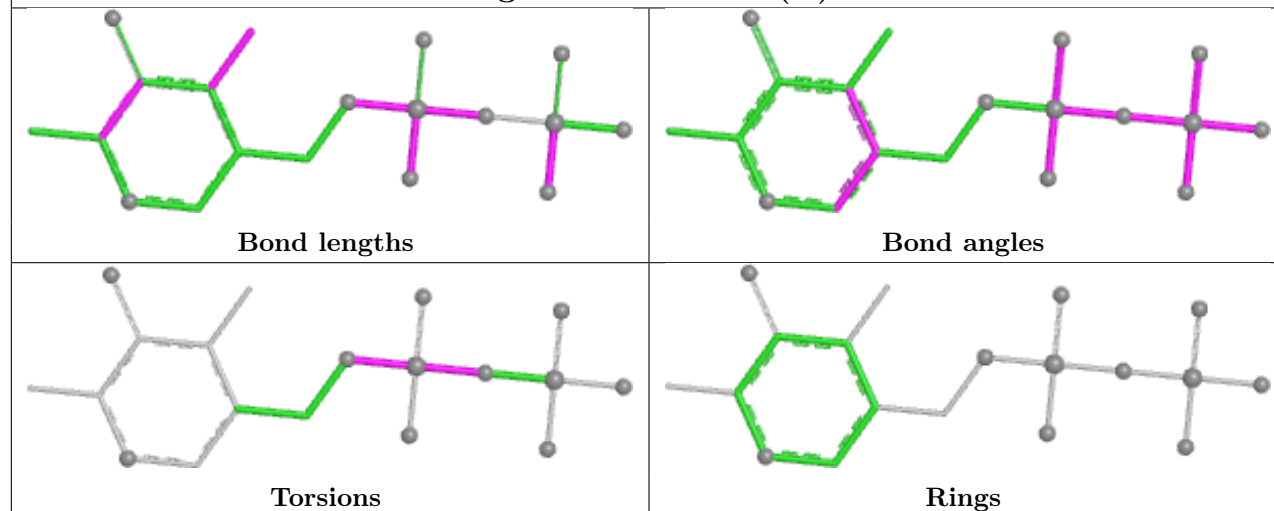
2 monomers are involved in 2 short contacts:

| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 2   | B     | 843    | AMP  | 1       | 0            |
| 3   | B     | 860[B] | PDP  | 1       | 0            |

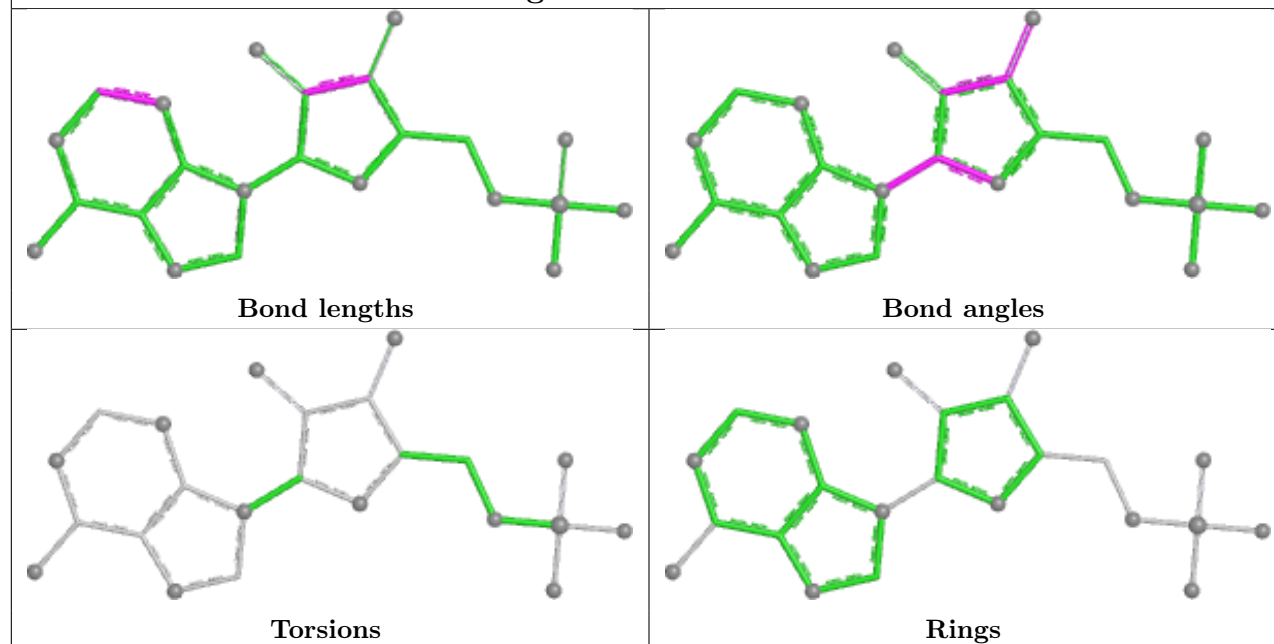
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



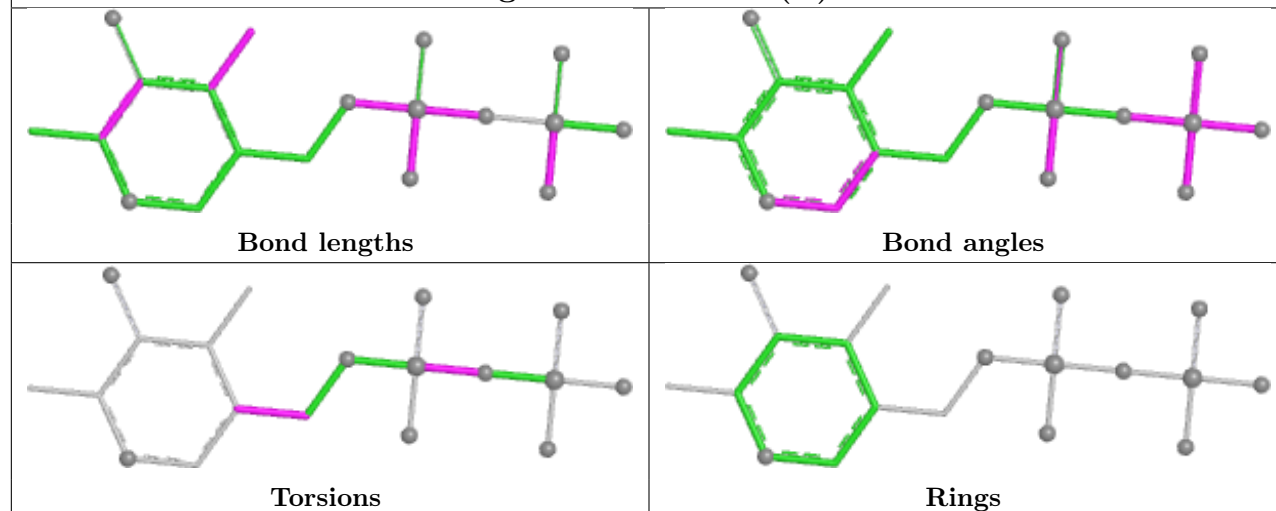
## Ligand PDP B 860 (A)



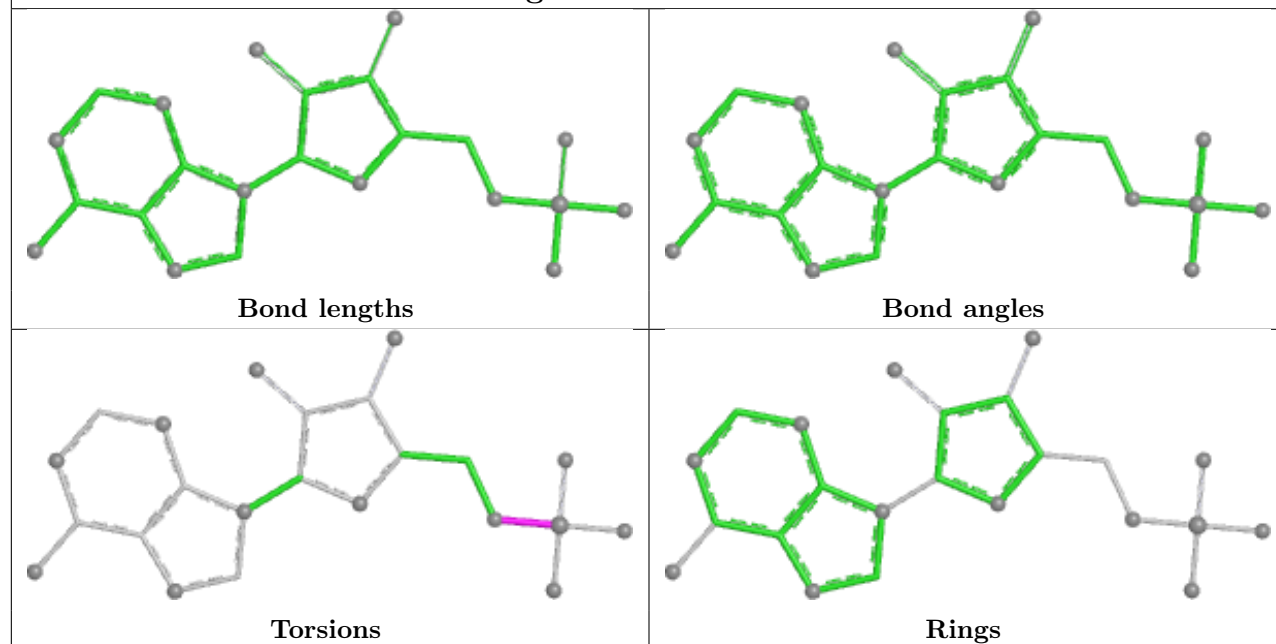
## Ligand AMP C 843



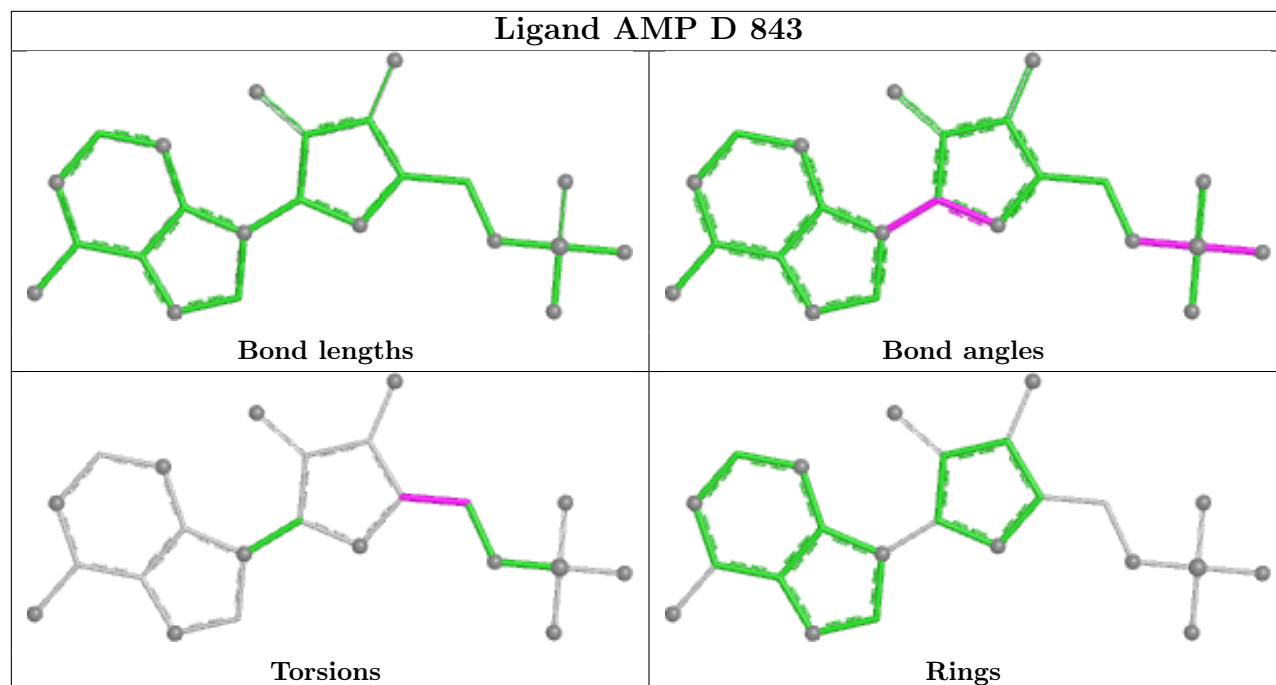
## Ligand PDP C 860 (B)



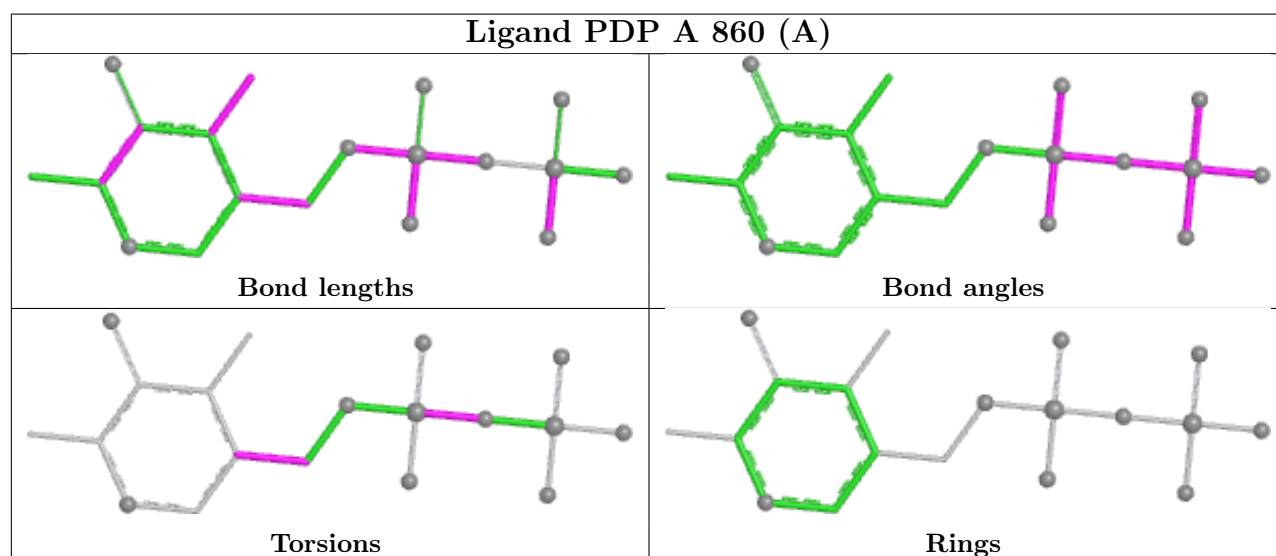
## Ligand AMP A 843



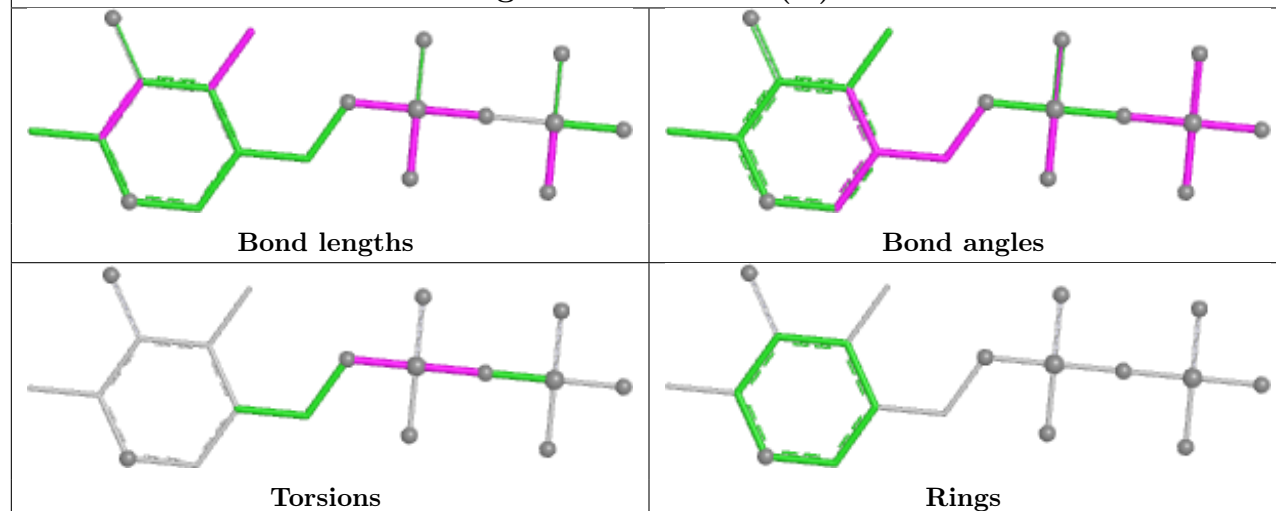
## Ligand AMP D 843



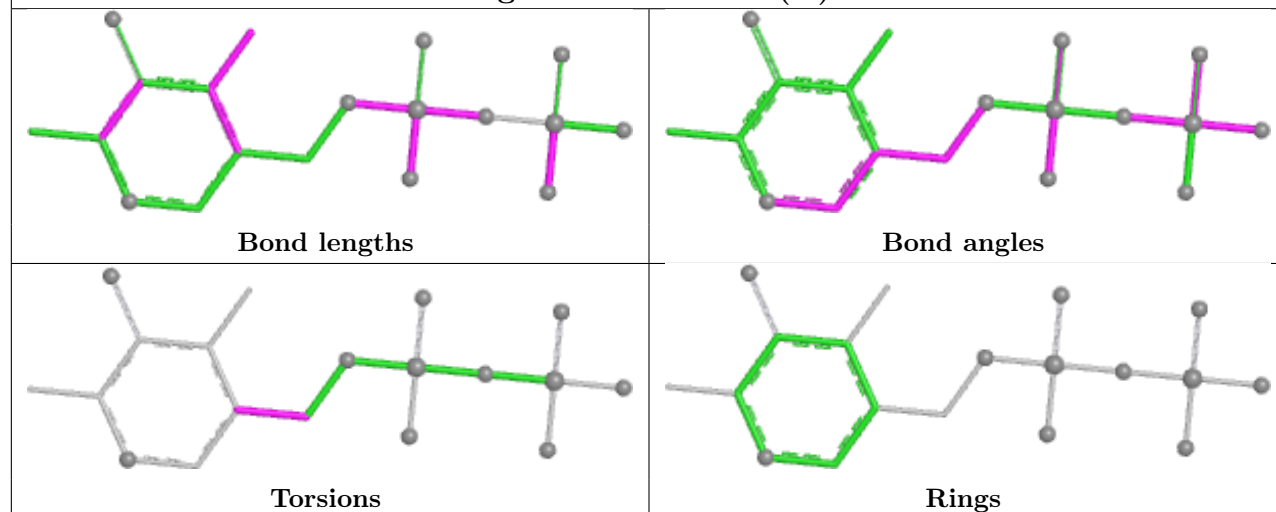
## Ligand PDP A 860 (A)



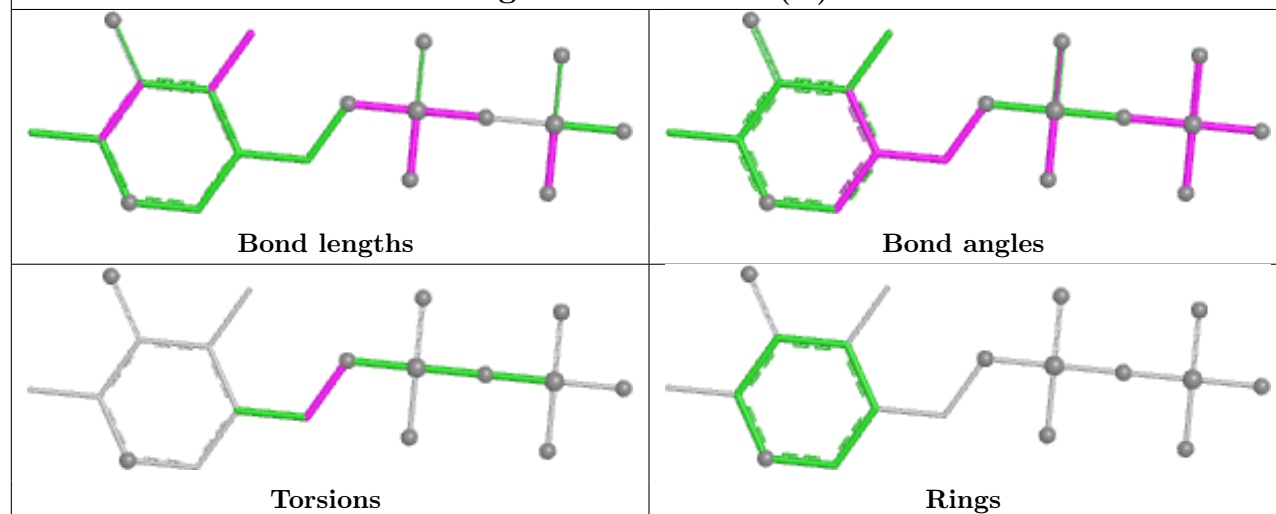
## Ligand PDP D 860 (A)

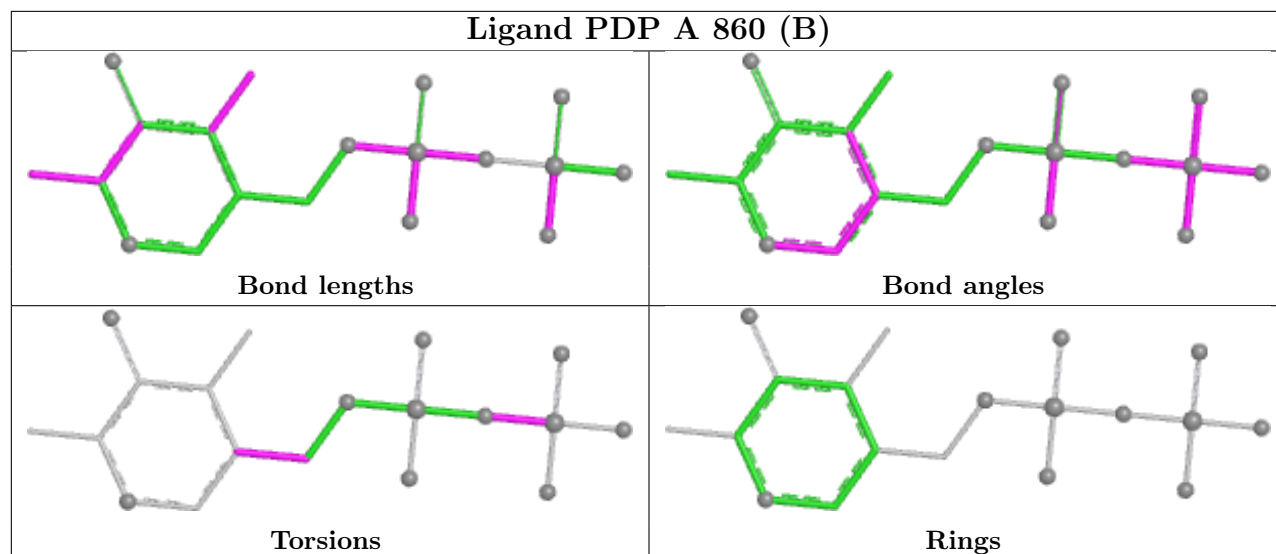


## Ligand PDP C 860 (A)



## Ligand PDP B 860 (B)





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.