



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:23 AM UTC

PDB ID : 1NOI / pdb\_00001noi  
Title : COMPLEX OF GLYCOGEN PHOSPHORYLASE WITH A TRANSITION  
STATE ANALOGUE NOJIRIMYCIN TETRAZOLE AND PHOSPHATE IN  
THE T AND R STATES  
Authors : Johnson, L.N.; Mitchell, E.P.  
Deposited on : 1996-03-12  
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

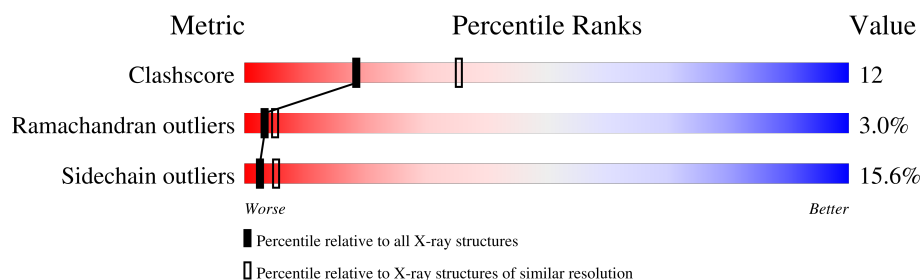
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



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

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

Note EDS was not executed.

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

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | PO4  | A     | 997 | -         | X        | -       | -                |
| 2   | PO4  | B     | 997 | -         | X        | -       | -                |
| 2   | PO4  | C     | 997 | -         | X        | -       | -                |
| 2   | PO4  | D     | 997 | -         | X        | -       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27788 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.

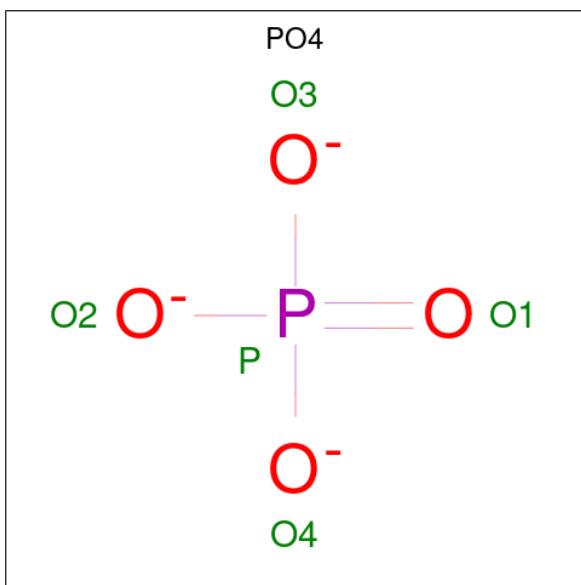
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 824      | Total | C    | N    | O    | S  | 0       | 0       | 1     |
|     |       |          | 6692  | 4264 | 1185 | 1213 | 30 |         |         |       |
| 1   | B     | 824      | Total | C    | N    | O    | S  | 0       | 0       | 1     |
|     |       |          | 6692  | 4264 | 1185 | 1213 | 30 |         |         |       |
| 1   | C     | 824      | Total | C    | N    | O    | S  | 0       | 0       | 1     |
|     |       |          | 6692  | 4264 | 1185 | 1213 | 30 |         |         |       |
| 1   | D     | 824      | Total | C    | N    | O    | S  | 0       | 0       | 1     |
|     |       |          | 6692  | 4264 | 1185 | 1213 | 30 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

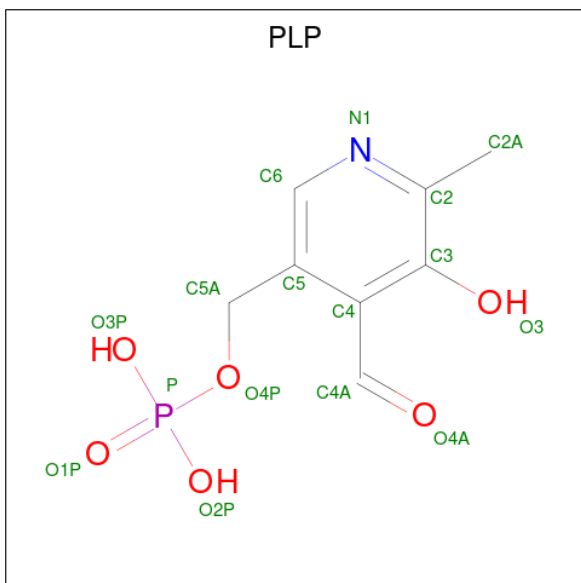
| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 380     | ILE      | LEU    | conflict | UNP P00489 |
| A     | 609     | PRO      | ALA    | conflict | UNP P00489 |
| B     | 380     | ILE      | LEU    | conflict | UNP P00489 |
| B     | 609     | PRO      | ALA    | conflict | UNP P00489 |
| C     | 380     | ILE      | LEU    | conflict | UNP P00489 |
| C     | 609     | PRO      | ALA    | conflict | UNP P00489 |
| D     | 380     | ILE      | LEU    | conflict | UNP P00489 |
| D     | 609     | PRO      | ALA    | conflict | UNP P00489 |

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



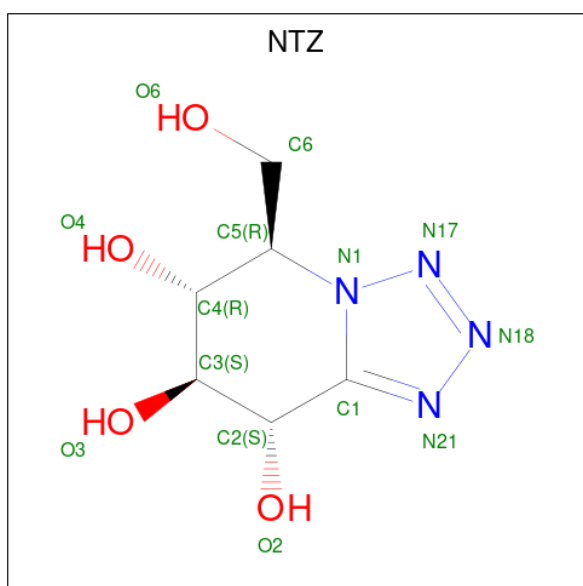
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 3   | B     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 3   | C     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 3   | D     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |

- Molecule 4 is NOJIRIMYCINE TETRAZOLE (CCD ID: NTZ) (formula:  $C_6H_{10}N_4O_4$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 6 | 4 | 4 |         |         |
| 4   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 6 | 4 | 4 |         |         |
| 4   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 6 | 4 | 4 |         |         |
| 4   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 6 | 4 | 4 |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 5   | A     | 223      | Total | O   | 0       | 0       |
|     |       |          | 223   | 223 |         |         |
| 5   | B     | 222      | Total | O   | 0       | 0       |
|     |       |          | 222   | 222 |         |         |

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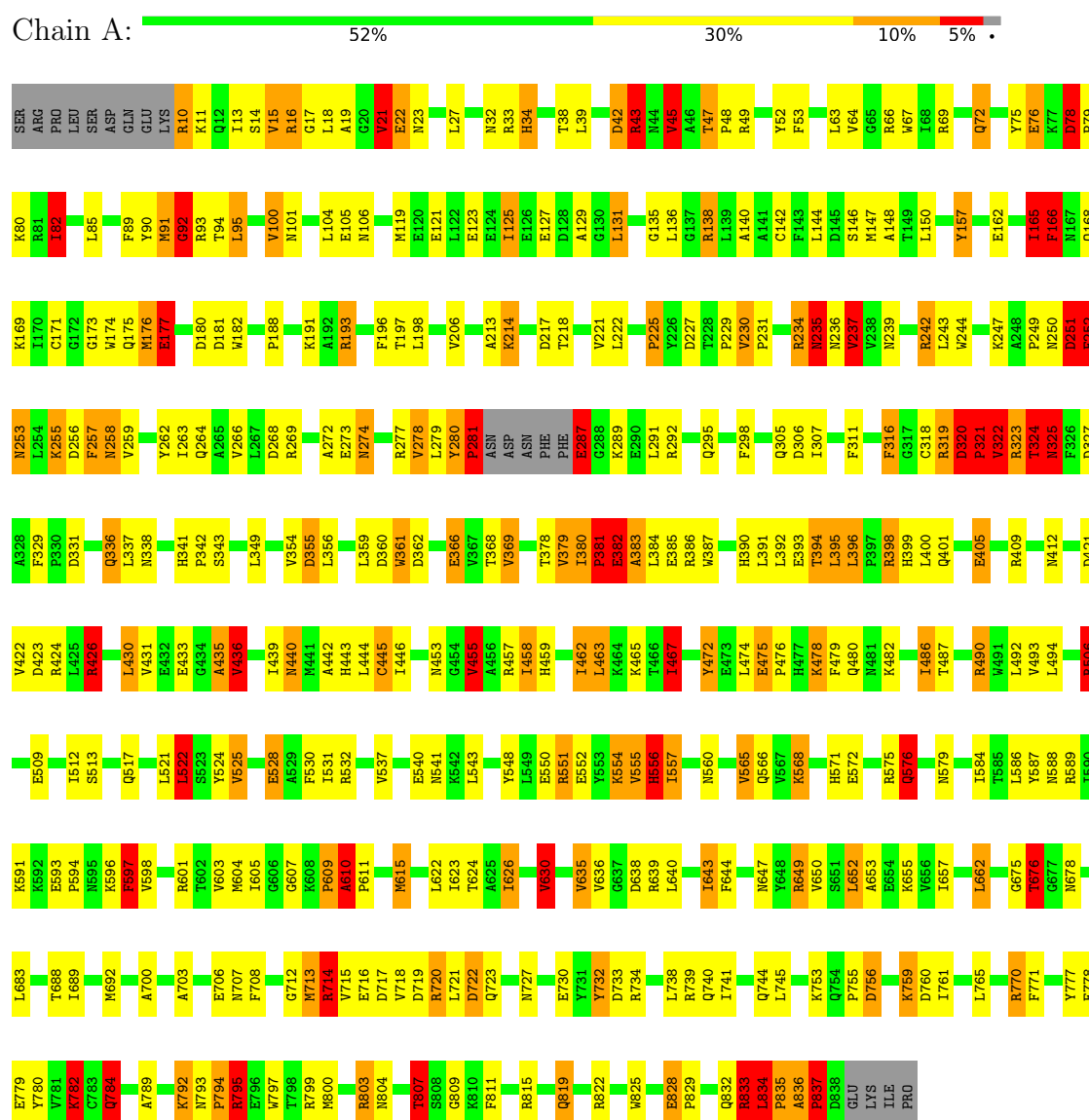
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | C     | 218      | Total<br>218 | O<br>218 | 0       | 0       |
| 5   | D     | 221      | Total<br>221 | O<br>221 | 0       | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

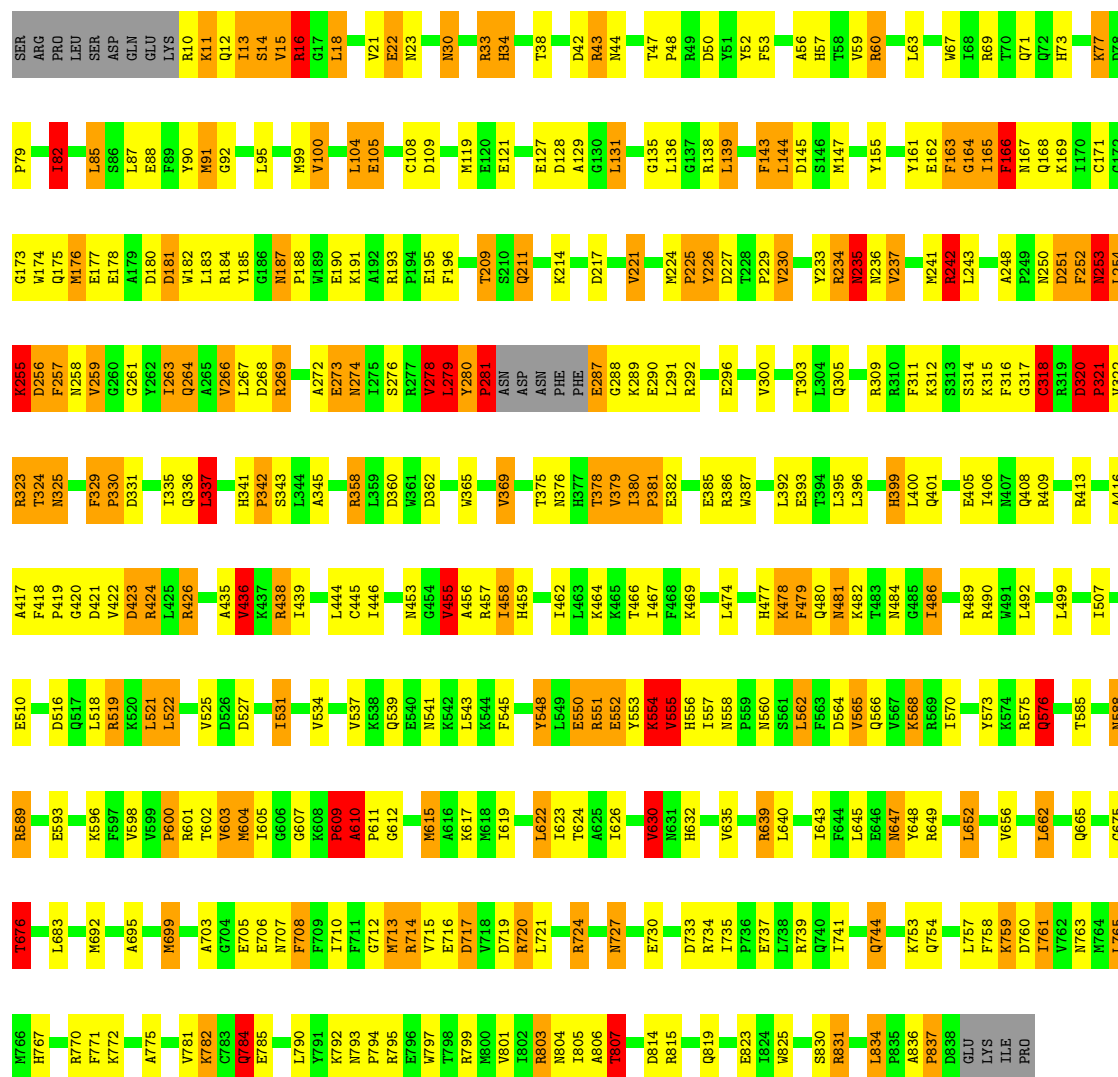
#### • Molecule 1: GLYCOGEN PHOSPHORYLASE



#### • Molecule 1: GLYCOGEN PHOSPHORYLASE

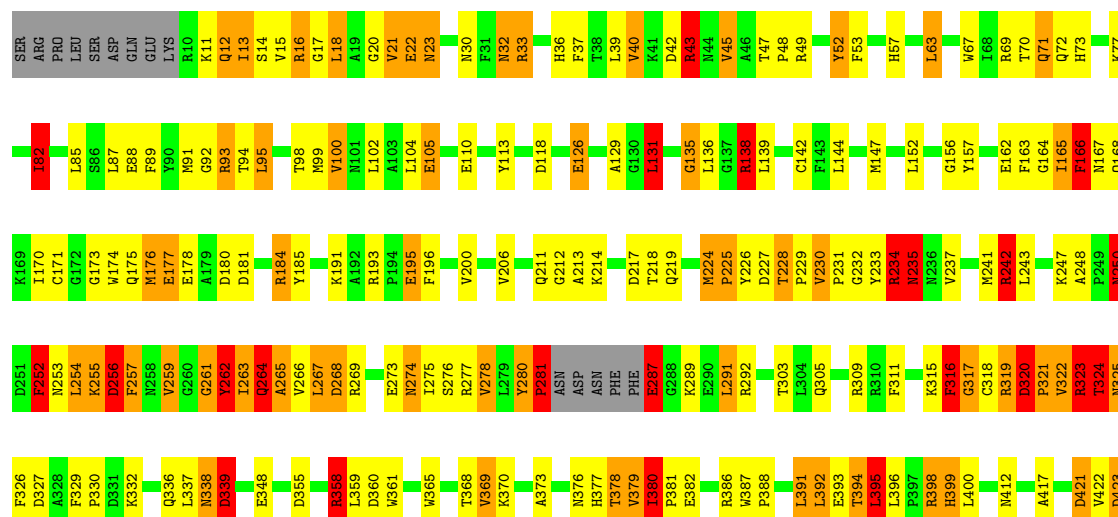






# Molecule 1: GLYCOGEN PHOSPHORYLASE

Chain C: 50% 31% 13%





## 4 Data and refinement statistics

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

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | P 1 21 1                                        | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 119.00Å 190.00Å 88.20Å<br>90.00° 109.35° 90.00° | Depositor |
| Resolution (Å)                                           | 8.00 – 2.50                                     | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (8.00-2.50)                     | Depositor |
| $R_{merge}$                                              | 0.07                                            | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | X-PLOR                                          | Depositor |
| R, $R_{free}$                                            | 0.171 , 0.273                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 27788                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 34.0                                            | 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: PLP, NTZ, PO4

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     | 1.18         | 25/6843 (0.4%)  | 2.16        | 279/9261 (3.0%)   |
| 1   | B     | 1.14         | 23/6843 (0.3%)  | 2.14        | 292/9261 (3.2%)   |
| 1   | C     | 1.15         | 18/6843 (0.3%)  | 2.10        | 281/9261 (3.0%)   |
| 1   | D     | 1.19         | 28/6843 (0.4%)  | 2.15        | 300/9261 (3.2%)   |
| All | All   | 1.16         | 94/27372 (0.3%) | 2.14        | 1152/37044 (3.1%) |

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                   | 9                   |
| 1   | B     | 0                   | 4                   |
| 1   | C     | 0                   | 7                   |
| 1   | D     | 0                   | 6                   |
| All | All   | 0                   | 26                  |

All (94) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 322 | VAL  | CA-CB | 12.51 | 1.71        | 1.54     |
| 1   | C     | 82  | ILE  | CA-CB | 11.17 | 1.68        | 1.54     |
| 1   | D     | 230 | VAL  | CA-CB | 10.57 | 1.63        | 1.54     |
| 1   | B     | 100 | VAL  | CA-CB | 9.90  | 1.67        | 1.54     |
| 1   | D     | 237 | VAL  | CA-CB | 9.86  | 1.67        | 1.54     |
| 1   | C     | 263 | ILE  | CA-CB | 9.53  | 1.67        | 1.54     |
| 1   | A     | 78  | ASP  | CA-CB | 9.24  | 1.68        | 1.53     |
| 1   | D     | 657 | ILE  | CA-CB | 8.75  | 1.59        | 1.54     |
| 1   | B     | 379 | VAL  | CA-CB | 8.74  | 1.66        | 1.54     |
| 1   | C     | 603 | VAL  | CA-CB | 8.43  | 1.64        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 436 | VAL  | CA-CB | 8.12  | 1.65        | 1.54     |
| 1   | D     | 565 | VAL  | CA-CB | 8.08  | 1.66        | 1.54     |
| 1   | D     | 630 | VAL  | CA-CB | 8.03  | 1.66        | 1.54     |
| 1   | C     | 380 | ILE  | CA-CB | 7.88  | 1.62        | 1.53     |
| 1   | D     | 555 | VAL  | CA-CB | 7.53  | 1.64        | 1.54     |
| 1   | C     | 165 | ILE  | CA-CB | 7.47  | 1.64        | 1.54     |
| 1   | A     | 509 | GLU  | CA-CB | -7.47 | 1.43        | 1.53     |
| 1   | B     | 237 | VAL  | CA-CB | 7.45  | 1.63        | 1.54     |
| 1   | B     | 165 | ILE  | CA-CB | 7.27  | 1.64        | 1.54     |
| 1   | C     | 230 | VAL  | CA-CB | 7.25  | 1.60        | 1.54     |
| 1   | D     | 468 | PHE  | CA-CB | 7.25  | 1.63        | 1.53     |
| 1   | D     | 827 | VAL  | CA-CB | 7.10  | 1.65        | 1.55     |
| 1   | D     | 78  | ASP  | CA-CB | 7.09  | 1.58        | 1.52     |
| 1   | D     | 787 | VAL  | CA-CB | 7.05  | 1.62        | 1.54     |
| 1   | A     | 657 | ILE  | CA-CB | 6.95  | 1.58        | 1.53     |
| 1   | A     | 263 | ILE  | CA-CB | 6.94  | 1.63        | 1.54     |
| 1   | D     | 735 | ILE  | CA-CB | 6.93  | 1.60        | 1.54     |
| 1   | A     | 165 | ILE  | CA-CB | 6.78  | 1.63        | 1.54     |
| 1   | B     | 486 | ILE  | CA-CB | 6.77  | 1.64        | 1.54     |
| 1   | A     | 237 | VAL  | CA-CB | 6.74  | 1.63        | 1.54     |
| 1   | C     | 565 | VAL  | CA-CB | 6.67  | 1.63        | 1.54     |
| 1   | D     | 165 | ILE  | CA-CB | 6.64  | 1.63        | 1.54     |
| 1   | D     | 462 | ILE  | CA-CB | 6.63  | 1.63        | 1.54     |
| 1   | A     | 100 | VAL  | CA-CB | 6.56  | 1.64        | 1.54     |
| 1   | C     | 466 | THR  | CA-CB | 6.47  | 1.64        | 1.53     |
| 1   | A     | 225 | PRO  | CA-CB | -6.21 | 1.47        | 1.54     |
| 1   | D     | 507 | ILE  | CA-CB | 6.14  | 1.62        | 1.54     |
| 1   | A     | 230 | VAL  | CA-CB | 6.12  | 1.62        | 1.54     |
| 1   | A     | 322 | VAL  | CA-CB | 6.09  | 1.62        | 1.54     |
| 1   | C     | 379 | VAL  | CA-CB | 6.08  | 1.62        | 1.54     |
| 1   | C     | 93  | ARG  | N-CA  | 6.02  | 1.53        | 1.46     |
| 1   | D     | 369 | VAL  | CA-CB | 6.02  | 1.63        | 1.54     |
| 1   | A     | 21  | VAL  | CA-CB | 6.00  | 1.62        | 1.54     |
| 1   | B     | 831 | ARG  | CA-CB | 5.96  | 1.61        | 1.52     |
| 1   | A     | 307 | ILE  | CA-CB | 5.94  | 1.60        | 1.54     |
| 1   | B     | 375 | THR  | CA-CB | -5.91 | 1.45        | 1.53     |
| 1   | A     | 259 | VAL  | CA-CB | 5.85  | 1.62        | 1.54     |
| 1   | A     | 82  | ILE  | CA-CB | 5.85  | 1.61        | 1.54     |
| 1   | D     | 837 | PRO  | C-N   | -5.81 | 1.25        | 1.33     |
| 1   | B     | 230 | VAL  | CA-CB | 5.76  | 1.61        | 1.54     |
| 1   | A     | 15  | VAL  | CA-CB | 5.76  | 1.62        | 1.54     |
| 1   | B     | 837 | PRO  | C-N   | -5.72 | 1.25        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 603 | VAL  | CA-CB | 5.71  | 1.61        | 1.54     |
| 1   | B     | 82  | ILE  | CA-CB | 5.69  | 1.61        | 1.54     |
| 1   | D     | 395 | LEU  | CB-CG | -5.69 | 1.42        | 1.53     |
| 1   | D     | 40  | VAL  | CA-CB | 5.68  | 1.62        | 1.54     |
| 1   | B     | 555 | VAL  | CA-CB | 5.67  | 1.62        | 1.54     |
| 1   | A     | 837 | PRO  | C-N   | -5.66 | 1.25        | 1.33     |
| 1   | B     | 406 | ILE  | CA-CB | 5.62  | 1.61        | 1.54     |
| 1   | A     | 555 | VAL  | CA-CB | 5.61  | 1.62        | 1.54     |
| 1   | B     | 603 | VAL  | CA-CB | 5.61  | 1.60        | 1.54     |
| 1   | B     | 565 | VAL  | CA-CB | 5.59  | 1.61        | 1.54     |
| 1   | B     | 209 | THR  | CA-CB | 5.47  | 1.62        | 1.53     |
| 1   | D     | 263 | ILE  | CA-CB | 5.46  | 1.62        | 1.54     |
| 1   | B     | 831 | ARG  | NE-CZ | 5.46  | 1.39        | 1.33     |
| 1   | D     | 629 | VAL  | CA-CB | 5.45  | 1.61        | 1.54     |
| 1   | B     | 15  | VAL  | CA-CB | 5.43  | 1.61        | 1.54     |
| 1   | B     | 630 | VAL  | CA-CB | 5.42  | 1.61        | 1.54     |
| 1   | A     | 369 | VAL  | CA-CB | 5.40  | 1.62        | 1.54     |
| 1   | A     | 338 | ASN  | CA-CB | -5.38 | 1.46        | 1.52     |
| 1   | D     | 379 | VAL  | CA-CB | 5.37  | 1.61        | 1.54     |
| 1   | C     | 100 | VAL  | CA-CB | 5.36  | 1.61        | 1.54     |
| 1   | B     | 656 | VAL  | CA-CB | 5.35  | 1.61        | 1.54     |
| 1   | C     | 324 | THR  | CA-CB | 5.35  | 1.61        | 1.53     |
| 1   | C     | 259 | VAL  | CA-CB | 5.35  | 1.59        | 1.54     |
| 1   | B     | 598 | VAL  | CA-CB | 5.33  | 1.61        | 1.54     |
| 1   | A     | 467 | ILE  | CA-CB | 5.32  | 1.60        | 1.54     |
| 1   | C     | 206 | VAL  | CA-CB | -5.29 | 1.47        | 1.54     |
| 1   | C     | 678 | ASN  | CA-CB | 5.28  | 1.61        | 1.53     |
| 1   | C     | 741 | ILE  | CA-CB | 5.26  | 1.60        | 1.54     |
| 1   | B     | 341 | HIS  | CA-CB | -5.24 | 1.46        | 1.53     |
| 1   | A     | 565 | VAL  | CA-CB | 5.21  | 1.62        | 1.54     |
| 1   | C     | 325 | ASN  | CA-C  | -5.21 | 1.46        | 1.52     |
| 1   | D     | 555 | VAL  | N-CA  | 5.18  | 1.52        | 1.46     |
| 1   | B     | 305 | GLN  | CA-CB | -5.14 | 1.45        | 1.53     |
| 1   | A     | 540 | GLU  | CA-CB | -5.13 | 1.44        | 1.53     |
| 1   | D     | 537 | VAL  | CA-CB | 5.10  | 1.60        | 1.54     |
| 1   | A     | 436 | VAL  | CA-CB | 5.10  | 1.61        | 1.54     |
| 1   | C     | 837 | PRO  | C-N   | -5.09 | 1.26        | 1.33     |
| 1   | D     | 583 | VAL  | CA-CB | 5.09  | 1.60        | 1.54     |
| 1   | A     | 253 | ASN  | CA-CB | 5.06  | 1.62        | 1.53     |
| 1   | B     | 436 | VAL  | CA-CB | 5.06  | 1.61        | 1.54     |
| 1   | A     | 379 | VAL  | CA-CB | 5.02  | 1.60        | 1.55     |
| 1   | D     | 678 | ASN  | CA-CB | 5.01  | 1.61        | 1.53     |

All (1152) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | B     | 280 | TYR  | N-CA-C    | 16.72  | 123.27      | 108.22   |
| 1   | A     | 455 | VAL  | N-CA-CB   | -15.27 | 92.57       | 112.26   |
| 1   | B     | 266 | VAL  | N-CA-C    | -14.40 | 96.85       | 110.82   |
| 1   | D     | 325 | ASN  | CA-CB-CG  | 14.37  | 126.97      | 112.60   |
| 1   | C     | 455 | VAL  | N-CA-CB   | -14.37 | 93.48       | 112.16   |
| 1   | C     | 324 | THR  | N-CA-C    | -13.73 | 93.21       | 111.74   |
| 1   | B     | 320 | ASP  | CA-CB-CG  | 13.51  | 126.11      | 112.60   |
| 1   | A     | 251 | ASP  | CA-CB-CG  | -13.45 | 99.15       | 112.60   |
| 1   | D     | 274 | ASN  | CA-CB-CG  | 13.44  | 126.04      | 112.60   |
| 1   | D     | 325 | ASN  | O-C-N     | 13.32  | 137.67      | 123.42   |
| 1   | D     | 378 | THR  | O-C-N     | 12.81  | 138.09      | 123.48   |
| 1   | B     | 455 | VAL  | N-CA-CB   | -12.65 | 95.71       | 112.16   |
| 1   | A     | 253 | ASN  | CA-CB-CG  | 12.59  | 125.19      | 112.60   |
| 1   | C     | 316 | PHE  | CA-CB-CG  | -12.37 | 101.43      | 113.80   |
| 1   | B     | 211 | GLN  | N-CA-C    | -11.78 | 98.47       | 111.07   |
| 1   | A     | 490 | ARG  | NE-CZ-NH2 | -11.58 | 108.78      | 119.20   |
| 1   | C     | 181 | ASP  | CA-CB-CG  | 11.58  | 124.18      | 112.60   |
| 1   | A     | 280 | TYR  | N-CA-C    | 11.54  | 121.64      | 108.25   |
| 1   | D     | 30  | ASN  | CA-CB-CG  | -11.30 | 101.30      | 112.60   |
| 1   | D     | 268 | ASP  | CA-CB-CG  | 11.27  | 123.86      | 112.60   |
| 1   | D     | 165 | ILE  | N-CA-C    | -11.25 | 91.92       | 108.12   |
| 1   | A     | 379 | VAL  | N-CA-C    | 11.14  | 122.25      | 111.67   |
| 1   | C     | 268 | ASP  | CA-CB-CG  | 10.95  | 123.55      | 112.60   |
| 1   | B     | 325 | ASN  | N-CA-C    | 10.82  | 127.42      | 109.46   |
| 1   | B     | 378 | THR  | O-C-N     | 10.43  | 135.17      | 123.48   |
| 1   | D     | 256 | ASP  | N-CA-C    | -10.41 | 88.64       | 110.80   |
| 1   | A     | 274 | ASN  | CA-CB-CG  | 10.38  | 122.98      | 112.60   |
| 1   | B     | 181 | ASP  | CA-CB-CG  | 10.34  | 122.94      | 112.60   |
| 1   | B     | 23  | ASN  | N-CA-C    | 10.31  | 126.37      | 108.02   |
| 1   | D     | 455 | VAL  | N-CA-CB   | -10.15 | 94.47       | 111.23   |
| 1   | D     | 281 | PRO  | N-CA-C    | 10.08  | 133.23      | 112.47   |
| 1   | A     | 615 | MET  | CG-SD-CE  | -10.07 | 78.74       | 100.90   |
| 1   | B     | 268 | ASP  | CA-CB-CG  | 10.04  | 122.64      | 112.60   |
| 1   | A     | 252 | PHE  | N-CA-C    | -9.92  | 88.33       | 107.57   |
| 1   | C     | 771 | PHE  | CA-CB-CG  | -9.87  | 103.93      | 113.80   |
| 1   | B     | 252 | PHE  | CA-CB-CG  | 9.84   | 123.64      | 113.80   |
| 1   | B     | 325 | ASN  | CA-C-O    | 9.76   | 131.57      | 120.54   |
| 1   | D     | 676 | THR  | N-CA-CB   | -9.65  | 94.18       | 110.49   |
| 1   | A     | 177 | GLU  | CA-CB-CG  | 9.60   | 133.29      | 114.10   |
| 1   | D     | 181 | ASP  | CA-CB-CG  | 9.59   | 122.19      | 112.60   |
| 1   | B     | 423 | ASP  | CA-CB-CG  | 9.58   | 122.18      | 112.60   |
| 1   | A     | 325 | ASN  | N-CA-C    | 9.40   | 123.84      | 108.52   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 320 | ASP  | N-CA-C     | 9.38  | 130.55      | 109.81   |
| 1   | A     | 321 | PRO  | N-CA-C     | 9.37  | 131.77      | 112.47   |
| 1   | A     | 551 | ARG  | N-CA-C     | -9.34 | 100.26      | 112.68   |
| 1   | A     | 486 | ILE  | CA-CB-CG1  | -9.26 | 94.67       | 110.40   |
| 1   | A     | 486 | ILE  | CA-CB-CG2  | 9.19  | 126.12      | 110.50   |
| 1   | B     | 378 | THR  | CA-C-N     | 9.17  | 138.48      | 121.97   |
| 1   | B     | 378 | THR  | C-N-CA     | 9.17  | 138.48      | 121.97   |
| 1   | C     | 274 | ASN  | CA-CB-CG   | 9.12  | 121.72      | 112.60   |
| 1   | B     | 727 | ASN  | OD1-CG-ND2 | -9.10 | 113.50      | 122.60   |
| 1   | B     | 325 | ASN  | O-C-N      | 9.08  | 133.57      | 123.22   |
| 1   | D     | 393 | GLU  | CA-CB-CG   | 9.01  | 132.11      | 114.10   |
| 1   | D     | 402 | ILE  | CA-C-O     | -8.99 | 111.59      | 120.95   |
| 1   | D     | 177 | GLU  | CA-CB-CG   | 8.92  | 131.94      | 114.10   |
| 1   | C     | 730 | GLU  | CA-CB-CG   | 8.91  | 131.93      | 114.10   |
| 1   | A     | 390 | HIS  | CA-CB-CG   | 8.84  | 122.64      | 113.80   |
| 1   | A     | 217 | ASP  | CA-CB-CG   | 8.82  | 121.42      | 112.60   |
| 1   | A     | 575 | ARG  | N-CA-C     | 8.81  | 123.85      | 111.52   |
| 1   | A     | 101 | ASN  | OD1-CG-ND2 | -8.70 | 113.90      | 122.60   |
| 1   | B     | 105 | GLU  | N-CA-C     | 8.67  | 120.35      | 111.07   |
| 1   | A     | 336 | GLN  | OE1-CD-NE2 | -8.67 | 113.93      | 122.60   |
| 1   | C     | 435 | ALA  | N-CA-C     | -8.65 | 94.49       | 108.41   |
| 1   | D     | 253 | ASN  | CA-CB-CG   | 8.64  | 121.24      | 112.60   |
| 1   | B     | 458 | ILE  | CB-CG1-CD1 | -8.61 | 95.72       | 113.80   |
| 1   | A     | 268 | ASP  | CA-CB-CG   | 8.61  | 121.21      | 112.60   |
| 1   | D     | 604 | MET  | CG-SD-CE   | -8.59 | 82.01       | 100.90   |
| 1   | B     | 421 | ASP  | CA-C-O     | 8.58  | 129.46      | 120.54   |
| 1   | B     | 733 | ASP  | CA-CB-CG   | 8.57  | 121.17      | 112.60   |
| 1   | B     | 325 | ASN  | CA-CB-CG   | -8.56 | 104.04      | 112.60   |
| 1   | D     | 378 | THR  | CA-C-N     | 8.52  | 137.31      | 121.97   |
| 1   | D     | 378 | THR  | C-N-CA     | 8.52  | 137.31      | 121.97   |
| 1   | C     | 455 | VAL  | CB-CA-C    | 8.48  | 122.00      | 111.65   |
| 1   | B     | 217 | ASP  | CA-CB-CG   | 8.46  | 121.06      | 112.60   |
| 1   | A     | 182 | TRP  | N-CA-C     | -8.45 | 102.07      | 112.38   |
| 1   | A     | 455 | VAL  | CB-CA-C    | 8.44  | 121.67      | 111.20   |
| 1   | A     | 121 | GLU  | CB-CG-CD   | 8.43  | 126.93      | 112.60   |
| 1   | B     | 834 | LEU  | N-CA-C     | -8.43 | 97.40       | 109.62   |
| 1   | D     | 321 | PRO  | N-CA-C     | 8.41  | 129.79      | 112.47   |
| 1   | C     | 458 | ILE  | CA-CB-CG2  | -8.40 | 96.22       | 110.50   |
| 1   | D     | 329 | PHE  | CA-CB-CG   | 8.39  | 122.19      | 113.80   |
| 1   | B     | 575 | ARG  | CB-CG-CD   | -8.39 | 92.01       | 111.30   |
| 1   | A     | 834 | LEU  | N-CA-C     | -8.37 | 99.20       | 109.83   |
| 1   | A     | 490 | ARG  | NE-CZ-NH1  | 8.36  | 129.86      | 121.50   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 575 | ARG  | CB-CG-CD  | -8.36 | 92.08       | 111.30   |
| 1   | D     | 490 | ARG  | NE-CZ-NH2 | -8.35 | 111.69      | 119.20   |
| 1   | B     | 44  | ASN  | CA-CB-CG  | 8.34  | 120.94      | 112.60   |
| 1   | C     | 135 | GLY  | CA-C-O    | -8.33 | 112.17      | 120.75   |
| 1   | D     | 255 | LYS  | O-C-N     | 8.32  | 133.66      | 122.59   |
| 1   | A     | 257 | PHE  | CA-C-N    | 8.28  | 131.71      | 120.44   |
| 1   | A     | 257 | PHE  | C-N-CA    | 8.28  | 131.71      | 120.44   |
| 1   | B     | 609 | PRO  | N-CA-CB   | 8.26  | 111.93      | 103.25   |
| 1   | D     | 787 | VAL  | N-CA-C    | -8.25 | 102.77      | 110.53   |
| 1   | C     | 165 | ILE  | N-CA-C    | -8.24 | 92.19       | 109.34   |
| 1   | A     | 100 | VAL  | N-CA-C    | -8.21 | 102.88      | 111.58   |
| 1   | C     | 320 | ASP  | CA-CB-CG  | 8.20  | 120.80      | 112.60   |
| 1   | A     | 165 | ILE  | N-CA-C    | -8.19 | 92.31       | 109.34   |
| 1   | A     | 166 | PHE  | N-CA-C    | 8.16  | 128.19      | 110.80   |
| 1   | C     | 380 | ILE  | CB-CA-C   | 8.14  | 119.42      | 110.71   |
| 1   | A     | 678 | ASN  | CB-CG-ND2 | 8.11  | 128.56      | 116.40   |
| 1   | D     | 248 | ALA  | CA-C-O    | -8.10 | 111.50      | 120.25   |
| 1   | A     | 255 | LYS  | O-C-N     | 8.08  | 132.96      | 123.02   |
| 1   | C     | 323 | ARG  | N-CA-C    | 8.07  | 128.00      | 110.80   |
| 1   | B     | 615 | MET  | CG-SD-CE  | -8.07 | 83.15       | 100.90   |
| 1   | D     | 13  | ILE  | N-CA-C    | -8.06 | 95.92       | 107.37   |
| 1   | D     | 181 | ASP  | CA-C-O    | 8.06  | 131.02      | 121.11   |
| 1   | C     | 217 | ASP  | CA-CB-CG  | 8.05  | 120.65      | 112.60   |
| 1   | A     | 180 | ASP  | CA-C-O    | -8.03 | 112.40      | 121.39   |
| 1   | A     | 258 | ASN  | N-CA-C    | -8.03 | 102.47      | 111.14   |
| 1   | D     | 633 | ASP  | CA-CB-CG  | -8.03 | 104.57      | 112.60   |
| 1   | B     | 253 | ASN  | CA-CB-CG  | 8.01  | 120.61      | 112.60   |
| 1   | B     | 399 | HIS  | CA-C-O    | -8.01 | 110.34      | 119.79   |
| 1   | D     | 575 | ARG  | N-CA-C    | 7.99  | 122.27      | 111.24   |
| 1   | C     | 552 | GLU  | N-CA-C    | -7.98 | 95.89       | 108.90   |
| 1   | C     | 720 | ARG  | CA-CB-CG  | 7.97  | 130.04      | 114.10   |
| 1   | C     | 455 | VAL  | N-CA-C    | 7.97  | 119.76      | 112.43   |
| 1   | B     | 274 | ASN  | CA-CB-CG  | 7.96  | 120.56      | 112.60   |
| 1   | D     | 180 | ASP  | CA-CB-CG  | 7.95  | 120.55      | 112.60   |
| 1   | B     | 255 | LYS  | O-C-N     | 7.91  | 132.92      | 123.27   |
| 1   | B     | 309 | ARG  | CA-CB-CG  | 7.90  | 129.90      | 114.10   |
| 1   | C     | 250 | ASN  | N-CA-C    | 7.84  | 127.50      | 110.80   |
| 1   | C     | 281 | PRO  | CA-N-CD   | -7.84 | 101.02      | 112.00   |
| 1   | B     | 455 | VAL  | CB-CA-C   | 7.84  | 121.21      | 111.65   |
| 1   | C     | 15  | VAL  | CB-CA-C   | -7.83 | 101.76      | 112.02   |
| 1   | B     | 379 | VAL  | O-C-N     | 7.83  | 132.35      | 122.57   |
| 1   | C     | 731 | TYR  | N-CA-C    | -7.79 | 102.87      | 111.36   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 280 | TYR  | CA-C-N     | 7.79  | 129.58      | 119.84   |
| 1   | D     | 280 | TYR  | C-N-CA     | 7.79  | 129.58      | 119.84   |
| 1   | D     | 256 | ASP  | CA-CB-CG   | 7.75  | 120.36      | 112.60   |
| 1   | A     | 793 | ASN  | CA-CB-CG   | 7.75  | 120.35      | 112.60   |
| 1   | A     | 572 | GLU  | CA-C-O     | -7.73 | 112.63      | 120.90   |
| 1   | B     | 831 | ARG  | N-CA-C     | -7.73 | 100.96      | 111.55   |
| 1   | C     | 708 | PHE  | CA-C-O     | -7.72 | 112.38      | 121.11   |
| 1   | D     | 797 | TRP  | CG-CD2-CE3 | -7.71 | 126.19      | 133.90   |
| 1   | C     | 281 | PRO  | N-CA-C     | 7.71  | 128.35      | 112.47   |
| 1   | D     | 320 | ASP  | O-C-N      | -7.70 | 112.47      | 121.32   |
| 1   | D     | 267 | LEU  | CA-C-O     | -7.69 | 111.70      | 120.24   |
| 1   | A     | 565 | VAL  | N-CA-C     | 7.67  | 119.89      | 108.46   |
| 1   | C     | 807 | THR  | N-CA-CB    | -7.64 | 99.32       | 110.70   |
| 1   | C     | 250 | ASN  | OD1-CG-ND2 | -7.64 | 114.96      | 122.60   |
| 1   | B     | 250 | ASN  | N-CA-C     | 7.61  | 119.97      | 109.54   |
| 1   | C     | 737 | GLU  | N-CA-CB    | 7.61  | 122.07      | 110.28   |
| 1   | C     | 615 | MET  | CG-SD-CE   | -7.58 | 84.22       | 100.90   |
| 1   | A     | 281 | PRO  | CA-N-CD    | -7.57 | 101.40      | 112.00   |
| 1   | B     | 589 | ARG  | CA-CB-CG   | 7.54  | 129.19      | 114.10   |
| 1   | C     | 376 | ASN  | O-C-N      | -7.53 | 114.77      | 123.27   |
| 1   | D     | 359 | LEU  | N-CA-C     | -7.52 | 99.39       | 110.52   |
| 1   | C     | 458 | ILE  | CA-CB-CG1  | 7.50  | 123.16      | 110.40   |
| 1   | C     | 212 | GLY  | O-C-N      | 7.50  | 131.01      | 123.88   |
| 1   | C     | 318 | CYS  | N-CA-C     | -7.50 | 104.74      | 114.04   |
| 1   | D     | 131 | LEU  | N-CA-CB    | -7.47 | 100.19      | 110.95   |
| 1   | B     | 251 | ASP  | N-CA-C     | -7.47 | 102.81      | 112.23   |
| 1   | D     | 650 | VAL  | CA-C-O     | -7.47 | 113.25      | 121.17   |
| 1   | A     | 833 | ARG  | CB-CG-CD   | 7.46  | 128.45      | 111.30   |
| 1   | C     | 647 | ASN  | OD1-CG-ND2 | -7.44 | 115.16      | 122.60   |
| 1   | C     | 235 | ASN  | OD1-CG-ND2 | -7.44 | 115.16      | 122.60   |
| 1   | D     | 743 | GLU  | CA-C-O     | -7.44 | 111.02      | 119.79   |
| 1   | A     | 807 | THR  | N-CA-CB    | -7.40 | 99.00       | 111.20   |
| 1   | D     | 564 | ASP  | CA-C-O     | -7.39 | 112.56      | 120.46   |
| 1   | A     | 274 | ASN  | CB-CG-ND2  | 7.38  | 127.47      | 116.40   |
| 1   | A     | 458 | ILE  | CA-CB-CG2  | -7.38 | 97.96       | 110.50   |
| 1   | B     | 164 | GLY  | O-C-N      | 7.37  | 132.28      | 122.70   |
| 1   | A     | 33  | ARG  | N-CA-CB    | 7.36  | 120.69      | 110.01   |
| 1   | D     | 42  | ASP  | CA-CB-CG   | 7.36  | 119.96      | 112.60   |
| 1   | A     | 280 | TYR  | O-C-N      | 7.34  | 127.01      | 121.65   |
| 1   | B     | 362 | ASP  | CA-CB-CG   | -7.34 | 105.26      | 112.60   |
| 1   | B     | 235 | ASN  | OD1-CG-ND2 | -7.33 | 115.27      | 122.60   |
| 1   | C     | 13  | ILE  | N-CA-C     | -7.33 | 95.92       | 106.55   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 376 | ASN  | O-C-N      | -7.32 | 114.67      | 123.16   |
| 1   | B     | 604 | MET  | CG-SD-CE   | -7.31 | 84.83       | 100.90   |
| 1   | D     | 166 | PHE  | N-CA-C     | 7.30  | 126.35      | 110.80   |
| 1   | C     | 241 | MET  | CG-SD-CE   | 7.30  | 116.96      | 100.90   |
| 1   | A     | 320 | ASP  | CA-C-N     | 7.29  | 128.95      | 119.84   |
| 1   | A     | 320 | ASP  | C-N-CA     | 7.29  | 128.95      | 119.84   |
| 1   | C     | 280 | TYR  | CA-C-N     | 7.28  | 128.94      | 119.84   |
| 1   | C     | 280 | TYR  | C-N-CA     | 7.28  | 128.94      | 119.84   |
| 1   | C     | 797 | TRP  | CG-CD2-CE3 | -7.28 | 126.62      | 133.90   |
| 1   | B     | 281 | PRO  | CA-N-CD    | -7.28 | 101.81      | 112.00   |
| 1   | B     | 823 | GLU  | N-CA-C     | 7.27  | 122.25      | 113.23   |
| 1   | B     | 324 | THR  | CA-C-N     | -7.27 | 111.94      | 122.19   |
| 1   | B     | 324 | THR  | C-N-CA     | -7.27 | 111.94      | 122.19   |
| 1   | D     | 105 | GLU  | N-CA-C     | 7.25  | 118.83      | 111.07   |
| 1   | D     | 162 | GLU  | N-CA-C     | 7.25  | 119.18      | 111.28   |
| 1   | A     | 324 | THR  | CA-C-N     | -7.25 | 112.90      | 123.05   |
| 1   | A     | 324 | THR  | C-N-CA     | -7.25 | 112.90      | 123.05   |
| 1   | D     | 275 | ILE  | N-CA-C     | -7.23 | 103.42      | 110.72   |
| 1   | C     | 326 | PHE  | CA-CB-CG   | -7.23 | 106.57      | 113.80   |
| 1   | A     | 732 | TYR  | O-C-N      | 7.23  | 129.78      | 122.12   |
| 1   | D     | 547 | ALA  | CA-C-O     | -7.22 | 113.22      | 120.80   |
| 1   | C     | 200 | VAL  | N-CA-C     | -7.22 | 98.08       | 108.48   |
| 1   | C     | 575 | ARG  | CB-CG-CD   | -7.21 | 94.71       | 111.30   |
| 1   | A     | 635 | VAL  | O-C-N      | 7.20  | 128.85      | 121.87   |
| 1   | B     | 91  | MET  | N-CA-C     | 7.19  | 120.16      | 111.82   |
| 1   | C     | 486 | ILE  | CA-CB-CG1  | -7.18 | 98.20       | 110.40   |
| 1   | D     | 615 | MET  | CG-SD-CE   | -7.17 | 85.14       | 100.90   |
| 1   | A     | 797 | TRP  | CG-CD2-CE3 | -7.16 | 126.74      | 133.90   |
| 1   | C     | 45  | VAL  | N-CA-CB    | -7.15 | 102.49      | 112.35   |
| 1   | A     | 21  | VAL  | CA-C-O     | -7.14 | 111.85      | 120.78   |
| 1   | D     | 33  | ARG  | CB-CG-CD   | -7.13 | 94.89       | 111.30   |
| 1   | A     | 34  | HIS  | CA-CB-CG   | -7.13 | 106.67      | 113.80   |
| 1   | A     | 42  | ASP  | CA-CB-CG   | 7.13  | 119.73      | 112.60   |
| 1   | D     | 314 | SER  | N-CA-C     | -7.13 | 99.11       | 109.59   |
| 1   | C     | 42  | ASP  | CA-CB-CG   | 7.12  | 119.72      | 112.60   |
| 1   | C     | 252 | PHE  | CA-CB-CG   | 7.12  | 120.92      | 113.80   |
| 1   | C     | 516 | ASP  | CA-CB-CG   | -7.10 | 105.50      | 112.60   |
| 1   | D     | 436 | VAL  | CA-C-O     | 7.10  | 129.65      | 120.78   |
| 1   | D     | 541 | ASN  | OD1-CG-ND2 | -7.09 | 115.51      | 122.60   |
| 1   | A     | 467 | ILE  | CB-CA-C    | -7.09 | 102.75      | 112.04   |
| 1   | C     | 759 | LYS  | CA-CB-CG   | 7.09  | 128.29      | 114.10   |
| 1   | C     | 18  | LEU  | N-CA-C     | 7.09  | 120.42      | 108.23   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 607 | GLY  | CA-C-O     | -7.08 | 114.61      | 121.83   |
| 1   | A     | 318 | CYS  | O-C-N      | -7.08 | 113.17      | 122.59   |
| 1   | C     | 741 | ILE  | CB-CA-C    | -7.07 | 102.97      | 111.81   |
| 1   | D     | 321 | PRO  | N-CA-CB    | -7.07 | 95.82       | 103.25   |
| 1   | A     | 435 | ALA  | N-CA-C     | -7.07 | 95.56       | 107.99   |
| 1   | B     | 486 | ILE  | CA-CB-CG2  | 7.07  | 122.51      | 110.50   |
| 1   | B     | 321 | PRO  | CA-N-CD    | -7.06 | 102.11      | 112.00   |
| 1   | D     | 426 | ARG  | CA-CB-CG   | 7.06  | 128.22      | 114.10   |
| 1   | A     | 218 | THR  | O-C-N      | -7.06 | 114.81      | 122.85   |
| 1   | A     | 537 | VAL  | N-CA-C     | -7.05 | 103.65      | 110.42   |
| 1   | D     | 23  | ASN  | CA-CB-CG   | -7.05 | 105.55      | 112.60   |
| 1   | A     | 393 | GLU  | CA-CB-CG   | 7.05  | 128.20      | 114.10   |
| 1   | B     | 714 | ARG  | CB-CG-CD   | 7.04  | 127.49      | 111.30   |
| 1   | C     | 14  | SER  | CA-C-N     | 7.04  | 129.57      | 120.56   |
| 1   | C     | 14  | SER  | C-N-CA     | 7.04  | 129.57      | 120.56   |
| 1   | C     | 730 | GLU  | N-CA-C     | 7.03  | 119.03      | 111.36   |
| 1   | D     | 322 | VAL  | CA-C-O     | 7.02  | 129.55      | 120.78   |
| 1   | A     | 45  | VAL  | N-CA-CB    | -7.01 | 99.85       | 111.98   |
| 1   | B     | 619 | ILE  | CA-C-O     | -7.01 | 113.74      | 121.17   |
| 1   | A     | 712 | GLY  | O-C-N      | 7.00  | 131.01      | 123.17   |
| 1   | B     | 639 | ARG  | N-CA-C     | -6.96 | 104.60      | 113.23   |
| 1   | B     | 16  | ARG  | CA-CB-CG   | 6.96  | 128.01      | 114.10   |
| 1   | B     | 269 | ARG  | CB-CA-C    | -6.96 | 100.25      | 110.96   |
| 1   | C     | 228 | THR  | CA-C-N     | 6.95  | 127.98      | 120.13   |
| 1   | C     | 228 | THR  | C-N-CA     | 6.95  | 127.98      | 120.13   |
| 1   | A     | 33  | ARG  | CB-CA-C    | -6.94 | 99.98       | 110.88   |
| 1   | A     | 643 | ILE  | CB-CG1-CD1 | -6.94 | 99.22       | 113.80   |
| 1   | A     | 21  | VAL  | CG1-CB-CG2 | -6.94 | 95.53       | 110.80   |
| 1   | A     | 777 | TYR  | N-CA-C     | 6.94  | 118.84      | 111.28   |
| 1   | A     | 325 | ASN  | OD1-CG-ND2 | -6.93 | 115.67      | 122.60   |
| 1   | D     | 78  | ASP  | CA-CB-CG   | 6.92  | 119.52      | 112.60   |
| 1   | A     | 584 | ILE  | CA-C-O     | -6.92 | 113.51      | 120.85   |
| 1   | A     | 528 | GLU  | N-CA-C     | 6.92  | 119.67      | 111.71   |
| 1   | A     | 445 | CYS  | CA-C-O     | -6.92 | 113.22      | 120.55   |
| 1   | A     | 579 | ASN  | CA-CB-CG   | 6.91  | 119.51      | 112.60   |
| 1   | D     | 435 | ALA  | N-CA-C     | -6.91 | 96.35       | 108.23   |
| 1   | D     | 714 | ARG  | CA-CB-CG   | -6.90 | 100.31      | 114.10   |
| 1   | C     | 715 | VAL  | CA-C-N     | 6.89  | 129.40      | 120.44   |
| 1   | C     | 715 | VAL  | C-N-CA     | 6.89  | 129.40      | 120.44   |
| 1   | B     | 181 | ASP  | O-C-N      | 6.89  | 130.33      | 122.55   |
| 1   | A     | 181 | ASP  | CA-CB-CG   | 6.88  | 119.48      | 112.60   |
| 1   | B     | 695 | ALA  | N-CA-C     | -6.88 | 104.86      | 113.18   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 167 | ASN  | CB-CG-ND2  | 6.87  | 126.71      | 116.40   |
| 1   | A     | 675 | GLY  | N-CA-C     | -6.86 | 103.73      | 112.65   |
| 1   | D     | 575 | ARG  | CB-CG-CD   | -6.86 | 95.52       | 111.30   |
| 1   | A     | 146 | SER  | CA-C-O     | -6.86 | 113.15      | 120.42   |
| 1   | A     | 458 | ILE  | CA-CB-CG1  | 6.85  | 122.05      | 110.40   |
| 1   | B     | 831 | ARG  | CA-CB-CG   | 6.85  | 127.81      | 114.10   |
| 1   | A     | 638 | ASP  | CA-CB-CG   | 6.85  | 119.45      | 112.60   |
| 1   | B     | 269 | ARG  | N-CA-CB    | 6.85  | 119.91      | 109.91   |
| 1   | C     | 486 | ILE  | CA-CB-CG2  | 6.85  | 122.14      | 110.50   |
| 1   | D     | 610 | ALA  | N-CA-C     | -6.85 | 94.68       | 109.81   |
| 1   | B     | 409 | ARG  | N-CA-C     | 6.84  | 119.76      | 111.82   |
| 1   | C     | 386 | ARG  | O-C-N      | 6.84  | 131.21      | 123.27   |
| 1   | B     | 469 | LYS  | CA-CB-CG   | 6.84  | 127.78      | 114.10   |
| 1   | C     | 32  | ASN  | CA-C-O     | -6.84 | 113.30      | 120.55   |
| 1   | C     | 565 | VAL  | N-CA-C     | 6.84  | 117.96      | 108.12   |
| 1   | D     | 676 | THR  | CB-CA-C    | 6.83  | 124.01      | 110.42   |
| 1   | C     | 177 | GLU  | CA-CB-CG   | 6.82  | 127.74      | 114.10   |
| 1   | A     | 47  | THR  | N-CA-C     | -6.82 | 100.14      | 110.50   |
| 1   | B     | 139 | LEU  | CA-C-O     | -6.81 | 113.67      | 120.82   |
| 1   | D     | 360 | ASP  | CA-CB-CG   | 6.80  | 119.40      | 112.60   |
| 1   | C     | 166 | PHE  | N-CA-C     | 6.77  | 125.23      | 110.80   |
| 1   | D     | 727 | ASN  | OD1-CG-ND2 | -6.76 | 115.84      | 122.60   |
| 1   | D     | 570 | ILE  | O-C-N      | -6.76 | 115.31      | 122.68   |
| 1   | A     | 611 | PRO  | N-CA-C     | -6.75 | 100.63      | 111.03   |
| 1   | A     | 733 | ASP  | CA-CB-CG   | 6.75  | 119.35      | 112.60   |
| 1   | B     | 554 | LYS  | CA-C-O     | -6.75 | 113.90      | 121.25   |
| 1   | D     | 323 | ARG  | CA-CB-CG   | 6.74  | 127.58      | 114.10   |
| 1   | B     | 424 | ARG  | CA-CB-CG   | 6.74  | 127.58      | 114.10   |
| 1   | A     | 521 | LEU  | N-CA-CB    | -6.74 | 99.89       | 110.46   |
| 1   | B     | 737 | GLU  | N-CA-C     | -6.73 | 104.01      | 111.82   |
| 1   | A     | 368 | THR  | CA-C-O     | -6.73 | 113.77      | 120.70   |
| 1   | B     | 420 | GLY  | CA-C-N     | -6.73 | 114.09      | 122.84   |
| 1   | B     | 420 | GLY  | C-N-CA     | -6.73 | 114.09      | 122.84   |
| 1   | C     | 536 | LYS  | N-CA-C     | -6.72 | 103.88      | 111.07   |
| 1   | D     | 602 | THR  | N-CA-C     | -6.71 | 96.07       | 108.02   |
| 1   | A     | 181 | ASP  | CA-C-O     | 6.70  | 128.90      | 121.39   |
| 1   | A     | 649 | ARG  | CG-CD-NE   | -6.70 | 97.27       | 112.00   |
| 1   | A     | 281 | PRO  | N-CA-C     | 6.70  | 126.26      | 112.47   |
| 1   | D     | 180 | ASP  | CA-C-N     | -6.69 | 112.72      | 123.23   |
| 1   | D     | 180 | ASP  | C-N-CA     | -6.69 | 112.72      | 123.23   |
| 1   | B     | 318 | CYS  | N-CA-C     | -6.68 | 103.69      | 110.97   |
| 1   | B     | 507 | ILE  | N-CA-C     | 6.68  | 119.58      | 113.10   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 280 | TYR  | N-CA-C     | 6.68  | 124.58      | 109.81   |
| 1   | C     | 647 | ASN  | CA-CB-CG   | 6.68  | 119.28      | 112.60   |
| 1   | D     | 236 | ASN  | OD1-CG-ND2 | -6.68 | 115.92      | 122.60   |
| 1   | C     | 650 | VAL  | CA-C-O     | -6.68 | 114.10      | 121.05   |
| 1   | B     | 145 | ASP  | N-CA-C     | -6.67 | 103.48      | 111.69   |
| 1   | A     | 383 | ALA  | CA-C-O     | 6.67  | 129.59      | 118.91   |
| 1   | C     | 250 | ASN  | CB-CG-ND2  | 6.67  | 126.41      | 116.40   |
| 1   | B     | 784 | GLN  | OE1-CD-NE2 | -6.67 | 115.93      | 122.60   |
| 1   | D     | 62  | HIS  | CA-CB-CG   | -6.67 | 107.13      | 113.80   |
| 1   | B     | 21  | VAL  | O-C-N      | 6.67  | 129.41      | 122.54   |
| 1   | D     | 494 | LEU  | CA-C-O     | -6.67 | 113.83      | 120.70   |
| 1   | A     | 193 | ARG  | CA-C-N     | 6.66  | 126.91      | 119.32   |
| 1   | A     | 193 | ARG  | C-N-CA     | 6.66  | 126.91      | 119.32   |
| 1   | C     | 777 | TYR  | N-CA-C     | 6.66  | 119.14      | 111.02   |
| 1   | D     | 261 | GLY  | O-C-N      | 6.66  | 128.63      | 122.17   |
| 1   | B     | 610 | ALA  | N-CA-C     | -6.65 | 95.11       | 109.81   |
| 1   | B     | 560 | ASN  | CA-CB-CG   | -6.65 | 105.95      | 112.60   |
| 1   | A     | 27  | LEU  | CA-C-O     | -6.65 | 113.37      | 120.42   |
| 1   | B     | 259 | VAL  | N-CA-C     | 6.64  | 118.00      | 109.30   |
| 1   | B     | 486 | ILE  | CA-CB-CG1  | -6.64 | 99.11       | 110.40   |
| 1   | D     | 575 | ARG  | NE-CZ-NH2  | -6.63 | 113.23      | 119.20   |
| 1   | A     | 490 | ARG  | CD-NE-CZ   | 6.63  | 133.68      | 124.40   |
| 1   | D     | 782 | LYS  | CB-CG-CD   | 6.62  | 126.52      | 111.30   |
| 1   | D     | 784 | GLN  | OE1-CD-NE2 | -6.62 | 115.98      | 122.60   |
| 1   | C     | 716 | GLU  | CB-CG-CD   | 6.61  | 123.84      | 112.60   |
| 1   | A     | 804 | ASN  | OD1-CG-ND2 | -6.61 | 115.99      | 122.60   |
| 1   | A     | 700 | ALA  | N-CA-C     | -6.61 | 104.08      | 111.28   |
| 1   | D     | 384 | LEU  | N-CA-C     | -6.61 | 97.59       | 108.76   |
| 1   | A     | 426 | ARG  | CA-CB-CG   | 6.59  | 127.29      | 114.10   |
| 1   | D     | 575 | ARG  | NE-CZ-NH1  | 6.59  | 128.09      | 121.50   |
| 1   | B     | 255 | LYS  | CA-C-N     | 6.59  | 134.12      | 121.54   |
| 1   | B     | 255 | LYS  | C-N-CA     | 6.59  | 134.12      | 121.54   |
| 1   | B     | 575 | ARG  | N-CA-C     | 6.58  | 120.74      | 111.52   |
| 1   | D     | 182 | TRP  | N-CA-C     | -6.58 | 104.14      | 111.71   |
| 1   | C     | 219 | GLN  | CB-CG-CD   | 6.58  | 123.78      | 112.60   |
| 1   | C     | 426 | ARG  | CA-CB-CG   | 6.58  | 127.26      | 114.10   |
| 1   | A     | 383 | ALA  | N-CA-C     | 6.58  | 121.01      | 113.19   |
| 1   | D     | 379 | VAL  | N-CA-CB    | -6.56 | 100.40      | 111.23   |
| 1   | C     | 167 | ASN  | CA-CB-CG   | -6.56 | 106.04      | 112.60   |
| 1   | A     | 16  | ARG  | N-CA-C     | 6.55  | 124.75      | 110.80   |
| 1   | D     | 490 | ARG  | N-CA-C     | 6.55  | 118.42      | 111.28   |
| 1   | C     | 700 | ALA  | N-CA-C     | -6.54 | 104.07      | 111.07   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 143 | PHE  | CA-C-O     | -6.54 | 113.62      | 120.55   |
| 1   | B     | 256 | ASP  | CA-C-N     | 6.54  | 134.03      | 121.54   |
| 1   | B     | 256 | ASP  | C-N-CA     | 6.54  | 134.03      | 121.54   |
| 1   | B     | 576 | GLN  | CG-CD-NE2  | 6.54  | 126.20      | 116.40   |
| 1   | B     | 712 | GLY  | O-C-N      | 6.53  | 129.78      | 123.05   |
| 1   | D     | 164 | GLY  | CA-C-N     | 6.53  | 132.07      | 122.99   |
| 1   | D     | 164 | GLY  | C-N-CA     | 6.53  | 132.07      | 122.99   |
| 1   | C     | 163 | PHE  | CA-CB-CG   | -6.53 | 107.27      | 113.80   |
| 1   | A     | 33  | ARG  | CA-CB-CG   | 6.52  | 127.14      | 114.10   |
| 1   | D     | 405 | GLU  | CB-CG-CD   | 6.52  | 123.68      | 112.60   |
| 1   | A     | 723 | GLN  | CB-CG-CD   | 6.51  | 123.67      | 112.60   |
| 1   | B     | 676 | THR  | N-CA-CB    | -6.51 | 99.49       | 110.49   |
| 1   | A     | 692 | MET  | CG-SD-CE   | -6.50 | 86.61       | 100.90   |
| 1   | C     | 673 | ALA  | CA-C-O     | -6.49 | 113.67      | 120.55   |
| 1   | D     | 490 | ARG  | CG-CD-NE   | -6.49 | 97.72       | 112.00   |
| 1   | B     | 253 | ASN  | N-CA-C     | -6.49 | 96.98       | 110.80   |
| 1   | D     | 514 | ASP  | CA-CB-CG   | 6.49  | 119.09      | 112.60   |
| 1   | A     | 21  | VAL  | CA-CB-CG1  | 6.49  | 121.43      | 110.40   |
| 1   | B     | 15  | VAL  | CB-CA-C    | -6.48 | 103.55      | 112.04   |
| 1   | C     | 458 | ILE  | CB-CA-C    | -6.47 | 103.29      | 112.22   |
| 1   | C     | 635 | VAL  | CB-CA-C    | -6.47 | 103.29      | 112.22   |
| 1   | A     | 652 | LEU  | N-CA-C     | -6.47 | 104.08      | 112.23   |
| 1   | B     | 555 | VAL  | CB-CA-C    | -6.47 | 100.68      | 111.29   |
| 1   | D     | 315 | LYS  | CA-C-O     | -6.47 | 111.26      | 120.51   |
| 1   | A     | 512 | ILE  | CB-CG1-CD1 | 6.46  | 127.37      | 113.80   |
| 1   | B     | 144 | LEU  | CD1-CG-CD2 | -6.46 | 96.58       | 110.80   |
| 1   | B     | 797 | TRP  | CG-CD2-CE3 | -6.46 | 127.44      | 133.90   |
| 1   | B     | 499 | LEU  | CA-C-O     | -6.46 | 113.57      | 120.42   |
| 1   | D     | 835 | PRO  | N-CA-C     | 6.46  | 120.27      | 111.22   |
| 1   | A     | 771 | PHE  | N-CA-C     | 6.46  | 121.21      | 112.88   |
| 1   | D     | 33  | ARG  | CA-CB-CG   | 6.45  | 127.01      | 114.10   |
| 1   | C     | 481 | ASN  | OD1-CG-ND2 | -6.45 | 116.15      | 122.60   |
| 1   | A     | 478 | LYS  | CA-CB-CG   | 6.45  | 127.00      | 114.10   |
| 1   | C     | 43  | ARG  | CA-CB-CG   | 6.45  | 127.00      | 114.10   |
| 1   | D     | 834 | LEU  | O-C-N      | -6.44 | 114.44      | 121.53   |
| 1   | B     | 108 | CYS  | O-C-N      | 6.44  | 130.19      | 122.27   |
| 1   | A     | 722 | ASP  | O-C-N      | 6.44  | 128.70      | 122.07   |
| 1   | B     | 565 | VAL  | N-CA-C     | 6.44  | 117.39      | 108.12   |
| 1   | B     | 759 | LYS  | CA-CB-CG   | 6.44  | 126.98      | 114.10   |
| 1   | A     | 280 | TYR  | CA-C-N     | 6.43  | 127.88      | 119.84   |
| 1   | A     | 280 | TYR  | C-N-CA     | 6.43  | 127.88      | 119.84   |
| 1   | D     | 262 | TYR  | O-C-N      | 6.43  | 131.14      | 122.59   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 281 | PRO  | CA-N-CD    | -6.43 | 103.00      | 112.00   |
| 1   | A     | 650 | VAL  | N-CA-C     | 6.42  | 117.17      | 110.62   |
| 1   | A     | 33  | ARG  | N-CA-C     | -6.42 | 104.20      | 111.07   |
| 1   | D     | 593 | GLU  | CA-C-N     | 6.42  | 126.11      | 119.82   |
| 1   | D     | 593 | GLU  | C-N-CA     | 6.42  | 126.11      | 119.82   |
| 1   | C     | 255 | LYS  | O-C-N      | 6.42  | 131.13      | 122.59   |
| 1   | B     | 548 | TYR  | O-C-N      | 6.40  | 128.90      | 122.12   |
| 1   | B     | 234 | ARG  | CD-NE-CZ   | 6.40  | 133.35      | 124.40   |
| 1   | B     | 552 | GLU  | N-CA-C     | -6.39 | 98.78       | 109.07   |
| 1   | D     | 477 | HIS  | CA-CB-CG   | 6.39  | 120.19      | 113.80   |
| 1   | B     | 34  | HIS  | CA-C-O     | -6.39 | 113.65      | 120.42   |
| 1   | A     | 47  | THR  | CB-CA-C    | 6.39  | 118.68      | 108.91   |
| 1   | C     | 325 | ASN  | OD1-CG-ND2 | -6.39 | 116.21      | 122.60   |
| 1   | A     | 457 | ARG  | CA-C-O     | -6.38 | 113.74      | 120.63   |
| 1   | C     | 361 | TRP  | CG-CD2-CE3 | -6.38 | 127.52      | 133.90   |
| 1   | A     | 101 | ASN  | CB-CG-ND2  | 6.37  | 125.96      | 116.40   |
| 1   | C     | 399 | HIS  | CA-CB-CG   | -6.37 | 107.43      | 113.80   |
| 1   | D     | 491 | TRP  | N-CA-C     | 6.37  | 120.06      | 112.93   |
| 1   | D     | 455 | VAL  | CB-CA-C    | 6.37  | 121.73      | 111.29   |
| 1   | B     | 269 | ARG  | CA-C-O     | -6.36 | 114.32      | 121.00   |
| 1   | D     | 578 | LEU  | N-CA-C     | -6.36 | 104.43      | 111.36   |
| 1   | D     | 727 | ASN  | CB-CG-ND2  | 6.36  | 125.94      | 116.40   |
| 1   | B     | 274 | ASN  | CB-CG-ND2  | 6.36  | 125.93      | 116.40   |
| 1   | A     | 475 | GLU  | CA-C-N     | 6.34  | 126.09      | 119.05   |
| 1   | A     | 475 | GLU  | C-N-CA     | 6.34  | 126.09      | 119.05   |
| 1   | C     | 15  | VAL  | N-CA-CB    | 6.34  | 118.69      | 110.57   |
| 1   | D     | 486 | ILE  | CA-CB-CG1  | -6.34 | 99.62       | 110.40   |
| 1   | D     | 391 | LEU  | N-CA-C     | -6.34 | 104.29      | 111.14   |
| 1   | A     | 604 | MET  | CG-SD-CE   | -6.34 | 86.96       | 100.90   |
| 1   | A     | 382 | GLU  | CB-CG-CD   | 6.32  | 123.35      | 112.60   |
| 1   | A     | 455 | VAL  | N-CA-C     | 6.32  | 118.97      | 112.90   |
| 1   | D     | 262 | TYR  | N-CA-C     | 6.32  | 124.26      | 110.80   |
| 1   | C     | 52  | TYR  | N-CA-C     | -6.32 | 104.39      | 111.28   |
| 1   | B     | 30  | ASN  | OD1-CG-ND2 | -6.31 | 116.29      | 122.60   |
| 1   | C     | 180 | ASP  | CA-C-N     | -6.31 | 113.53      | 123.12   |
| 1   | C     | 180 | ASP  | C-N-CA     | -6.31 | 113.53      | 123.12   |
| 1   | B     | 537 | VAL  | CA-C-O     | -6.31 | 114.71      | 121.27   |
| 1   | A     | 321 | PRO  | CA-N-CD    | -6.30 | 103.19      | 112.00   |
| 1   | B     | 793 | ASN  | CA-CB-CG   | 6.30  | 118.90      | 112.60   |
| 1   | C     | 176 | MET  | CA-C-N     | -6.30 | 114.66      | 122.84   |
| 1   | C     | 176 | MET  | C-N-CA     | -6.30 | 114.66      | 122.84   |
| 1   | B     | 647 | ASN  | CA-CB-CG   | 6.29  | 118.89      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 717 | ASP  | N-CA-C     | 6.29  | 119.11      | 111.82   |
| 1   | B     | 14  | SER  | CA-C-N     | 6.28  | 129.72      | 120.74   |
| 1   | B     | 14  | SER  | C-N-CA     | 6.28  | 129.72      | 120.74   |
| 1   | D     | 272 | ALA  | N-CA-C     | -6.28 | 103.14      | 111.24   |
| 1   | D     | 458 | ILE  | CB-CG1-CD1 | -6.28 | 100.61      | 113.80   |
| 1   | A     | 278 | VAL  | N-CA-CB    | -6.28 | 100.74      | 112.36   |
| 1   | A     | 277 | ARG  | CA-CB-CG   | -6.28 | 101.54      | 114.10   |
| 1   | B     | 13  | ILE  | N-CA-C     | -6.28 | 97.55       | 107.15   |
| 1   | D     | 394 | THR  | CA-C-O     | -6.28 | 113.83      | 120.55   |
| 1   | A     | 795 | ARG  | N-CA-C     | -6.28 | 103.73      | 112.45   |
| 1   | A     | 381 | PRO  | CA-C-N     | 6.27  | 128.59      | 120.44   |
| 1   | A     | 381 | PRO  | C-N-CA     | 6.27  | 128.59      | 120.44   |
| 1   | B     | 562 | LEU  | N-CA-C     | -6.25 | 98.98       | 108.67   |
| 1   | A     | 530 | PHE  | N-CA-C     | -6.25 | 104.39      | 111.14   |
| 1   | D     | 322 | VAL  | CA-C-N     | 6.25  | 131.03      | 122.34   |
| 1   | D     | 322 | VAL  | C-N-CA     | 6.25  | 131.03      | 122.34   |
| 1   | C     | 652 | LEU  | N-CA-C     | -6.24 | 104.56      | 111.36   |
| 1   | A     | 462 | ILE  | CB-CG1-CD1 | -6.23 | 100.71      | 113.80   |
| 1   | C     | 604 | MET  | CG-SD-CE   | -6.23 | 87.19       | 100.90   |
| 1   | D     | 252 | PHE  | CA-CB-CG   | 6.23  | 120.03      | 113.80   |
| 1   | B     | 622 | LEU  | CA-C-O     | -6.23 | 114.28      | 120.82   |
| 1   | B     | 60  | ARG  | CA-CB-CG   | -6.22 | 101.66      | 114.10   |
| 1   | C     | 118 | ASP  | CA-CB-CG   | 6.22  | 118.82      | 112.60   |
| 1   | D     | 474 | LEU  | CA-C-O     | -6.22 | 114.30      | 120.70   |
| 1   | A     | 72  | GLN  | OE1-CD-NE2 | -6.21 | 116.39      | 122.60   |
| 1   | C     | 811 | PHE  | CA-CB-CG   | -6.20 | 107.60      | 113.80   |
| 1   | B     | 555 | VAL  | N-CA-CB    | 6.19  | 121.44      | 111.23   |
| 1   | C     | 477 | HIS  | CA-CB-CG   | 6.19  | 119.99      | 113.80   |
| 1   | C     | 486 | ILE  | CB-CG1-CD1 | -6.19 | 100.80      | 113.80   |
| 1   | A     | 323 | ARG  | N-CA-C     | 6.18  | 123.97      | 110.80   |
| 1   | A     | 780 | TYR  | CA-C-O     | -6.18 | 114.33      | 120.70   |
| 1   | C     | 737 | GLU  | CA-CB-CG   | 6.18  | 126.46      | 114.10   |
| 1   | B     | 727 | ASN  | CB-CG-ND2  | 6.17  | 125.66      | 116.40   |
| 1   | A     | 100 | VAL  | CA-C-O     | -6.16 | 113.62      | 120.46   |
| 1   | A     | 678 | ASN  | CA-CB-CG   | 6.16  | 118.76      | 112.60   |
| 1   | C     | 655 | LYS  | CA-CB-CG   | 6.16  | 126.42      | 114.10   |
| 1   | D     | 720 | ARG  | CA-CB-CG   | 6.16  | 126.41      | 114.10   |
| 1   | B     | 257 | PHE  | CA-C-O     | 6.15  | 129.30      | 120.51   |
| 1   | C     | 770 | ARG  | CG-CD-NE   | 6.15  | 125.52      | 112.00   |
| 1   | B     | 576 | GLN  | N-CA-C     | -6.14 | 104.65      | 111.71   |
| 1   | C     | 71  | GLN  | OE1-CD-NE2 | -6.14 | 116.46      | 122.60   |
| 1   | B     | 235 | ASN  | CB-CG-ND2  | 6.14  | 125.61      | 116.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 219 | GLN  | N-CA-C     | -6.14 | 102.26      | 110.55   |
| 1   | A     | 239 | ASN  | OD1-CG-ND2 | -6.13 | 116.47      | 122.60   |
| 1   | A     | 316 | PHE  | N-CA-C     | 6.13  | 120.49      | 113.19   |
| 1   | A     | 439 | ILE  | N-CA-C     | -6.13 | 98.91       | 107.80   |
| 1   | B     | 85  | LEU  | CD1-CG-CD2 | -6.12 | 97.33       | 110.80   |
| 1   | C     | 218 | THR  | CA-C-O     | -6.12 | 114.02      | 121.36   |
| 1   | C     | 454 | GLY  | N-CA-C     | -6.12 | 102.92      | 112.58   |
| 1   | D     | 824 | ILE  | N-CA-C     | -6.12 | 106.79      | 111.62   |
| 1   | C     | 329 | PHE  | CA-CB-CG   | 6.11  | 119.91      | 113.80   |
| 1   | C     | 184 | ARG  | CA-CB-CG   | 6.11  | 126.31      | 114.10   |
| 1   | C     | 265 | ALA  | CA-C-N     | 6.10  | 129.09      | 120.42   |
| 1   | C     | 265 | ALA  | C-N-CA     | 6.10  | 129.09      | 120.42   |
| 1   | C     | 770 | ARG  | CD-NE-CZ   | 6.10  | 132.94      | 124.40   |
| 1   | B     | 252 | PHE  | O-C-N      | 6.10  | 130.64      | 122.96   |
| 1   | A     | 278 | VAL  | CB-CA-C    | 6.10  | 120.60      | 110.30   |
| 1   | B     | 273 | GLU  | CB-CG-CD   | 6.09  | 122.95      | 112.60   |
| 1   | C     | 575 | ARG  | N-CA-C     | 6.09  | 119.79      | 111.39   |
| 1   | C     | 387 | TRP  | CA-C-N     | 6.08  | 126.03      | 119.76   |
| 1   | C     | 387 | TRP  | C-N-CA     | 6.08  | 126.03      | 119.76   |
| 1   | D     | 793 | ASN  | CA-C-N     | 6.08  | 126.25      | 119.32   |
| 1   | D     | 793 | ASN  | C-N-CA     | 6.08  | 126.25      | 119.32   |
| 1   | A     | 486 | ILE  | N-CA-CB    | -6.08 | 101.48      | 111.45   |
| 1   | C     | 741 | ILE  | N-CA-CB    | 6.07  | 117.24      | 110.62   |
| 1   | C     | 464 | LYS  | CG-CD-CE   | 6.07  | 125.25      | 111.30   |
| 1   | A     | 405 | GLU  | CB-CG-CD   | 6.07  | 122.91      | 112.60   |
| 1   | B     | 720 | ARG  | CA-CB-CG   | 6.07  | 126.23      | 114.10   |
| 1   | B     | 278 | VAL  | O-C-N      | 6.06  | 129.67      | 123.00   |
| 1   | D     | 388 | PRO  | CA-C-O     | -6.06 | 114.51      | 121.36   |
| 1   | A     | 819 | GLN  | CG-CD-NE2  | -6.05 | 107.33      | 116.40   |
| 1   | D     | 319 | ARG  | N-CA-C     | -6.05 | 100.55      | 109.62   |
| 1   | A     | 325 | ASN  | CB-CG-ND2  | 6.05  | 125.47      | 116.40   |
| 1   | C     | 564 | ASP  | CA-C-O     | -6.05 | 113.99      | 120.46   |
| 1   | D     | 250 | ASN  | OD1-CG-ND2 | -6.05 | 116.55      | 122.60   |
| 1   | A     | 435 | ALA  | O-C-N      | 6.04  | 130.35      | 122.68   |
| 1   | B     | 393 | GLU  | CA-CB-CG   | 6.04  | 126.19      | 114.10   |
| 1   | A     | 653 | ALA  | N-CA-C     | -6.04 | 104.81      | 111.82   |
| 1   | A     | 745 | LEU  | O-C-N      | 6.04  | 128.61      | 122.09   |
| 1   | B     | 807 | THR  | N-CA-CB    | -6.04 | 101.37      | 110.73   |
| 1   | A     | 552 | GLU  | N-CA-C     | -6.04 | 99.05       | 108.90   |
| 1   | B     | 782 | LYS  | CA-CB-CG   | 6.04  | 126.18      | 114.10   |
| 1   | B     | 784 | GLN  | CG-CD-NE2  | 6.04  | 125.46      | 116.40   |
| 1   | D     | 622 | LEU  | CA-C-O     | -6.04 | 114.48      | 120.82   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 135 | GLY  | CA-C-O     | -6.04 | 114.53      | 120.75   |
| 1   | D     | 552 | GLU  | N-CA-C     | -6.03 | 98.56       | 108.76   |
| 1   | B     | 289 | LYS  | CA-CB-CG   | 6.03  | 126.16      | 114.10   |
| 1   | B     | 539 | GLN  | OE1-CD-NE2 | -6.03 | 116.57      | 122.60   |
| 1   | C     | 105 | GLU  | N-CA-C     | 6.03  | 117.85      | 111.28   |
| 1   | C     | 423 | ASP  | CA-CB-CG   | 6.02  | 118.62      | 112.60   |
| 1   | C     | 234 | ARG  | O-C-N      | -6.02 | 114.58      | 122.59   |
| 1   | D     | 639 | ARG  | N-CA-C     | -6.02 | 105.43      | 112.89   |
| 1   | D     | 652 | LEU  | N-CA-C     | -6.02 | 104.29      | 111.69   |
| 1   | B     | 280 | TYR  | CA-C-N     | 6.02  | 127.36      | 119.84   |
| 1   | B     | 280 | TYR  | C-N-CA     | 6.02  | 127.36      | 119.84   |
| 1   | D     | 579 | ASN  | CB-CG-ND2  | 6.01  | 125.42      | 116.40   |
| 1   | A     | 94  | THR  | CA-C-O     | -6.01 | 112.54      | 118.97   |
| 1   | A     | 165 | ILE  | CB-CG1-CD1 | 6.01  | 126.43      | 113.80   |
| 1   | B     | 236 | ASN  | CA-C-N     | -6.01 | 115.36      | 122.93   |
| 1   | B     | 236 | ASN  | C-N-CA     | -6.01 | 115.36      | 122.93   |
| 1   | D     | 180 | ASP  | CA-C-O     | -6.01 | 114.66      | 121.39   |
| 1   | D     | 443 | HIS  | CA-CB-CG   | -6.01 | 107.79      | 113.80   |
| 1   | C     | 33  | ARG  | CB-CA-C    | -6.00 | 99.14       | 110.67   |
| 1   | C     | 156 | GLY  | CA-C-O     | -6.00 | 115.64      | 120.81   |
| 1   | D     | 36  | HIS  | CA-C-O     | -6.00 | 114.50      | 120.80   |
| 1   | D     | 562 | LEU  | N-CA-C     | -6.00 | 100.95      | 109.96   |
| 1   | C     | 470 | ASP  | N-CA-C     | -6.00 | 104.82      | 111.36   |
| 1   | D     | 474 | LEU  | CB-CA-C    | -6.00 | 101.42      | 110.90   |
| 1   | C     | 277 | ARG  | CA-CB-CG   | -5.99 | 102.11      | 114.10   |
| 1   | A     | 127 | GLU  | CB-CA-C    | -5.99 | 99.41       | 109.53   |
| 1   | A     | 325 | ASN  | CA-C-O     | 5.99  | 126.91      | 120.32   |
| 1   | D     | 614 | HIS  | O-C-N      | 5.99  | 128.24      | 122.07   |
| 1   | D     | 729 | GLN  | N-CA-C     | -5.99 | 104.87      | 111.82   |
| 1   | A     | 828 | GLU  | CB-CA-C    | -5.99 | 102.41      | 109.47   |
| 1   | B     | 760 | ASP  | N-CA-C     | 5.99  | 117.48      | 111.07   |
| 1   | A     | 176 | MET  | N-CA-C     | -5.98 | 98.65       | 108.76   |
| 1   | B     | 165 | ILE  | N-CA-C     | -5.98 | 96.90       | 109.34   |
| 1   | C     | 77  | LYS  | CB-CG-CD   | 5.97  | 125.04      | 111.30   |
| 1   | B     | 801 | VAL  | N-CA-C     | -5.97 | 104.69      | 110.42   |
| 1   | C     | 256 | ASP  | CA-C-N     | 5.97  | 131.06      | 122.40   |
| 1   | C     | 256 | ASP  | C-N-CA     | 5.97  | 131.06      | 122.40   |
| 1   | B     | 11  | LYS  | CA-CB-CG   | 5.97  | 126.03      | 114.10   |
| 1   | B     | 88  | GLU  | CA-CB-CG   | 5.96  | 126.03      | 114.10   |
| 1   | D     | 235 | ASN  | OD1-CG-ND2 | -5.96 | 116.64      | 122.60   |
| 1   | B     | 378 | THR  | OG1-CB-CG2 | -5.96 | 97.37       | 109.30   |
| 1   | D     | 135 | GLY  | CA-C-O     | -5.96 | 112.46      | 119.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 541 | ASN  | OD1-CG-ND2 | -5.96 | 116.64      | 122.60   |
| 1   | B     | 438 | ARG  | CB-CG-CD   | -5.96 | 97.60       | 111.30   |
| 1   | C     | 275 | ILE  | N-CA-C     | -5.96 | 104.71      | 110.72   |
| 1   | C     | 339 | ASP  | CA-CB-CG   | 5.95  | 118.55      | 112.60   |
| 1   | B     | 477 | HIS  | CA-CB-CG   | 5.95  | 119.75      | 113.80   |
| 1   | B     | 713 | MET  | CG-SD-CE   | -5.95 | 87.82       | 100.90   |
| 1   | B     | 264 | GLN  | CA-C-N     | 5.95  | 129.33      | 120.17   |
| 1   | B     | 264 | GLN  | C-N-CA     | 5.95  | 129.33      | 120.17   |
| 1   | D     | 325 | ASN  | CA-C-N     | 5.95  | 132.05      | 120.99   |
| 1   | D     | 325 | ASN  | C-N-CA     | 5.95  | 132.05      | 120.99   |
| 1   | D     | 554 | LYS  | N-CA-C     | 5.94  | 117.52      | 108.07   |
| 1   | B     | 274 | ASN  | N-CA-C     | 5.94  | 120.22      | 113.15   |
| 1   | D     | 735 | ILE  | CA-C-O     | 5.94  | 124.92      | 120.88   |
| 1   | B     | 602 | THR  | CA-C-N     | -5.92 | 115.47      | 122.93   |
| 1   | B     | 602 | THR  | C-N-CA     | -5.92 | 115.47      | 122.93   |
| 1   | B     | 323 | ARG  | O-C-N      | 5.92  | 130.47      | 122.59   |
| 1   | D     | 353 | LEU  | O-C-N      | -5.92 | 115.69      | 122.09   |
| 1   | C     | 507 | ILE  | N-CA-C     | 5.92  | 117.88      | 112.43   |
| 1   | B     | 758 | PHE  | N-CA-CB    | -5.91 | 102.40      | 110.56   |
| 1   | C     | 834 | LEU  | N-CA-C     | -5.91 | 101.61      | 110.24   |
| 1   | D     | 588 | ASN  | CA-C-N     | 5.91  | 128.47      | 120.44   |
| 1   | D     | 588 | ASN  | C-N-CA     | 5.91  | 128.47      | 120.44   |
| 1   | A     | 258 | ASN  | CA-CB-CG   | 5.90  | 118.50      | 112.60   |
| 1   | C     | 378 | THR  | N-CA-C     | 5.90  | 119.17      | 109.85   |
| 1   | D     | 252 | PHE  | CA-C-O     | 5.89  | 127.42      | 120.58   |
| 1   | D     | 655 | LYS  | N-CA-C     | -5.89 | 105.75      | 113.12   |
| 1   | C     | 471 | PHE  | CA-CB-CG   | -5.89 | 107.91      | 113.80   |
| 1   | A     | 556 | HIS  | N-CA-C     | -5.89 | 98.26       | 110.80   |
| 1   | B     | 280 | TYR  | CB-CA-C    | -5.89 | 102.45      | 110.22   |
| 1   | B     | 632 | HIS  | CA-CB-CG   | 5.89  | 119.69      | 113.80   |
| 1   | A     | 258 | ASN  | OD1-CG-ND2 | -5.88 | 116.72      | 122.60   |
| 1   | D     | 384 | LEU  | CA-C-O     | -5.88 | 113.79      | 120.32   |
| 1   | C     | 40  | VAL  | CG1-CB-CG2 | -5.88 | 97.86       | 110.80   |
| 1   | A     | 349 | LEU  | O-C-N      | 5.88  | 128.85      | 122.15   |
| 1   | A     | 235 | ASN  | OD1-CG-ND2 | -5.88 | 116.72      | 122.60   |
| 1   | C     | 213 | ALA  | O-C-N      | 5.88  | 130.04      | 122.81   |
| 1   | C     | 255 | LYS  | CA-C-N     | 5.87  | 132.75      | 121.54   |
| 1   | C     | 255 | LYS  | C-N-CA     | 5.87  | 132.75      | 121.54   |
| 1   | D     | 264 | GLN  | CA-CB-CG   | 5.87  | 125.83      | 114.10   |
| 1   | B     | 466 | THR  | CA-C-N     | 5.87  | 132.53      | 121.97   |
| 1   | B     | 466 | THR  | C-N-CA     | 5.87  | 132.53      | 121.97   |
| 1   | B     | 464 | LYS  | CA-CB-CG   | 5.86  | 125.83      | 114.10   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 767 | HIS  | N-CA-C     | 5.86  | 120.70      | 113.50   |
| 1   | B     | 699 | MET  | CA-C-N     | 5.85  | 128.71      | 120.28   |
| 1   | B     | 699 | MET  | C-N-CA     | 5.85  | 128.71      | 120.28   |
| 1   | A     | 568 | LYS  | O-C-N      | -5.85 | 117.76      | 123.26   |
| 1   | C     | 234 | ARG  | CG-CD-NE   | -5.85 | 99.14       | 112.00   |
| 1   | D     | 239 | ASN  | OD1-CG-ND2 | -5.85 | 116.75      | 122.60   |
| 1   | D     | 458 | ILE  | CA-C-O     | -5.84 | 114.66      | 120.85   |
| 1   | D     | 720 | ARG  | N-CA-CB    | 5.84  | 118.44      | 109.91   |
| 1   | B     | 309 | ARG  | CD-NE-CZ   | 5.84  | 132.57      | 124.40   |
| 1   | B     | 611 | PRO  | CA-C-N     | -5.83 | 112.92      | 122.20   |
| 1   | B     | 611 | PRO  | C-N-CA     | -5.83 | 112.92      | 122.20   |
| 1   | C     | 602 | THR  | CA-C-N     | -5.83 | 115.43      | 122.90   |
| 1   | C     | 602 | THR  | C-N-CA     | -5.83 | 115.43      | 122.90   |
| 1   | B     | 598 | VAL  | N-CA-CB    | -5.83 | 103.01      | 111.52   |
| 1   | C     | 94  | THR  | CA-CB-OG1  | -5.83 | 100.85      | 109.60   |
| 1   | D     | 212 | GLY  | O-C-N      | 5.83  | 128.64      | 123.80   |
| 1   | B     | 11  | LYS  | N-CA-C     | -5.82 | 106.02      | 113.01   |
| 1   | C     | 227 | ASP  | O-C-N      | 5.82  | 130.16      | 123.29   |
| 1   | C     | 89  | PHE  | O-C-N      | -5.82 | 115.44      | 123.12   |
| 1   | D     | 138 | ARG  | NE-CZ-NH1  | 5.82  | 127.32      | 121.50   |
| 1   | C     | 311 | PHE  | CA-CB-CG   | 5.82  | 119.62      | 113.80   |
| 1   | D     | 326 | PHE  | CA-C-O     | -5.81 | 111.78      | 119.10   |
| 1   | A     | 92  | GLY  | O-C-N      | -5.81 | 115.15      | 122.70   |
| 1   | A     | 323 | ARG  | CA-C-N     | 5.81  | 132.63      | 121.54   |
| 1   | A     | 323 | ARG  | C-N-CA     | 5.81  | 132.63      | 121.54   |
| 1   | C     | 261 | GLY  | O-C-N      | 5.80  | 130.24      | 122.70   |
| 1   | C     | 639 | ARG  | N-CA-C     | -5.80 | 105.47      | 112.54   |
| 1   | A     | 630 | VAL  | CA-C-O     | -5.80 | 114.21      | 120.47   |
| 1   | B     | 195 | GLU  | CB-CA-C    | -5.80 | 98.89       | 110.42   |
| 1   | D     | 88  | GLU  | CA-CB-CG   | 5.79  | 125.69      | 114.10   |
| 1   | A     | 387 | TRP  | CA-C-N     | 5.79  | 126.13      | 119.93   |
| 1   | A     | 387 | TRP  | C-N-CA     | 5.79  | 126.13      | 119.93   |
| 1   | B     | 771 | PHE  | CA-CB-CG   | -5.79 | 108.01      | 113.80   |
| 1   | D     | 764 | MET  | N-CA-C     | -5.79 | 105.05      | 111.36   |
| 1   | A     | 727 | ASN  | CB-CG-ND2  | 5.79  | 125.09      | 116.40   |
| 1   | A     | 325 | ASN  | O-C-N      | 5.79  | 130.10      | 123.27   |
| 1   | C     | 566 | GLN  | CA-CB-CG   | -5.79 | 102.53      | 114.10   |
| 1   | B     | 22  | GLU  | CA-C-N     | -5.78 | 114.65      | 122.86   |
| 1   | B     | 22  | GLU  | C-N-CA     | -5.78 | 114.65      | 122.86   |
| 1   | B     | 708 | PHE  | CA-C-O     | -5.78 | 113.66      | 120.60   |
| 1   | A     | 834 | LEU  | CB-CA-C    | 5.78  | 118.49      | 109.42   |
| 1   | A     | 782 | LYS  | CB-CG-CD   | 5.78  | 124.58      | 111.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 754 | GLN  | CA-C-N     | 5.78  | 125.91      | 119.32   |
| 1   | B     | 754 | GLN  | C-N-CA     | 5.78  | 125.91      | 119.32   |
| 1   | A     | 718 | VAL  | N-CA-C     | -5.77 | 104.89      | 110.72   |
| 1   | B     | 737 | GLU  | N-CA-CB    | 5.77  | 119.22      | 110.28   |
| 1   | A     | 807 | THR  | CB-CA-C    | 5.77  | 120.37      | 111.02   |
| 1   | C     | 368 | THR  | CA-C-O     | -5.77 | 114.76      | 120.82   |
| 1   | C     | 458 | ILE  | CB-CG1-CD1 | -5.77 | 101.68      | 113.80   |
| 1   | D     | 554 | LYS  | CA-C-O     | -5.77 | 114.66      | 121.06   |
| 1   | C     | 719 | ASP  | CA-C-O     | -5.76 | 114.73      | 120.90   |
| 1   | B     | 385 | GLU  | N-CA-C     | 5.76  | 118.68      | 110.10   |
| 1   | A     | 832 | GLN  | O-C-N      | 5.76  | 129.78      | 123.22   |
| 1   | B     | 108 | CYS  | CA-CB-SG   | -5.76 | 101.16      | 114.40   |
| 1   | D     | 755 | PRO  | CA-N-CD    | -5.76 | 103.94      | 112.00   |
| 1   | A     | 610 | ALA  | N-CA-C     | -5.76 | 97.09       | 109.81   |
| 1   | C     | 12  | GLN  | N-CA-C     | -5.76 | 105.89      | 114.64   |
| 1   | A     | 713 | MET  | CG-SD-CE   | -5.75 | 88.24       | 100.90   |
| 1   | D     | 314 | SER  | CA-CB-OG   | 5.74  | 122.58      | 111.10   |
| 1   | C     | 162 | GLU  | N-CA-C     | 5.74  | 117.53      | 111.28   |
| 1   | C     | 478 | LYS  | CA-CB-CG   | 5.74  | 125.57      | 114.10   |
| 1   | C     | 164 | GLY  | CA-C-N     | 5.73  | 132.29      | 121.97   |
| 1   | C     | 164 | GLY  | C-N-CA     | 5.73  | 132.29      | 121.97   |
| 1   | D     | 576 | GLN  | OE1-CD-NE2 | -5.73 | 116.87      | 122.60   |
| 1   | B     | 263 | ILE  | CA-CB-CG2  | -5.73 | 100.75      | 110.50   |
| 1   | B     | 12  | GLN  | OE1-CD-NE2 | 5.73  | 128.33      | 122.60   |
| 1   | C     | 615 | MET  | N-CA-C     | -5.73 | 104.94      | 111.07   |
| 1   | B     | 67  | TRP  | CA-C-N     | 5.73  | 127.99      | 120.60   |
| 1   | B     | 67  | TRP  | C-N-CA     | 5.73  | 127.99      | 120.60   |
| 1   | C     | 744 | GLN  | OE1-CD-NE2 | -5.73 | 116.87      | 122.60   |
| 1   | C     | 377 | HIS  | CA-CB-CG   | 5.72  | 119.53      | 113.80   |
| 1   | B     | 782 | LYS  | N-CA-C     | -5.72 | 105.12      | 111.36   |
| 1   | D     | 45  | VAL  | N-CA-CB    | -5.72 | 104.39      | 112.12   |
| 1   | C     | 545 | PHE  | CA-CB-CG   | -5.72 | 108.08      | 113.80   |
| 1   | D     | 579 | ASN  | CA-CB-CG   | 5.72  | 118.32      | 112.60   |
| 1   | A     | 274 | ASN  | OD1-CG-ND2 | -5.71 | 116.89      | 122.60   |
| 1   | A     | 655 | LYS  | CA-CB-CG   | 5.71  | 125.53      | 114.10   |
| 1   | D     | 34  | HIS  | CA-CB-CG   | -5.71 | 108.09      | 113.80   |
| 1   | A     | 517 | GLN  | CA-CB-CG   | -5.70 | 102.70      | 114.10   |
| 1   | C     | 737 | GLU  | CB-CA-C    | -5.69 | 99.74       | 110.67   |
| 1   | B     | 713 | MET  | CA-CB-CG   | 5.69  | 125.49      | 114.10   |
| 1   | B     | 180 | ASP  | CA-C-N     | -5.69 | 114.39      | 122.41   |
| 1   | B     | 180 | ASP  | C-N-CA     | -5.69 | 114.39      | 122.41   |
| 1   | D     | 540 | GLU  | CB-CA-C    | -5.69 | 101.18      | 110.85   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 517 | GLN  | CG-CD-NE2 | -5.69 | 107.87      | 116.40   |
| 1   | C     | 348 | GLU  | CA-C-O    | -5.69 | 114.39      | 120.42   |
| 1   | A     | 140 | ALA  | CA-C-O    | -5.68 | 114.53      | 120.55   |
| 1   | A     | 741 | ILE  | N-CA-C    | -5.68 | 104.79      | 110.30   |
| 1   | D     | 280 | TYR  | O-C-N     | 5.68  | 127.85      | 121.32   |
| 1   | D     | 423 | ASP  | CA-CB-CG  | 5.68  | 118.28      | 112.60   |
| 1   | B     | 329 | PHE  | CA-C-N    | 5.68  | 125.30      | 119.56   |
| 1   | B     | 329 | PHE  | C-N-CA    | 5.68  | 125.30      | 119.56   |
| 1   | B     | 486 | ILE  | O-C-N     | -5.67 | 116.75      | 123.05   |
| 1   | A     | 329 | PHE  | CA-C-N    | 5.67  | 125.34      | 119.56   |
| 1   | A     | 329 | PHE  | C-N-CA    | 5.67  | 125.34      | 119.56   |
| 1   | A     | 531 | ILE  | CA-C-O    | -5.67 | 115.37      | 121.27   |
| 1   | C     | 88  | GLU  | CA-CB-CG  | 5.67  | 125.44      | 114.10   |
| 1   | D     | 187 | ASN  | CA-C-N    | 5.67  | 125.77      | 119.87   |
| 1   | D     | 187 | ASN  | C-N-CA    | 5.67  | 125.77      | 119.87   |
| 1   | B     | 221 | VAL  | N-CA-C    | -5.67 | 100.06      | 108.45   |
| 1   | B     | 585 | THR  | N-CA-C    | -5.67 | 104.79      | 110.97   |
| 1   | A     | 362 | ASP  | CA-CB-CG  | -5.67 | 106.93      | 112.60   |
| 1   | C     | 588 | ASN  | N-CA-C    | 5.66  | 117.13      | 111.07   |
| 1   | D     | 732 | TYR  | O-C-N     | 5.66  | 128.12      | 122.12   |
| 1   | D     | 486 | ILE  | CA-CB-CG2 | 5.66  | 120.11      | 110.50   |
| 1   | D     | 715 | VAL  | CB-CA-C   | -5.66 | 104.51      | 112.14   |
| 1   | B     | 269 | ARG  | N-CA-C    | -5.65 | 104.81      | 110.97   |
| 1   | D     | 735 | ILE  | N-CA-C    | 5.65  | 113.75      | 108.15   |
| 1   | C     | 142 | CYS  | N-CA-C    | -5.65 | 105.12      | 111.28   |
| 1   | C     | 72  | GLN  | N-CA-C    | -5.64 | 105.21      | 111.36   |
| 1   | A     | 609 | PRO  | CA-C-N    | 5.63  | 135.55      | 121.80   |
| 1   | A     | 609 | PRO  | C-N-CA    | 5.63  | 135.55      | 121.80   |
| 1   | B     | 600 | PRO  | CB-CA-C   | 5.63  | 118.36      | 110.98   |
| 1   | C     | 287 | GLU  | CA-CB-CG  | 5.63  | 125.37      | 114.10   |
| 1   | D     | 256 | ASP  | CA-C-N    | 5.63  | 132.29      | 121.54   |
| 1   | D     | 256 | ASP  | C-N-CA    | 5.63  | 132.29      | 121.54   |
| 1   | C     | 458 | ILE  | N-CA-CB   | 5.63  | 119.02      | 110.58   |
| 1   | D     | 823 | GLU  | N-CA-C    | 5.63  | 120.42      | 113.50   |
| 1   | B     | 259 | VAL  | O-C-N     | 5.62  | 128.25      | 122.79   |
| 1   | C     | 93  | ARG  | CB-CA-C   | -5.62 | 99.23       | 110.42   |
| 1   | C     | 675 | GLY  | N-CA-C    | -5.62 | 105.59      | 112.68   |
| 1   | B     | 648 | TYR  | O-C-N     | 5.62  | 129.78      | 122.87   |
| 1   | B     | 30  | ASN  | CB-CG-ND2 | 5.62  | 124.82      | 116.40   |
| 1   | C     | 131 | LEU  | N-CA-CB   | -5.62 | 102.86      | 110.95   |
| 1   | C     | 739 | ARG  | CG-CD-NE  | 5.61  | 124.33      | 112.00   |
| 1   | A     | 760 | ASP  | O-C-N     | 5.60  | 127.84      | 122.07   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 241 | MET  | O-C-N      | -5.60 | 116.66      | 123.27   |
| 1   | C     | 490 | ARG  | CG-CD-NE   | -5.60 | 99.68       | 112.00   |
| 1   | B     | 534 | VAL  | N-CA-C     | -5.60 | 104.48      | 110.36   |
| 1   | C     | 811 | PHE  | N-CA-CB    | -5.60 | 101.03      | 110.49   |
| 1   | D     | 321 | PRO  | CA-C-O     | -5.60 | 110.42      | 120.60   |
| 1   | A     | 426 | ARG  | CG-CD-NE   | 5.59  | 124.31      | 112.00   |
| 1   | A     | 453 | ASN  | CA-CB-CG   | 5.59  | 118.19      | 112.60   |
| 1   | D     | 692 | MET  | CG-SD-CE   | -5.59 | 88.59       | 100.90   |
| 1   | C     | 224 | MET  | CA-C-O     | -5.59 | 113.35      | 119.61   |
| 1   | C     | 609 | PRO  | N-CA-CB    | 5.59  | 109.12      | 103.25   |
| 1   | C     | 727 | ASN  | OD1-CG-ND2 | -5.59 | 117.01      | 122.60   |
| 1   | C     | 138 | ARG  | NE-CZ-NH2  | -5.59 | 114.17      | 119.20   |
| 1   | C     | 392 | LEU  | CA-C-N     | 5.59  | 127.70      | 120.44   |
| 1   | C     | 392 | LEU  | C-N-CA     | 5.59  | 127.70      | 120.44   |
| 1   | A     | 525 | VAL  | CA-C-O     | 5.59  | 126.55      | 120.57   |
| 1   | D     | 234 | ARG  | O-C-N      | -5.59 | 115.16      | 122.59   |
| 1   | D     | 213 | ALA  | N-CA-C     | 5.58  | 118.33      | 110.23   |
| 1   | B     | 337 | LEU  | N-CA-CB    | -5.58 | 101.33      | 110.42   |
| 1   | B     | 42  | ASP  | CA-C-O     | -5.58 | 114.97      | 121.10   |
| 1   | C     | 311 | PHE  | N-CA-C     | -5.58 | 105.11      | 111.07   |
| 1   | B     | 417 | ALA  | N-CA-C     | 5.57  | 117.16      | 111.14   |
| 1   | D     | 92  | GLY  | O-C-N      | -5.57 | 115.45      | 122.70   |
| 1   | B     | 267 | LEU  | CA-C-O     | -5.57 | 114.97      | 120.82   |
| 1   | A     | 401 | GLN  | O-C-N      | 5.57  | 128.02      | 122.12   |
| 1   | A     | 593 | GLU  | CA-C-N     | 5.57  | 126.80      | 119.84   |
| 1   | A     | 593 | GLU  | C-N-CA     | 5.57  | 126.80      | 119.84   |
| 1   | A     | 789 | ALA  | N-CA-C     | -5.57 | 105.13      | 111.14   |
| 1   | B     | 724 | ARG  | N-CA-C     | -5.57 | 105.61      | 112.90   |
| 1   | C     | 242 | ARG  | CB-CG-CD   | -5.57 | 98.49       | 111.30   |
| 1   | D     | 184 | ARG  | CA-CB-CG   | 5.57  | 125.24      | 114.10   |
| 1   | C     | 16  | ARG  | CA-CB-CG   | 5.56  | 125.23      | 114.10   |
| 1   | D     | 429 | SER  | O-C-N      | 5.56  | 129.65      | 122.81   |
| 1   | C     | 248 | ALA  | CA-C-N     | 5.56  | 126.79      | 119.84   |
| 1   | C     | 248 | ALA  | C-N-CA     | 5.56  | 126.79      | 119.84   |
| 1   | B     | 257 | PHE  | N-CA-C     | -5.56 | 98.96       | 110.80   |
| 1   | B     | 490 | ARG  | CG-CD-NE   | -5.56 | 99.78       | 112.00   |
| 1   | B     | 564 | ASP  | CA-CB-CG   | 5.56  | 118.16      | 112.60   |
| 1   | C     | 139 | LEU  | CA-C-O     | -5.55 | 114.98      | 120.70   |
| 1   | A     | 331 | ASP  | CA-CB-CG   | 5.55  | 118.15      | 112.60   |
| 1   | B     | 744 | GLN  | OE1-CD-NE2 | -5.55 | 117.05      | 122.60   |
| 1   | A     | 678 | ASN  | OD1-CG-ND2 | -5.55 | 117.05      | 122.60   |
| 1   | A     | 770 | ARG  | CD-NE-CZ   | 5.55  | 132.17      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 21  | VAL  | N-CA-C      | -5.55 | 103.94      | 110.21   |
| 1   | C     | 126 | GLU  | CB-CG-CD    | 5.55  | 122.03      | 112.60   |
| 1   | D     | 629 | VAL  | CG1-CB-CG2  | -5.54 | 98.61       | 110.80   |
| 1   | A     | 257 | PHE  | O-C-N       | 5.54  | 129.96      | 122.59   |
| 1   | A     | 676 | THR  | OG1-CB-CG2  | 5.54  | 120.38      | 109.30   |
| 1   | B     | 479 | PHE  | CA-CB-CG    | -5.54 | 108.26      | 113.80   |
| 1   | C     | 469 | LYS  | N-CA-C      | 5.54  | 119.14      | 112.38   |
| 1   | B     | 401 | GLN  | CA-C-O      | -5.54 | 115.19      | 121.00   |
| 1   | D     | 250 | ASN  | CB-CG-ND2   | 5.53  | 124.70      | 116.40   |
| 1   | C     | 702 | GLU  | CA-C-O      | -5.53 | 114.11      | 120.24   |
| 1   | A     | 797 | TRP  | CE2-CD2-CE3 | 5.52  | 124.32      | 118.80   |
| 1   | B     | 675 | GLY  | N-CA-C      | -5.52 | 105.72      | 112.68   |
| 1   | A     | 361 | TRP  | CG-CD2-CE3  | -5.52 | 128.38      | 133.90   |
| 1   | B     | 481 | ASN  | OD1-CG-ND2  | -5.52 | 117.08      | 122.60   |
| 1   | C     | 678 | ASN  | CA-CB-CG    | 5.52  | 118.12      | 112.60   |
| 1   | C     | 832 | GLN  | N-CA-C      | 5.52  | 118.64      | 110.48   |
| 1   | B     | 248 | ALA  | CA-C-O      | -5.51 | 114.29      | 120.25   |
| 1   | B     | 256 | ASP  | N-CA-C      | -5.51 | 99.06       | 110.80   |
| 1   | A     | 47  | THR  | N-CA-CB     | -5.51 | 99.74       | 110.10   |
| 1   | B     | 44  | ASN  | CB-CA-C     | -5.51 | 100.09      | 110.67   |
| 1   | C     | 421 | ASP  | CA-C-N      | 5.51  | 127.61      | 120.56   |
| 1   | C     | 421 | ASP  | C-N-CA      | 5.51  | 127.61      | 120.56   |
| 1   | A     | 18  | LEU  | CA-C-N      | 5.51  | 132.06      | 121.54   |
| 1   | A     | 18  | LEU  | C-N-CA      | 5.51  | 132.06      | 121.54   |
| 1   | D     | 484 | ASN  | O-C-N       | 5.51  | 129.18      | 122.68   |
| 1   | A     | 465 | LYS  | CA-CB-CG    | 5.50  | 125.11      | 114.10   |
| 1   | C     | 735 | ILE  | CA-C-N      | 5.50  | 124.85      | 118.85   |
| 1   | C     | 735 | ILE  | C-N-CA      | 5.50  | 124.85      | 118.85   |
| 1   | D     | 333 | VAL  | N-CA-C      | 5.50  | 116.66      | 108.46   |
| 1   | B     | 33  | ARG  | CB-CA-C     | -5.50 | 101.66      | 110.79   |
| 1   | D     | 187 | ASN  | CA-C-O      | -5.50 | 113.83      | 119.49   |
| 1   | B     | 400 | LEU  | CB-CA-C     | -5.50 | 100.46      | 110.63   |
| 1   | C     | 322 | VAL  | CB-CA-C     | 5.50  | 121.07      | 111.18   |
| 1   | B     | 163 | PHE  | CA-C-O      | 5.50  | 126.07      | 119.59   |
| 1   | C     | 329 | PHE  | CA-C-N      | 5.49  | 125.58      | 119.87   |
| 1   | C     | 329 | PHE  | C-N-CA      | 5.49  | 125.58      | 119.87   |
| 1   | D     | 551 | ARG  | N-CA-C      | -5.49 | 104.81      | 112.45   |
| 1   | D     | 88  | GLU  | CB-CA-C     | -5.49 | 98.81       | 109.68   |
| 1   | A     | 148 | ALA  | N-CA-C      | 5.49  | 117.26      | 111.28   |
| 1   | A     | 355 | ASP  | CA-C-O      | -5.49 | 114.73      | 120.55   |
| 1   | C     | 358 | ARG  | CA-CB-CG    | 5.49  | 125.07      | 114.10   |
| 1   | C     | 579 | ASN  | CA-CB-CG    | 5.49  | 118.09      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 715 | VAL  | CA-C-O     | -5.48 | 115.36      | 121.17   |
| 1   | B     | 281 | PRO  | N-CA-C     | 5.48  | 123.76      | 112.47   |
| 1   | D     | 469 | LYS  | N-CA-C     | 5.48  | 118.01      | 111.71   |
| 1   | C     | 602 | THR  | N-CA-C     | -5.48 | 98.43       | 108.02   |
| 1   | C     | 644 | PHE  | CA-CB-CG   | -5.48 | 108.32      | 113.80   |
| 1   | A     | 180 | ASP  | O-C-N      | -5.48 | 115.95      | 122.63   |
| 1   | B     | 720 | ARG  | N-CA-CB    | 5.47  | 118.17      | 110.12   |
| 1   | C     | 438 | ARG  | CA-C-O     | -5.47 | 114.70      | 121.11   |
| 1   | D     | 739 | ARG  | CG-CD-NE   | 5.47  | 124.04      | 112.00   |
| 1   | D     | 380 | ILE  | CB-CA-C    | -5.47 | 104.39      | 110.68   |
| 1   | A     | 506 | ARG  | CB-CA-C    | -5.47 | 101.61      | 110.79   |
| 1   | B     | 187 | ASN  | CA-CB-CG   | 5.47  | 118.07      | 112.60   |
| 1   | B     | 831 | ARG  | CD-NE-CZ   | 5.47  | 132.05      | 124.40   |
| 1   | A     | 269 | ARG  | CB-CA-C    | -5.46 | 102.55      | 110.96   |
| 1   | C     | 589 | ARG  | CB-CG-CD   | 5.46  | 123.87      | 111.30   |
| 1   | A     | 597 | PHE  | CA-CB-CG   | -5.46 | 108.34      | 113.80   |
| 1   | C     | 184 | ARG  | CD-NE-CZ   | 5.46  | 132.05      | 124.40   |
| 1   | D     | 144 | LEU  | CA-C-O     | -5.46 | 114.76      | 120.55   |
| 1   | D     | 665 | GLN  | CG-CD-NE2  | 5.46  | 124.59      | 116.40   |
| 1   | A     | 784 | GLN  | OE1-CD-NE2 | -5.46 | 117.14      | 122.60   |
| 1   | C     | 264 | GLN  | CA-C-N     | 5.46  | 131.99      | 121.18   |
| 1   | C     | 264 | GLN  | C-N-CA     | 5.46  | 131.99      | 121.18   |
| 1   | C     | 589 | ARG  | CA-C-N     | 5.46  | 128.17      | 120.42   |
| 1   | C     | 589 | ARG  | C-N-CA     | 5.46  | 128.17      | 120.42   |
| 1   | D     | 554 | LYS  | CA-C-N     | 5.45  | 131.78      | 121.97   |
| 1   | D     | 554 | LYS  | C-N-CA     | 5.45  | 131.78      | 121.97   |
| 1   | B     | 607 | GLY  | CA-C-O     | -5.45 | 116.27      | 121.83   |
| 1   | A     | 720 | ARG  | CB-CA-C    | -5.44 | 102.33      | 110.88   |
| 1   | D     | 82  | ILE  | O-C-N      | 5.44  | 128.89      | 123.18   |
| 1   | D     | 665 | GLN  | OE1-CD-NE2 | -5.44 | 117.16      | 122.60   |
| 1   | A     | 72  | GLN  | N-CA-C     | -5.44 | 105.25      | 111.07   |
| 1   | A     | 490 | ARG  | CG-CD-NE   | -5.44 | 100.03      | 112.00   |
| 1   | C     | 287 | GLU  | N-CA-C     | 5.44  | 122.39      | 110.80   |
| 1   | D     | 657 | ILE  | O-C-N      | -5.44 | 116.94      | 120.42   |
| 1   | B     | 490 | ARG  | N-CA-C     | 5.44  | 117.91      | 111.33   |
| 1   | B     | 166 | PHE  | N-CA-C     | 5.44  | 122.38      | 110.80   |
| 1   | C     | 45  | VAL  | CB-CA-C    | 5.44  | 116.81      | 110.88   |
| 1   | D     | 815 | ARG  | CA-C-O     | -5.44 | 115.10      | 120.70   |
| 1   | D     | 60  | ARG  | NE-CZ-NH2  | -5.44 | 114.31      | 119.20   |
| 1   | C     | 380 | ILE  | N-CA-C     | -5.43 | 102.27      | 107.76   |
| 1   | D     | 484 | ASN  | OD1-CG-ND2 | 5.43  | 128.03      | 122.60   |
| 1   | C     | 422 | VAL  | N-CA-CB    | -5.43 | 103.62      | 110.57   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 771 | PHE  | CA-CB-CG  | -5.43 | 108.37      | 113.80   |
| 1   | C     | 176 | MET  | N-CA-C    | -5.43 | 99.56       | 108.41   |
| 1   | C     | 486 | ILE  | CA-C-O    | -5.43 | 114.59      | 120.67   |
| 1   | D     | 770 | ARG  | CD-NE-CZ  | 5.42  | 131.99      | 124.40   |
| 1   | B     | 279 | LEU  | CA-C-O    | -5.42 | 115.81      | 121.99   |
| 1   | A     | 298 | PHE  | CA-CB-CG  | 5.42  | 119.22      | 113.80   |
| 1   | D     | 584 | ILE  | CA-C-O    | -5.42 | 115.11      | 120.85   |
| 1   | D     | 750 | PHE  | CA-CB-CG  | -5.42 | 108.38      | 113.80   |
| 1   | A     | 714 | ARG  | N-CA-C    | -5.42 | 102.03      | 110.42   |
| 1   | C     | 278 | VAL  | N-CA-CB   | -5.42 | 102.34      | 112.36   |
| 1   | C     | 280 | TYR  | N-CA-C    | 5.42  | 121.78      | 109.81   |
| 1   | A     | 91  | MET  | N-CA-C    | 5.41  | 118.10      | 111.82   |
| 1   | D     | 229 | PRO  | O-C-N     | -5.41 | 116.61      | 123.10   |
| 1   | D     | 275 | ILE  | O-C-N     | -5.41 | 116.26      | 121.83   |
| 1   | B     | 453 | ASN  | CA-CB-CG  | 5.41  | 118.01      | 112.60   |
| 1   | D     | 309 | ARG  | N-CA-C    | -5.41 | 105.47      | 111.36   |
| 1   | D     | 474 | LEU  | N-CA-CB   | 5.41  | 117.91      | 110.07   |
| 1   | A     | 560 | ASN  | CA-CB-CG  | -5.41 | 107.19      | 112.60   |
| 1   | D     | 351 | ARG  | CA-C-O    | -5.39 | 115.16      | 120.82   |
| 1   | B     | 342 | PRO  | N-CA-CB   | -5.39 | 97.59       | 103.25   |
| 1   | C     | 793 | ASN  | CB-CG-ND2 | -5.39 | 108.32      | 116.40   |
| 1   | A     | 385 | GLU  | N-CA-C    | 5.38  | 117.83      | 110.24   |
| 1   | D     | 287 | GLU  | N-CA-C    | 5.38  | 122.27      | 110.80   |
| 1   | C     | 178 | GLU  | O-C-N     | -5.38 | 116.91      | 122.94   |
| 1   | D     | 402 | ILE  | CA-C-N    | 5.38  | 127.83      | 120.46   |
| 1   | D     | 402 | ILE  | C-N-CA    | 5.38  | 127.83      | 120.46   |
| 1   | C     | 309 | ARG  | N-CA-C    | -5.38 | 105.33      | 111.14   |
| 1   | B     | 167 | ASN  | CB-CG-ND2 | 5.38  | 124.46      | 116.40   |
| 1   | A     | 611 | PRO  | CA-C-N    | -5.37 | 113.66      | 122.20   |
| 1   | A     | 611 | PRO  | C-N-CA    | -5.37 | 113.66      | 122.20   |
| 1   | D     | 191 | LYS  | CG-CD-CE  | -5.37 | 98.94       | 111.30   |
| 1   | D     | 193 | ARG  | NE-CZ-NH2 | -5.37 | 114.37      | 119.20   |
| 1   | D     | 555 | VAL  | CA-C-N    | 5.37  | 131.79      | 121.54   |
| 1   | D     | 555 | VAL  | C-N-CA    | 5.37  | 131.79      | 121.54   |
| 1   | D     | 216 | VAL  | CA-C-N    | 5.37  | 131.79      | 121.54   |
| 1   | D     | 216 | VAL  | C-N-CA    | 5.37  | 131.79      | 121.54   |
| 1   | D     | 236 | ASN  | CB-CG-ND2 | 5.37  | 124.45      | 116.40   |
| 1   | A     | 506 | ARG  | N-CA-CB   | 5.36  | 118.07      | 110.13   |
| 1   | C     | 737 | GLU  | N-CA-C    | -5.36 | 105.60      | 111.82   |
| 1   | C     | 615 | MET  | CA-C-O    | -5.35 | 115.20      | 120.82   |
| 1   | C     | 512 | ILE  | CA-C-O    | -5.35 | 115.49      | 121.05   |
| 1   | D     | 394 | THR  | CA-C-N    | -5.35 | 112.25      | 121.66   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 394 | THR  | C-N-CA     | -5.35 | 112.25      | 121.66   |
| 1   | A     | 230 | VAL  | CA-C-N     | 5.35  | 125.76      | 119.99   |
| 1   | A     | 230 | VAL  | C-N-CA     | 5.35  | 125.76      | 119.99   |
| 1   | B     | 805 | ILE  | CB-CA-C    | -5.34 | 105.04      | 112.04   |
| 1   | B     | 234 | ARG  | N-CA-C     | 5.34  | 119.09      | 112.47   |
| 1   | A     | 541 | ASN  | OD1-CG-ND2 | -5.34 | 117.26      | 122.60   |
| 1   | C     | 765 | LEU  | N-CA-CB    | -5.34 | 102.28      | 110.12   |
| 1   | D     | 67  | TRP  | CA-C-O     | -5.34 | 115.19      | 120.90   |
| 1   | D     | 696 | ASN  | CA-CB-CG   | 5.34  | 117.94      | 112.60   |
| 1   | D     | 121 | GLU  | CB-CG-CD   | 5.33  | 121.67      | 112.60   |
| 1   | D     | 264 | GLN  | CB-CG-CD   | 5.33  | 121.67      | 112.60   |
| 1   | C     | 23  | ASN  | CA-C-N     | 5.33  | 127.28      | 120.56   |
| 1   | C     | 23  | ASN  | C-N-CA     | 5.33  | 127.28      | 120.56   |
| 1   | D     | 47  | THR  | CA-C-O     | -5.33 | 115.17      | 120.66   |
| 1   | D     | 255 | LYS  | CA-C-N     | 5.33  | 131.72      | 121.54   |
| 1   | D     | 255 | LYS  | C-N-CA     | 5.33  | 131.72      | 121.54   |
| 1   | A     | 626 | ILE  | CA-C-O     | -5.33 | 115.51      | 121.05   |
| 1   | A     | 809 | GLY  | N-CA-C     | 5.33  | 120.22      | 113.24   |
| 1   | C     | 445 | CYS  | CA-C-O     | -5.33 | 114.90      | 120.55   |
| 1   | B     | 719 | ASP  | CA-C-O     | -5.33 | 115.23      | 120.82   |
| 1   | A     | 380 | ILE  | CA-C-N     | 5.33  | 126.50      | 119.84   |
| 1   | A     | 380 | ILE  | C-N-CA     | 5.33  | 126.50      | 119.84   |
| 1   | C     | 195 | GLU  | CB-CA-C    | -5.33 | 100.13      | 110.46   |
| 1   | A     | 263 | ILE  | CA-C-O     | 5.32  | 126.79      | 120.72   |
| 1   | A     | 426 | ARG  | CB-CG-CD   | 5.32  | 123.54      | 111.30   |
| 1   | B     | 164 | GLY  | CA-C-N     | 5.32  | 131.55      | 121.97   |
| 1   | B     | 164 | GLY  | C-N-CA     | 5.32  | 131.55      | 121.97   |
| 1   | B     | 100 | VAL  | CA-C-O     | -5.32 | 114.50      | 120.25   |
| 1   | B     | 797 | TRP  | N-CA-C     | -5.32 | 105.38      | 111.07   |
| 1   | D     | 386 | ARG  | CA-C-O     | -5.32 | 114.54      | 120.66   |
| 1   | A     | 251 | ASP  | O-C-N      | 5.32  | 129.67      | 122.59   |
| 1   | A     | 649 | ARG  | NE-CZ-NH1  | -5.32 | 116.18      | 121.50   |
| 1   | D     | 77  | LYS  | CA-C-N     | 5.32  | 128.21      | 123.10   |
| 1   | D     | 77  | LYS  | C-N-CA     | 5.32  | 128.21      | 123.10   |
| 1   | C     | 796 | GLU  | O-C-N      | 5.32  | 129.14      | 122.23   |
| 1   | C     | 720 | ARG  | CB-CA-C    | -5.32 | 102.31      | 110.81   |
| 1   | A     | 273 | GLU  | CA-C-O     | -5.31 | 114.92      | 120.55   |
| 1   | D     | 554 | LYS  | CA-CB-CG   | 5.31  | 124.73      | 114.10   |
| 1   | D     | 828 | GLU  | CB-CG-CD   | 5.31  | 121.63      | 112.60   |
| 1   | A     | 394 | THR  | CA-C-N     | -5.31 | 112.74      | 121.92   |
| 1   | A     | 394 | THR  | C-N-CA     | -5.31 | 112.74      | 121.92   |
| 1   | C     | 30  | ASN  | CA-CB-CG   | -5.31 | 107.29      | 112.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | D     | 133 | ASN  | O-C-N       | -5.31 | 115.53      | 122.59   |
| 1   | D     | 435 | ALA  | CA-C-O      | -5.30 | 115.25      | 120.98   |
| 1   | A     | 105 | GLU  | CA-C-N      | 5.30  | 127.33      | 120.44   |
| 1   | A     | 105 | GLU  | C-N-CA      | 5.30  | 127.33      | 120.44   |
| 1   | D     | 292 | ARG  | N-CA-C      | -5.30 | 105.58      | 111.36   |
| 1   | A     | 76  | GLU  | CB-CG-CD    | 5.30  | 121.61      | 112.60   |
| 1   | B     | 226 | TYR  | N-CA-C      | -5.30 | 101.24      | 109.72   |
| 1   | A     | 250 | ASN  | O-C-N       | 5.30  | 129.53      | 123.02   |
| 1   | C     | 162 | GLU  | CA-CB-CG    | -5.30 | 103.51      | 114.10   |
| 1   | D     | 718 | VAL  | CA-C-O      | -5.30 | 115.44      | 120.95   |
| 1   | D     | 570 | ILE  | CB-CG1-CD1  | 5.29  | 124.92      | 113.80   |
| 1   | A     | 412 | ASN  | OD1-CG-ND2  | -5.29 | 117.31      | 122.60   |
| 1   | A     | 72  | GLN  | CG-CD-NE2   | 5.29  | 124.33      | 116.40   |
| 1   | D     | 27  | LEU  | N-CA-C      | -5.29 | 105.59      | 111.36   |
| 1   | A     | 354 | VAL  | O-C-N       | -5.29 | 115.96      | 122.57   |
| 1   | D     | 323 | ARG  | N-CA-C      | -5.29 | 104.12      | 111.52   |
| 1   | B     | 457 | ARG  | CA-C-O      | -5.28 | 115.25      | 120.90   |
| 1   | B     | 12  | GLN  | CA-C-N      | -5.28 | 115.88      | 122.48   |
| 1   | B     | 12  | GLN  | C-N-CA      | -5.28 | 115.88      | 122.48   |
| 1   | B     | 598 | VAL  | CB-CA-C     | 5.28  | 118.04      | 110.33   |
| 1   | B     | 531 | ILE  | CA-C-O      | -5.28 | 115.92      | 121.41   |
| 1   | A     | 440 | ASN  | OD1-CG-ND2  | -5.28 | 117.33      | 122.60   |
| 1   | B     | 593 | GLU  | CA-C-N      | 5.27  | 124.98      | 119.82   |
| 1   | B     | 593 | GLU  | C-N-CA      | 5.27  | 124.98      | 119.82   |
| 1   | C     | 330 | PRO  | CA-N-CD     | -5.27 | 104.62      | 112.00   |
| 1   | C     | 359 | LEU  | N-CA-C      | -5.27 | 102.95      | 110.59   |
| 1   | B     | 436 | VAL  | CA-CB-CG1   | 5.27  | 119.35      | 110.40   |
| 1   | B     | 772 | LYS  | N-CA-C      | 5.27  | 118.60      | 111.17   |
| 1   | C     | 759 | LYS  | CA-C-O      | 5.27  | 126.86      | 121.07   |
| 1   | D     | 156 | GLY  | CA-C-O      | -5.27 | 116.28      | 120.81   |
| 1   | C     | 432 | GLU  | CA-CB-CG    | 5.27  | 124.63      | 114.10   |
| 1   | C     | 758 | PHE  | N-CA-C      | 5.26  | 118.55      | 112.97   |
| 1   | B     | 176 | MET  | N-CA-C      | -5.26 | 100.32      | 108.90   |
| 1   | D     | 575 | ARG  | N-CA-CB     | -5.26 | 103.34      | 111.65   |
| 1   | A     | 493 | VAL  | CA-C-O      | 5.26  | 126.42      | 120.95   |
| 1   | A     | 395 | LEU  | CA-CB-CG    | 5.26  | 134.69      | 116.30   |
| 1   | A     | 770 | ARG  | CA-CB-CG    | 5.25  | 124.61      | 114.10   |
| 1   | A     | 571 | HIS  | CE1-NE2-CD2 | 5.25  | 114.25      | 109.00   |
| 1   | B     | 405 | GLU  | CA-C-O      | -5.25 | 114.86      | 120.42   |
| 1   | D     | 143 | PHE  | O-C-N       | -5.25 | 116.08      | 122.22   |
| 1   | B     | 290 | GLU  | CA-C-O      | -5.24 | 114.97      | 120.63   |
| 1   | C     | 39  | LEU  | N-CA-C      | 5.24  | 119.73      | 113.23   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 720 | ARG  | CB-CA-C    | -5.24 | 102.89      | 110.96   |
| 1   | D     | 480 | GLN  | CG-CD-NE2  | 5.24  | 124.25      | 116.40   |
| 1   | B     | 376 | ASN  | CA-C-O     | -5.23 | 114.90      | 120.92   |
| 1   | C     | 412 | ASN  | N-CA-C     | -5.23 | 105.69      | 111.71   |
| 1   | D     | 607 | GLY  | CA-C-O     | -5.23 | 116.63      | 121.96   |
| 1   | A     | 366 | GLU  | N-CA-C     | -5.23 | 105.47      | 111.07   |
| 1   | B     | 761 | ILE  | N-CA-C     | -5.23 | 105.62      | 110.53   |
| 1   | D     | 484 | ASN  | CB-CG-ND2  | -5.23 | 108.56      | 116.40   |
| 1   | A     | 463 | LEU  | N-CA-C     | -5.23 | 105.50      | 111.14   |
| 1   | B     | 564 | ASP  | CA-C-O     | -5.22 | 115.11      | 120.54   |
| 1   | A     | 255 | LYS  | N-CA-C     | 5.22  | 117.23      | 109.25   |
| 1   | B     | 331 | ASP  | CA-CB-CG   | 5.22  | 117.82      | 112.60   |
| 1   | C     | 338 | ASN  | CA-C-N     | 5.21  | 131.50      | 121.54   |
| 1   | C     | 338 | ASN  | C-N-CA     | 5.21  | 131.50      | 121.54   |
| 1   | D     | 734 | ARG  | CA-CB-CG   | 5.21  | 124.53      | 114.10   |
| 1   | A     | 64  | VAL  | CG1-CB-CG2 | -5.21 | 99.34       | 110.80   |
| 1   | C     | 379 | VAL  | CA-C-N     | -5.21 | 118.84      | 122.59   |
| 1   | C     | 379 | VAL  | C-N-CA     | -5.21 | 118.84      | 122.59   |
| 1   | B     | 256 | ASP  | CA-CB-CG   | 5.21  | 117.81      | 112.60   |
| 1   | C     | 773 | VAL  | CA-C-O     | -5.21 | 115.64      | 121.05   |
| 1   | B     | 814 | ASP  | CA-CB-CG   | 5.21  | 117.81      | 112.60   |
| 1   | C     | 812 | SER  | N-CA-C     | -5.20 | 101.23      | 109.76   |
| 1   | B     | 135 | GLY  | CA-C-O     | -5.20 | 113.36      | 119.50   |
| 1   | C     | 417 | ALA  | N-CA-C     | -5.20 | 106.09      | 112.90   |
| 1   | C     | 824 | ILE  | CA-C-O     | -5.20 | 116.17      | 120.80   |
| 1   | D     | 770 | ARG  | NE-CZ-NH1  | 5.20  | 126.70      | 121.50   |
| 1   | B     | 252 | PHE  | CA-C-N     | 5.20  | 131.47      | 121.54   |
| 1   | B     | 252 | PHE  | C-N-CA     | 5.20  | 131.47      | 121.54   |
| 1   | C     | 394 | THR  | CA-C-N     | -5.19 | 112.40      | 122.06   |
| 1   | C     | 394 | THR  | C-N-CA     | -5.19 | 112.40      | 122.06   |
| 1   | A     | 383 | ALA  | N-CA-CB    | -5.19 | 101.29      | 110.42   |
| 1   | D     | 585 | THR  | CA-C-N     | 5.19  | 127.69      | 120.63   |
| 1   | D     | 585 | THR  | C-N-CA     | 5.19  | 127.69      | 120.63   |
| 1   | A     | 287 | GLU  | CA-CB-CG   | 5.19  | 124.48      | 114.10   |
| 1   | C     | 388 | PRO  | CA-C-O     | -5.18 | 115.43      | 121.34   |
| 1   | D     | 159 | ILE  | N-CA-C     | -5.18 | 100.87      | 108.85   |
| 1   | C     | 720 | ARG  | N-CA-CB    | 5.18  | 117.66      | 109.94   |
| 1   | D     | 622 | LEU  | N-CA-C     | -5.18 | 105.53      | 111.07   |
| 1   | A     | 338 | ASN  | CA-CB-CG   | -5.18 | 107.42      | 112.60   |
| 1   | A     | 730 | GLU  | CA-CB-CG   | 5.18  | 124.45      | 114.10   |
| 1   | B     | 100 | VAL  | N-CA-C     | -5.18 | 104.50      | 111.44   |
| 1   | D     | 47  | THR  | CA-C-N     | 5.18  | 126.31      | 119.84   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 47  | THR  | C-N-CA     | 5.18  | 126.31      | 119.84   |
| 1   | B     | 165 | ILE  | CB-CG1-CD1 | 5.17  | 124.67      | 113.80   |
| 1   | C     | 276 | SER  | CB-CA-C    | -5.17 | 101.16      | 110.37   |
| 1   | D     | 251 | ASP  | CA-CB-CG   | 5.17  | 117.77      | 112.60   |
| 1   | D     | 758 | PHE  | CA-C-N     | 5.17  | 127.52      | 120.54   |
| 1   | D     | 758 | PHE  | C-N-CA     | 5.17  | 127.52      | 120.54   |
| 1   | A     | 522 | LEU  | N-CA-CB    | -5.17 | 102.51      | 110.16   |
| 1   | B     | 128 | ASP  | N-CA-C     | -5.17 | 101.54      | 109.76   |
| 1   | C     | 325 | ASN  | O-C-N      | 5.17  | 129.23      | 122.87   |
| 1   | D     | 395 | LEU  | CA-CB-CG   | 5.17  | 134.39      | 116.30   |
| 1   | C     | 263 | ILE  | CA-CB-CG1  | 5.17  | 119.18      | 110.40   |
| 1   | C     | 267 | LEU  | CA-C-O     | -5.17 | 115.38      | 120.70   |
| 1   | B     | 527 | ASP  | CA-CB-CG   | 5.16  | 117.76      | 112.60   |
| 1   | A     | 43  | ARG  | NE-CZ-NH2  | 5.16  | 123.84      | 119.20   |
| 1   | A     | 234 | ARG  | N-CA-C     | 5.16  | 119.15      | 112.86   |
| 1   | B     | 90  | TYR  | N-CA-CB    | -5.16 | 104.24      | 110.53   |
| 1   | B     | 715 | VAL  | CA-C-N     | 5.16  | 127.14      | 120.44   |
| 1   | B     | 715 | VAL  | C-N-CA     | 5.16  | 127.14      | 120.44   |
| 1   | D     | 262 | TYR  | CA-C-O     | 5.15  | 127.88      | 120.51   |
| 1   | D     | 242 | ARG  | NE-CZ-NH1  | 5.15  | 126.65      | 121.50   |
| 1   | C     | 257 | PHE  | N-CA-C     | 5.15  | 118.83      | 112.24   |
| 1   | D     | 597 | PHE  | CA-CB-CG   | -5.15 | 108.65      | 113.80   |
| 1   | B     | 408 | GLN  | N-CA-C     | -5.14 | 104.94      | 111.11   |
| 1   | C     | 527 | ASP  | N-CA-C     | -5.14 | 100.92      | 109.46   |
| 1   | A     | 610 | ALA  | N-CA-CB    | 5.14  | 119.52      | 110.37   |
| 1   | D     | 36  | HIS  | CA-CB-CG   | -5.14 | 108.66      | 113.80   |
| 1   | A     | 106 | ASN  | O-C-N      | 5.13  | 127.36      | 122.07   |
| 1   | D     | 240 | THR  | N-CA-C     | 5.13  | 117.85      | 109.59   |
| 1   | A     | 727 | ASN  | OD1-CG-ND2 | -5.13 | 117.47      | 122.60   |
| 1   | B     | 510 | GLU  | CA-CB-CG   | 5.13  | 124.36      | 114.10   |
| 1   | C     | 737 | GLU  | CA-C-O     | -5.13 | 114.07      | 119.97   |
| 1   | A     | 106 | ASN  | CA-CB-CG   | 5.13  | 117.73      | 112.60   |
| 1   | D     | 47  | THR  | CA-CB-OG1  | -5.13 | 101.91      | 109.60   |
| 1   | D     | 358 | ARG  | N-CA-C     | 5.13  | 118.46      | 111.39   |
| 1   | D     | 384 | LEU  | N-CA-CB    | -5.12 | 101.93      | 110.80   |
| 1   | C     | 715 | VAL  | CB-CA-C    | -5.12 | 105.33      | 112.04   |
| 1   | D     | 317 | GLY  | N-CA-C     | -5.12 | 101.04      | 113.18   |
| 1   | D     | 490 | ARG  | NE-CZ-NH1  | 5.12  | 126.62      | 121.50   |
| 1   | B     | 558 | ASN  | N-CA-C     | -5.12 | 98.49       | 109.81   |
| 1   | C     | 322 | VAL  | CA-C-N     | 5.12  | 131.32      | 121.54   |
| 1   | C     | 322 | VAL  | C-N-CA     | 5.12  | 131.32      | 121.54   |
| 1   | D     | 262 | TYR  | CA-C-N     | 5.12  | 129.94      | 121.54   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 262 | TYR  | C-N-CA     | 5.12  | 129.94      | 121.54   |
| 1   | D     | 318 | CYS  | O-C-N      | -5.12 | 115.39      | 122.30   |
| 1   | C     | 556 | HIS  | N-CA-C     | -5.12 | 99.89       | 110.80   |
| 1   | A     | 362 | ASP  | N-CA-C     | 5.12  | 116.94      | 111.36   |
| 1   | B     | 588 | ASN  | CA-C-N     | 5.12  | 127.09      | 120.44   |
| 1   | B     | 588 | ASN  | C-N-CA     | 5.12  | 127.09      | 120.44   |
| 1   | B     | 180 | ASP  | O-C-N      | -5.11 | 116.77      | 122.55   |
| 1   | D     | 573 | TYR  | CA-CB-CG   | 5.11  | 123.09      | 113.90   |
| 1   | C     | 761 | ILE  | N-CA-C     | -5.11 | 105.73      | 110.53   |
| 1   | D     | 648 | TYR  | O-C-N      | 5.11  | 129.21      | 122.93   |
| 1   | B     | 241 | MET  | CA-C-N     | 5.10  | 130.20      | 123.05   |
| 1   | B     | 241 | MET  | C-N-CA     | 5.10  | 130.20      | 123.05   |
| 1   | D     | 676 | THR  | OG1-CB-CG2 | 5.10  | 119.51      | 109.30   |
| 1   | B     | 165 | ILE  | CA-C-N     | 5.10  | 131.28      | 121.54   |
| 1   | B     | 165 | ILE  | C-N-CA     | 5.10  | 131.28      | 121.54   |
| 1   | D     | 309 | ARG  | CA-CB-CG   | 5.10  | 124.30      | 114.10   |
| 1   | D     | 138 | ARG  | O-C-N      | -5.10 | 116.71      | 122.12   |
| 1   | B     | 635 | VAL  | O-C-N      | 5.10  | 127.08      | 121.83   |
| 1   | A     | 479 | PHE  | CA-C-O     | -5.09 | 114.78      | 120.54   |
| 1   | C     | 434 | GLY  | N-CA-C     | -5.09 | 103.70      | 110.58   |
| 1   | D     | 400 | LEU  | N-CA-C     | -5.09 | 105.91      | 111.82   |
| 1   | D     | 556 | HIS  | N-CA-CB    | 5.09  | 119.09      | 110.49   |
| 1   | D     | 758 | PHE  | N-CA-C     | 5.09  | 118.32      | 112.57   |
| 1   | B     | 255 | LYS  | N-CA-C     | 5.09  | 117.74      | 109.24   |
| 1   | A     | 147 | MET  | CA-CB-CG   | -5.09 | 103.93      | 114.10   |
| 1   | B     | 551 | ARG  | N-CA-C     | -5.09 | 105.19      | 111.40   |
| 1   | C     | 763 | ASN  | CB-CA-C    | -5.09 | 102.03      | 110.68   |
| 1   | D     | 675 | GLY  | N-CA-C     | -5.09 | 106.27      | 112.68   |
| 1   | A     | 197 | THR  | OG1-CB-CG2 | -5.08 | 99.13       | 109.30   |
| 1   | C     | 633 | ASP  | CA-C-N     | 5.08  | 125.37      | 119.47   |
| 1   | C     | 633 | ASP  | C-N-CA     | 5.08  | 125.37      | 119.47   |
| 1   | B     | 330 | PRO  | CA-N-CD    | -5.08 | 104.88      | 112.00   |
| 1   | B     | 724 | ARG  | CA-CB-CG   | 5.08  | 124.27      | 114.10   |
| 1   | B     | 163 | PHE  | N-CA-CB    | -5.08 | 102.85      | 110.73   |
| 1   | C     | 305 | GLN  | N-CA-C     | -5.08 | 105.65      | 111.14   |
| 1   | A     | 707 | ASN  | CA-CB-CG   | -5.08 | 107.52      | 112.60   |
| 1   | B     | 793 | ASN  | CA-C-N     | 5.08  | 126.19      | 119.84   |
| 1   | B     | 793 | ASN  | C-N-CA     | 5.08  | 126.19      | 119.84   |
| 1   | D     | 110 | GLU  | CA-C-O     | -5.08 | 115.04      | 120.42   |
| 1   | C     | 16  | ARG  | N-CA-C     | 5.07  | 121.60      | 110.80   |
| 1   | C     | 395 | LEU  | N-CA-C     | 5.07  | 119.47      | 113.28   |
| 1   | C     | 823 | GLU  | N-CA-C     | 5.07  | 119.74      | 113.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 770 | ARG  | CG-CD-NE    | 5.07  | 123.15      | 112.00   |
| 1   | A     | 576 | GLN  | N-CA-C      | -5.07 | 105.94      | 111.82   |
| 1   | D     | 455 | VAL  | CG1-CB-CG2  | 5.07  | 121.95      | 110.80   |
| 1   | B     | 236 | ASN  | OD1-CG-ND2  | -5.07 | 117.53      | 122.60   |
| 1   | C     | 280 | TYR  | O-C-N       | 5.07  | 127.14      | 121.32   |
| 1   | D     | 715 | VAL  | CA-C-N      | 5.07  | 127.02      | 120.44   |
| 1   | D     | 715 | VAL  | C-N-CA      | 5.07  | 127.02      | 120.44   |
| 1   | D     | 164 | GLY  | O-C-N       | 5.06  | 129.54      | 122.55   |
| 1   | B     | 252 | PHE  | CA-C-O      | 5.06  | 126.45      | 120.58   |
| 1   | D     | 555 | VAL  | CB-CA-C     | -5.06 | 103.00      | 111.29   |
| 1   | A     | 359 | LEU  | N-CA-C      | -5.05 | 104.01      | 110.53   |
| 1   | B     | 739 | ARG  | CG-CD-NE    | 5.05  | 123.12      | 112.00   |
| 1   | D     | 455 | VAL  | CA-CB-CG2   | -5.05 | 101.81      | 110.40   |
| 1   | D     | 798 | THR  | N-CA-C      | 5.05  | 116.79      | 111.28   |
| 1   | D     | 824 | ILE  | CA-C-O      | -5.05 | 116.30      | 120.80   |
| 1   | B     | 735 | ILE  | CA-C-N      | 5.05  | 124.66      | 119.05   |
| 1   | B     | 735 | ILE  | C-N-CA      | 5.05  | 124.66      | 119.05   |
| 1   | B     | 744 | GLN  | CG-CD-NE2   | 5.05  | 123.98      | 116.40   |
| 1   | C     | 522 | LEU  | O-C-N       | -5.05 | 116.31      | 122.22   |
| 1   | A     | 214 | LYS  | N-CA-C      | -5.05 | 100.81      | 109.24   |
| 1   | C     | 33  | ARG  | N-CA-CB     | 5.05  | 118.11      | 110.28   |
| 1   | A     | 95  | LEU  | CB-CA-C     | -5.04 | 103.14      | 110.95   |
| 1   | B     | 167 | ASN  | OD1-CG-ND2  | -5.04 | 117.56      | 122.60   |
| 1   | B     | 257 | PHE  | O-C-N       | 5.04  | 129.30      | 122.59   |
| 1   | C     | 393 | GLU  | CB-CG-CD    | -5.04 | 104.03      | 112.60   |
| 1   | B     | 782 | LYS  | CB-CG-CD    | 5.04  | 122.89      | 111.30   |
| 1   | C     | 361 | TRP  | CE2-CD2-CE3 | 5.04  | 123.84      | 118.80   |
| 1   | B     | 652 | LEU  | CA-C-O      | -5.04 | 114.65      | 120.24   |
| 1   | D     | 655 | LYS  | CA-CB-CG    | 5.04  | 124.17      | 114.10   |
| 1   | A     | 257 | PHE  | CA-CB-CG    | -5.04 | 108.77      | 113.80   |
| 1   | C     | 370 | LYS  | CB-CG-CD    | -5.03 | 99.72       | 111.30   |
| 1   | B     | 401 | GLN  | CB-CA-C     | -5.03 | 103.21      | 110.96   |
| 1   | D     | 78  | ASP  | CA-C-O      | -5.03 | 117.00      | 120.47   |
| 1   | A     | 794 | PRO  | N-CA-C      | 5.03  | 120.38      | 113.84   |
| 1   | B     | 22  | GLU  | CA-CB-CG    | 5.03  | 124.16      | 114.10   |
| 1   | A     | 405 | GLU  | CA-CB-CG    | 5.03  | 124.15      | 114.10   |
| 1   | C     | 595 | ASN  | CA-CB-CG    | 5.03  | 117.63      | 112.60   |
| 1   | A     | 623 | ILE  | N-CA-C      | -5.03 | 105.49      | 110.62   |
| 1   | C     | 291 | LEU  | O-C-N       | 5.03  | 127.45      | 122.12   |
| 1   | D     | 506 | ARG  | CA-CB-CG    | 5.03  | 124.15      | 114.10   |
| 1   | D     | 641 | ARG  | CB-CG-CD    | -5.02 | 99.75       | 111.30   |
| 1   | A     | 716 | GLU  | CB-CG-CD    | 5.02  | 121.14      | 112.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 797 | TRP  | CE2-CD2-CE3 | 5.02  | 123.82      | 118.80   |
| 1   | C     | 733 | ASP  | N-CA-C      | 5.02  | 116.75      | 111.28   |
| 1   | D     | 534 | VAL  | N-CA-C      | -5.02 | 105.50      | 110.62   |
| 1   | D     | 681 | PHE  | O-C-N       | 5.02  | 127.44      | 122.12   |
| 1   | D     | 155 | TYR  | CA-C-N      | 5.02  | 126.76      | 122.29   |
| 1   | D     | 155 | TYR  | C-N-CA      | 5.02  | 126.76      | 122.29   |
| 1   | C     | 778 | GLU  | CA-C-O      | -5.02 | 115.53      | 120.70   |
| 1   | D     | 713 | MET  | CA-CB-CG    | 5.02  | 124.13      | 114.10   |
| 1   | A     | 295 | GLN  | O-C-N       | 5.02  | 127.24      | 122.07   |
| 1   | A     | 688 | THR  | CA-C-O      | -5.02 | 114.94      | 120.36   |
| 1   | D     | 32  | ASN  | CB-CG-ND2   | 5.01  | 123.92      | 116.40   |
| 1   | B     | 14  | SER  | N-CA-C      | 5.01  | 116.86      | 108.99   |
| 1   | B     | 707 | ASN  | CA-CB-CG    | -5.01 | 107.59      | 112.60   |
| 1   | D     | 629 | VAL  | CA-C-O      | -5.01 | 114.52      | 120.78   |
| 1   | A     | 644 | PHE  | O-C-N       | -5.01 | 117.51      | 123.22   |
| 1   | B     | 242 | ARG  | CB-CG-CD    | -5.01 | 99.78       | 111.30   |
| 1   | B     | 790 | LEU  | N-CA-C      | -5.00 | 106.02      | 111.82   |
| 1   | C     | 638 | ASP  | CA-CB-CG    | 5.00  | 117.60      | 112.60   |

There are no chirality outliers.

All (26) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 157 | TYR  | Sidechain         |
| 1   | A     | 252 | PHE  | Sidechain         |
| 1   | A     | 262 | TYR  | Sidechain         |
| 1   | A     | 472 | TYR  | Sidechain         |
| 1   | A     | 52  | TYR  | Sidechain         |
| 1   | A     | 597 | PHE  | Sidechain         |
| 1   | A     | 811 | PHE  | Sidechain         |
| 1   | A     | 836 | ALA  | Mainchain,Peptide |
| 1   | B     | 155 | TYR  | Sidechain         |
| 1   | B     | 320 | ASP  | Peptide           |
| 1   | B     | 380 | ILE  | Peptide           |
| 1   | B     | 52  | TYR  | Sidechain         |
| 1   | C     | 262 | TYR  | Sidechain         |
| 1   | C     | 280 | TYR  | Peptide           |
| 1   | C     | 316 | PHE  | Sidechain         |
| 1   | C     | 320 | ASP  | Peptide           |
| 1   | C     | 324 | THR  | Peptide           |
| 1   | C     | 52  | TYR  | Sidechain         |
| 1   | C     | 836 | ALA  | Peptide           |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | D     | 262 | TYR  | Sidechain |
| 1   | D     | 297 | TYR  | Sidechain |
| 1   | D     | 320 | ASP  | Peptide   |
| 1   | D     | 52  | TYR  | Sidechain |
| 1   | D     | 597 | PHE  | Sidechain |
| 1   | D     | 836 | ALA  | Peptide   |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 6692  | 0        | 6650     | 149     | 0            |
| 1   | B     | 6692  | 0        | 6650     | 166     | 1            |
| 1   | C     | 6692  | 0        | 6650     | 188     | 0            |
| 1   | D     | 6692  | 0        | 6650     | 167     | 0            |
| 2   | A     | 5     | 0        | 0        | 0       | 0            |
| 2   | B     | 5     | 0        | 0        | 0       | 0            |
| 2   | C     | 5     | 0        | 0        | 1       | 0            |
| 2   | D     | 5     | 0        | 0        | 0       | 0            |
| 3   | A     | 15    | 0        | 7        | 0       | 0            |
| 3   | B     | 15    | 0        | 6        | 1       | 0            |
| 3   | C     | 15    | 0        | 7        | 0       | 0            |
| 3   | D     | 15    | 0        | 6        | 0       | 0            |
| 4   | A     | 14    | 0        | 10       | 0       | 0            |
| 4   | B     | 14    | 0        | 10       | 0       | 0            |
| 4   | C     | 14    | 0        | 10       | 0       | 0            |
| 4   | D     | 14    | 0        | 10       | 0       | 0            |
| 5   | A     | 223   | 0        | 0        | 14      | 1            |
| 5   | B     | 222   | 0        | 0        | 18      | 0            |
| 5   | C     | 218   | 0        | 0        | 16      | 1            |
| 5   | D     | 221   | 0        | 0        | 16      | 1            |
| All | All   | 27788 | 0        | 26666    | 644     | 2            |

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 12.

All (644) 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:322:VAL:HG13 | 1:D:325:ASN:HB3  | 1.43                     | 0.98              |
| 1:C:171:CYS:SG   | 1:C:176:MET:HG3  | 2.09                     | 0.92              |
| 1:B:85:LEU:HD21  | 1:B:303:THR:HG21 | 1.54                     | 0.90              |
| 1:A:615:MET:HE1  | 1:A:761:ILE:HG12 | 1.57                     | 0.86              |
| 1:D:225:PRO:HB2  | 1:D:242:ARG:HD2  | 1.58                     | 0.86              |
| 1:C:325:ASN:HB3  | 1:C:327:ASP:HB2  | 1.58                     | 0.84              |
| 1:A:676:THR:HG21 | 5:A:1022:HOH:O   | 1.78                     | 0.84              |
| 1:B:144:LEU:HD12 | 5:B:1135:HOH:O   | 1.79                     | 0.82              |
| 1:C:713:MET:HE1  | 1:C:775:ALA:HB1  | 1.61                     | 0.82              |
| 1:A:381:PRO:HA   | 1:A:384:LEU:HD13 | 1.60                     | 0.82              |
| 1:D:82:ILE:HB    | 5:D:1150:HOH:O   | 1.79                     | 0.81              |
| 1:C:604:MET:HE2  | 1:C:645:LEU:HD21 | 1.62                     | 0.81              |
| 1:C:254:LEU:HA   | 1:C:259:VAL:HG21 | 1.62                     | 0.81              |
| 1:B:692:MET:SD   | 1:B:710:ILE:HD12 | 2.20                     | 0.80              |
| 1:C:173:GLY:HA3  | 1:C:624:THR:HG21 | 1.63                     | 0.79              |
| 1:B:168:GLN:HE21 | 1:B:647:ASN:H    | 1.28                     | 0.79              |
| 1:B:676:THR:HG21 | 5:B:1031:HOH:O   | 1.83                     | 0.78              |
| 1:B:10:ARG:HG3   | 1:B:13:ILE:HD12  | 1.66                     | 0.78              |
| 1:D:703:ALA:HA   | 1:D:807:THR:HG21 | 1.66                     | 0.78              |
| 1:C:676:THR:HG21 | 5:C:1022:HOH:O   | 1.82                     | 0.77              |
| 1:C:381:PRO:HG3  | 1:C:467:ILE:HG12 | 1.64                     | 0.77              |
| 1:C:85:LEU:HD21  | 1:C:303:THR:HG21 | 1.66                     | 0.77              |
| 1:B:703:ALA:HA   | 1:B:807:THR:HG21 | 1.66                     | 0.77              |
| 1:A:225:PRO:HB2  | 1:A:242:ARG:HD2  | 1.67                     | 0.76              |
| 1:A:455:VAL:H    | 1:A:459:HIS:HD2  | 1.32                     | 0.76              |
| 1:C:566:GLN:HE22 | 1:C:576:GLN:HA   | 1.51                     | 0.76              |
| 1:A:703:ALA:HA   | 1:A:807:THR:HG21 | 1.66                     | 0.75              |
| 1:B:550:GLU:HG3  | 1:B:554:LYS:HA   | 1.68                     | 0.75              |
| 1:D:168:GLN:HG3  | 1:D:175:GLN:HG3  | 1.68                     | 0.75              |
| 1:D:254:LEU:HA   | 1:D:259:VAL:HG22 | 1.69                     | 0.75              |
| 1:A:168:GLN:HG3  | 1:A:175:GLN:HG3  | 1.69                     | 0.74              |
| 1:A:320:ASP:HB2  | 1:A:324:THR:HA   | 1.67                     | 0.74              |
| 1:B:315:LYS:HA   | 1:B:318:CYS:SG   | 2.28                     | 0.74              |
| 1:C:545:PHE:CE2  | 1:C:604:MET:HE1  | 2.23                     | 0.74              |
| 1:C:766:MET:HE3  | 1:C:774:PHE:HE2  | 1.52                     | 0.74              |
| 1:A:336:GLN:HE21 | 1:A:825:TRP:HE1  | 1.34                     | 0.73              |
| 1:D:615:MET:HE1  | 1:D:761:ILE:HG12 | 1.70                     | 0.73              |
| 1:D:550:GLU:HG3  | 1:D:554:LYS:HA   | 1.70                     | 0.73              |
| 1:C:597:PHE:HE2  | 1:C:792:LYS:HD2  | 1.54                     | 0.73              |
| 1:B:225:PRO:HB2  | 1:B:242:ARG:HD2  | 1.69                     | 0.73              |
| 1:C:545:PHE:HE2  | 1:C:604:MET:HE1  | 1.54                     | 0.72              |
| 1:B:193:ARG:HB2  | 1:B:225:PRO:HG2  | 1.70                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:588:ASN:HD21 | 1:C:744:GLN:HE22 | 1.36                     | 0.72              |
| 1:D:676:THR:HG21 | 5:D:1032:HOH:O   | 1.89                     | 0.71              |
| 1:B:588:ASN:HD21 | 1:B:744:GLN:HE22 | 1.35                     | 0.71              |
| 1:B:378:THR:HG23 | 5:B:1038:HOH:O   | 1.89                     | 0.71              |
| 1:D:381:PRO:HG2  | 1:D:382:GLU:HG3  | 1.72                     | 0.71              |
| 1:C:267:LEU:HD23 | 1:D:266:VAL:HG11 | 1.73                     | 0.71              |
| 1:A:557:ILE:HD11 | 1:A:643:ILE:HD11 | 1.71                     | 0.71              |
| 1:D:91:MET:SD    | 5:D:1137:HOH:O   | 2.49                     | 0.71              |
| 1:A:222:LEU:HB2  | 1:A:247:LYS:HB2  | 1.71                     | 0.71              |
| 1:B:713:MET:HE1  | 1:B:775:ALA:HB1  | 1.73                     | 0.70              |
| 1:C:168:GLN:HG3  | 1:C:175:GLN:HG3  | 1.74                     | 0.70              |
| 1:B:615:MET:HE1  | 1:B:761:ILE:HG12 | 1.73                     | 0.70              |
| 1:C:703:ALA:HA   | 1:C:807:THR:HG21 | 1.74                     | 0.69              |
| 1:B:287:GLU:O    | 1:B:292:ARG:HD3  | 1.91                     | 0.69              |
| 1:C:336:GLN:NE2  | 1:C:825:TRP:HE1  | 1.90                     | 0.69              |
| 1:C:322:VAL:HG22 | 1:C:325:ASN:HD22 | 1.57                     | 0.68              |
| 1:D:322:VAL:CG1  | 1:D:325:ASN:HB3  | 2.21                     | 0.68              |
| 1:D:173:GLY:CA   | 1:D:624:THR:HG21 | 2.22                     | 0.68              |
| 1:B:548:TYR:HD1  | 1:B:551:ARG:HH21 | 1.41                     | 0.68              |
| 1:A:236:ASN:HB2  | 1:A:834:LEU:O    | 1.94                     | 0.68              |
| 1:C:336:GLN:HE21 | 1:C:825:TRP:HE1  | 1.41                     | 0.68              |
| 1:B:168:GLN:HG3  | 1:B:175:GLN:HG3  | 1.76                     | 0.68              |
| 1:A:10:ARG:HG3   | 1:B:43:ARG:HD3   | 1.75                     | 0.68              |
| 1:C:319:ARG:HE   | 1:C:321:PRO:HD2  | 1.56                     | 0.68              |
| 1:A:193:ARG:HB3  | 1:A:196:PHE:HD2  | 1.57                     | 0.67              |
| 1:A:601:ARG:HH22 | 1:A:784:GLN:NE2  | 1.92                     | 0.67              |
| 1:C:597:PHE:CE2  | 1:C:792:LYS:HD2  | 2.29                     | 0.67              |
| 1:A:168:GLN:HE21 | 1:A:647:ASN:H    | 1.42                     | 0.67              |
| 1:B:59:VAL:HG13  | 1:B:104:LEU:HD23 | 1.76                     | 0.67              |
| 1:C:211:GLN:HG2  | 1:C:358:ARG:HD2  | 1.76                     | 0.67              |
| 1:C:795:ARG:O    | 1:C:799:ARG:HG3  | 1.94                     | 0.67              |
| 1:D:791:TYR:HA   | 1:D:797:TRP:CD1  | 2.30                     | 0.67              |
| 1:C:322:VAL:HG22 | 1:C:325:ASN:ND2  | 2.10                     | 0.67              |
| 1:A:144:LEU:HD12 | 5:A:1128:HOH:O   | 1.95                     | 0.66              |
| 1:A:463:LEU:HD23 | 1:A:467:ILE:HD13 | 1.78                     | 0.66              |
| 1:A:173:GLY:HA2  | 1:A:624:THR:HG21 | 1.77                     | 0.65              |
| 1:C:168:GLN:HE21 | 1:C:647:ASN:H    | 1.44                     | 0.65              |
| 1:D:713:MET:HE1  | 1:D:775:ALA:HB1  | 1.78                     | 0.65              |
| 1:B:836:ALA:HB1  | 1:B:837:PRO:HA   | 1.77                     | 0.65              |
| 1:C:322:VAL:HG13 | 1:C:325:ASN:HB2  | 1.78                     | 0.65              |
| 1:D:289:LYS:HG2  | 1:D:291:LEU:H    | 1.62                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:343:SER:HB3  | 1:A:445:CYS:SG   | 2.36                     | 0.65              |
| 1:A:426:ARG:NH1  | 1:D:755:PRO:HB2  | 2.11                     | 0.65              |
| 1:D:129:ALA:HB1  | 1:D:131:LEU:HD22 | 1.77                     | 0.65              |
| 1:D:593:GLU:HB3  | 1:D:596:LYS:HB2  | 1.77                     | 0.65              |
| 1:C:225:PRO:HB2  | 1:C:242:ARG:HD2  | 1.79                     | 0.64              |
| 1:C:480:GLN:HE21 | 1:C:482:LYS:HZ3  | 1.44                     | 0.64              |
| 1:C:550:GLU:HG3  | 1:C:554:LYS:HA   | 1.79                     | 0.64              |
| 1:A:142:CYS:SG   | 1:A:487:THR:HG22 | 2.37                     | 0.64              |
| 1:A:426:ARG:NE   | 1:D:755:PRO:HD2  | 2.12                     | 0.64              |
| 1:A:91:MET:SD    | 5:A:1128:HOH:O   | 2.55                     | 0.64              |
| 1:B:193:ARG:HB3  | 1:B:196:PHE:HD2  | 1.62                     | 0.64              |
| 1:D:322:VAL:HG23 | 1:D:323:ARG:NH1  | 2.13                     | 0.64              |
| 1:A:168:GLN:NE2  | 1:A:647:ASN:H    | 1.96                     | 0.64              |
| 1:A:235:ASN:HA   | 1:A:833:ARG:HG3  | 1.80                     | 0.64              |
| 1:D:568:LYS:HZ1  | 1:D:665:GLN:HE22 | 1.45                     | 0.64              |
| 1:C:168:GLN:NE2  | 1:C:647:ASN:H    | 1.96                     | 0.64              |
| 1:D:311:PHE:O    | 1:D:316:PHE:HB2  | 1.98                     | 0.64              |
| 1:B:676:THR:HG22 | 3:B:999:PLP:H5A1 | 1.78                     | 0.63              |
| 1:D:545:PHE:O    | 1:D:549:LEU:HB2  | 1.98                     | 0.63              |
| 1:D:316:PHE:C    | 1:D:320:ASP:HA   | 2.24                     | 0.63              |
| 1:B:235:ASN:H    | 1:B:235:ASN:HD22 | 1.44                     | 0.63              |
| 1:A:21:VAL:HG12  | 1:A:22:GLU:H     | 1.64                     | 0.62              |
| 1:A:336:GLN:NE2  | 1:A:825:TRP:HE1  | 1.97                     | 0.62              |
| 1:D:144:LEU:HD12 | 5:D:1137:HOH:O   | 1.99                     | 0.62              |
| 1:D:358:ARG:HD3  | 1:D:358:ARG:N    | 2.14                     | 0.62              |
| 1:A:480:GLN:HE21 | 1:A:482:LYS:HZ3  | 1.47                     | 0.62              |
| 1:B:795:ARG:O    | 1:B:799:ARG:HG3  | 1.99                     | 0.62              |
| 1:C:480:GLN:HE21 | 1:C:482:LYS:NZ   | 1.98                     | 0.62              |
| 1:D:173:GLY:HA2  | 1:D:624:THR:HG21 | 1.81                     | 0.62              |
| 1:B:34:HIS:HD2   | 1:B:38:THR:OG1   | 1.82                     | 0.62              |
| 1:B:455:VAL:HG22 | 1:B:484:ASN:OD1  | 1.99                     | 0.61              |
| 1:A:138:ARG:HB3  | 5:A:1022:HOH:O   | 1.99                     | 0.61              |
| 1:C:378:THR:O    | 1:C:459:HIS:HE1  | 1.83                     | 0.61              |
| 1:A:467:ILE:HD12 | 1:A:467:ILE:H    | 1.66                     | 0.61              |
| 1:A:734:ARG:HD2  | 5:A:1161:HOH:O   | 1.99                     | 0.61              |
| 1:B:263:ILE:HG13 | 1:C:262:TYR:OH   | 2.01                     | 0.61              |
| 1:C:193:ARG:HB3  | 1:C:196:PHE:HD2  | 1.66                     | 0.61              |
| 1:D:550:GLU:HA   | 1:D:553:TYR:O    | 2.00                     | 0.61              |
| 1:D:610:ALA:N    | 5:D:1158:HOH:O   | 2.33                     | 0.61              |
| 1:D:336:GLN:NE2  | 1:D:825:TRP:HE1  | 1.97                     | 0.61              |
| 1:B:615:MET:CE   | 1:B:761:ILE:HG12 | 2.31                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:721:LEU:HD23 | 1:C:772:LYS:HD3  | 1.83                     | 0.61              |
| 1:B:161:TYR:HA   | 1:B:276:SER:O    | 2.01                     | 0.60              |
| 1:B:803:ARG:HH11 | 1:B:803:ARG:HB2  | 1.64                     | 0.60              |
| 1:C:365:TRP:O    | 1:C:369:VAL:HG13 | 2.01                     | 0.60              |
| 1:D:601:ARG:HD2  | 5:D:1172:HOH:O   | 2.01                     | 0.60              |
| 1:A:383:ALA:HA   | 5:A:1160:HOH:O   | 1.99                     | 0.60              |
| 1:D:173:GLY:HA3  | 1:D:624:THR:HG21 | 1.84                     | 0.60              |
| 1:B:71:GLN:HG3   | 5:B:1162:HOH:O   | 2.00                     | 0.60              |
| 1:C:317:GLY:HA2  | 1:C:324:THR:OG1  | 2.01                     | 0.60              |
| 1:B:144:LEU:HD23 | 1:B:147:MET:CE   | 2.32                     | 0.60              |
| 1:B:545:PHE:HE2  | 1:B:604:MET:HE1  | 1.65                     | 0.60              |
| 1:C:615:MET:HE1  | 1:C:761:ILE:HG12 | 1.83                     | 0.60              |
| 1:D:322:VAL:O    | 1:D:325:ASN:HB2  | 2.01                     | 0.60              |
| 5:A:1108:HOH:O   | 1:B:33:ARG:HD2   | 2.02                     | 0.60              |
| 1:A:173:GLY:CA   | 1:A:624:THR:HG21 | 2.32                     | 0.60              |
| 1:B:615:MET:HE1  | 1:B:761:ILE:HA   | 1.84                     | 0.59              |
| 1:C:739:ARG:HG3  | 1:C:739:ARG:HH11 | 1.67                     | 0.59              |
| 1:A:138:ARG:NH2  | 1:A:490:ARG:HD3  | 2.17                     | 0.59              |
| 1:A:713:MET:HE1  | 1:A:721:LEU:HD22 | 1.84                     | 0.59              |
| 1:D:734:ARG:HD2  | 5:D:1168:HOH:O   | 2.03                     | 0.59              |
| 1:B:320:ASP:HA   | 1:B:324:THR:HA   | 1.84                     | 0.59              |
| 1:B:588:ASN:HD21 | 1:B:744:GLN:NE2  | 2.00                     | 0.59              |
| 1:C:588:ASN:HD21 | 1:C:744:GLN:NE2  | 1.99                     | 0.59              |
| 1:A:198:LEU:HD13 | 1:A:305:GLN:HB2  | 1.82                     | 0.59              |
| 1:A:550:GLU:HG2  | 1:A:554:LYS:HA   | 1.85                     | 0.59              |
| 1:C:33:ARG:HD2   | 5:C:1214:HOH:O   | 2.01                     | 0.59              |
| 1:C:32:ASN:OD1   | 1:D:13:ILE:HA    | 2.02                     | 0.59              |
| 1:C:193:ARG:HB2  | 1:C:225:PRO:HG2  | 1.85                     | 0.59              |
| 1:B:47:THR:HG22  | 1:B:50:ASP:OD2   | 2.03                     | 0.59              |
| 1:B:610:ALA:N    | 5:B:1155:HOH:O   | 2.35                     | 0.59              |
| 1:A:138:ARG:O    | 1:A:138:ARG:HD3  | 2.02                     | 0.59              |
| 1:B:173:GLY:CA   | 1:B:624:THR:HG21 | 2.32                     | 0.59              |
| 1:C:486:ILE:HD11 | 1:C:676:THR:HG23 | 1.85                     | 0.59              |
| 1:B:381:PRO:HG3  | 1:B:467:ILE:HG12 | 1.84                     | 0.58              |
| 1:B:741:ILE:HA   | 1:B:744:GLN:HE21 | 1.68                     | 0.58              |
| 1:C:184:ARG:HD2  | 1:C:185:TYR:CE2  | 2.38                     | 0.58              |
| 1:D:601:ARG:HH22 | 1:D:784:GLN:NE2  | 2.01                     | 0.58              |
| 1:A:480:GLN:HE21 | 1:A:482:LYS:NZ   | 2.01                     | 0.58              |
| 1:B:435:ALA:O    | 1:B:436:VAL:HG12 | 2.04                     | 0.58              |
| 1:A:601:ARG:NH2  | 1:A:784:GLN:NE2  | 2.52                     | 0.58              |
| 1:C:144:LEU:HD12 | 5:C:1130:HOH:O   | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:92:GLY:O     | 1:A:93:ARG:HB2   | 2.04                     | 0.58              |
| 1:B:63:LEU:HD13  | 1:B:229:PRO:HG2  | 1.86                     | 0.58              |
| 1:B:480:GLN:HE21 | 1:B:482:LYS:NZ   | 2.01                     | 0.58              |
| 1:A:21:VAL:O     | 1:A:23:ASN:N     | 2.37                     | 0.58              |
| 1:B:163:PHE:HB2  | 1:B:278:VAL:HG23 | 1.85                     | 0.58              |
| 1:C:323:ARG:HB3  | 1:C:325:ASN:HA   | 1.83                     | 0.58              |
| 1:C:555:VAL:HG21 | 1:C:643:ILE:HG12 | 1.86                     | 0.58              |
| 1:C:610:ALA:N    | 5:C:1153:HOH:O   | 2.36                     | 0.57              |
| 1:D:171:CYS:SG   | 1:D:176:MET:HG3  | 2.44                     | 0.57              |
| 1:D:336:GLN:HE21 | 1:D:825:TRP:HE1  | 1.52                     | 0.57              |
| 1:A:67:TRP:CZ3   | 1:A:229:PRO:HG3  | 2.38                     | 0.57              |
| 1:A:587:TYR:O    | 1:A:591:LYS:HG2  | 2.03                     | 0.57              |
| 1:A:714:ARG:HD3  | 5:A:1185:HOH:O   | 2.04                     | 0.57              |
| 1:D:458:ILE:HG23 | 5:D:1129:HOH:O   | 2.05                     | 0.57              |
| 1:B:254:LEU:HA   | 1:B:259:VAL:HG11 | 1.86                     | 0.57              |
| 1:B:455:VAL:H    | 1:B:459:HIS:HD2  | 1.53                     | 0.57              |
| 1:A:13:ILE:O     | 1:B:43:ARG:HG2   | 2.05                     | 0.57              |
| 1:A:43:ARG:HE    | 1:B:11:LYS:HA    | 1.69                     | 0.57              |
| 1:D:522:LEU:O    | 1:D:525:VAL:HG23 | 2.05                     | 0.57              |
| 1:A:588:ASN:HD21 | 1:A:744:GLN:NE2  | 2.03                     | 0.57              |
| 1:B:601:ARG:HH22 | 1:B:784:GLN:NE2  | 2.03                     | 0.57              |
| 1:B:763:ASN:O    | 1:B:767:HIS:HB2  | 2.05                     | 0.57              |
| 1:C:287:GLU:O    | 1:C:292:ARG:HD3  | 2.05                     | 0.57              |
| 1:C:455:VAL:H    | 1:C:459:HIS:HD2  | 1.52                     | 0.57              |
| 1:B:18:LEU:HD12  | 5:B:1008:HOH:O   | 2.04                     | 0.57              |
| 1:A:430:LEU:HD22 | 1:A:443:HIS:HB3  | 1.87                     | 0.56              |
| 1:C:528:GLU:O    | 1:C:532:ARG:HG2  | 2.05                     | 0.56              |
| 1:A:566:GLN:HE22 | 1:A:576:GLN:HA   | 1.68                     | 0.56              |
| 1:D:143:PHE:O    | 1:D:147:MET:HG3  | 2.04                     | 0.56              |
| 1:B:605:ILE:HG21 | 1:B:623:ILE:HD13 | 1.86                     | 0.56              |
| 1:D:235:ASN:HD22 | 1:D:235:ASN:H    | 1.53                     | 0.56              |
| 1:C:224:MET:HE2  | 1:C:226:TYR:CE1  | 2.40                     | 0.56              |
| 1:D:545:PHE:HE2  | 1:D:604:MET:HE1  | 1.70                     | 0.56              |
| 1:B:129:ALA:HB1  | 1:B:131:LEU:HD22 | 1.87                     | 0.56              |
| 1:D:455:VAL:H    | 1:D:459:HIS:HD2  | 1.51                     | 0.56              |
| 1:B:703:ALA:CA   | 1:B:807:THR:HG21 | 2.35                     | 0.56              |
| 1:A:82:ILE:HB    | 5:A:1142:HOH:O   | 2.06                     | 0.56              |
| 1:B:734:ARG:HD2  | 5:B:1166:HOH:O   | 2.05                     | 0.56              |
| 1:C:224:MET:HB2  | 1:C:247:LYS:NZ   | 2.22                     | 0.55              |
| 1:C:573:TYR:CZ   | 1:C:574:LYS:HE2  | 2.41                     | 0.55              |
| 1:B:525:VAL:O    | 1:B:531:ILE:HD11 | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:601:ARG:HD2  | 5:B:1170:HOH:O   | 2.07                     | 0.55              |
| 1:B:727:ASN:O    | 1:B:730:GLU:HG2  | 2.06                     | 0.55              |
| 1:D:184:ARG:HD2  | 1:D:185:TYR:CE2  | 2.42                     | 0.55              |
| 1:A:795:ARG:O    | 1:A:799:ARG:HG3  | 2.06                     | 0.55              |
| 1:D:157:TYR:CE1  | 1:D:242:ARG:HG2  | 2.42                     | 0.55              |
| 1:B:423:ASP:O    | 1:B:426:ARG:HD3  | 2.07                     | 0.55              |
| 1:D:193:ARG:HB2  | 1:D:225:PRO:HG2  | 1.89                     | 0.55              |
| 1:C:550:GLU:HA   | 1:C:554:LYS:HA   | 1.89                     | 0.54              |
| 1:B:600:PRO:HB3  | 1:B:639:ARG:HA   | 1.89                     | 0.54              |
| 1:D:355:ASP:OD2  | 1:D:398:ARG:HD3  | 2.07                     | 0.54              |
| 1:A:53:PHE:CE1   | 1:A:188:PRO:HD3  | 2.42                     | 0.54              |
| 1:A:227:ASP:OD1  | 1:A:242:ARG:HD3  | 2.08                     | 0.54              |
| 1:C:548:TYR:HD1  | 1:C:551:ARG:NH2  | 2.04                     | 0.54              |
| 1:B:480:GLN:HE21 | 1:B:482:LYS:HZ3  | 1.55                     | 0.54              |
| 1:C:791:TYR:HA   | 1:C:797:TRP:CD1  | 2.42                     | 0.54              |
| 1:A:311:PHE:O    | 1:A:316:PHE:CD1  | 2.61                     | 0.54              |
| 1:B:14:SER:OG    | 1:B:16:ARG:HG3   | 2.08                     | 0.54              |
| 1:C:11:LYS:HA    | 1:D:43:ARG:HE    | 1.72                     | 0.54              |
| 1:D:227:ASP:OD1  | 1:D:242:ARG:HD3  | 2.08                     | 0.54              |
| 1:A:610:ALA:N    | 5:A:1149:HOH:O   | 2.37                     | 0.54              |
| 1:C:391:LEU:O    | 1:C:395:LEU:HD23 | 2.08                     | 0.54              |
| 1:B:395:LEU:HD23 | 1:B:395:LEU:H    | 1.72                     | 0.54              |
| 1:C:727:ASN:O    | 1:C:730:GLU:HG2  | 2.08                     | 0.54              |
| 1:B:336:GLN:NE2  | 1:B:825:TRP:HE1  | 2.06                     | 0.53              |
| 1:D:692:MET:SD   | 1:D:710:ILE:HD12 | 2.48                     | 0.53              |
| 1:D:250:ASN:HD22 | 1:D:269:ARG:HH22 | 1.56                     | 0.53              |
| 1:B:336:GLN:HE21 | 1:B:825:TRP:HE1  | 1.55                     | 0.53              |
| 1:D:21:VAL:HG22  | 1:D:62:HIS:HD2   | 1.73                     | 0.53              |
| 1:D:545:PHE:CE2  | 1:D:604:MET:HE1  | 2.43                     | 0.53              |
| 1:A:717:ASP:HA   | 1:A:720:ARG:HG2  | 1.91                     | 0.53              |
| 1:B:164:GLY:O    | 1:B:279:LEU:HB2  | 2.09                     | 0.53              |
| 1:D:289:LYS:HD3  | 1:D:291:LEU:HB2  | 1.90                     | 0.53              |
| 1:A:719:ASP:O    | 1:A:722:ASP:HB2  | 2.09                     | 0.53              |
| 1:B:168:GLN:NE2  | 1:B:647:ASN:H    | 2.02                     | 0.53              |
| 1:D:641:ARG:HG3  | 5:D:1128:HOH:O   | 2.08                     | 0.53              |
| 1:A:458:ILE:O    | 1:A:462:ILE:HG23 | 2.08                     | 0.53              |
| 1:A:756:ASP:HB2  | 1:A:759:LYS:HG3  | 1.91                     | 0.53              |
| 1:A:778:GLU:O    | 1:A:782:LYS:HG2  | 2.09                     | 0.53              |
| 1:D:562:LEU:HD21 | 1:D:662:LEU:HB2  | 1.91                     | 0.53              |
| 1:D:583:VAL:HG22 | 1:D:603:VAL:HG11 | 1.91                     | 0.53              |
| 1:B:173:GLY:HA2  | 1:B:624:THR:HG21 | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:322:VAL:HG13 | 1:C:325:ASN:CB   | 2.38                     | 0.52              |
| 1:C:82:ILE:HB    | 5:C:1145:HOH:O   | 2.08                     | 0.52              |
| 1:D:133:ASN:OD1  | 1:D:165:ILE:HG21 | 2.08                     | 0.52              |
| 1:A:69:ARG:HE    | 1:A:837:PRO:HB2  | 1.75                     | 0.52              |
| 1:D:280:TYR:HB3  | 1:D:292:ARG:HD2  | 1.90                     | 0.52              |
| 1:D:597:PHE:CE2  | 1:D:792:LYS:HD2  | 2.43                     | 0.52              |
| 1:A:322:VAL:HG13 | 1:A:325:ASN:CG   | 2.35                     | 0.52              |
| 1:C:157:TYR:CE1  | 1:C:242:ARG:HG2  | 2.45                     | 0.52              |
| 1:D:316:PHE:HB3  | 1:D:320:ASP:O    | 2.09                     | 0.52              |
| 1:A:792:LYS:O    | 1:A:794:PRO:HD3  | 2.10                     | 0.52              |
| 1:C:110:GLU:O    | 1:C:113:TYR:HB3  | 2.10                     | 0.52              |
| 1:A:528:GLU:OE2  | 1:A:795:ARG:HD2  | 2.10                     | 0.52              |
| 1:C:322:VAL:O    | 1:C:325:ASN:HB2  | 2.09                     | 0.52              |
| 1:C:525:VAL:O    | 1:C:799:ARG:HD2  | 2.09                     | 0.52              |
| 1:D:480:GLN:HE21 | 1:D:482:LYS:NZ   | 2.08                     | 0.52              |
| 1:D:568:LYS:NZ   | 1:D:665:GLN:HE22 | 2.08                     | 0.52              |
| 1:B:804:ASN:O    | 1:B:807:THR:HG22 | 2.09                     | 0.52              |
| 1:D:144:LEU:HD23 | 1:D:147:MET:CE   | 2.38                     | 0.52              |
| 1:D:803:ARG:HH11 | 1:D:803:ARG:HB2  | 1.74                     | 0.52              |
| 1:B:184:ARG:HD2  | 1:B:185:TYR:CE2  | 2.45                     | 0.52              |
| 1:C:584:ILE:HG21 | 1:C:741:ILE:HG23 | 1.91                     | 0.52              |
| 1:D:386:ARG:HB3  | 1:D:438:ARG:HD3  | 1.91                     | 0.51              |
| 1:D:727:ASN:O    | 1:D:730:GLU:HG2  | 2.10                     | 0.51              |
| 1:B:171:CYS:SG   | 1:B:176:MET:HG3  | 2.50                     | 0.51              |
| 1:C:423:ASP:OD1  | 1:C:426:ARG:HD2  | 2.09                     | 0.51              |
| 1:A:129:ALA:HB1  | 1:A:131:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:396:LEU:HB3  | 1:A:399:HIS:HB2  | 1.91                     | 0.51              |
| 1:A:435:ALA:HB2  | 1:D:174:TRP:CE3  | 2.46                     | 0.51              |
| 1:A:588:ASN:HD21 | 1:A:744:GLN:HE22 | 1.59                     | 0.51              |
| 1:C:463:LEU:HD23 | 1:C:467:ILE:HD12 | 1.91                     | 0.51              |
| 1:C:568:LYS:NZ   | 1:C:665:GLN:HE22 | 2.09                     | 0.51              |
| 1:A:594:PRO:HB3  | 1:A:635:VAL:HG13 | 1.93                     | 0.51              |
| 1:C:268:ASP:HB2  | 5:C:1104:HOH:O   | 2.09                     | 0.51              |
| 1:C:319:ARG:HH21 | 1:C:320:ASP:HA   | 1.76                     | 0.51              |
| 1:D:293:LEU:HD23 | 1:D:395:LEU:HD21 | 1.92                     | 0.51              |
| 1:D:699:MET:HE2  | 1:D:708:PHE:HZ   | 1.76                     | 0.51              |
| 1:C:261:GLY:O    | 1:C:262:TYR:HB2  | 2.11                     | 0.51              |
| 1:D:168:GLN:NE2  | 1:D:647:ASN:H    | 2.08                     | 0.51              |
| 1:C:93:ARG:HG2   | 1:C:126:GLU:HG2  | 1.93                     | 0.51              |
| 1:B:300:VAL:HG13 | 1:B:345:ALA:HA   | 1.92                     | 0.51              |
| 1:C:475:GLU:CD   | 1:C:478:LYS:HE2  | 2.36                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:316:PHE:HA   | 1:D:319:ARG:O    | 2.11                     | 0.51              |
| 1:B:626:ILE:O    | 1:B:630:VAL:HG13 | 2.11                     | 0.50              |
| 1:A:322:VAL:HG22 | 1:A:325:ASN:ND2  | 2.26                     | 0.50              |
| 1:B:566:GLN:HE22 | 1:B:576:GLN:HA   | 1.75                     | 0.50              |
| 1:C:235:ASN:H    | 1:C:235:ASN:ND2  | 2.09                     | 0.50              |
| 1:B:426:ARG:CZ   | 1:C:755:PRO:HD2  | 2.42                     | 0.50              |
| 1:C:421:ASP:OD2  | 1:C:424:ARG:HD2  | 2.11                     | 0.50              |
| 1:B:173:GLY:HA3  | 1:B:624:THR:HG21 | 1.93                     | 0.50              |
| 1:A:138:ARG:HD3  | 1:A:138:ARG:C    | 2.37                     | 0.50              |
| 1:A:522:LEU:O    | 1:A:525:VAL:HG23 | 2.11                     | 0.50              |
| 1:D:130:GLY:O    | 1:D:164:GLY:HA2  | 2.10                     | 0.50              |
| 1:D:446:ILE:O    | 1:D:478:LYS:HE3  | 2.12                     | 0.50              |
| 1:A:166:PHE:CD1  | 1:A:177:GLU:HB3  | 2.47                     | 0.50              |
| 1:A:193:ARG:HB3  | 1:A:196:PHE:CD2  | 2.44                     | 0.50              |
| 1:B:699:MET:HE2  | 1:B:708:PHE:HZ   | 1.77                     | 0.50              |
| 1:B:456:ALA:C    | 1:B:481:ASN:HD21 | 2.19                     | 0.50              |
| 1:C:95:LEU:HD22  | 1:C:99:MET:HE2   | 1.94                     | 0.50              |
| 1:C:571:HIS:ND1  | 1:C:573:TYR:HD1  | 2.09                     | 0.50              |
| 1:B:568:LYS:HZ1  | 1:B:665:GLN:HE22 | 1.58                     | 0.49              |
| 1:B:716:GLU:OE2  | 1:B:720:ARG:HD3  | 2.12                     | 0.49              |
| 1:C:235:ASN:HD22 | 1:C:235:ASN:N    | 2.10                     | 0.49              |
| 1:A:426:ARG:CZ   | 1:D:755:PRO:HD2  | 2.41                     | 0.49              |
| 1:A:426:ARG:CD   | 1:D:755:PRO:HD2  | 2.42                     | 0.49              |
| 1:B:235:ASN:H    | 1:B:235:ASN:ND2  | 2.10                     | 0.49              |
| 1:D:170:ILE:HG12 | 1:D:646:GLU:HG3  | 1.94                     | 0.49              |
| 1:B:548:TYR:HD1  | 1:B:551:ARG:NH2  | 2.08                     | 0.49              |
| 1:C:232:GLY:HA3  | 1:C:235:ASN:HD21 | 1.76                     | 0.49              |
| 1:A:34:HIS:HD2   | 1:A:38:THR:OG1   | 1.94                     | 0.49              |
| 1:B:386:ARG:HB3  | 1:B:438:ARG:HD3  | 1.94                     | 0.49              |
| 1:C:254:LEU:HD11 | 1:C:257:PHE:CZ   | 2.47                     | 0.49              |
| 1:D:752:PRO:O    | 1:D:755:PRO:HD3  | 2.13                     | 0.49              |
| 1:C:144:LEU:HD23 | 1:C:147:MET:HE3  | 1.94                     | 0.49              |
| 1:C:266:VAL:HG11 | 1:D:267:LEU:HD23 | 1.94                     | 0.49              |
| 1:C:57:HIS:HE1   | 5:C:1129:HOH:O   | 1.95                     | 0.49              |
| 1:A:435:ALA:HB2  | 1:D:174:TRP:CZ3  | 2.48                     | 0.49              |
| 1:B:717:ASP:HA   | 1:B:720:ARG:HG2  | 1.95                     | 0.49              |
| 1:C:13:ILE:HA    | 1:D:32:ASN:OD1   | 2.13                     | 0.49              |
| 1:D:70:THR:O     | 1:D:73:HIS:HB3   | 2.13                     | 0.49              |
| 1:A:150:LEU:HB3  | 1:A:829:PRO:HB3  | 1.95                     | 0.49              |
| 1:A:235:ASN:HD22 | 1:A:235:ASN:H    | 1.60                     | 0.49              |
| 1:D:241:MET:HG2  | 1:D:243:LEU:HD13 | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:252:PHE:CE2  | 1:D:269:ARG:HG3  | 2.47                     | 0.49              |
| 1:B:73:HIS:O     | 1:B:77:LYS:HB2   | 2.13                     | 0.49              |
| 1:B:311:PHE:O    | 1:B:316:PHE:HB2  | 2.13                     | 0.49              |
| 1:C:138:ARG:O    | 1:C:138:ARG:HD3  | 2.13                     | 0.49              |
| 1:A:423:ASP:O    | 1:A:426:ARG:HD3  | 2.13                     | 0.48              |
| 1:B:280:TYR:HB3  | 1:B:292:ARG:HD2  | 1.95                     | 0.48              |
| 1:C:250:ASN:ND2  | 1:C:269:ARG:HG2  | 2.28                     | 0.48              |
| 1:C:355:ASP:OD2  | 1:C:398:ARG:HD3  | 2.12                     | 0.48              |
| 1:D:618:MET:O    | 1:D:621:LYS:HB3  | 2.12                     | 0.48              |
| 1:A:171:CYS:SG   | 1:A:176:MET:HG3  | 2.53                     | 0.48              |
| 1:A:280:TYR:HB3  | 1:A:292:ARG:HD2  | 1.95                     | 0.48              |
| 1:A:676:THR:HB   | 5:A:1043:HOH:O   | 2.13                     | 0.48              |
| 1:C:325:ASN:C    | 1:C:327:ASP:N    | 2.70                     | 0.48              |
| 1:B:601:ARG:NH2  | 1:B:784:GLN:NE2  | 2.60                     | 0.48              |
| 1:D:82:ILE:HG12  | 1:D:83:TYR:N     | 2.28                     | 0.48              |
| 1:D:492:LEU:HD22 | 1:D:500:ALA:HB2  | 1.95                     | 0.48              |
| 1:A:528:GLU:O    | 1:A:532:ARG:HG2  | 2.13                     | 0.48              |
| 1:B:57:HIS:HE1   | 5:B:1134:HOH:O   | 1.96                     | 0.48              |
| 1:B:69:ARG:HG2   | 1:B:69:ARG:HH11  | 1.79                     | 0.48              |
| 1:A:548:TYR:HD2  | 1:A:551:ARG:HH21 | 1.62                     | 0.48              |
| 1:C:224:MET:HB2  | 1:C:247:LYS:HZ3  | 1.77                     | 0.48              |
| 1:C:252:PHE:CD2  | 1:C:265:ALA:HB1  | 2.48                     | 0.48              |
| 1:D:322:VAL:HG23 | 1:D:323:ARG:HH11 | 1.76                     | 0.48              |
| 1:D:568:LYS:NZ   | 1:D:665:GLN:NE2  | 2.62                     | 0.48              |
| 1:D:797:TRP:HZ3  | 5:D:1114:HOH:O   | 1.94                     | 0.48              |
| 1:B:53:PHE:CE2   | 1:B:188:PRO:HD3  | 2.49                     | 0.48              |
| 1:B:550:GLU:HA   | 1:B:554:LYS:HA   | 1.96                     | 0.48              |
| 1:B:600:PRO:HA   | 1:B:639:ARG:O    | 2.14                     | 0.48              |
| 1:C:152:LEU:HD22 | 1:C:827:VAL:HG21 | 1.95                     | 0.48              |
| 1:D:60:ARG:O     | 1:D:64:VAL:HG22  | 2.13                     | 0.48              |
| 1:D:235:ASN:OD1  | 1:D:237:VAL:HG13 | 2.14                     | 0.48              |
| 1:A:49:ARG:HA    | 1:A:125:ILE:HG21 | 1.96                     | 0.48              |
| 1:B:56:ALA:O     | 1:B:60:ARG:HB2   | 2.14                     | 0.48              |
| 1:C:18:LEU:HG    | 1:D:33:ARG:NH1   | 2.28                     | 0.48              |
| 1:C:584:ILE:CG2  | 1:C:741:ILE:HD12 | 2.44                     | 0.48              |
| 1:D:251:ASP:HB3  | 1:D:255:LYS:HD3  | 1.96                     | 0.48              |
| 1:A:21:VAL:HG21  | 1:A:66:ARG:HH22  | 1.79                     | 0.47              |
| 1:A:11:LYS:HA    | 1:B:43:ARG:HH21  | 1.79                     | 0.47              |
| 1:B:761:ILE:HG22 | 1:B:765:LEU:HD22 | 1.95                     | 0.47              |
| 1:C:235:ASN:H    | 1:C:235:ASN:HD22 | 1.61                     | 0.47              |
| 1:D:160:ARG:HB2  | 1:D:243:LEU:HB3  | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:168:GLN:HE21 | 1:D:647:ASN:H    | 1.62                     | 0.47              |
| 1:D:338:ASN:O    | 1:D:339:ASP:HB2  | 2.13                     | 0.47              |
| 1:A:32:ASN:HB3   | 1:B:18:LEU:HD11  | 1.95                     | 0.47              |
| 1:A:316:PHE:O    | 1:A:324:THR:HG23 | 2.14                     | 0.47              |
| 1:C:777:TYR:O    | 1:C:781:VAL:HG13 | 2.14                     | 0.47              |
| 1:A:235:ASN:H    | 1:A:235:ASN:ND2  | 2.13                     | 0.47              |
| 1:B:211:GLN:HG2  | 1:B:358:ARG:HD2  | 1.97                     | 0.47              |
| 1:C:583:VAL:HG21 | 1:C:603:VAL:HG21 | 1.96                     | 0.47              |
| 1:A:703:ALA:CA   | 1:A:807:THR:HG21 | 2.41                     | 0.47              |
| 1:B:604:MET:HE2  | 1:B:645:LEU:HD21 | 1.95                     | 0.47              |
| 1:C:442:ALA:O    | 1:C:446:ILE:HG13 | 2.14                     | 0.47              |
| 1:D:241:MET:HE3  | 1:D:243:LEU:HD22 | 1.96                     | 0.47              |
| 1:A:636:VAL:O    | 1:A:639:ARG:HD3  | 2.14                     | 0.47              |
| 1:B:127:GLU:HG3  | 1:B:182:TRP:HA   | 1.97                     | 0.47              |
| 1:D:316:PHE:O    | 1:D:320:ASP:HA   | 2.15                     | 0.47              |
| 1:A:446:ILE:O    | 1:A:478:LYS:HE3  | 2.15                     | 0.47              |
| 1:C:822:ARG:HD3  | 1:C:828:GLU:OE2  | 2.15                     | 0.47              |
| 1:D:557:ILE:N    | 1:D:557:ILE:HD12 | 2.30                     | 0.47              |
| 1:D:604:MET:HA   | 1:D:643:ILE:O    | 2.14                     | 0.47              |
| 1:C:170:ILE:HA   | 1:C:174:TRP:O    | 2.15                     | 0.47              |
| 1:D:486:ILE:HD11 | 1:D:680:LYS:HE3  | 1.96                     | 0.47              |
| 1:A:235:ASN:ND2  | 1:A:237:VAL:H    | 2.13                     | 0.47              |
| 1:A:266:VAL:HG12 | 1:B:266:VAL:HG12 | 1.96                     | 0.47              |
| 1:B:224:MET:HE2  | 1:B:226:TYR:CE1  | 2.50                     | 0.47              |
| 1:B:568:LYS:NZ   | 1:B:665:GLN:HE22 | 2.13                     | 0.47              |
| 1:C:105:GLU:HB3  | 5:C:1090:HOH:O   | 2.14                     | 0.47              |
| 1:B:144:LEU:HD23 | 1:B:147:MET:HE2  | 1.97                     | 0.46              |
| 1:D:803:ARG:HG3  | 5:D:1147:HOH:O   | 2.14                     | 0.46              |
| 1:B:233:TYR:CZ   | 1:B:234:ARG:HD3  | 2.51                     | 0.46              |
| 1:C:20:GLY:O     | 1:C:23:ASN:HB3   | 2.15                     | 0.46              |
| 1:D:803:ARG:NE   | 5:D:1117:HOH:O   | 2.47                     | 0.46              |
| 1:B:292:ARG:O    | 1:B:296:GLU:HG3  | 2.15                     | 0.46              |
| 1:B:480:GLN:NE2  | 1:B:482:LYS:NZ   | 2.64                     | 0.46              |
| 1:C:316:PHE:HE1  | 1:C:332:LYS:NZ   | 2.13                     | 0.46              |
| 1:D:322:VAL:HG13 | 1:D:325:ASN:CB   | 2.31                     | 0.46              |
| 1:A:119:MET:O    | 1:A:123:GLU:HG3  | 2.16                     | 0.46              |
| 1:C:173:GLY:CA   | 1:C:624:THR:HG21 | 2.38                     | 0.46              |
| 1:C:601:ARG:HH22 | 1:C:784:GLN:NE2  | 2.14                     | 0.46              |
| 1:D:253:ASN:O    | 1:D:259:VAL:HG21 | 2.15                     | 0.46              |
| 1:D:193:ARG:HB3  | 1:D:196:PHE:HD2  | 1.80                     | 0.46              |
| 1:C:566:GLN:NE2  | 1:C:576:GLN:HA   | 2.25                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:800:MET:HA   | 1:A:803:ARG:NH1  | 2.31                     | 0.46              |
| 1:B:221:VAL:HG13 | 1:B:272:ALA:HB1  | 1.97                     | 0.46              |
| 1:C:582:HIS:HB2  | 1:C:780:TYR:CE2  | 2.51                     | 0.46              |
| 1:C:803:ARG:HG3  | 5:C:1141:HOH:O   | 2.14                     | 0.46              |
| 1:D:557:ILE:HA   | 5:D:1128:HOH:O   | 2.16                     | 0.46              |
| 1:A:380:ILE:O    | 1:A:382:GLU:N    | 2.49                     | 0.46              |
| 1:C:584:ILE:HG22 | 1:C:741:ILE:HD12 | 1.97                     | 0.46              |
| 1:C:717:ASP:HA   | 1:C:720:ARG:HG2  | 1.98                     | 0.46              |
| 1:D:713:MET:HE1  | 1:D:775:ALA:CB   | 2.46                     | 0.46              |
| 1:B:82:ILE:HB    | 5:B:1148:HOH:O   | 2.15                     | 0.45              |
| 1:C:316:PHE:C    | 1:C:324:THR:HG23 | 2.41                     | 0.45              |
| 1:A:221:VAL:HG13 | 1:A:272:ALA:HB1  | 1.98                     | 0.45              |
| 1:C:699:MET:HE2  | 1:C:708:PHE:HZ   | 1.80                     | 0.45              |
| 1:D:47:THR:HG22  | 1:D:50:ASP:OD2   | 2.17                     | 0.45              |
| 1:C:43:ARG:HE    | 1:D:11:LYS:HG3   | 1.81                     | 0.45              |
| 1:A:506:ARG:HB3  | 1:A:524:TYR:CZ   | 2.52                     | 0.45              |
| 1:B:18:LEU:HA    | 5:B:1008:HOH:O   | 2.16                     | 0.45              |
| 1:C:336:GLN:HE22 | 1:C:373:ALA:HB3  | 1.80                     | 0.45              |
| 1:C:525:VAL:O    | 1:C:531:ILE:HD11 | 2.16                     | 0.45              |
| 1:C:726:TYR:OH   | 1:C:774:PHE:HB2  | 2.17                     | 0.45              |
| 1:D:99:MET:HE1   | 1:D:119:MET:SD   | 2.56                     | 0.45              |
| 1:A:480:GLN:NE2  | 1:A:482:LYS:NZ   | 2.63                     | 0.45              |
| 1:C:262:TYR:HB3  | 1:C:264:GLN:OE1  | 2.17                     | 0.45              |
| 1:D:343:SER:HB3  | 1:D:445:CYS:SG   | 2.56                     | 0.45              |
| 1:C:67:TRP:CZ3   | 1:C:229:PRO:HG3  | 2.50                     | 0.45              |
| 1:C:91:MET:HE1   | 5:C:1130:HOH:O   | 2.15                     | 0.45              |
| 1:C:479:PHE:CD1  | 1:C:479:PHE:N    | 2.83                     | 0.45              |
| 1:C:522:LEU:O    | 1:C:525:VAL:HG23 | 2.16                     | 0.45              |
| 1:C:548:TYR:HD1  | 1:C:551:ARG:HH21 | 1.63                     | 0.45              |
| 1:A:80:LYS:HE2   | 1:A:825:TRP:O    | 2.17                     | 0.45              |
| 1:A:174:TRP:CH2  | 1:D:435:ALA:HB2  | 2.51                     | 0.45              |
| 1:B:479:PHE:CD1  | 1:B:479:PHE:N    | 2.85                     | 0.45              |
| 1:B:724:ARG:O    | 1:C:729:GLN:HG2  | 2.17                     | 0.45              |
| 1:C:67:TRP:O     | 1:C:71:GLN:HG2   | 2.17                     | 0.45              |
| 1:C:69:ARG:HD2   | 1:C:836:ALA:HA   | 1.99                     | 0.45              |
| 1:C:568:LYS:HZ3  | 1:C:665:GLN:HE22 | 1.65                     | 0.45              |
| 1:C:817:ILE:HD13 | 1:C:817:ILE:HA   | 1.74                     | 0.45              |
| 1:D:795:ARG:O    | 1:D:799:ARG:HG3  | 2.16                     | 0.45              |
| 1:A:319:ARG:HE   | 1:A:320:ASP:HA   | 1.80                     | 0.45              |
| 1:A:784:GLN:HE21 | 1:A:784:GLN:HA   | 1.82                     | 0.45              |
| 1:D:736:PRO:HG3  | 1:D:739:ARG:NH2  | 2.31                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:53:PHE:HE1   | 1:A:188:PRO:HD3  | 1.80                     | 0.45              |
| 1:A:355:ASP:OD2  | 1:A:398:ARG:HD3  | 2.16                     | 0.45              |
| 1:A:361:TRP:CH2  | 1:A:409:ARG:HD2  | 2.51                     | 0.45              |
| 1:A:740:GLN:O    | 1:A:744:GLN:HG3  | 2.16                     | 0.45              |
| 1:B:516:ASP:O    | 1:B:519:ARG:HB2  | 2.17                     | 0.45              |
| 1:C:592:LYS:HG2  | 1:C:593:GLU:HG3  | 1.98                     | 0.45              |
| 1:C:797:TRP:HZ3  | 5:C:1105:HOH:O   | 1.98                     | 0.45              |
| 1:D:423:ASP:OD1  | 1:D:426:ARG:HD2  | 2.16                     | 0.45              |
| 1:A:426:ARG:HD2  | 1:D:755:PRO:HD2  | 1.98                     | 0.45              |
| 1:D:379:VAL:HG11 | 1:D:671:THR:HA   | 1.98                     | 0.45              |
| 1:A:475:GLU:OE1  | 1:A:478:LYS:HE2  | 2.18                     | 0.44              |
| 1:B:252:PHE:HE1  | 1:B:269:ARG:HG2  | 1.82                     | 0.44              |
| 1:B:269:ARG:O    | 1:B:273:GLU:HG3  | 2.17                     | 0.44              |
| 1:B:365:TRP:O    | 1:B:369:VAL:HG13 | 2.18                     | 0.44              |
| 1:C:475:GLU:OE1  | 1:C:478:LYS:HE2  | 2.17                     | 0.44              |
| 1:C:815:ARG:O    | 1:C:819:GLN:HG3  | 2.17                     | 0.44              |
| 1:D:34:HIS:HD2   | 1:D:38:THR:OG1   | 1.99                     | 0.44              |
| 1:A:472:TYR:O    | 1:A:476:PRO:HG3  | 2.17                     | 0.44              |
| 1:B:322:VAL:HG23 | 1:B:323:ARG:NH2  | 2.32                     | 0.44              |
| 1:C:338:ASN:O    | 1:C:339:ASP:HB2  | 2.18                     | 0.44              |
| 1:B:91:MET:SD    | 5:B:1135:HOH:O   | 2.60                     | 0.44              |
| 1:B:518:LEU:O    | 1:B:521:LEU:HB2  | 2.17                     | 0.44              |
| 1:C:70:THR:O     | 1:C:73:HIS:HB3   | 2.17                     | 0.44              |
| 1:C:480:GLN:NE2  | 1:C:482:LYS:NZ   | 2.65                     | 0.44              |
| 1:C:549:LEU:O    | 1:C:550:GLU:HG3  | 2.17                     | 0.44              |
| 1:A:626:ILE:O    | 1:A:630:VAL:HG13 | 2.18                     | 0.44              |
| 1:A:566:GLN:O    | 1:A:605:ILE:HA   | 2.17                     | 0.44              |
| 1:C:166:PHE:CG   | 1:C:177:GLU:HB2  | 2.52                     | 0.44              |
| 1:A:399:HIS:HD2  | 5:A:1129:HOH:O   | 2.00                     | 0.44              |
| 1:D:34:HIS:HE1   | 1:D:61:ASP:OD2   | 1.99                     | 0.44              |
| 1:A:548:TYR:HD2  | 1:A:551:ARG:NH2  | 2.16                     | 0.44              |
| 1:D:332:LYS:HA   | 1:D:332:LYS:HD3  | 1.69                     | 0.44              |
| 1:A:662:LEU:HD22 | 1:A:689:ILE:HG22 | 1.99                     | 0.44              |
| 1:B:335:ILE:HG22 | 1:B:337:LEU:HD13 | 1.99                     | 0.44              |
| 1:D:504:ALA:HA   | 1:D:508:GLY:O    | 2.18                     | 0.44              |
| 1:A:319:ARG:HH21 | 1:A:320:ASP:HA   | 1.83                     | 0.43              |
| 1:B:382:GLU:HA   | 1:B:386:ARG:HH12 | 1.83                     | 0.43              |
| 1:C:82:ILE:HD12  | 1:C:147:MET:SD   | 2.58                     | 0.43              |
| 1:C:380:ILE:HD12 | 1:C:380:ILE:HA   | 1.73                     | 0.43              |
| 1:C:739:ARG:HH11 | 1:C:739:ARG:CG   | 2.31                     | 0.43              |
| 1:C:741:ILE:O    | 1:C:744:GLN:HB2  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:741:ILE:HA   | 1:C:744:GLN:HE21 | 1.82                     | 0.43              |
| 1:B:16:ARG:NH2   | 1:B:18:LEU:HD13  | 2.34                     | 0.43              |
| 1:B:343:SER:HB3  | 1:B:445:CYS:SG   | 2.57                     | 0.43              |
| 1:C:49:ARG:O     | 1:C:53:PHE:HD1   | 2.00                     | 0.43              |
| 1:C:499:LEU:O    | 1:C:503:ILE:HG13 | 2.18                     | 0.43              |
| 1:D:456:ALA:C    | 1:D:481:ASN:HD21 | 2.26                     | 0.43              |
| 1:A:341:HIS:HB2  | 1:A:342:PRO:HD3  | 2.01                     | 0.43              |
| 1:B:399:HIS:HD2  | 5:B:1136:HOH:O   | 2.00                     | 0.43              |
| 1:D:269:ARG:O    | 1:D:273:GLU:HG3  | 2.18                     | 0.43              |
| 1:A:89:PHE:O     | 1:A:131:LEU:HB3  | 2.19                     | 0.43              |
| 1:B:395:LEU:HD23 | 1:B:395:LEU:N    | 2.33                     | 0.43              |
| 1:C:456:ALA:C    | 1:C:481:ASN:HD21 | 2.27                     | 0.43              |
| 1:C:676:THR:HB   | 5:C:1044:HOH:O   | 2.18                     | 0.43              |
| 1:D:196:PHE:HB3  | 5:D:1183:HOH:O   | 2.17                     | 0.43              |
| 1:D:790:LEU:HG   | 1:D:797:TRP:CD1  | 2.53                     | 0.43              |
| 1:D:268:ASP:HB2  | 5:D:1113:HOH:O   | 2.18                     | 0.43              |
| 1:A:386:ARG:HH21 | 1:A:440:ASN:ND2  | 2.17                     | 0.43              |
| 1:A:732:TYR:O    | 1:A:739:ARG:NH1  | 2.52                     | 0.43              |
| 1:C:399:HIS:HD2  | 5:C:1131:HOH:O   | 2.02                     | 0.43              |
| 1:D:469:LYS:HE2  | 1:D:469:LYS:HB2  | 1.86                     | 0.43              |
| 1:D:703:ALA:CA   | 1:D:807:THR:HG21 | 2.43                     | 0.43              |
| 1:D:736:PRO:O    | 1:D:739:ARG:HB3  | 2.19                     | 0.43              |
| 1:A:596:LYS:HD3  | 1:A:597:PHE:H    | 1.84                     | 0.43              |
| 1:B:489:ARG:HB3  | 5:B:1154:HOH:O   | 2.19                     | 0.43              |
| 1:B:562:LEU:HD21 | 1:B:662:LEU:HB2  | 2.00                     | 0.43              |
| 1:B:604:MET:HA   | 1:B:643:ILE:O    | 2.18                     | 0.43              |
| 1:D:21:VAL:HG22  | 1:D:62:HIS:CD2   | 2.53                     | 0.43              |
| 1:B:174:TRP:HH2  | 1:B:757:LEU:HD11 | 1.84                     | 0.43              |
| 1:C:233:TYR:CE1  | 1:C:234:ARG:HD3  | 2.54                     | 0.43              |
| 1:C:269:ARG:O    | 1:C:273:GLU:HG3  | 2.18                     | 0.43              |
| 1:C:536:LYS:HA   | 1:C:536:LYS:HD2  | 1.86                     | 0.43              |
| 1:D:34:HIS:CD2   | 1:D:38:THR:OG1   | 2.72                     | 0.43              |
| 1:D:225:PRO:CB   | 1:D:242:ARG:HD2  | 2.39                     | 0.43              |
| 1:A:421:ASP:O    | 1:A:424:ARG:HB3  | 2.19                     | 0.43              |
| 1:C:713:MET:HB3  | 5:C:1148:HOH:O   | 2.18                     | 0.43              |
| 1:A:442:ALA:O    | 1:A:446:ILE:HG13 | 2.19                     | 0.42              |
| 1:B:99:MET:HE1   | 1:B:119:MET:SD   | 2.58                     | 0.42              |
| 1:B:174:TRP:CH2  | 1:B:757:LEU:HD11 | 2.54                     | 0.42              |
| 1:B:557:ILE:N    | 1:B:557:ILE:HD12 | 2.34                     | 0.42              |
| 1:C:43:ARG:HG3   | 1:C:43:ARG:HH11  | 1.83                     | 0.42              |
| 1:C:129:ALA:HB1  | 1:C:131:LEU:HD22 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:168:GLN:HE21 | 1:C:647:ASN:N    | 2.14                     | 0.42              |
| 1:C:651:SER:HB3  | 5:C:1026:HOH:O   | 2.18                     | 0.42              |
| 1:C:703:ALA:CA   | 1:C:807:THR:HG21 | 2.47                     | 0.42              |
| 1:D:565:VAL:HG22 | 1:D:681:PHE:CZ   | 2.53                     | 0.42              |
| 1:A:815:ARG:O    | 1:A:819:GLN:HG3  | 2.18                     | 0.42              |
| 1:B:190:GLU:HA   | 1:B:227:ASP:O    | 2.19                     | 0.42              |
| 1:C:135:GLY:HA3  | 2:C:997:PO4:O3   | 2.19                     | 0.42              |
| 1:D:316:PHE:HA   | 1:D:319:ARG:C    | 2.44                     | 0.42              |
| 1:D:322:VAL:CB   | 1:D:325:ASN:HB3  | 2.48                     | 0.42              |
| 1:D:548:TYR:C    | 1:D:550:GLU:H    | 2.27                     | 0.42              |
| 1:D:698:GLU:O    | 1:D:702:GLU:HG2  | 2.18                     | 0.42              |
| 1:A:601:ARG:HD2  | 5:A:1166:HOH:O   | 2.19                     | 0.42              |
| 1:D:289:LYS:HG2  | 1:D:291:LEU:N    | 2.31                     | 0.42              |
| 1:D:432:GLU:O    | 1:D:437:LYS:HA   | 2.19                     | 0.42              |
| 1:B:329:PHE:HB3  | 1:B:330:PRO:HD3  | 2.01                     | 0.42              |
| 1:C:450:HIS:HE1  | 1:C:824:ILE:O    | 2.03                     | 0.42              |
| 1:D:480:GLN:HE21 | 1:D:482:LYS:HZ3  | 1.66                     | 0.42              |
| 1:D:761:ILE:HG22 | 1:D:765:LEU:HD22 | 2.01                     | 0.42              |
| 1:B:166:PHE:HB2  | 1:B:178:GLU:O    | 2.19                     | 0.42              |
| 1:D:519:ARG:O    | 1:D:522:LEU:HB2  | 2.19                     | 0.42              |
| 1:D:754:GLN:O    | 1:D:756:ASP:N    | 2.52                     | 0.42              |
| 1:B:181:ASP:O    | 1:B:184:ARG:HB2  | 2.20                     | 0.42              |
| 1:C:320:ASP:CB   | 1:C:324:THR:H    | 2.33                     | 0.42              |
| 1:D:459:HIS:HB2  | 1:D:673:ALA:O    | 2.19                     | 0.42              |
| 1:D:569:ARG:O    | 1:D:574:LYS:HD2  | 2.20                     | 0.42              |
| 1:D:676:THR:HB   | 5:D:1053:HOH:O   | 2.20                     | 0.42              |
| 1:B:233:TYR:CE1  | 1:B:234:ARG:HD3  | 2.55                     | 0.42              |
| 1:B:785:GLU:HG3  | 5:B:1130:HOH:O   | 2.19                     | 0.42              |
| 1:C:319:ARG:O    | 1:C:324:THR:HA   | 2.20                     | 0.42              |
| 1:C:756:ASP:O    | 1:C:759:LYS:HB2  | 2.19                     | 0.42              |
| 1:A:42:ASP:H     | 1:A:45:VAL:HG12  | 1.85                     | 0.42              |
| 1:A:168:GLN:HE21 | 1:A:647:ASN:N    | 2.14                     | 0.42              |
| 1:A:713:MET:HG2  | 1:A:717:ASP:HB2  | 2.01                     | 0.42              |
| 1:B:30:ASN:HB3   | 5:B:1003:HOH:O   | 2.19                     | 0.42              |
| 1:D:102:LEU:HD23 | 1:D:104:LEU:HD22 | 2.02                     | 0.42              |
| 1:D:585:THR:O    | 1:D:589:ARG:HD3  | 2.20                     | 0.42              |
| 1:B:251:ASP:HB2  | 1:B:255:LYS:HG3  | 2.02                     | 0.42              |
| 1:C:432:GLU:O    | 1:C:437:LYS:HA   | 2.19                     | 0.42              |
| 1:C:446:ILE:O    | 1:C:478:LYS:HE3  | 2.20                     | 0.42              |
| 1:D:161:TYR:HA   | 1:D:276:SER:O    | 2.20                     | 0.42              |
| 1:D:758:PHE:O    | 1:D:762:VAL:HG23 | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:196:PHE:HB3  | 5:B:1182:HOH:O   | 2.20                     | 0.41              |
| 1:A:739:ARG:HG3  | 1:A:739:ARG:HH11 | 1.85                     | 0.41              |
| 1:B:413:ARG:O    | 1:B:416:ALA:HB3  | 2.20                     | 0.41              |
| 1:B:418:PHE:CG   | 1:B:424:ARG:HD3  | 2.55                     | 0.41              |
| 1:B:612:GLY:H    | 1:B:617:LYS:HE3  | 1.85                     | 0.41              |
| 1:C:784:GLN:O    | 1:C:787:VAL:HB   | 2.20                     | 0.41              |
| 1:A:138:ARG:NH1  | 1:A:142:CYS:SG   | 2.81                     | 0.41              |
| 1:B:525:VAL:O    | 1:B:799:ARG:HD2  | 2.21                     | 0.41              |
| 1:C:228:THR:HA   | 1:C:229:PRO:HD3  | 1.85                     | 0.41              |
| 1:C:758:PHE:CD1  | 1:C:761:ILE:HD12 | 2.55                     | 0.41              |
| 1:D:793:ASN:HD21 | 1:D:796:GLU:HG2  | 1.85                     | 0.41              |
| 1:A:738:LEU:HD12 | 1:A:738:LEU:HA   | 1.81                     | 0.41              |
| 1:B:386:ARG:HA   | 1:B:439:ILE:O    | 2.19                     | 0.41              |
| 1:C:550:GLU:CG   | 1:C:554:LYS:HA   | 2.50                     | 0.41              |
| 1:A:433:GLU:HB2  | 1:D:754:GLN:HG2  | 2.02                     | 0.41              |
| 1:B:105:GLU:O    | 1:B:109:ASP:HB2  | 2.21                     | 0.41              |
| 1:B:162:GLU:HG2  | 1:B:183:LEU:HD12 | 2.02                     | 0.41              |
| 1:C:380:ILE:HG13 | 1:C:382:GLU:OE1  | 2.21                     | 0.41              |
| 1:C:709:PHE:HB3  | 1:C:783:CYS:SG   | 2.60                     | 0.41              |
| 1:D:386:ARG:HA   | 1:D:439:ILE:O    | 2.20                     | 0.41              |
| 1:D:790:LEU:HG   | 1:D:797:TRP:HD1  | 1.84                     | 0.41              |
| 1:A:225:PRO:HB3  | 1:A:244:TRP:CZ3  | 2.56                     | 0.41              |
| 1:B:15:VAL:O     | 1:B:18:LEU:HD22  | 2.20                     | 0.41              |
| 1:B:288:GLY:HA2  | 1:B:387:TRP:CH2  | 2.56                     | 0.41              |
| 1:B:522:LEU:O    | 1:B:525:VAL:HG23 | 2.20                     | 0.41              |
| 1:C:734:ARG:HD2  | 5:C:1165:HOH:O   | 2.20                     | 0.41              |
| 1:C:761:ILE:O    | 1:C:765:LEU:HB2  | 2.21                     | 0.41              |
| 1:A:556:HIS:C    | 1:A:557:ILE:HD12 | 2.45                     | 0.41              |
| 1:B:570:ILE:HB   | 1:B:609:PRO:HA   | 2.03                     | 0.41              |
| 1:C:594:PRO:HB3  | 1:C:635:VAL:CG1  | 2.51                     | 0.41              |
| 1:C:818:ALA:O    | 1:C:822:ARG:HG3  | 2.21                     | 0.41              |
| 1:D:604:MET:HE2  | 1:D:645:LEU:HD21 | 2.03                     | 0.41              |
| 1:A:72:GLN:O     | 1:A:75:TYR:HB3   | 2.21                     | 0.41              |
| 1:B:458:ILE:O    | 1:B:462:ILE:HG23 | 2.21                     | 0.41              |
| 1:C:37:PHE:CZ    | 1:D:18:LEU:HB3   | 2.56                     | 0.41              |
| 1:C:636:VAL:O    | 1:C:639:ARG:HD3  | 2.21                     | 0.41              |
| 1:D:738:LEU:O    | 1:D:742:ILE:HG12 | 2.21                     | 0.41              |
| 1:A:157:TYR:CE1  | 1:A:242:ARG:HG2  | 2.56                     | 0.41              |
| 1:A:206:VAL:CG1  | 1:A:213:ALA:HB1  | 2.51                     | 0.41              |
| 1:A:596:LYS:HD3  | 1:A:597:PHE:N    | 2.36                     | 0.41              |
| 1:B:522:LEU:HD13 | 1:B:806:ALA:HB3  | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:554:LYS:O    | 1:B:555:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:568:LYS:NZ   | 1:B:665:GLN:NE2  | 2.69                     | 0.41              |
| 1:C:85:LEU:HD23  | 1:C:157:TYR:HB2  | 2.03                     | 0.41              |
| 1:C:235:ASN:ND2  | 1:C:235:ASN:N    | 2.69                     | 0.41              |
| 1:D:49:ARG:O     | 1:D:53:PHE:HD1   | 2.03                     | 0.41              |
| 1:D:287:GLU:H    | 1:D:292:ARG:CD   | 2.34                     | 0.41              |
| 1:B:467:ILE:H    | 1:B:467:ILE:HG13 | 1.57                     | 0.41              |
| 1:B:803:ARG:HG3  | 5:B:1145:HOH:O   | 2.20                     | 0.41              |
| 1:C:63:LEU:HG    | 1:C:98:THR:HG23  | 2.03                     | 0.41              |
| 1:A:322:VAL:HG13 | 1:A:325:ASN:CB   | 2.51                     | 0.40              |
| 1:C:481:ASN:O    | 1:C:482:LYS:HG2  | 2.21                     | 0.40              |
| 1:A:399:HIS:CD2  | 5:A:1129:HOH:O   | 2.73                     | 0.40              |
| 1:A:803:ARG:O    | 1:A:807:THR:HB   | 2.20                     | 0.40              |
| 1:A:822:ARG:HH11 | 1:A:828:GLU:CD   | 2.29                     | 0.40              |
| 1:B:312:LYS:O    | 1:B:317:GLY:N    | 2.55                     | 0.40              |
| 1:B:548:TYR:CD1  | 1:B:551:ARG:NH2  | 2.88                     | 0.40              |
| 1:B:815:ARG:O    | 1:B:819:GLN:HG3  | 2.21                     | 0.40              |
| 1:C:36:HIS:O     | 1:C:40:VAL:HA    | 2.21                     | 0.40              |
| 1:C:224:MET:HE2  | 1:C:226:TYR:CZ   | 2.56                     | 0.40              |
| 1:A:249:PRO:O    | 1:A:252:PHE:CE2  | 2.74                     | 0.40              |
| 1:B:139:LEU:HD11 | 1:B:143:PHE:CE1  | 2.57                     | 0.40              |
| 1:C:319:ARG:NH2  | 1:C:322:VAL:O    | 2.54                     | 0.40              |
| 1:D:49:ARG:HA    | 1:D:125:ILE:HG21 | 2.02                     | 0.40              |
| 1:B:446:ILE:O    | 1:B:478:LYS:HE3  | 2.21                     | 0.40              |
| 1:C:615:MET:HE1  | 1:C:761:ILE:HA   | 2.04                     | 0.40              |
| 1:C:623:ILE:H    | 1:C:623:ILE:HG13 | 1.76                     | 0.40              |
| 1:D:713:MET:HB2  | 1:D:713:MET:HE3  | 1.87                     | 0.40              |
| 1:D:287:GLU:H    | 1:D:292:ARG:HD3  | 1.87                     | 0.40              |

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

| Atom-1          | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 5:A:1030:HOH:O  | 5:D:1049:HOH:O[2_646] | 1.46                     | 0.74              |
| 1:B:550:GLU:OE2 | 5:C:1030:HOH:O[2_746] | 2.04                     | 0.16              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|----------|----------|-------------|---|
| 1   | A     | 822/842 (98%)   | 741 (90%)  | 52 (6%)  | 29 (4%)  | 3           | 4 |
| 1   | B     | 822/842 (98%)   | 743 (90%)  | 59 (7%)  | 20 (2%)  | 4           | 8 |
| 1   | C     | 822/842 (98%)   | 751 (91%)  | 46 (6%)  | 25 (3%)  | 3           | 5 |
| 1   | D     | 822/842 (98%)   | 746 (91%)  | 51 (6%)  | 25 (3%)  | 3           | 5 |
| All | All   | 3288/3368 (98%) | 2981 (91%) | 208 (6%) | 99 (3%)  | 3           | 5 |

All (99) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 16  | ARG  |
| 1   | A     | 19  | ALA  |
| 1   | A     | 22  | GLU  |
| 1   | A     | 166 | PHE  |
| 1   | A     | 253 | ASN  |
| 1   | A     | 281 | PRO  |
| 1   | A     | 321 | PRO  |
| 1   | A     | 323 | ARG  |
| 1   | A     | 381 | PRO  |
| 1   | A     | 555 | VAL  |
| 1   | A     | 610 | ALA  |
| 1   | A     | 837 | PRO  |
| 1   | B     | 16  | ARG  |
| 1   | B     | 166 | PHE  |
| 1   | B     | 256 | ASP  |
| 1   | B     | 257 | PHE  |
| 1   | B     | 261 | GLY  |
| 1   | B     | 281 | PRO  |
| 1   | B     | 321 | PRO  |
| 1   | B     | 380 | ILE  |
| 1   | B     | 555 | VAL  |
| 1   | B     | 556 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 609 | PRO  |
| 1   | B     | 610 | ALA  |
| 1   | C     | 16  | ARG  |
| 1   | C     | 166 | PHE  |
| 1   | C     | 234 | ARG  |
| 1   | C     | 254 | LEU  |
| 1   | C     | 262 | TYR  |
| 1   | C     | 264 | GLN  |
| 1   | C     | 281 | PRO  |
| 1   | C     | 315 | LYS  |
| 1   | C     | 323 | ARG  |
| 1   | C     | 555 | VAL  |
| 1   | C     | 556 | HIS  |
| 1   | C     | 609 | PRO  |
| 1   | C     | 610 | ALA  |
| 1   | D     | 16  | ARG  |
| 1   | D     | 166 | PHE  |
| 1   | D     | 256 | ASP  |
| 1   | D     | 257 | PHE  |
| 1   | D     | 321 | PRO  |
| 1   | D     | 324 | THR  |
| 1   | D     | 555 | VAL  |
| 1   | D     | 556 | HIS  |
| 1   | D     | 609 | PRO  |
| 1   | D     | 610 | ALA  |
| 1   | A     | 21  | VAL  |
| 1   | A     | 287 | GLU  |
| 1   | A     | 436 | VAL  |
| 1   | A     | 556 | HIS  |
| 1   | A     | 609 | PRO  |
| 1   | B     | 92  | GLY  |
| 1   | B     | 258 | ASN  |
| 1   | B     | 436 | VAL  |
| 1   | C     | 17  | GLY  |
| 1   | C     | 22  | GLU  |
| 1   | C     | 250 | ASN  |
| 1   | C     | 256 | ASP  |
| 1   | D     | 264 | GLN  |
| 1   | D     | 755 | PRO  |
| 1   | D     | 836 | ALA  |
| 1   | A     | 17  | GLY  |
| 1   | A     | 165 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 256 | ASP  |
| 1   | A     | 264 | GLN  |
| 1   | A     | 835 | PRO  |
| 1   | B     | 22  | GLU  |
| 1   | B     | 253 | ASN  |
| 1   | B     | 314 | SER  |
| 1   | C     | 317 | GLY  |
| 1   | C     | 436 | VAL  |
| 1   | D     | 21  | VAL  |
| 1   | D     | 92  | GLY  |
| 1   | D     | 93  | ARG  |
| 1   | D     | 254 | LEU  |
| 1   | D     | 436 | VAL  |
| 1   | D     | 549 | LEU  |
| 1   | A     | 78  | ASP  |
| 1   | A     | 251 | ASP  |
| 1   | A     | 320 | ASP  |
| 1   | A     | 324 | THR  |
| 1   | A     | 836 | ALA  |
| 1   | B     | 209 | THR  |
| 1   | C     | 21  | VAL  |
| 1   | C     | 263 | ILE  |
| 1   | D     | 255 | LYS  |
| 1   | D     | 262 | TYR  |
| 1   | A     | 676 | THR  |
| 1   | D     | 281 | PRO  |
| 1   | D     | 315 | LYS  |
| 1   | B     | 381 | PRO  |
| 1   | C     | 339 | ASP  |
| 1   | D     | 249 | PRO  |
| 1   | D     | 837 | PRO  |
| 1   | C     | 594 | PRO  |
| 1   | A     | 92  | GLY  |
| 1   | C     | 92  | GLY  |
| 1   | C     | 836 | ALA  |

### 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     | 712/732 (97%)   | 590 (83%)  | 122 (17%) | 2           | 4 |
| 1   | B     | 712/732 (97%)   | 613 (86%)  | 99 (14%)  | 3           | 7 |
| 1   | C     | 712/732 (97%)   | 607 (85%)  | 105 (15%) | 3           | 6 |
| 1   | D     | 712/732 (97%)   | 594 (83%)  | 118 (17%) | 2           | 4 |
| All | All   | 2848/2928 (97%) | 2404 (84%) | 444 (16%) | 2           | 5 |

All (444) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | ARG  |
| 1   | A     | 14  | SER  |
| 1   | A     | 15  | VAL  |
| 1   | A     | 39  | LEU  |
| 1   | A     | 43  | ARG  |
| 1   | A     | 45  | VAL  |
| 1   | A     | 47  | THR  |
| 1   | A     | 48  | PRO  |
| 1   | A     | 63  | LEU  |
| 1   | A     | 76  | GLU  |
| 1   | A     | 78  | ASP  |
| 1   | A     | 79  | PRO  |
| 1   | A     | 82  | ILE  |
| 1   | A     | 85  | LEU  |
| 1   | A     | 90  | TYR  |
| 1   | A     | 95  | LEU  |
| 1   | A     | 100 | VAL  |
| 1   | A     | 104 | LEU  |
| 1   | A     | 125 | ILE  |
| 1   | A     | 131 | LEU  |
| 1   | A     | 136 | LEU  |
| 1   | A     | 138 | ARG  |
| 1   | A     | 162 | GLU  |
| 1   | A     | 165 | ILE  |
| 1   | A     | 169 | LYS  |
| 1   | A     | 177 | GLU  |
| 1   | A     | 191 | LYS  |
| 1   | A     | 214 | LYS  |
| 1   | A     | 230 | VAL  |
| 1   | A     | 231 | PRO  |
| 1   | A     | 234 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 235 | ASN  |
| 1   | A     | 237 | VAL  |
| 1   | A     | 242 | ARG  |
| 1   | A     | 243 | LEU  |
| 1   | A     | 251 | ASP  |
| 1   | A     | 255 | LYS  |
| 1   | A     | 257 | PHE  |
| 1   | A     | 258 | ASN  |
| 1   | A     | 274 | ASN  |
| 1   | A     | 278 | VAL  |
| 1   | A     | 279 | LEU  |
| 1   | A     | 281 | PRO  |
| 1   | A     | 287 | GLU  |
| 1   | A     | 289 | LYS  |
| 1   | A     | 291 | LEU  |
| 1   | A     | 306 | ASP  |
| 1   | A     | 319 | ARG  |
| 1   | A     | 321 | PRO  |
| 1   | A     | 322 | VAL  |
| 1   | A     | 325 | ASN  |
| 1   | A     | 327 | ASP  |
| 1   | A     | 337 | LEU  |
| 1   | A     | 356 | LEU  |
| 1   | A     | 360 | ASP  |
| 1   | A     | 366 | GLU  |
| 1   | A     | 369 | VAL  |
| 1   | A     | 378 | THR  |
| 1   | A     | 379 | VAL  |
| 1   | A     | 381 | PRO  |
| 1   | A     | 382 | GLU  |
| 1   | A     | 391 | LEU  |
| 1   | A     | 392 | LEU  |
| 1   | A     | 394 | THR  |
| 1   | A     | 395 | LEU  |
| 1   | A     | 396 | LEU  |
| 1   | A     | 398 | ARG  |
| 1   | A     | 400 | LEU  |
| 1   | A     | 405 | GLU  |
| 1   | A     | 422 | VAL  |
| 1   | A     | 426 | ARG  |
| 1   | A     | 430 | LEU  |
| 1   | A     | 431 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 436 | VAL  |
| 1   | A     | 444 | LEU  |
| 1   | A     | 455 | VAL  |
| 1   | A     | 467 | ILE  |
| 1   | A     | 474 | LEU  |
| 1   | A     | 486 | ILE  |
| 1   | A     | 492 | LEU  |
| 1   | A     | 494 | LEU  |
| 1   | A     | 506 | ARG  |
| 1   | A     | 513 | SER  |
| 1   | A     | 522 | LEU  |
| 1   | A     | 543 | LEU  |
| 1   | A     | 554 | LYS  |
| 1   | A     | 557 | ILE  |
| 1   | A     | 565 | VAL  |
| 1   | A     | 568 | LYS  |
| 1   | A     | 576 | GLN  |
| 1   | A     | 586 | LEU  |
| 1   | A     | 589 | ARG  |
| 1   | A     | 598 | VAL  |
| 1   | A     | 603 | VAL  |
| 1   | A     | 622 | LEU  |
| 1   | A     | 630 | VAL  |
| 1   | A     | 640 | LEU  |
| 1   | A     | 649 | ARG  |
| 1   | A     | 652 | LEU  |
| 1   | A     | 662 | LEU  |
| 1   | A     | 676 | THR  |
| 1   | A     | 683 | LEU  |
| 1   | A     | 706 | GLU  |
| 1   | A     | 708 | PHE  |
| 1   | A     | 714 | ARG  |
| 1   | A     | 753 | LYS  |
| 1   | A     | 755 | PRO  |
| 1   | A     | 756 | ASP  |
| 1   | A     | 759 | LYS  |
| 1   | A     | 765 | LEU  |
| 1   | A     | 770 | ARG  |
| 1   | A     | 779 | GLU  |
| 1   | A     | 782 | LYS  |
| 1   | A     | 784 | GLN  |
| 1   | A     | 792 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 795 | ARG  |
| 1   | A     | 803 | ARG  |
| 1   | A     | 807 | THR  |
| 1   | A     | 833 | ARG  |
| 1   | A     | 834 | LEU  |
| 1   | A     | 835 | PRO  |
| 1   | A     | 837 | PRO  |
| 1   | B     | 16  | ARG  |
| 1   | B     | 18  | LEU  |
| 1   | B     | 43  | ARG  |
| 1   | B     | 48  | PRO  |
| 1   | B     | 77  | LYS  |
| 1   | B     | 79  | PRO  |
| 1   | B     | 82  | ILE  |
| 1   | B     | 87  | LEU  |
| 1   | B     | 95  | LEU  |
| 1   | B     | 100 | VAL  |
| 1   | B     | 104 | LEU  |
| 1   | B     | 121 | GLU  |
| 1   | B     | 131 | LEU  |
| 1   | B     | 136 | LEU  |
| 1   | B     | 138 | ARG  |
| 1   | B     | 165 | ILE  |
| 1   | B     | 169 | LYS  |
| 1   | B     | 177 | GLU  |
| 1   | B     | 187 | ASN  |
| 1   | B     | 191 | LYS  |
| 1   | B     | 214 | LYS  |
| 1   | B     | 225 | PRO  |
| 1   | B     | 230 | VAL  |
| 1   | B     | 235 | ASN  |
| 1   | B     | 237 | VAL  |
| 1   | B     | 242 | ARG  |
| 1   | B     | 243 | LEU  |
| 1   | B     | 253 | ASN  |
| 1   | B     | 254 | LEU  |
| 1   | B     | 255 | LYS  |
| 1   | B     | 264 | GLN  |
| 1   | B     | 274 | ASN  |
| 1   | B     | 278 | VAL  |
| 1   | B     | 279 | LEU  |
| 1   | B     | 281 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 287 | GLU  |
| 1   | B     | 291 | LEU  |
| 1   | B     | 318 | CYS  |
| 1   | B     | 320 | ASP  |
| 1   | B     | 321 | PRO  |
| 1   | B     | 325 | ASN  |
| 1   | B     | 337 | LEU  |
| 1   | B     | 342 | PRO  |
| 1   | B     | 358 | ARG  |
| 1   | B     | 360 | ASP  |
| 1   | B     | 369 | VAL  |
| 1   | B     | 379 | VAL  |
| 1   | B     | 392 | LEU  |
| 1   | B     | 396 | LEU  |
| 1   | B     | 419 | PRO  |
| 1   | B     | 422 | VAL  |
| 1   | B     | 426 | ARG  |
| 1   | B     | 444 | LEU  |
| 1   | B     | 455 | VAL  |
| 1   | B     | 474 | LEU  |
| 1   | B     | 478 | LYS  |
| 1   | B     | 486 | ILE  |
| 1   | B     | 492 | LEU  |
| 1   | B     | 519 | ARG  |
| 1   | B     | 521 | LEU  |
| 1   | B     | 522 | LEU  |
| 1   | B     | 543 | LEU  |
| 1   | B     | 550 | GLU  |
| 1   | B     | 552 | GLU  |
| 1   | B     | 553 | TYR  |
| 1   | B     | 554 | LYS  |
| 1   | B     | 565 | VAL  |
| 1   | B     | 568 | LYS  |
| 1   | B     | 573 | TYR  |
| 1   | B     | 576 | GLN  |
| 1   | B     | 589 | ARG  |
| 1   | B     | 596 | LYS  |
| 1   | B     | 603 | VAL  |
| 1   | B     | 622 | LEU  |
| 1   | B     | 630 | VAL  |
| 1   | B     | 640 | LEU  |
| 1   | B     | 649 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 652 | LEU  |
| 1   | B     | 662 | LEU  |
| 1   | B     | 676 | THR  |
| 1   | B     | 683 | LEU  |
| 1   | B     | 705 | GLU  |
| 1   | B     | 706 | GLU  |
| 1   | B     | 714 | ARG  |
| 1   | B     | 721 | LEU  |
| 1   | B     | 753 | LYS  |
| 1   | B     | 759 | LYS  |
| 1   | B     | 765 | LEU  |
| 1   | B     | 770 | ARG  |
| 1   | B     | 781 | VAL  |
| 1   | B     | 782 | LYS  |
| 1   | B     | 784 | GLN  |
| 1   | B     | 792 | LYS  |
| 1   | B     | 794 | PRO  |
| 1   | B     | 803 | ARG  |
| 1   | B     | 807 | THR  |
| 1   | B     | 830 | SER  |
| 1   | B     | 831 | ARG  |
| 1   | B     | 834 | LEU  |
| 1   | C     | 12  | GLN  |
| 1   | C     | 21  | VAL  |
| 1   | C     | 22  | GLU  |
| 1   | C     | 43  | ARG  |
| 1   | C     | 45  | VAL  |
| 1   | C     | 47  | THR  |
| 1   | C     | 48  | PRO  |
| 1   | C     | 63  | LEU  |
| 1   | C     | 82  | ILE  |
| 1   | C     | 87  | LEU  |
| 1   | C     | 95  | LEU  |
| 1   | C     | 100 | VAL  |
| 1   | C     | 102 | LEU  |
| 1   | C     | 104 | LEU  |
| 1   | C     | 131 | LEU  |
| 1   | C     | 136 | LEU  |
| 1   | C     | 138 | ARG  |
| 1   | C     | 165 | ILE  |
| 1   | C     | 191 | LYS  |
| 1   | C     | 195 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 214 | LYS  |
| 1   | C     | 225 | PRO  |
| 1   | C     | 230 | VAL  |
| 1   | C     | 231 | PRO  |
| 1   | C     | 235 | ASN  |
| 1   | C     | 237 | VAL  |
| 1   | C     | 242 | ARG  |
| 1   | C     | 243 | LEU  |
| 1   | C     | 252 | PHE  |
| 1   | C     | 253 | ASN  |
| 1   | C     | 255 | LYS  |
| 1   | C     | 256 | ASP  |
| 1   | C     | 262 | TYR  |
| 1   | C     | 264 | GLN  |
| 1   | C     | 274 | ASN  |
| 1   | C     | 278 | VAL  |
| 1   | C     | 281 | PRO  |
| 1   | C     | 287 | GLU  |
| 1   | C     | 289 | LYS  |
| 1   | C     | 291 | LEU  |
| 1   | C     | 319 | ARG  |
| 1   | C     | 321 | PRO  |
| 1   | C     | 323 | ARG  |
| 1   | C     | 337 | LEU  |
| 1   | C     | 358 | ARG  |
| 1   | C     | 360 | ASP  |
| 1   | C     | 369 | VAL  |
| 1   | C     | 379 | VAL  |
| 1   | C     | 380 | ILE  |
| 1   | C     | 391 | LEU  |
| 1   | C     | 392 | LEU  |
| 1   | C     | 394 | THR  |
| 1   | C     | 395 | LEU  |
| 1   | C     | 396 | LEU  |
| 1   | C     | 398 | ARG  |
| 1   | C     | 400 | LEU  |
| 1   | C     | 425 | LEU  |
| 1   | C     | 426 | ARG  |
| 1   | C     | 436 | VAL  |
| 1   | C     | 444 | LEU  |
| 1   | C     | 455 | VAL  |
| 1   | C     | 462 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 466 | THR  |
| 1   | C     | 474 | LEU  |
| 1   | C     | 486 | ILE  |
| 1   | C     | 492 | LEU  |
| 1   | C     | 513 | SER  |
| 1   | C     | 521 | LEU  |
| 1   | C     | 522 | LEU  |
| 1   | C     | 525 | VAL  |
| 1   | C     | 543 | LEU  |
| 1   | C     | 550 | GLU  |
| 1   | C     | 552 | GLU  |
| 1   | C     | 553 | TYR  |
| 1   | C     | 554 | LYS  |
| 1   | C     | 565 | VAL  |
| 1   | C     | 568 | LYS  |
| 1   | C     | 586 | LEU  |
| 1   | C     | 593 | GLU  |
| 1   | C     | 603 | VAL  |
| 1   | C     | 605 | ILE  |
| 1   | C     | 622 | LEU  |
| 1   | C     | 624 | THR  |
| 1   | C     | 630 | VAL  |
| 1   | C     | 640 | LEU  |
| 1   | C     | 643 | ILE  |
| 1   | C     | 649 | ARG  |
| 1   | C     | 652 | LEU  |
| 1   | C     | 662 | LEU  |
| 1   | C     | 676 | THR  |
| 1   | C     | 706 | GLU  |
| 1   | C     | 708 | PHE  |
| 1   | C     | 714 | ARG  |
| 1   | C     | 716 | GLU  |
| 1   | C     | 753 | LYS  |
| 1   | C     | 755 | PRO  |
| 1   | C     | 759 | LYS  |
| 1   | C     | 766 | MET  |
| 1   | C     | 779 | GLU  |
| 1   | C     | 781 | VAL  |
| 1   | C     | 782 | LYS  |
| 1   | C     | 792 | LYS  |
| 1   | C     | 803 | ARG  |
| 1   | C     | 807 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 833 | ARG  |
| 1   | D     | 11  | LYS  |
| 1   | D     | 12  | GLN  |
| 1   | D     | 15  | VAL  |
| 1   | D     | 22  | GLU  |
| 1   | D     | 23  | ASN  |
| 1   | D     | 43  | ARG  |
| 1   | D     | 45  | VAL  |
| 1   | D     | 48  | PRO  |
| 1   | D     | 66  | ARG  |
| 1   | D     | 77  | LYS  |
| 1   | D     | 82  | ILE  |
| 1   | D     | 85  | LEU  |
| 1   | D     | 87  | LEU  |
| 1   | D     | 95  | LEU  |
| 1   | D     | 100 | VAL  |
| 1   | D     | 102 | LEU  |
| 1   | D     | 104 | LEU  |
| 1   | D     | 121 | GLU  |
| 1   | D     | 131 | LEU  |
| 1   | D     | 136 | LEU  |
| 1   | D     | 138 | ARG  |
| 1   | D     | 144 | LEU  |
| 1   | D     | 165 | ILE  |
| 1   | D     | 177 | GLU  |
| 1   | D     | 191 | LYS  |
| 1   | D     | 195 | GLU  |
| 1   | D     | 199 | PRO  |
| 1   | D     | 214 | LYS  |
| 1   | D     | 217 | ASP  |
| 1   | D     | 230 | VAL  |
| 1   | D     | 235 | ASN  |
| 1   | D     | 237 | VAL  |
| 1   | D     | 242 | ARG  |
| 1   | D     | 243 | LEU  |
| 1   | D     | 257 | PHE  |
| 1   | D     | 259 | VAL  |
| 1   | D     | 262 | TYR  |
| 1   | D     | 263 | ILE  |
| 1   | D     | 274 | ASN  |
| 1   | D     | 278 | VAL  |
| 1   | D     | 279 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 281 | PRO  |
| 1   | D     | 287 | GLU  |
| 1   | D     | 289 | LYS  |
| 1   | D     | 309 | ARG  |
| 1   | D     | 319 | ARG  |
| 1   | D     | 322 | VAL  |
| 1   | D     | 323 | ARG  |
| 1   | D     | 337 | LEU  |
| 1   | D     | 358 | ARG  |
| 1   | D     | 360 | ASP  |
| 1   | D     | 366 | GLU  |
| 1   | D     | 369 | VAL  |
| 1   | D     | 378 | THR  |
| 1   | D     | 379 | VAL  |
| 1   | D     | 380 | ILE  |
| 1   | D     | 382 | GLU  |
| 1   | D     | 389 | VAL  |
| 1   | D     | 392 | LEU  |
| 1   | D     | 395 | LEU  |
| 1   | D     | 396 | LEU  |
| 1   | D     | 398 | ARG  |
| 1   | D     | 400 | LEU  |
| 1   | D     | 422 | VAL  |
| 1   | D     | 424 | ARG  |
| 1   | D     | 426 | ARG  |
| 1   | D     | 436 | VAL  |
| 1   | D     | 437 | LYS  |
| 1   | D     | 444 | LEU  |
| 1   | D     | 455 | VAL  |
| 1   | D     | 462 | ILE  |
| 1   | D     | 474 | LEU  |
| 1   | D     | 475 | GLU  |
| 1   | D     | 486 | ILE  |
| 1   | D     | 492 | LEU  |
| 1   | D     | 506 | ARG  |
| 1   | D     | 521 | LEU  |
| 1   | D     | 522 | LEU  |
| 1   | D     | 543 | LEU  |
| 1   | D     | 550 | GLU  |
| 1   | D     | 553 | TYR  |
| 1   | D     | 554 | LYS  |
| 1   | D     | 565 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 568 | LYS  |
| 1   | D     | 573 | TYR  |
| 1   | D     | 583 | VAL  |
| 1   | D     | 586 | LEU  |
| 1   | D     | 589 | ARG  |
| 1   | D     | 603 | VAL  |
| 1   | D     | 622 | LEU  |
| 1   | D     | 630 | VAL  |
| 1   | D     | 640 | LEU  |
| 1   | D     | 649 | ARG  |
| 1   | D     | 652 | LEU  |
| 1   | D     | 662 | LEU  |
| 1   | D     | 676 | THR  |
| 1   | D     | 683 | LEU  |
| 1   | D     | 705 | GLU  |
| 1   | D     | 706 | GLU  |
| 1   | D     | 708 | PHE  |
| 1   | D     | 714 | ARG  |
| 1   | D     | 715 | VAL  |
| 1   | D     | 716 | GLU  |
| 1   | D     | 741 | ILE  |
| 1   | D     | 753 | LYS  |
| 1   | D     | 755 | PRO  |
| 1   | D     | 756 | ASP  |
| 1   | D     | 765 | LEU  |
| 1   | D     | 766 | MET  |
| 1   | D     | 770 | ARG  |
| 1   | D     | 782 | LYS  |
| 1   | D     | 784 | GLN  |
| 1   | D     | 792 | LYS  |
| 1   | D     | 797 | TRP  |
| 1   | D     | 803 | ARG  |
| 1   | D     | 807 | THR  |
| 1   | D     | 832 | GLN  |
| 1   | D     | 837 | PRO  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | GLN  |
| 1   | A     | 34  | HIS  |
| 1   | A     | 62  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 168 | GLN  |
| 1   | A     | 235 | ASN  |
| 1   | A     | 264 | GLN  |
| 1   | A     | 336 | GLN  |
| 1   | A     | 390 | HIS  |
| 1   | A     | 399 | HIS  |
| 1   | A     | 412 | ASN  |
| 1   | A     | 459 | HIS  |
| 1   | A     | 477 | HIS  |
| 1   | A     | 480 | GLN  |
| 1   | A     | 481 | ASN  |
| 1   | A     | 556 | HIS  |
| 1   | A     | 566 | GLN  |
| 1   | A     | 576 | GLN  |
| 1   | A     | 579 | ASN  |
| 1   | A     | 665 | GLN  |
| 1   | A     | 727 | ASN  |
| 1   | A     | 744 | GLN  |
| 1   | A     | 784 | GLN  |
| 1   | B     | 34  | HIS  |
| 1   | B     | 167 | ASN  |
| 1   | B     | 168 | GLN  |
| 1   | B     | 235 | ASN  |
| 1   | B     | 336 | GLN  |
| 1   | B     | 399 | HIS  |
| 1   | B     | 480 | GLN  |
| 1   | B     | 481 | ASN  |
| 1   | B     | 541 | ASN  |
| 1   | B     | 566 | GLN  |
| 1   | B     | 576 | GLN  |
| 1   | B     | 579 | ASN  |
| 1   | B     | 614 | HIS  |
| 1   | B     | 665 | GLN  |
| 1   | B     | 744 | GLN  |
| 1   | B     | 784 | GLN  |
| 1   | C     | 12  | GLN  |
| 1   | C     | 30  | ASN  |
| 1   | C     | 34  | HIS  |
| 1   | C     | 57  | HIS  |
| 1   | C     | 62  | HIS  |
| 1   | C     | 114 | GLN  |
| 1   | C     | 167 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 168 | GLN  |
| 1   | C     | 208 | HIS  |
| 1   | C     | 235 | ASN  |
| 1   | C     | 270 | ASN  |
| 1   | C     | 336 | GLN  |
| 1   | C     | 399 | HIS  |
| 1   | C     | 412 | ASN  |
| 1   | C     | 453 | ASN  |
| 1   | C     | 459 | HIS  |
| 1   | C     | 480 | GLN  |
| 1   | C     | 481 | ASN  |
| 1   | C     | 496 | ASN  |
| 1   | C     | 517 | GLN  |
| 1   | C     | 541 | ASN  |
| 1   | C     | 566 | GLN  |
| 1   | C     | 576 | GLN  |
| 1   | C     | 579 | ASN  |
| 1   | C     | 665 | GLN  |
| 1   | C     | 707 | ASN  |
| 1   | C     | 727 | ASN  |
| 1   | C     | 744 | GLN  |
| 1   | C     | 754 | GLN  |
| 1   | C     | 767 | HIS  |
| 1   | C     | 768 | HIS  |
| 1   | C     | 784 | GLN  |
| 1   | C     | 793 | ASN  |
| 1   | D     | 12  | GLN  |
| 1   | D     | 34  | HIS  |
| 1   | D     | 62  | HIS  |
| 1   | D     | 73  | HIS  |
| 1   | D     | 168 | GLN  |
| 1   | D     | 235 | ASN  |
| 1   | D     | 250 | ASN  |
| 1   | D     | 336 | GLN  |
| 1   | D     | 390 | HIS  |
| 1   | D     | 399 | HIS  |
| 1   | D     | 412 | ASN  |
| 1   | D     | 453 | ASN  |
| 1   | D     | 477 | HIS  |
| 1   | D     | 480 | GLN  |
| 1   | D     | 481 | ASN  |
| 1   | D     | 541 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 566 | GLN  |
| 1   | D     | 576 | GLN  |
| 1   | D     | 588 | ASN  |
| 1   | D     | 665 | GLN  |
| 1   | D     | 727 | ASN  |
| 1   | D     | 744 | GLN  |
| 1   | D     | 754 | GLN  |
| 1   | D     | 784 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

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   | PLP  | A     | 999 | 1    | 15,15,16     | 1.05 | 1 (6%)      | 21,22,23    | 1.28 | 2 (9%)      |
| 4   | NTZ  | B     | 998 | -    | 13,15,15     | 2.59 | 6 (46%)     | 14,22,22    | 3.60 | 5 (35%)     |
| 3   | PLP  | D     | 999 | 1    | 15,15,16     | 1.54 | 2 (13%)     | 21,22,23    | 1.14 | 1 (4%)      |
| 4   | NTZ  | C     | 998 | -    | 13,15,15     | 3.68 | 5 (38%)     | 14,22,22    | 3.53 | 4 (28%)     |
| 2   | PO4  | D     | 997 | -    | 4,4,4        | 3.62 | 3 (75%)     | 6,6,6       | 2.39 | 4 (66%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NTZ  | A     | 998 | -    | 13,15,15     | 2.06 | 3 (23%)  | 14,22,22    | 3.92 | 3 (21%)  |
| 2   | PO4  | B     | 997 | -    | 4,4,4        | 3.80 | 4 (100%) | 6,6,6       | 2.23 | 2 (33%)  |
| 4   | NTZ  | D     | 998 | -    | 13,15,15     | 3.07 | 5 (38%)  | 14,22,22    | 4.36 | 5 (35%)  |
| 2   | PO4  | C     | 997 | -    | 4,4,4        | 3.92 | 4 (100%) | 6,6,6       | 2.56 | 4 (66%)  |
| 3   | PLP  | B     | 999 | 1    | 15,15,16     | 1.46 | 3 (20%)  | 21,22,23    | 1.12 | 1 (4%)   |
| 2   | PO4  | A     | 997 | -    | 4,4,4        | 3.57 | 4 (100%) | 6,6,6       | 2.78 | 4 (66%)  |
| 3   | PLP  | C     | 999 | 1    | 15,15,16     | 1.73 | 3 (20%)  | 21,22,23    | 1.19 | 2 (9%)   |

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   | PLP  | A     | 999 | 1    | -       | 1/6/6/8   | 0/1/1/1 |
| 4   | NTZ  | B     | 998 | -    | -       | 0/2/22/22 | 0/2/2/2 |
| 3   | PLP  | D     | 999 | 1    | -       | 1/6/6/8   | 0/1/1/1 |
| 4   | NTZ  | C     | 998 | -    | -       | 1/2/22/22 | 0/2/2/2 |
| 4   | NTZ  | A     | 998 | -    | -       | 1/2/22/22 | 0/2/2/2 |
| 4   | NTZ  | D     | 998 | -    | -       | 0/2/22/22 | 0/2/2/2 |
| 3   | PLP  | B     | 999 | 1    | -       | 1/6/6/8   | 0/1/1/1 |
| 3   | PLP  | C     | 999 | 1    | -       | 1/6/6/8   | 0/1/1/1 |

All (43) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | C     | 998 | NTZ  | C1-N21  | 8.26  | 1.40        | 1.32     |
| 4   | D     | 998 | NTZ  | C1-N21  | 7.94  | 1.40        | 1.32     |
| 4   | C     | 998 | NTZ  | C1-N1   | 7.35  | 1.40        | 1.34     |
| 4   | B     | 998 | NTZ  | C1-N1   | 6.03  | 1.39        | 1.34     |
| 4   | A     | 998 | NTZ  | C1-N1   | 5.07  | 1.38        | 1.34     |
| 2   | C     | 997 | PO4  | P-O2    | -4.94 | 1.40        | 1.54     |
| 2   | D     | 997 | PO4  | P-O2    | -4.59 | 1.41        | 1.54     |
| 4   | C     | 998 | NTZ  | N17-N18 | 4.52  | 1.40        | 1.30     |
| 3   | D     | 999 | PLP  | C3-C2   | -4.44 | 1.36        | 1.41     |
| 2   | B     | 997 | PO4  | P-O2    | -4.42 | 1.41        | 1.54     |
| 2   | B     | 997 | PO4  | P-O3    | -4.35 | 1.42        | 1.54     |
| 4   | D     | 998 | NTZ  | N17-N18 | 4.16  | 1.39        | 1.30     |
| 2   | C     | 997 | PO4  | P-O4    | -4.07 | 1.42        | 1.54     |
| 4   | B     | 998 | NTZ  | N17-N18 | 4.05  | 1.39        | 1.30     |
| 2   | A     | 997 | PO4  | P-O2    | -4.05 | 1.42        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | A     | 998 | NTZ  | C1-N21  | 4.04  | 1.36        | 1.32     |
| 2   | A     | 997 | PO4  | P-O3    | -3.98 | 1.43        | 1.54     |
| 2   | D     | 997 | PO4  | P-O3    | -3.97 | 1.43        | 1.54     |
| 2   | D     | 997 | PO4  | P-O4    | -3.84 | 1.43        | 1.54     |
| 4   | D     | 998 | NTZ  | N1-N17  | 3.83  | 1.40        | 1.35     |
| 4   | C     | 998 | NTZ  | N1-N17  | 3.82  | 1.40        | 1.35     |
| 2   | B     | 997 | PO4  | P-O4    | -3.79 | 1.43        | 1.54     |
| 4   | B     | 998 | NTZ  | C1-N21  | 3.74  | 1.35        | 1.32     |
| 2   | C     | 997 | PO4  | P-O3    | -3.71 | 1.43        | 1.54     |
| 3   | C     | 999 | PLP  | C3-C2   | -3.69 | 1.37        | 1.41     |
| 2   | A     | 997 | PO4  | P-O4    | -3.60 | 1.44        | 1.54     |
| 4   | D     | 998 | NTZ  | C1-N1   | 3.34  | 1.37        | 1.34     |
| 4   | C     | 998 | NTZ  | N21-N18 | 3.32  | 1.41        | 1.36     |
| 3   | C     | 999 | PLP  | C4A-C4  | 2.99  | 1.57        | 1.51     |
| 4   | D     | 998 | NTZ  | C3-C2   | 2.85  | 1.57        | 1.53     |
| 4   | B     | 998 | NTZ  | N1-N17  | 2.67  | 1.39        | 1.35     |
| 3   | B     | 999 | PLP  | C3-C2   | -2.66 | 1.38        | 1.41     |
| 2   | C     | 997 | PO4  | P-O1    | 2.59  | 1.56        | 1.50     |
| 4   | A     | 998 | NTZ  | N17-N18 | 2.55  | 1.35        | 1.30     |
| 3   | A     | 999 | PLP  | C3-C2   | -2.44 | 1.38        | 1.41     |
| 2   | A     | 997 | PO4  | P-O1    | 2.39  | 1.56        | 1.50     |
| 3   | B     | 999 | PLP  | C5-C4   | -2.31 | 1.37        | 1.40     |
| 4   | B     | 998 | NTZ  | N21-N18 | 2.29  | 1.39        | 1.36     |
| 3   | C     | 999 | PLP  | C5-C4   | -2.29 | 1.38        | 1.40     |
| 4   | B     | 998 | NTZ  | C4-C5   | -2.27 | 1.49        | 1.53     |
| 2   | B     | 997 | PO4  | P-O1    | 2.21  | 1.55        | 1.50     |
| 3   | B     | 999 | PLP  | C2A-C2  | 2.13  | 1.53        | 1.50     |
| 3   | D     | 999 | PLP  | C6-N1   | 2.04  | 1.38        | 1.34     |

All (37) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | D     | 998 | NTZ  | N1-N17-N18  | 9.81  | 113.51      | 106.00   |
| 4   | A     | 998 | NTZ  | C1-N1-N17   | -9.67 | 102.05      | 108.47   |
| 4   | B     | 998 | NTZ  | N1-C1-N21   | 9.63  | 113.11      | 108.45   |
| 4   | C     | 998 | NTZ  | N1-C1-N21   | 8.75  | 112.68      | 108.45   |
| 4   | D     | 998 | NTZ  | C1-N1-N17   | -8.69 | 102.70      | 108.47   |
| 4   | A     | 998 | NTZ  | N1-C1-N21   | 8.56  | 112.59      | 108.45   |
| 4   | C     | 998 | NTZ  | C1-N1-N17   | -7.04 | 103.79      | 108.47   |
| 4   | B     | 998 | NTZ  | C1-N1-N17   | -6.97 | 103.84      | 108.47   |
| 4   | D     | 998 | NTZ  | N21-N18-N17 | -6.35 | 104.04      | 111.07   |
| 4   | A     | 998 | NTZ  | N1-N17-N18  | 6.13  | 110.69      | 106.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | D     | 998 | NTZ  | N1-C1-N21   | 5.70  | 111.20      | 108.45   |
| 4   | C     | 998 | NTZ  | N1-N17-N18  | 5.67  | 110.34      | 106.00   |
| 4   | B     | 998 | NTZ  | N1-N17-N18  | 4.40  | 109.37      | 106.00   |
| 4   | D     | 998 | NTZ  | C1-N21-N18  | 4.03  | 108.54      | 105.81   |
| 2   | A     | 997 | PO4  | O3-P-O1     | -3.98 | 96.86       | 110.95   |
| 2   | A     | 997 | PO4  | O4-P-O2     | 3.97  | 120.25      | 107.91   |
| 2   | B     | 997 | PO4  | O4-P-O2     | 3.61  | 119.14      | 107.91   |
| 2   | D     | 997 | PO4  | O4-P-O2     | 3.57  | 119.02      | 107.91   |
| 2   | C     | 997 | PO4  | O4-P-O1     | -3.49 | 98.61       | 110.95   |
| 2   | C     | 997 | PO4  | O4-P-O2     | 3.29  | 118.14      | 107.91   |
| 3   | A     | 999 | PLP  | O2P-P-O4P   | -3.25 | 98.19       | 106.67   |
| 2   | B     | 997 | PO4  | O3-P-O1     | -3.10 | 99.97       | 110.95   |
| 3   | A     | 999 | PLP  | O3P-P-O4P   | 3.00  | 114.49      | 106.67   |
| 2   | C     | 997 | PO4  | O3-P-O1     | -2.84 | 100.92      | 110.95   |
| 3   | C     | 999 | PLP  | O4P-C5A-C5  | -2.80 | 104.11      | 109.36   |
| 4   | B     | 998 | NTZ  | C6-C5-C4    | 2.79  | 117.14      | 112.93   |
| 2   | A     | 997 | PO4  | O4-P-O1     | -2.77 | 101.14      | 110.95   |
| 3   | B     | 999 | PLP  | O3P-P-O1P   | 2.65  | 121.18      | 110.83   |
| 3   | D     | 999 | PLP  | O3P-P-O4P   | 2.63  | 113.53      | 106.67   |
| 2   | D     | 997 | PO4  | O3-P-O1     | -2.51 | 102.08      | 110.95   |
| 2   | A     | 997 | PO4  | O4-P-O3     | 2.38  | 115.31      | 107.91   |
| 2   | C     | 997 | PO4  | O4-P-O3     | 2.27  | 114.97      | 107.91   |
| 3   | C     | 999 | PLP  | O3P-P-O1P   | 2.22  | 119.50      | 110.83   |
| 2   | D     | 997 | PO4  | O4-P-O1     | -2.18 | 103.26      | 110.95   |
| 4   | B     | 998 | NTZ  | N21-N18-N17 | -2.17 | 108.67      | 111.07   |
| 4   | C     | 998 | NTZ  | N21-N18-N17 | -2.17 | 108.67      | 111.07   |
| 2   | D     | 997 | PO4  | O2-P-O1     | -2.17 | 103.28      | 110.95   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 3   | C     | 999 | PLP  | C4-C5-C5A-O4P |
| 3   | D     | 999 | PLP  | C4-C5-C5A-O4P |
| 4   | A     | 998 | NTZ  | C4-C5-C6-O6   |
| 4   | C     | 998 | NTZ  | C4-C5-C6-O6   |
| 3   | A     | 999 | PLP  | C6-C5-C5A-O4P |
| 3   | B     | 999 | PLP  | C6-C5-C5A-O4P |

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | C     | 997 | PO4  | 1       | 0            |
| 3   | B     | 999 | PLP  | 1       | 0            |

## 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.