



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:35 PM UTC

PDB ID : 1B65 / pdb\_00001b65  
Title : Structure of l-aminopeptidase d-ala-esterase/amidase from ochrobactrum anthropi, a prototype for the serine aminopeptidases, reveals a new variant among the ntn hydrolase fold  
Authors : Bompard-Gilles, C.; Villeret, V.; Davies, G.J.; Fanuel, L.; Joris, B.; Frere, J.M.; Van Beeumen, J.  
Deposited on : 1999-01-20  
Resolution : 1.82 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : **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

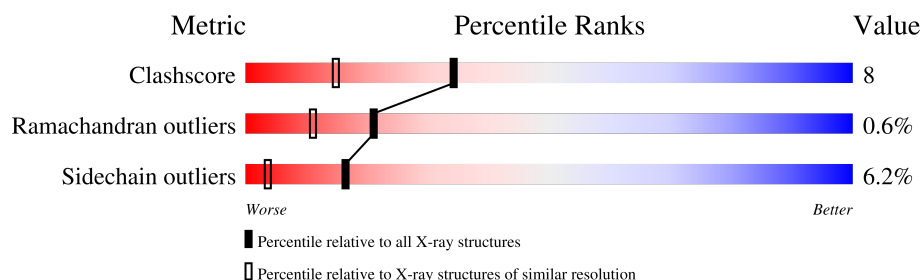
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.82 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                      | 1148 (1.82-1.82)                                      |
| Ramachandran outliers | 187476                      | 1140 (1.82-1.82)                                      |
| Sidechain outliers    | 187428                      | 1140 (1.82-1.82)                                      |

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     | 375    |  80% 12% . . . |
| 1   | B     | 375    |  80% 13% . . . |
| 1   | C     | 375    |  79% 14% . . . |
| 1   | D     | 375    |  79% 13% . . . |
| 1   | E     | 375    |  80% 13% . . . |
| 1   | F     | 375    |  79% 13% . . . |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17786 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 PROTEIN (AMINOPEPTIDASE).

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 363      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2747  | 1719 | 499 | 516 | 13 |         |         |       |
| 1   | B     | 363      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2747  | 1719 | 499 | 516 | 13 |         |         |       |
| 1   | C     | 363      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2747  | 1719 | 499 | 516 | 13 |         |         |       |
| 1   | D     | 363      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2747  | 1719 | 499 | 516 | 13 |         |         |       |
| 1   | E     | 363      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2747  | 1719 | 499 | 516 | 13 |         |         |       |
| 1   | F     | 363      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2747  | 1719 | 499 | 516 | 13 |         |         |       |

- Molecule 2 is water.

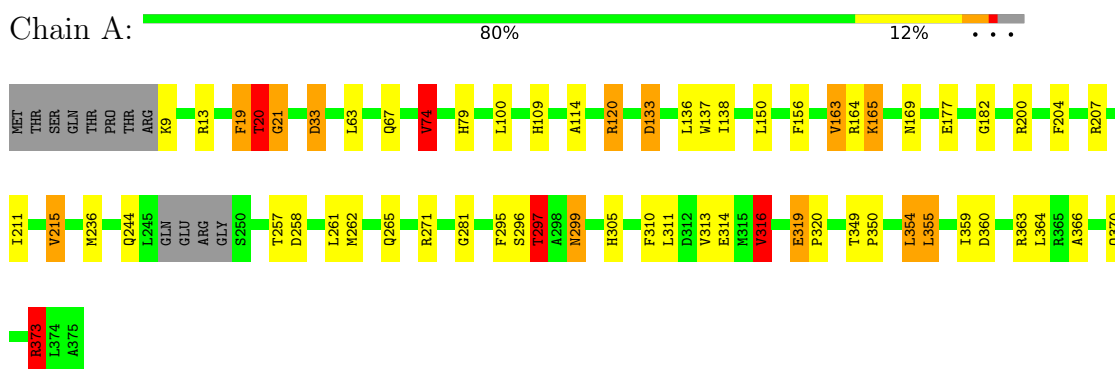
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 2   | A     | 220      | Total | O   | 0       | 0       |
|     |       |          | 220   | 220 |         |         |
| 2   | B     | 220      | Total | O   | 0       | 0       |
|     |       |          | 220   | 220 |         |         |
| 2   | C     | 230      | Total | O   | 0       | 0       |
|     |       |          | 230   | 230 |         |         |
| 2   | D     | 216      | Total | O   | 0       | 0       |
|     |       |          | 216   | 216 |         |         |
| 2   | E     | 207      | Total | O   | 0       | 0       |
|     |       |          | 207   | 207 |         |         |
| 2   | F     | 211      | Total | O   | 0       | 0       |
|     |       |          | 211   | 211 |         |         |

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

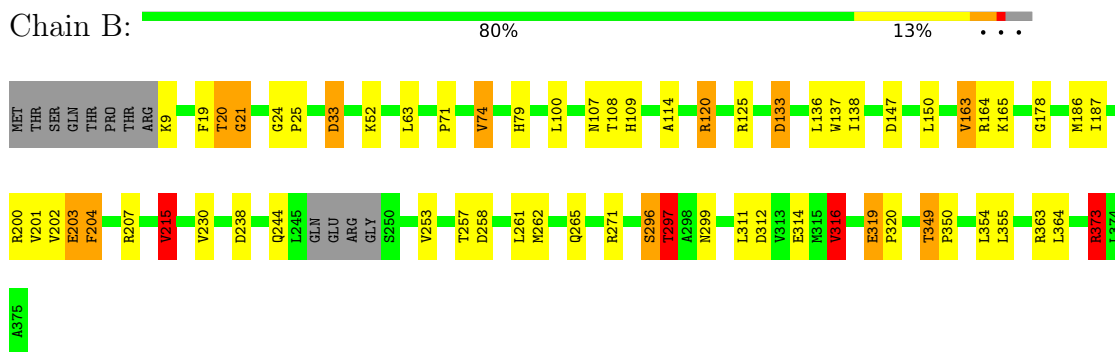
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

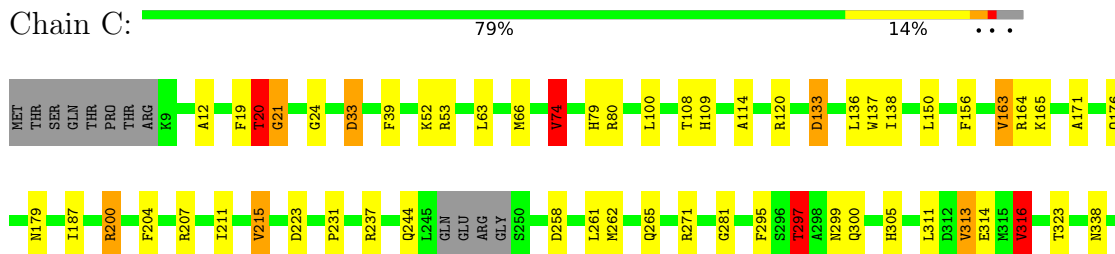
- Molecule 1: PROTEIN (AMINOPEPTIDASE)



- Molecule 1: PROTEIN (AMINOPEPTIDASE)



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• Molecule 1: PROTEIN (AMINOPEPTIDASE)

Chain D: 79% 13%



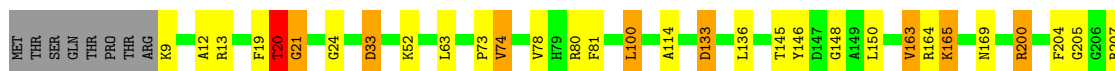
• Molecule 1: PROTEIN (AMINOPEPTIDASE)

Chain E: 80% 13%



• Molecule 1: PROTEIN (AMINOPEPTIDASE)

Chain F: 79% 13%



## 4 Data and refinement statistics

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

| Property                                                 | Value                                          | Source    |
|----------------------------------------------------------|------------------------------------------------|-----------|
| Space group                                              | P 21 21 2                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 156.97Å 96.22Å 154.41Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 12.50 – 1.82                                   | Depositor |
| % Data completeness<br>(in resolution range)             | 95.8 (12.50-1.82)                              | Depositor |
| $R_{merge}$                                              | (Not available)                                | Depositor |
| $R_{sym}$                                                | 0.06                                           | Depositor |
| Refinement program                                       | REFMAC                                         | Depositor |
| R, $R_{free}$                                            | 0.169 , 0.206                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 17786                                          | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 21.0                                           | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.81         | 3/2808 (0.1%)   | 1.75        | 44/3820 (1.2%)   |
| 1   | B     | 0.82         | 0/2808          | 1.80        | 45/3820 (1.2%)   |
| 1   | C     | 0.82         | 1/2808 (0.0%)   | 1.81        | 51/3820 (1.3%)   |
| 1   | D     | 0.86         | 4/2808 (0.1%)   | 1.89        | 61/3820 (1.6%)   |
| 1   | E     | 0.88         | 4/2808 (0.1%)   | 1.84        | 51/3820 (1.3%)   |
| 1   | F     | 0.83         | 1/2808 (0.0%)   | 1.78        | 42/3820 (1.1%)   |
| All | All   | 0.84         | 13/16848 (0.1%) | 1.81        | 294/22920 (1.3%) |

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                   | 1                   |
| 1   | D     | 0                   | 2                   |
| 1   | E     | 0                   | 3                   |
| All | All   | 0                   | 6                   |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | E     | 317 | ASN  | CA-CB   | 15.18 | 1.76        | 1.53     |
| 1   | D     | 25  | PRO  | CA-CB   | 9.41  | 1.67        | 1.53     |
| 1   | E     | 92  | TRP  | CZ2-CH2 | 6.34  | 1.49        | 1.37     |
| 1   | A     | 20  | THR  | N-CA    | -5.95 | 1.38        | 1.46     |
| 1   | D     | 206 | GLY  | C-N     | 5.86  | 1.41        | 1.33     |
| 1   | D     | 20  | THR  | N-CA    | -5.68 | 1.38        | 1.46     |
| 1   | E     | 20  | THR  | N-CA    | -5.60 | 1.39        | 1.46     |
| 1   | E     | 92  | TRP  | CZ3-CH2 | 5.51  | 1.54        | 1.40     |
| 1   | A     | 207 | ARG  | CD-NE   | -5.42 | 1.38        | 1.46     |
| 1   | F     | 207 | ARG  | CD-NE   | -5.40 | 1.38        | 1.46     |
| 1   | D     | 25  | PRO  | N-CA    | -5.28 | 1.40        | 1.47     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 156 | PHE  | CA-CB | 5.15  | 1.56        | 1.52     |
| 1   | C     | 20  | THR  | N-CA  | -5.10 | 1.39        | 1.46     |

All (294) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | C     | 164 | ARG  | CD-NE-CZ  | 23.48  | 157.27      | 124.40   |
| 1   | E     | 164 | ARG  | CD-NE-CZ  | 23.11  | 156.75      | 124.40   |
| 1   | F     | 207 | ARG  | CD-NE-CZ  | 21.17  | 154.04      | 124.40   |
| 1   | A     | 19  | PHE  | CA-C-N    | 20.41  | 160.52      | 121.54   |
| 1   | A     | 19  | PHE  | C-N-CA    | 20.41  | 160.52      | 121.54   |
| 1   | D     | 19  | PHE  | CA-C-N    | 18.98  | 157.80      | 121.54   |
| 1   | D     | 19  | PHE  | C-N-CA    | 18.98  | 157.80      | 121.54   |
| 1   | E     | 317 | ASN  | CB-CA-C   | -18.23 | 70.46       | 110.19   |
| 1   | E     | 19  | PHE  | CA-C-N    | 18.03  | 155.97      | 121.54   |
| 1   | E     | 19  | PHE  | C-N-CA    | 18.03  | 155.97      | 121.54   |
| 1   | C     | 19  | PHE  | CA-C-N    | 16.89  | 153.80      | 121.54   |
| 1   | C     | 19  | PHE  | C-N-CA    | 16.89  | 153.80      | 121.54   |
| 1   | F     | 19  | PHE  | CA-C-N    | 16.73  | 153.49      | 121.54   |
| 1   | F     | 19  | PHE  | C-N-CA    | 16.73  | 153.49      | 121.54   |
| 1   | B     | 19  | PHE  | CA-C-N    | 16.57  | 153.19      | 121.54   |
| 1   | B     | 19  | PHE  | C-N-CA    | 16.57  | 153.19      | 121.54   |
| 1   | A     | 164 | ARG  | CD-NE-CZ  | 15.83  | 146.56      | 124.40   |
| 1   | F     | 373 | ARG  | NE-CZ-NH2 | -15.35 | 105.39      | 119.20   |
| 1   | D     | 19  | PHE  | CA-C-O    | 15.22  | 138.21      | 121.16   |
| 1   | E     | 19  | PHE  | CA-C-O    | 14.94  | 138.08      | 121.05   |
| 1   | D     | 25  | PRO  | N-CA-C    | 14.91  | 143.19      | 112.47   |
| 1   | E     | 373 | ARG  | NE-CZ-NH2 | -14.57 | 106.08      | 119.20   |
| 1   | E     | 317 | ASN  | O-C-N     | 14.42  | 140.25      | 122.65   |
| 1   | D     | 373 | ARG  | NE-CZ-NH2 | -14.39 | 106.25      | 119.20   |
| 1   | A     | 207 | ARG  | CD-NE-CZ  | 14.05  | 144.07      | 124.40   |
| 1   | F     | 74  | VAL  | N-CA-CB   | -13.92 | 93.55       | 111.64   |
| 1   | A     | 297 | THR  | N-CA-CB   | -13.90 | 89.92       | 110.49   |
| 1   | E     | 297 | THR  | N-CA-CB   | -13.86 | 90.33       | 110.56   |
| 1   | B     | 19  | PHE  | CA-C-O    | 13.80  | 137.34      | 121.47   |
| 1   | E     | 317 | ASN  | N-CA-CB   | 13.78  | 129.25      | 110.38   |
| 1   | D     | 164 | ARG  | CD-NE-CZ  | 13.74  | 143.63      | 124.40   |
| 1   | A     | 373 | ARG  | NE-CZ-NH2 | -13.73 | 106.84      | 119.20   |
| 1   | F     | 297 | THR  | N-CA-CB   | -13.66 | 90.62       | 110.56   |
| 1   | B     | 297 | THR  | N-CA-CB   | -13.31 | 91.13       | 110.56   |
| 1   | C     | 297 | THR  | N-CA-CB   | -13.31 | 90.80       | 110.49   |
| 1   | D     | 25  | PRO  | N-CA-CB   | -13.23 | 89.36       | 103.25   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | C     | 373 | ARG  | NE-CZ-NH2  | -13.23 | 107.29      | 119.20   |
| 1   | D     | 205 | GLY  | CA-C-N     | 13.18  | 144.21      | 122.86   |
| 1   | D     | 205 | GLY  | C-N-CA     | 13.18  | 144.21      | 122.86   |
| 1   | D     | 297 | THR  | N-CA-CB    | -13.12 | 91.08       | 110.49   |
| 1   | B     | 164 | ARG  | CD-NE-CZ   | 12.76  | 142.26      | 124.40   |
| 1   | F     | 164 | ARG  | CD-NE-CZ   | 12.65  | 142.10      | 124.40   |
| 1   | A     | 120 | ARG  | CD-NE-CZ   | 12.61  | 142.05      | 124.40   |
| 1   | D     | 207 | ARG  | CA-C-O     | -12.56 | 107.03      | 121.47   |
| 1   | B     | 74  | VAL  | N-CA-CB    | -12.31 | 95.64       | 111.64   |
| 1   | C     | 19  | PHE  | CA-C-O     | 11.81  | 134.51      | 121.05   |
| 1   | A     | 19  | PHE  | CA-C-O     | 11.64  | 134.32      | 121.05   |
| 1   | B     | 373 | ARG  | NE-CZ-NH2  | -11.59 | 108.77      | 119.20   |
| 1   | A     | 74  | VAL  | N-CA-CB    | -11.48 | 96.71       | 111.64   |
| 1   | D     | 207 | ARG  | CD-NE-CZ   | 10.96  | 139.74      | 124.40   |
| 1   | E     | 19  | PHE  | O-C-N      | -10.94 | 110.10      | 123.01   |
| 1   | A     | 373 | ARG  | NH1-CZ-NH2 | 10.94  | 133.52      | 119.30   |
| 1   | F     | 373 | ARG  | NH1-CZ-NH2 | 10.83  | 133.38      | 119.30   |
| 1   | D     | 19  | PHE  | O-C-N      | -10.79 | 109.72      | 122.89   |
| 1   | F     | 19  | PHE  | CA-C-O     | 10.68  | 133.22      | 121.05   |
| 1   | E     | 317 | ASN  | CA-C-O     | -10.60 | 109.90      | 121.99   |
| 1   | A     | 207 | ARG  | NE-CZ-NH2  | -10.45 | 109.80      | 119.20   |
| 1   | C     | 74  | VAL  | N-CA-CB    | -10.37 | 98.16       | 111.64   |
| 1   | E     | 74  | VAL  | N-CA-CB    | -9.96  | 98.69       | 111.64   |
| 1   | D     | 74  | VAL  | N-CA-CB    | -9.75  | 97.96       | 111.41   |
| 1   | B     | 207 | ARG  | CD-NE-CZ   | 9.70   | 137.98      | 124.40   |
| 1   | E     | 373 | ARG  | NH1-CZ-NH2 | 9.67   | 131.88      | 119.30   |
| 1   | E     | 316 | VAL  | N-CA-CB    | -9.43  | 93.99       | 110.49   |
| 1   | A     | 19  | PHE  | O-C-N      | -9.31  | 112.02      | 123.01   |
| 1   | E     | 215 | VAL  | N-CA-CB    | -9.28  | 94.76       | 111.93   |
| 1   | F     | 164 | ARG  | NE-CZ-NH2  | -9.27  | 110.86      | 119.20   |
| 1   | F     | 74  | VAL  | CB-CA-C    | 9.23   | 123.87      | 110.77   |
| 1   | C     | 373 | ARG  | NH1-CZ-NH2 | 9.22   | 131.28      | 119.30   |
| 1   | B     | 120 | ARG  | CD-NE-CZ   | 9.07   | 137.09      | 124.40   |
| 1   | B     | 19  | PHE  | O-C-N      | -9.06  | 112.72      | 122.96   |
| 1   | C     | 316 | VAL  | N-CA-CB    | -9.04  | 94.67       | 110.49   |
| 1   | B     | 33  | ASP  | CB-CG-OD1  | -9.03  | 97.63       | 118.40   |
| 1   | A     | 271 | ARG  | CD-NE-CZ   | 8.91   | 136.87      | 124.40   |
| 1   | C     | 297 | THR  | OG1-CB-CG2 | 8.78   | 126.85      | 109.30   |
| 1   | F     | 316 | VAL  | N-CA-CB    | -8.70  | 95.26       | 110.49   |
| 1   | D     | 316 | VAL  | N-CA-CB    | -8.69  | 93.51       | 110.45   |
| 1   | E     | 297 | THR  | OG1-CB-CG2 | 8.68   | 126.66      | 109.30   |
| 1   | D     | 215 | VAL  | N-CA-CB    | -8.67  | 93.96       | 111.91   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 297 | THR  | OG1-CB-CG2 | 8.67  | 126.64      | 109.30   |
| 1   | B     | 215 | VAL  | N-CA-CB    | -8.60 | 96.03       | 111.93   |
| 1   | F     | 215 | VAL  | N-CA-CB    | -8.50 | 96.21       | 111.93   |
| 1   | B     | 33  | ASP  | CB-CG-OD2  | 8.46  | 137.85      | 118.40   |
| 1   | A     | 215 | VAL  | N-CA-CB    | -8.34 | 96.50       | 111.93   |
| 1   | D     | 33  | ASP  | CB-CG-OD1  | -8.28 | 99.36       | 118.40   |
| 1   | B     | 316 | VAL  | N-CA-CB    | -8.26 | 96.03       | 110.49   |
| 1   | C     | 271 | ARG  | NE-CZ-NH2  | -8.08 | 111.93      | 119.20   |
| 1   | C     | 33  | ASP  | CB-CG-OD1  | -8.06 | 99.85       | 118.40   |
| 1   | F     | 33  | ASP  | CA-CB-CG   | -8.06 | 104.54      | 112.60   |
| 1   | E     | 96  | GLY  | O-C-N      | 8.02  | 131.56      | 122.34   |
| 1   | A     | 74  | VAL  | CB-CA-C    | 8.02  | 122.15      | 110.77   |
| 1   | B     | 297 | THR  | OG1-CB-CG2 | 7.99  | 125.29      | 109.30   |
| 1   | C     | 215 | VAL  | N-CA-CB    | -7.96 | 95.43       | 111.91   |
| 1   | F     | 207 | ARG  | NE-CZ-NH1  | -7.96 | 113.54      | 121.50   |
| 1   | F     | 207 | ARG  | NE-CZ-NH2  | 7.90  | 126.31      | 119.20   |
| 1   | A     | 316 | VAL  | N-CA-CB    | -7.89 | 96.68       | 110.49   |
| 1   | C     | 24  | GLY  | N-CA-C     | -7.87 | 102.71      | 112.23   |
| 1   | D     | 297 | THR  | OG1-CB-CG2 | 7.81  | 124.91      | 109.30   |
| 1   | E     | 33  | ASP  | CB-CG-OD1  | -7.78 | 100.50      | 118.40   |
| 1   | A     | 297 | THR  | OG1-CB-CG2 | 7.77  | 124.84      | 109.30   |
| 1   | D     | 203 | GLU  | CB-CG-CD   | 7.76  | 125.79      | 112.60   |
| 1   | D     | 206 | GLY  | CA-C-N     | 7.72  | 134.21      | 121.39   |
| 1   | D     | 206 | GLY  | C-N-CA     | 7.72  | 134.21      | 121.39   |
| 1   | B     | 74  | VAL  | CB-CA-C    | 7.68  | 121.68      | 110.77   |
| 1   | C     | 19  | PHE  | CA-CB-CG   | -7.67 | 106.13      | 113.80   |
| 1   | B     | 207 | ARG  | NE-CZ-NH1  | 7.64  | 129.14      | 121.50   |
| 1   | C     | 207 | ARG  | NE-CZ-NH2  | -7.60 | 112.36      | 119.20   |
| 1   | D     | 25  | PRO  | CA-C-O     | 7.56  | 134.35      | 120.60   |
| 1   | B     | 349 | THR  | N-CA-CB    | 7.52  | 117.99      | 109.49   |
| 1   | C     | 200 | ARG  | NE-CZ-NH1  | 7.52  | 129.02      | 121.50   |
| 1   | A     | 133 | ASP  | CA-CB-CG   | -7.52 | 105.08      | 112.60   |
| 1   | B     | 120 | ARG  | NE-CZ-NH1  | 7.50  | 129.00      | 121.50   |
| 1   | C     | 237 | ARG  | CD-NE-CZ   | 7.49  | 134.88      | 124.40   |
| 1   | D     | 74  | VAL  | CB-CA-C    | 7.43  | 121.62      | 110.63   |
| 1   | F     | 271 | ARG  | CD-NE-CZ   | 7.43  | 134.80      | 124.40   |
| 1   | C     | 187 | ILE  | CA-C-O     | -7.40 | 112.52      | 120.36   |
| 1   | E     | 74  | VAL  | CB-CA-C    | 7.31  | 121.16      | 110.77   |
| 1   | E     | 317 | ASN  | OD1-CG-ND2 | -7.29 | 115.31      | 122.60   |
| 1   | F     | 19  | PHE  | CA-CB-CG   | -7.29 | 106.51      | 113.80   |
| 1   | B     | 24  | GLY  | N-CA-C     | -7.25 | 103.46      | 112.23   |
| 1   | D     | 164 | ARG  | NE-CZ-NH2  | -7.18 | 112.74      | 119.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 373 | ARG  | NH1-CZ-NH2 | 7.15  | 128.60      | 119.30   |
| 1   | E     | 317 | ASN  | CA-C-N     | -7.07 | 109.21      | 121.66   |
| 1   | E     | 317 | ASN  | C-N-CA     | -7.07 | 109.21      | 121.66   |
| 1   | B     | 20  | THR  | N-CA-CB    | -7.03 | 98.61       | 110.49   |
| 1   | A     | 120 | ARG  | NE-CZ-NH1  | 7.02  | 128.52      | 121.50   |
| 1   | B     | 33  | ASP  | CA-C-O     | 6.98  | 128.57      | 120.96   |
| 1   | E     | 72  | VAL  | CA-C-O     | -6.95 | 114.00      | 119.98   |
| 1   | B     | 373 | ARG  | NH1-CZ-NH2 | 6.85  | 128.21      | 119.30   |
| 1   | C     | 19  | PHE  | O-C-N      | -6.84 | 114.94      | 123.01   |
| 1   | F     | 24  | GLY  | N-CA-C     | -6.76 | 104.05      | 112.23   |
| 1   | E     | 279 | ARG  | NE-CZ-NH2  | -6.74 | 113.14      | 119.20   |
| 1   | C     | 74  | VAL  | CB-CA-C    | 6.70  | 120.29      | 110.77   |
| 1   | D     | 281 | GLY  | N-CA-C     | 6.67  | 122.41      | 114.48   |
| 1   | D     | 33  | ASP  | CA-CB-CG   | -6.63 | 105.97      | 112.60   |
| 1   | E     | 67  | GLN  | CB-CG-CD   | 6.63  | 123.86      | 112.60   |
| 1   | D     | 363 | ARG  | CD-NE-CZ   | 6.59  | 133.62      | 124.40   |
| 1   | C     | 164 | ARG  | NE-CZ-NH2  | -6.58 | 113.28      | 119.20   |
| 1   | C     | 223 | ASP  | CA-CB-CG   | 6.54  | 119.14      | 112.60   |
| 1   | C     | 33  | ASP  | CA-C-O     | 6.52  | 128.06      | 120.96   |
| 1   | A     | 164 | ARG  | NE-CZ-NH2  | -6.50 | 113.35      | 119.20   |
| 1   | E     | 207 | ARG  | CD-NE-CZ   | 6.49  | 133.49      | 124.40   |
| 1   | F     | 311 | LEU  | CA-C-O     | -6.36 | 113.92      | 121.11   |
| 1   | F     | 21  | GLY  | N-CA-C     | 6.35  | 128.22      | 113.18   |
| 1   | C     | 297 | THR  | CB-CA-C    | 6.33  | 120.67      | 110.09   |
| 1   | F     | 164 | ARG  | NE-CZ-NH1  | 6.30  | 127.81      | 121.50   |
| 1   | E     | 72  | VAL  | O-C-N      | 6.30  | 128.29      | 120.66   |
| 1   | C     | 21  | GLY  | N-CA-C     | 6.30  | 128.10      | 113.18   |
| 1   | D     | 297 | THR  | CB-CA-C    | 6.26  | 120.54      | 110.09   |
| 1   | D     | 133 | ASP  | CA-CB-CG   | -6.23 | 106.37      | 112.60   |
| 1   | C     | 207 | ARG  | CD-NE-CZ   | 6.21  | 133.09      | 124.40   |
| 1   | B     | 312 | ASP  | CA-CB-CG   | -6.20 | 106.41      | 112.60   |
| 1   | D     | 24  | GLY  | N-CA-C     | -6.18 | 99.73       | 112.34   |
| 1   | F     | 80  | ARG  | NE-CZ-NH2  | -6.18 | 113.64      | 119.20   |
| 1   | E     | 33  | ASP  | CB-CG-OD2  | 6.17  | 132.59      | 118.40   |
| 1   | F     | 373 | ARG  | CG-CD-NE   | -6.17 | 98.43       | 112.00   |
| 1   | C     | 171 | ALA  | CA-C-O     | -6.16 | 114.68      | 121.33   |
| 1   | E     | 39  | PHE  | CA-CB-CG   | 6.15  | 119.95      | 113.80   |
| 1   | A     | 21  | GLY  | N-CA-C     | 6.15  | 127.75      | 113.18   |
| 1   | D     | 33  | ASP  | CB-CG-OD2  | 6.13  | 132.50      | 118.40   |
| 1   | B     | 133 | ASP  | CA-CB-CG   | -6.12 | 106.48      | 112.60   |
| 1   | E     | 207 | ARG  | NE-CZ-NH2  | -6.11 | 113.70      | 119.20   |
| 1   | D     | 207 | ARG  | N-CA-CB    | 6.10  | 119.56      | 110.29   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 33  | ASP  | CB-CG-OD2  | 6.09  | 132.42      | 118.40   |
| 1   | C     | 271 | ARG  | CD-NE-CZ   | 6.09  | 132.92      | 124.40   |
| 1   | D     | 66  | MET  | CA-C-O     | -6.07 | 112.14      | 119.49   |
| 1   | F     | 345 | ASP  | CA-C-O     | 6.04  | 127.80      | 121.15   |
| 1   | E     | 272 | ARG  | CD-NE-CZ   | 6.04  | 132.85      | 124.40   |
| 1   | C     | 176 | GLN  | OE1-CD-NE2 | -6.03 | 116.57      | 122.60   |
| 1   | A     | 67  | GLN  | OE1-CD-NE2 | -6.02 | 116.58      | 122.60   |
| 1   | D     | 211 | ILE  | CA-C-N     | -6.01 | 116.98      | 121.61   |
| 1   | D     | 211 | ILE  | C-N-CA     | -6.01 | 116.98      | 121.61   |
| 1   | A     | 281 | GLY  | N-CA-C     | 6.00  | 121.62      | 114.48   |
| 1   | F     | 133 | ASP  | CA-CB-CG   | -5.99 | 106.61      | 112.60   |
| 1   | B     | 164 | ARG  | NE-CZ-NH2  | -5.97 | 113.83      | 119.20   |
| 1   | C     | 20  | THR  | N-CA-CB    | -5.96 | 100.42      | 110.49   |
| 1   | B     | 74  | VAL  | CA-CB-CG1  | 5.94  | 120.49      | 110.40   |
| 1   | A     | 316 | VAL  | CA-CB-CG1  | 5.93  | 120.47      | 110.40   |
| 1   | D     | 215 | VAL  | CA-CB-CG1  | 5.92  | 120.46      | 110.40   |
| 1   | F     | 200 | ARG  | NE-CZ-NH1  | 5.91  | 127.41      | 121.50   |
| 1   | E     | 271 | ARG  | NE-CZ-NH1  | 5.91  | 127.41      | 121.50   |
| 1   | A     | 79  | HIS  | CA-CB-CG   | -5.91 | 107.89      | 113.80   |
| 1   | E     | 297 | THR  | CB-CA-C    | 5.90  | 120.54      | 110.56   |
| 1   | F     | 20  | THR  | N-CA-CB    | -5.90 | 100.52      | 110.49   |
| 1   | D     | 206 | GLY  | O-C-N      | -5.88 | 116.29      | 122.52   |
| 1   | A     | 355 | LEU  | CA-C-N     | -5.87 | 115.39      | 122.90   |
| 1   | A     | 355 | LEU  | C-N-CA     | -5.87 | 115.39      | 122.90   |
| 1   | D     | 25  | PRO  | CB-CA-C    | -5.86 | 101.90      | 111.56   |
| 1   | E     | 74  | VAL  | CA-CB-CG1  | 5.86  | 120.36      | 110.40   |
| 1   | D     | 25  | PRO  | CA-N-CD    | 5.84  | 120.18      | 112.00   |
| 1   | A     | 360 | ASP  | CA-CB-CG   | -5.84 | 106.76      | 112.60   |
| 1   | E     | 120 | ARG  | CG-CD-NE   | 5.83  | 124.83      | 112.00   |
| 1   | D     | 279 | ARG  | NE-CZ-NH1  | 5.81  | 127.31      | 121.50   |
| 1   | C     | 300 | GLN  | OE1-CD-NE2 | 5.78  | 128.38      | 122.60   |
| 1   | E     | 21  | GLY  | N-CA-C     | 5.77  | 126.86      | 113.18   |
| 1   | A     | 310 | PHE  | CA-CB-CG   | -5.76 | 108.04      | 113.80   |
| 1   | D     | 316 | VAL  | CG1-CB-CG2 | 5.76  | 123.47      | 110.80   |
| 1   | D     | 21  | GLY  | N-CA-C     | 5.76  | 126.83      | 113.18   |
| 1   | C     | 313 | VAL  | N-CA-CB    | -5.74 | 102.80      | 112.44   |
| 1   | E     | 164 | ARG  | NE-CZ-NH2  | -5.74 | 114.04      | 119.20   |
| 1   | B     | 202 | VAL  | CA-C-O     | -5.73 | 115.65      | 121.67   |
| 1   | C     | 215 | VAL  | CA-CB-CG1  | 5.73  | 120.14      | 110.40   |
| 1   | A     | 215 | VAL  | CG1-CB-CG2 | 5.72  | 123.39      | 110.80   |
| 1   | B     | 19  | PHE  | CA-CB-CG   | -5.71 | 108.09      | 113.80   |
| 1   | B     | 79  | HIS  | CA-CB-CG   | -5.71 | 108.09      | 113.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | E     | 33  | ASP  | N-CA-CB    | 5.71  | 118.77      | 109.69   |
| 1   | F     | 215 | VAL  | CA-CB-CG1  | 5.70  | 120.09      | 110.40   |
| 1   | E     | 24  | GLY  | N-CA-C     | -5.65 | 105.39      | 112.23   |
| 1   | F     | 19  | PHE  | O-C-N      | -5.65 | 116.34      | 123.01   |
| 1   | B     | 296 | SER  | CA-C-O     | 5.65  | 127.49      | 121.11   |
| 1   | D     | 297 | THR  | CA-CB-OG1  | 5.64  | 118.06      | 109.60   |
| 1   | D     | 26  | TYR  | N-CA-C     | -5.63 | 106.17      | 113.16   |
| 1   | B     | 187 | ILE  | CA-C-O     | -5.63 | 114.39      | 120.36   |
| 1   | B     | 25  | PRO  | O-C-N      | -5.61 | 115.79      | 122.24   |
| 1   | C     | 66  | MET  | CA-C-O     | -5.61 | 112.70      | 119.49   |
| 1   | E     | 19  | PHE  | CA-CB-CG   | -5.61 | 108.19      | 113.80   |
| 1   | C     | 211 | ILE  | CA-C-N     | -5.59 | 118.32      | 122.18   |
| 1   | C     | 211 | ILE  | C-N-CA     | -5.59 | 118.32      | 122.18   |
| 1   | E     | 147 | ASP  | CA-CB-CG   | 5.59  | 118.19      | 112.60   |
| 1   | B     | 201 | VAL  | CA-C-O     | -5.58 | 114.36      | 120.84   |
| 1   | F     | 245 | LEU  | CD1-CG-CD2 | -5.57 | 98.54       | 110.80   |
| 1   | E     | 280 | ASN  | CA-C-N     | -5.57 | 117.40      | 123.30   |
| 1   | E     | 280 | ASN  | C-N-CA     | -5.57 | 117.40      | 123.30   |
| 1   | A     | 373 | ARG  | CG-CD-NE   | -5.55 | 99.79       | 112.00   |
| 1   | D     | 147 | ASP  | CA-CB-CG   | 5.50  | 118.10      | 112.60   |
| 1   | C     | 79  | HIS  | CA-CB-CG   | -5.49 | 108.31      | 113.80   |
| 1   | C     | 311 | LEU  | CA-C-O     | -5.48 | 114.92      | 121.11   |
| 1   | F     | 355 | LEU  | N-CA-C     | -5.47 | 99.50       | 108.41   |
| 1   | B     | 204 | PHE  | CA-C-O     | -5.46 | 113.54      | 120.20   |
| 1   | A     | 177 | GLU  | CA-C-N     | -5.46 | 117.22      | 121.86   |
| 1   | A     | 177 | GLU  | C-N-CA     | -5.46 | 117.22      | 121.86   |
| 1   | F     | 145 | THR  | N-CA-CB    | 5.43  | 121.14      | 111.69   |
| 1   | C     | 39  | PHE  | CA-CB-CG   | 5.41  | 119.21      | 113.80   |
| 1   | E     | 373 | ARG  | CG-CD-NE   | -5.41 | 100.09      | 112.00   |
| 1   | D     | 19  | PHE  | CA-CB-CG   | -5.39 | 108.41      | 113.80   |
| 1   | D     | 237 | ARG  | CD-NE-CZ   | 5.38  | 131.93      | 124.40   |
| 1   | A     | 19  | PHE  | CA-CB-CG   | -5.38 | 108.42      | 113.80   |
| 1   | D     | 79  | HIS  | CA-CB-CG   | -5.36 | 108.44      | 113.80   |
| 1   | D     | 355 | LEU  | N-CA-C     | -5.36 | 99.55       | 108.34   |
| 1   | E     | 318 | ASP  | N-CA-CB    | -5.35 | 102.09      | 110.44   |
| 1   | C     | 373 | ARG  | CG-CD-NE   | -5.35 | 100.23      | 112.00   |
| 1   | A     | 299 | ASN  | OD1-CG-ND2 | -5.34 | 117.25      | 122.60   |
| 1   | D     | 207 | ARG  | NE-CZ-NH1  | 5.34  | 126.84      | 121.50   |
| 1   | E     | 312 | ASP  | CA-CB-CG   | -5.34 | 107.26      | 112.60   |
| 1   | A     | 297 | THR  | CA-CB-OG1  | 5.33  | 117.60      | 109.60   |
| 1   | C     | 281 | GLY  | N-CA-C     | 5.33  | 119.28      | 113.58   |
| 1   | D     | 73  | PRO  | CA-C-N     | -5.32 | 116.17      | 123.14   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 73  | PRO  | C-N-CA     | -5.32 | 116.17      | 123.14   |
| 1   | E     | 207 | ARG  | CA-C-O     | -5.32 | 115.23      | 121.46   |
| 1   | A     | 363 | ARG  | NE-CZ-NH2  | -5.32 | 114.42      | 119.20   |
| 1   | E     | 215 | VAL  | CA-CB-CG1  | 5.32  | 119.44      | 110.40   |
| 1   | D     | 297 | THR  | N-CA-C     | -5.31 | 106.48      | 113.17   |
| 1   | B     | 271 | ARG  | CD-NE-CZ   | 5.30  | 131.82      | 124.40   |
| 1   | A     | 215 | VAL  | CA-CB-CG1  | 5.28  | 119.38      | 110.40   |
| 1   | C     | 53  | ARG  | NH1-CZ-NH2 | 5.28  | 126.17      | 119.30   |
| 1   | F     | 280 | ASN  | CA-CB-CG   | -5.28 | 107.32      | 112.60   |
| 1   | C     | 120 | ARG  | NE-CZ-NH1  | 5.27  | 126.77      | 121.50   |
| 1   | F     | 205 | GLY  | CA-C-O     | -5.25 | 113.45      | 119.80   |
| 1   | D     | 120 | ARG  | NE-CZ-NH1  | 5.25  | 126.75      | 121.50   |
| 1   | D     | 283 | PRO  | N-CA-C     | -5.24 | 107.33      | 114.98   |
| 1   | D     | 371 | TYR  | CA-C-O     | -5.23 | 113.56      | 119.78   |
| 1   | A     | 311 | LEU  | CA-C-O     | -5.22 | 115.06      | 120.70   |
| 1   | A     | 120 | ARG  | CG-CD-NE   | 5.22  | 123.48      | 112.00   |
| 1   | B     | 71  | PRO  | CA-C-O     | -5.22 | 115.39      | 121.34   |
| 1   | D     | 26  | TYR  | CA-C-O     | -5.21 | 112.98      | 119.28   |
| 1   | C     | 133 | ASP  | CA-CB-CG   | -5.21 | 107.39      | 112.60   |
| 1   | B     | 125 | ARG  | NE-CZ-NH2  | -5.20 | 114.52      | 119.20   |
| 1   | B     | 311 | LEU  | CA-C-O     | -5.20 | 115.24      | 121.11   |
| 1   | A     | 207 | ARG  | NE-CZ-NH1  | 5.19  | 126.69      | 121.50   |
| 1   | F     | 81  | PHE  | CA-CB-CG   | -5.19 | 108.61      | 113.80   |
| 1   | C     | 316 | VAL  | CB-CA-C    | 5.17  | 118.77      | 111.63   |
| 1   | C     | 179 | ASN  | OD1-CG-ND2 | -5.14 | 117.46      | 122.60   |
| 1   | B     | 21  | GLY  | N-CA-C     | 5.13  | 125.34      | 113.18   |
| 1   | F     | 78  | VAL  | O-C-N      | -5.13 | 117.65      | 123.03   |
| 1   | F     | 20  | THR  | CA-C-N     | 5.12  | 131.46      | 121.41   |
| 1   | F     | 20  | THR  | C-N-CA     | 5.12  | 131.46      | 121.41   |
| 1   | C     | 231 | PRO  | CA-C-N     | 5.12  | 127.47      | 120.46   |
| 1   | C     | 231 | PRO  | C-N-CA     | 5.12  | 127.47      | 120.46   |
| 1   | F     | 307 | SER  | CA-C-O     | -5.12 | 115.22      | 121.36   |
| 1   | B     | 33  | ASP  | CA-CB-CG   | -5.12 | 107.48      | 112.60   |
| 1   | A     | 211 | ILE  | CA-C-N     | -5.11 | 118.60      | 122.33   |
| 1   | A     | 211 | ILE  | C-N-CA     | -5.11 | 118.60      | 122.33   |
| 1   | D     | 280 | ASN  | CA-CB-CG   | -5.10 | 107.50      | 112.60   |
| 1   | B     | 207 | ARG  | NE-CZ-NH2  | -5.10 | 114.61      | 119.20   |
| 1   | E     | 79  | HIS  | CA-CB-CG   | -5.09 | 108.71      | 113.80   |
| 1   | D     | 37  | VAL  | CA-C-N     | -5.08 | 117.69      | 121.61   |
| 1   | D     | 37  | VAL  | C-N-CA     | -5.08 | 117.69      | 121.61   |
| 1   | B     | 178 | GLY  | CA-C-O     | 5.08  | 125.10      | 120.53   |
| 1   | B     | 107 | ASN  | OD1-CG-ND2 | -5.07 | 117.53      | 122.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 111 | ILE  | N-CA-C    | 5.07  | 115.28      | 110.42   |
| 1   | A     | 182 | GLY  | O-C-N     | -5.06 | 116.88      | 122.24   |
| 1   | E     | 97  | GLY  | CA-C-O    | -5.06 | 113.40      | 119.01   |
| 1   | F     | 272 | ARG  | CG-CD-NE  | 5.03  | 123.07      | 112.00   |
| 1   | C     | 80  | ARG  | NE-CZ-NH2 | -5.01 | 114.69      | 119.20   |
| 1   | B     | 203 | GLU  | CA-C-O    | -5.01 | 114.97      | 120.43   |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group               |
|-----|-------|-----|------|---------------------|
| 1   | A     | 19  | PHE  | Peptide             |
| 1   | D     | 19  | PHE  | Peptide             |
| 1   | D     | 206 | GLY  | Mainchain           |
| 1   | E     | 19  | PHE  | Peptide             |
| 1   | E     | 317 | ASN  | Mainchain,Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2747  | 0        | 2683     | 43      | 0            |
| 1   | B     | 2747  | 0        | 2683     | 41      | 0            |
| 1   | C     | 2747  | 0        | 2683     | 42      | 0            |
| 1   | D     | 2747  | 0        | 2683     | 53      | 5            |
| 1   | E     | 2747  | 0        | 2683     | 70      | 3            |
| 1   | F     | 2747  | 0        | 2683     | 38      | 0            |
| 2   | A     | 220   | 0        | 0        | 2       | 0            |
| 2   | B     | 220   | 0        | 0        | 5       | 0            |
| 2   | C     | 230   | 0        | 0        | 8       | 5            |
| 2   | D     | 216   | 0        | 0        | 10      | 0            |
| 2   | E     | 207   | 0        | 0        | 10      | 4            |
| 2   | F     | 211   | 0        | 0        | 5       | 1            |
| All | All   | 17786 | 0        | 16098    | 247     | 9            |

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 8.

All (247) 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:E:317:ASN:CB   | 1:E:317:ASN:CA   | 1.76                     | 1.55              |
| 1:E:317:ASN:CB   | 1:E:317:ASN:C    | 1.90                     | 1.43              |
| 1:E:317:ASN:HB3  | 1:E:318:ASP:N    | 1.42                     | 1.31              |
| 1:D:25:PRO:HB2   | 1:D:31:ASP:OD1   | 1.43                     | 1.18              |
| 1:E:317:ASN:CB   | 1:E:318:ASP:N    | 2.01                     | 1.17              |
| 1:E:92:TRP:CH2   | 2:E:798:HOH:O    | 2.03                     | 1.10              |
| 1:A:373:ARG:NH2  | 1:C:373:ARG:HH22 | 1.50                     | 1.09              |
| 1:B:373:ARG:NH2  | 1:D:373:ARG:HH22 | 1.51                     | 1.08              |
| 1:A:373:ARG:HH22 | 1:C:373:ARG:NH2  | 1.52                     | 1.06              |
| 1:E:373:ARG:NH2  | 1:F:373:ARG:HH22 | 1.56                     | 1.03              |
| 1:B:373:ARG:HH22 | 1:D:373:ARG:NH2  | 1.57                     | 1.01              |
| 1:E:92:TRP:CH2   | 1:E:96:GLY:HA2   | 1.94                     | 1.01              |
| 1:E:373:ARG:HH22 | 1:F:373:ARG:NH2  | 1.58                     | 1.01              |
| 1:E:92:TRP:CZ3   | 2:E:798:HOH:O    | 2.16                     | 0.99              |
| 1:E:317:ASN:C    | 1:E:317:ASN:HB3  | 1.73                     | 0.95              |
| 1:F:244:GLN:HE22 | 1:F:355:LEU:H    | 1.16                     | 0.94              |
| 1:D:262:MET:HB3  | 2:D:459:HOH:O    | 1.69                     | 0.93              |
| 1:D:25:PRO:CB    | 1:D:31:ASP:OD1   | 2.19                     | 0.91              |
| 1:A:109:HIS:HE1  | 1:D:138:ILE:H    | 1.18                     | 0.88              |
| 1:A:299:ASN:HD21 | 1:A:314:GLU:H    | 1.18                     | 0.88              |
| 1:F:20:THR:OG1   | 1:F:200:ARG:NH2  | 2.07                     | 0.88              |
| 1:E:299:ASN:HD21 | 1:E:314:GLU:H    | 1.21                     | 0.87              |
| 1:E:373:ARG:HH22 | 1:F:373:ARG:HH22 | 0.86                     | 0.86              |
| 1:B:33:ASP:OD1   | 2:B:422:HOH:O    | 1.94                     | 0.85              |
| 1:B:138:ILE:H    | 1:C:109:HIS:HE1  | 1.20                     | 0.85              |
| 1:A:138:ILE:H    | 1:D:109:HIS:HE1  | 1.23                     | 0.85              |
| 1:B:109:HIS:HE1  | 1:C:138:ILE:H    | 1.22                     | 0.84              |
| 1:D:33:ASP:OD1   | 2:D:427:HOH:O    | 1.95                     | 0.83              |
| 1:E:92:TRP:CH2   | 1:E:96:GLY:CA    | 2.60                     | 0.83              |
| 1:E:112:GLY:N    | 2:E:868:HOH:O    | 2.06                     | 0.83              |
| 1:B:349:THR:HB   | 1:B:350:PRO:HD2  | 1.60                     | 0.83              |
| 1:B:299:ASN:HD21 | 1:B:314:GLU:H    | 1.26                     | 0.82              |
| 1:C:299:ASN:HD21 | 1:C:314:GLU:H    | 1.27                     | 0.82              |
| 1:E:92:TRP:CZ2   | 2:E:798:HOH:O    | 2.24                     | 0.82              |
| 1:B:244:GLN:HE22 | 1:B:355:LEU:H    | 1.25                     | 0.81              |
| 1:C:244:GLN:HE22 | 1:C:355:LEU:H    | 1.28                     | 0.81              |
| 1:D:258:ASP:HA   | 1:D:297:THR:HG22 | 1.63                     | 0.81              |
| 1:A:244:GLN:HE22 | 1:A:355:LEU:H    | 1.29                     | 0.80              |
| 1:D:244:GLN:HE22 | 1:D:355:LEU:H    | 1.31                     | 0.79              |
| 1:C:33:ASP:OD1   | 2:C:425:HOH:O    | 2.00                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:299:ASN:HD21 | 1:D:314:GLU:H    | 1.28                     | 0.78              |
| 1:E:317:ASN:HB3  | 1:E:318:ASP:CA   | 2.12                     | 0.78              |
| 1:F:262:MET:H    | 1:F:265:GLN:HE21 | 1.30                     | 0.78              |
| 1:E:244:GLN:HE22 | 1:E:355:LEU:H    | 1.32                     | 0.77              |
| 1:E:262:MET:H    | 1:E:265:GLN:HE21 | 1.33                     | 0.77              |
| 1:B:20:THR:OG1   | 1:B:200:ARG:NH2  | 2.17                     | 0.77              |
| 1:E:33:ASP:OD1   | 2:E:788:HOH:O    | 2.02                     | 0.77              |
| 1:F:299:ASN:HD21 | 1:F:314:GLU:H    | 1.31                     | 0.76              |
| 1:C:20:THR:OG1   | 1:C:200:ARG:NH2  | 2.18                     | 0.76              |
| 1:A:373:ARG:NH1  | 1:C:373:ARG:NH1  | 2.33                     | 0.76              |
| 1:D:20:THR:OG1   | 1:D:200:ARG:NH2  | 2.20                     | 0.75              |
| 1:E:317:ASN:HB3  | 1:E:319:GLU:N    | 2.01                     | 0.75              |
| 1:E:92:TRP:CZ3   | 1:E:96:GLY:N     | 2.56                     | 0.74              |
| 1:C:258:ASP:HA   | 1:C:297:THR:HG22 | 1.71                     | 0.73              |
| 1:E:317:ASN:CB   | 1:E:317:ASN:O    | 2.36                     | 0.73              |
| 1:A:262:MET:H    | 1:A:265:GLN:HE21 | 1.35                     | 0.73              |
| 1:B:262:MET:H    | 1:B:265:GLN:HE21 | 1.36                     | 0.73              |
| 1:C:297:THR:HG21 | 2:C:425:HOH:O    | 1.89                     | 0.73              |
| 1:E:258:ASP:HA   | 1:E:297:THR:HG22 | 1.71                     | 0.73              |
| 1:C:33:ASP:OD1   | 2:C:538:HOH:O    | 2.07                     | 0.72              |
| 1:C:262:MET:H    | 1:C:265:GLN:HE21 | 1.36                     | 0.72              |
| 1:A:373:ARG:NH1  | 1:C:373:ARG:HH12 | 1.87                     | 0.72              |
| 1:B:297:THR:HG21 | 2:B:422:HOH:O    | 1.90                     | 0.71              |
| 1:A:258:ASP:HA   | 1:A:297:THR:HG22 | 1.71                     | 0.71              |
| 1:A:373:ARG:HH12 | 1:C:373:ARG:NH1  | 1.89                     | 0.70              |
| 1:A:373:ARG:HH22 | 1:C:373:ARG:HH22 | 0.75                     | 0.70              |
| 1:B:33:ASP:OD1   | 2:B:532:HOH:O    | 2.09                     | 0.70              |
| 1:B:258:ASP:HA   | 1:B:297:THR:HG22 | 1.74                     | 0.70              |
| 1:E:20:THR:OG1   | 1:E:200:ARG:NH2  | 2.25                     | 0.69              |
| 1:E:33:ASP:OD1   | 2:E:906:HOH:O    | 2.10                     | 0.69              |
| 1:A:20:THR:OG1   | 1:A:200:ARG:NH2  | 2.26                     | 0.68              |
| 1:A:109:HIS:CE1  | 1:D:138:ILE:H    | 2.08                     | 0.68              |
| 1:D:297:THR:HG21 | 2:D:427:HOH:O    | 1.94                     | 0.68              |
| 1:D:262:MET:H    | 1:D:265:GLN:HE21 | 1.39                     | 0.67              |
| 1:E:297:THR:HG21 | 2:E:788:HOH:O    | 1.95                     | 0.67              |
| 1:D:203:GLU:OE2  | 1:D:206:GLY:HA2  | 1.95                     | 0.67              |
| 1:E:317:ASN:HB3  | 1:E:319:GLU:H    | 1.61                     | 0.66              |
| 1:F:258:ASP:HA   | 1:F:297:THR:HG22 | 1.78                     | 0.66              |
| 1:B:109:HIS:CE1  | 1:C:138:ILE:H    | 2.11                     | 0.66              |
| 1:C:20:THR:CB    | 1:C:200:ARG:HH21 | 2.09                     | 0.66              |
| 1:B:297:THR:CG2  | 2:B:422:HOH:O    | 2.44                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:317:ASN:HB3  | 1:E:318:ASP:C    | 2.21                     | 0.65              |
| 1:E:373:ARG:NH1  | 1:F:373:ARG:NH1  | 2.45                     | 0.65              |
| 1:A:20:THR:CB    | 1:A:200:ARG:HH21 | 2.09                     | 0.65              |
| 1:D:297:THR:CG2  | 2:D:427:HOH:O    | 2.46                     | 0.64              |
| 1:C:323:THR:HG23 | 2:C:603:HOH:O    | 1.98                     | 0.63              |
| 1:F:242:GLN:HB2  | 2:F:581:HOH:O    | 1.99                     | 0.63              |
| 1:D:25:PRO:CG    | 1:D:31:ASP:OD1   | 2.47                     | 0.62              |
| 1:D:25:PRO:HG2   | 1:D:31:ASP:OD1   | 2.00                     | 0.62              |
| 1:C:204:PHE:CE1  | 1:C:316:VAL:HG22 | 2.35                     | 0.61              |
| 1:C:349:THR:HB   | 1:C:350:PRO:HD2  | 1.83                     | 0.60              |
| 1:B:138:ILE:H    | 1:C:109:HIS:CE1  | 2.12                     | 0.59              |
| 1:B:349:THR:HB   | 1:B:350:PRO:CD   | 2.29                     | 0.59              |
| 1:B:20:THR:HG1   | 1:B:200:ARG:NH2  | 2.00                     | 0.59              |
| 1:E:297:THR:CG2  | 2:E:788:HOH:O    | 2.51                     | 0.59              |
| 1:D:20:THR:CB    | 1:D:200:ARG:HH21 | 2.16                     | 0.59              |
| 1:E:20:THR:CB    | 1:E:200:ARG:HH21 | 2.16                     | 0.58              |
| 1:E:92:TRP:CE2   | 1:E:96:GLY:HA3   | 2.38                     | 0.58              |
| 1:E:373:ARG:NH2  | 1:F:373:ARG:NH2  | 2.32                     | 0.58              |
| 1:E:92:TRP:HZ3   | 1:E:95:ASP:HB3   | 1.68                     | 0.58              |
| 1:E:92:TRP:CZ2   | 1:E:96:GLY:CA    | 2.87                     | 0.58              |
| 1:B:204:PHE:CE1  | 1:B:316:VAL:HG22 | 2.38                     | 0.58              |
| 1:D:204:PHE:CE1  | 1:D:316:VAL:HG22 | 2.39                     | 0.58              |
| 1:F:20:THR:HG1   | 1:F:200:ARG:NH2  | 2.01                     | 0.58              |
| 1:C:262:MET:H    | 1:C:265:GLN:NE2  | 2.01                     | 0.57              |
| 1:E:204:PHE:CE1  | 1:E:316:VAL:HG22 | 2.39                     | 0.57              |
| 1:C:297:THR:CG2  | 2:C:425:HOH:O    | 2.47                     | 0.57              |
| 1:A:138:ILE:H    | 1:D:109:HIS:CE1  | 2.13                     | 0.56              |
| 1:E:92:TRP:HA    | 1:E:92:TRP:CE3   | 2.41                     | 0.56              |
| 1:F:204:PHE:CE1  | 1:F:316:VAL:HG22 | 2.40                     | 0.56              |
| 1:D:25:PRO:HG3   | 2:D:490:HOH:O    | 2.04                     | 0.56              |
| 1:E:317:ASN:CB   | 1:E:319:GLU:H    | 2.18                     | 0.56              |
| 1:D:25:PRO:CG    | 2:D:490:HOH:O    | 2.53                     | 0.55              |
| 1:A:319:GLU:HB3  | 1:A:320:PRO:HD3  | 1.88                     | 0.55              |
| 1:D:323:THR:HG23 | 2:D:590:HOH:O    | 2.05                     | 0.55              |
| 1:C:20:THR:HG1   | 1:C:200:ARG:NH2  | 2.04                     | 0.55              |
| 1:E:92:TRP:CE2   | 2:E:798:HOH:O    | 2.57                     | 0.55              |
| 1:E:272:ARG:HD2  | 1:F:283:PRO:O    | 2.07                     | 0.54              |
| 1:D:114:ALA:HA   | 1:D:163:VAL:HG11 | 1.90                     | 0.54              |
| 1:B:373:ARG:HH22 | 1:D:373:ARG:HH22 | 0.71                     | 0.54              |
| 1:F:319:GLU:HB3  | 1:F:320:PRO:HD3  | 1.90                     | 0.54              |
| 1:A:262:MET:HA   | 1:A:262:MET:HE2  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:349:THR:HB   | 1:D:350:PRO:CD   | 2.37                     | 0.54              |
| 1:E:165:LYS:HD3  | 1:E:169:ASN:HD21 | 1.73                     | 0.54              |
| 1:F:20:THR:CB    | 1:F:200:ARG:HH21 | 2.21                     | 0.53              |
| 1:C:349:THR:HB   | 1:C:350:PRO:CD   | 2.38                     | 0.53              |
| 1:E:92:TRP:CZ2   | 1:E:96:GLY:HA3   | 2.44                     | 0.53              |
| 1:B:137:TRP:HB2  | 1:C:108:THR:HG21 | 1.90                     | 0.53              |
| 1:D:349:THR:HB   | 1:D:350:PRO:HD2  | 1.89                     | 0.53              |
| 1:A:204:PHE:CE1  | 1:A:316:VAL:HG22 | 2.45                     | 0.52              |
| 1:D:262:MET:H    | 1:D:265:GLN:NE2  | 2.07                     | 0.52              |
| 1:A:262:MET:H    | 1:A:265:GLN:NE2  | 2.05                     | 0.52              |
| 1:F:262:MET:H    | 1:F:265:GLN:NE2  | 2.01                     | 0.52              |
| 1:D:20:THR:HG21  | 2:D:419:HOH:O    | 2.08                     | 0.52              |
| 1:C:366:ALA:O    | 1:C:370:GLN:HG3  | 2.10                     | 0.52              |
| 1:E:317:ASN:CB   | 1:E:318:ASP:H    | 2.16                     | 0.52              |
| 1:B:262:MET:HE2  | 1:B:262:MET:HA   | 1.92                     | 0.52              |
| 1:A:33:ASP:HB2   | 2:F:572:HOH:O    | 2.09                     | 0.51              |
| 1:E:92:TRP:CZ3   | 1:E:96:GLY:CA    | 2.93                     | 0.51              |
| 1:D:33:ASP:OD1   | 1:D:33:ASP:N     | 2.43                     | 0.51              |
| 1:C:262:MET:HA   | 1:C:262:MET:HE2  | 1.93                     | 0.51              |
| 1:B:319:GLU:HB3  | 1:B:320:PRO:HD3  | 1.93                     | 0.51              |
| 1:E:66:MET:HE3   | 2:E:1260:HOH:O   | 2.10                     | 0.51              |
| 1:B:230:VAL:HG22 | 1:B:373:ARG:NH1  | 2.26                     | 0.51              |
| 1:A:299:ASN:ND2  | 1:A:314:GLU:H    | 1.96                     | 0.51              |
| 1:F:20:THR:HG21  | 2:F:420:HOH:O    | 2.10                     | 0.50              |
| 1:E:92:TRP:CZ2   | 1:E:96:GLY:HA2   | 2.41                     | 0.50              |
| 1:E:114:ALA:HA   | 1:E:163:VAL:HG11 | 1.94                     | 0.50              |
| 1:A:373:ARG:NH2  | 1:C:373:ARG:NH2  | 2.30                     | 0.50              |
| 1:A:137:TRP:HB2  | 1:D:108:THR:HG21 | 1.94                     | 0.50              |
| 1:A:305:HIS:HE1  | 2:A:436:HOH:O    | 1.95                     | 0.50              |
| 1:D:73:PRO:HA    | 1:D:100:LEU:HD13 | 1.94                     | 0.50              |
| 1:B:20:THR:CB    | 1:B:200:ARG:HH21 | 2.25                     | 0.49              |
| 1:E:262:MET:H    | 1:E:265:GLN:NE2  | 2.04                     | 0.49              |
| 1:E:349:THR:HB   | 1:E:350:PRO:CD   | 2.42                     | 0.49              |
| 1:B:373:ARG:NH2  | 1:D:373:ARG:NH2  | 2.34                     | 0.49              |
| 1:D:262:MET:CB   | 2:D:459:HOH:O    | 2.42                     | 0.49              |
| 1:F:165:LYS:HD3  | 1:F:169:ASN:HD21 | 1.77                     | 0.49              |
| 1:C:12:ALA:H     | 1:C:338:ASN:ND2  | 2.11                     | 0.48              |
| 1:E:13:ARG:NH2   | 1:E:20:THR:O     | 2.46                     | 0.48              |
| 1:F:238:ASP:CG   | 1:F:363:ARG:HH22 | 2.21                     | 0.48              |
| 1:E:262:MET:HE2  | 1:E:262:MET:HA   | 1.95                     | 0.48              |
| 1:F:12:ALA:H     | 1:F:338:ASN:ND2  | 2.11                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:230:VAL:HG22 | 1:E:373:ARG:NH1  | 2.28                     | 0.48              |
| 1:E:74:VAL:HG13  | 1:E:295:PHE:HB2  | 1.95                     | 0.48              |
| 1:B:262:MET:H    | 1:B:265:GLN:NE2  | 2.06                     | 0.48              |
| 1:D:40:GLN:OE1   | 1:D:165:LYS:HD2  | 2.14                     | 0.48              |
| 1:E:317:ASN:CB   | 1:E:319:GLU:N    | 2.75                     | 0.48              |
| 1:E:165:LYS:HD3  | 1:E:169:ASN:ND2  | 2.28                     | 0.47              |
| 1:F:354:LEU:N    | 1:F:354:LEU:HD12 | 2.29                     | 0.47              |
| 1:D:12:ALA:H     | 1:D:338:ASN:ND2  | 2.12                     | 0.47              |
| 1:E:20:THR:HG1   | 1:E:200:ARG:NH2  | 2.13                     | 0.47              |
| 1:E:92:TRP:CE3   | 1:E:96:GLY:N     | 2.81                     | 0.47              |
| 1:A:20:THR:HG1   | 1:A:200:ARG:NH2  | 2.12                     | 0.47              |
| 1:A:236:MET:HE1  | 1:A:359:ILE:HG13 | 1.97                     | 0.47              |
| 1:A:354:LEU:N    | 1:A:354:LEU:HD12 | 2.30                     | 0.47              |
| 1:B:120:ARG:HG2  | 1:C:156:PHE:CZ   | 2.50                     | 0.47              |
| 1:C:114:ALA:HA   | 1:C:163:VAL:HG11 | 1.95                     | 0.47              |
| 1:D:203:GLU:HG3  | 1:D:206:GLY:C    | 2.39                     | 0.47              |
| 1:A:20:THR:HG21  | 2:A:409:HOH:O    | 2.15                     | 0.47              |
| 1:A:373:ARG:CZ   | 1:C:373:ARG:HH12 | 2.27                     | 0.47              |
| 1:E:299:ASN:ND2  | 1:E:314:GLU:H    | 2.00                     | 0.46              |
| 1:F:165:LYS:HD3  | 1:F:169:ASN:ND2  | 2.30                     | 0.46              |
| 1:A:109:HIS:HE1  | 1:D:138:ILE:N    | 2.00                     | 0.46              |
| 1:F:306:ARG:NH1  | 2:F:554:HOH:O    | 2.48                     | 0.46              |
| 1:E:92:TRP:CZ3   | 1:E:95:ASP:HB3   | 2.50                     | 0.46              |
| 1:B:138:ILE:N    | 1:C:109:HIS:HE1  | 2.01                     | 0.45              |
| 1:D:165:LYS:HD3  | 1:D:169:ASN:ND2  | 2.31                     | 0.45              |
| 1:B:108:THR:HG21 | 1:C:137:TRP:HB2  | 1.97                     | 0.45              |
| 1:C:20:THR:HG21  | 2:C:417:HOH:O    | 2.16                     | 0.45              |
| 1:B:373:ARG:NH1  | 1:D:373:ARG:NH1  | 2.64                     | 0.45              |
| 1:D:305:HIS:HE1  | 2:D:448:HOH:O    | 1.99                     | 0.45              |
| 1:F:114:ALA:HA   | 1:F:163:VAL:HG11 | 1.99                     | 0.45              |
| 1:F:262:MET:HA   | 1:F:262:MET:HE2  | 1.98                     | 0.45              |
| 1:A:349:THR:HB   | 1:A:350:PRO:CD   | 2.47                     | 0.45              |
| 1:B:373:ARG:HH12 | 1:D:373:ARG:CZ   | 2.30                     | 0.45              |
| 1:E:349:THR:HB   | 1:E:350:PRO:HD2  | 1.98                     | 0.45              |
| 1:D:165:LYS:HD3  | 1:D:169:ASN:HD21 | 1.82                     | 0.45              |
| 1:B:215:VAL:HG22 | 1:B:253:VAL:HG22 | 1.98                     | 0.44              |
| 1:A:257:THR:O    | 1:A:296:SER:HA   | 2.17                     | 0.44              |
| 1:F:73:PRO:HA    | 1:F:100:LEU:HD13 | 1.98                     | 0.44              |
| 1:F:146:TYR:CZ   | 1:F:148:GLY:HA3  | 2.52                     | 0.44              |
| 1:F:349:THR:HB   | 1:F:350:PRO:HD2  | 1.98                     | 0.44              |
| 1:B:33:ASP:CG    | 2:B:422:HOH:O    | 2.56                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:74:VAL:HG13  | 1:A:295:PHE:HB2  | 2.00                     | 0.44              |
| 1:A:373:ARG:HH12 | 1:C:373:ARG:CZ   | 2.31                     | 0.44              |
| 1:D:20:THR:HG1   | 1:D:200:ARG:NH2  | 2.15                     | 0.44              |
| 1:D:73:PRO:HG3   | 1:D:100:LEU:HD11 | 1.99                     | 0.44              |
| 1:C:354:LEU:HD12 | 1:C:354:LEU:N    | 2.33                     | 0.43              |
| 1:E:317:ASN:CA   | 1:E:317:ASN:CG   | 2.81                     | 0.43              |
| 1:E:20:THR:HB    | 1:E:200:ARG:HH21 | 1.83                     | 0.43              |
| 1:E:373:ARG:NH1  | 1:F:373:ARG:HH12 | 2.16                     | 0.43              |
| 1:F:374:LEU:HD12 | 1:F:374:LEU:HA   | 1.88                     | 0.43              |
| 1:A:20:THR:HG1   | 1:A:200:ARG:HH21 | 1.65                     | 0.43              |
| 1:C:74:VAL:HG13  | 1:C:295:PHE:HB2  | 1.99                     | 0.43              |
| 1:E:33:ASP:OD1   | 1:E:33:ASP:N     | 2.51                     | 0.42              |
| 1:E:373:ARG:HH12 | 1:F:373:ARG:NH1  | 2.16                     | 0.42              |
| 1:A:13:ARG:NH2   | 1:A:20:THR:O     | 2.50                     | 0.42              |
| 1:B:114:ALA:HA   | 1:B:163:VAL:HG11 | 2.01                     | 0.42              |
| 1:E:374:LEU:HD12 | 1:E:374:LEU:HA   | 1.93                     | 0.42              |
| 1:A:349:THR:HB   | 1:A:350:PRO:HD2  | 2.02                     | 0.42              |
| 1:D:25:PRO:HB2   | 1:D:26:TYR:H     | 1.07                     | 0.42              |
| 1:B:299:ASN:ND2  | 1:B:314:GLU:H    | 2.06                     | 0.42              |
| 1:F:230:VAL:HG22 | 1:F:373:ARG:NH1  | 2.35                     | 0.42              |
| 1:B:257:THR:O    | 1:B:296:SER:HA   | 2.20                     | 0.41              |
| 1:E:12:ALA:H     | 1:E:338:ASN:ND2  | 2.17                     | 0.41              |
| 1:E:373:ARG:HH12 | 1:F:373:ARG:CZ   | 2.33                     | 0.41              |
| 1:B:238:ASP:CG   | 1:B:363:ARG:HH22 | 2.28                     | 0.41              |
| 1:E:92:TRP:CZ3   | 1:E:95:ASP:C     | 2.98                     | 0.41              |
| 1:D:374:LEU:HD12 | 1:D:374:LEU:HA   | 1.88                     | 0.41              |
| 1:A:120:ARG:HG2  | 1:D:156:PHE:CZ   | 2.55                     | 0.41              |
| 1:C:305:HIS:HE1  | 2:C:446:HOH:O    | 2.03                     | 0.41              |
| 1:D:349:THR:CB   | 1:D:350:PRO:CD   | 2.99                     | 0.41              |
| 1:F:13:ARG:NH2   | 1:F:20:THR:O     | 2.46                     | 0.41              |
| 1:A:114:ALA:HA   | 1:A:163:VAL:HG11 | 2.02                     | 0.41              |
| 1:A:165:LYS:HD3  | 1:A:169:ASN:HD21 | 1.86                     | 0.41              |
| 1:C:354:LEU:HD12 | 2:C:514:HOH:O    | 2.20                     | 0.41              |
| 1:A:165:LYS:HD3  | 1:A:169:ASN:ND2  | 2.36                     | 0.41              |
| 1:F:354:LEU:HD12 | 1:F:354:LEU:H    | 1.86                     | 0.41              |
| 1:B:33:ASP:OD1   | 1:B:33:ASP:N     | 2.54                     | 0.41              |
| 1:E:317:ASN:CG   | 1:E:319:GLU:H    | 2.29                     | 0.41              |
| 1:B:147:ASP:HB3  | 1:B:186:MET:CE   | 2.51                     | 0.40              |
| 1:A:366:ALA:O    | 1:A:370:GLN:HG3  | 2.21                     | 0.40              |
| 1:D:74:VAL:HG13  | 1:D:295:PHE:HB2  | 2.04                     | 0.40              |
| 1:B:373:ARG:CZ   | 1:D:373:ARG:HH22 | 2.26                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:33:ASP:HA    | 2:F:572:HOH:O   | 2.22                     | 0.40              |
| 1:F:265:GLN:HE22 | 1:F:315:MET:HG3 | 1.86                     | 0.40              |

All (9) 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) |
|----------------|----------------------|--------------------------|-------------------|
| 1:E:317:ASN:CA | 2:E:899:HOH:O[2_665] | 1.71                     | 0.49              |
| 1:D:25:PRO:CA  | 2:C:573:HOH:O[3_545] | 1.88                     | 0.32              |
| 1:E:317:ASN:CB | 2:E:899:HOH:O[2_665] | 1.94                     | 0.26              |
| 1:D:33:ASP:OD1 | 2:C:589:HOH:O[3_545] | 1.95                     | 0.25              |
| 2:E:868:HOH:O  | 2:F:511:HOH:O[2_665] | 1.95                     | 0.25              |
| 1:D:25:PRO:CB  | 2:C:573:HOH:O[3_545] | 2.03                     | 0.17              |
| 1:D:207:ARG:N  | 2:C:566:HOH:O[3_545] | 2.10                     | 0.10              |
| 1:D:206:GLY:O  | 2:C:566:HOH:O[3_545] | 2.15                     | 0.05              |
| 1:E:317:ASN:CG | 2:E:899:HOH:O[2_665] | 2.15                     | 0.05              |

## 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     | 359/375 (96%)   | 348 (97%)  | 9 (2%)  | 2 (1%)   | 21          | 11 |
| 1   | B     | 359/375 (96%)   | 349 (97%)  | 9 (2%)  | 1 (0%)   | 36          | 26 |
| 1   | C     | 359/375 (96%)   | 347 (97%)  | 10 (3%) | 2 (1%)   | 21          | 11 |
| 1   | D     | 359/375 (96%)   | 348 (97%)  | 8 (2%)  | 3 (1%)   | 16          | 6  |
| 1   | E     | 359/375 (96%)   | 346 (96%)  | 11 (3%) | 2 (1%)   | 21          | 11 |
| 1   | F     | 359/375 (96%)   | 350 (98%)  | 7 (2%)  | 2 (1%)   | 21          | 11 |
| All | All   | 2154/2250 (96%) | 2088 (97%) | 54 (2%) | 12 (1%)  | 21          | 11 |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 25  | PRO  |
| 1   | A     | 21  | GLY  |
| 1   | B     | 21  | GLY  |
| 1   | C     | 21  | GLY  |
| 1   | D     | 20  | THR  |
| 1   | D     | 21  | GLY  |
| 1   | E     | 20  | THR  |
| 1   | E     | 21  | GLY  |
| 1   | F     | 21  | GLY  |
| 1   | A     | 20  | THR  |
| 1   | C     | 20  | THR  |
| 1   | F     | 20  | THR  |

### 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     | 286/297 (96%)   | 266 (93%)  | 20 (7%)  | 14          | 2 |
| 1   | B     | 286/297 (96%)   | 267 (93%)  | 19 (7%)  | 15          | 3 |
| 1   | C     | 286/297 (96%)   | 269 (94%)  | 17 (6%)  | 18          | 4 |
| 1   | D     | 286/297 (96%)   | 270 (94%)  | 16 (6%)  | 19          | 4 |
| 1   | E     | 286/297 (96%)   | 270 (94%)  | 16 (6%)  | 19          | 4 |
| 1   | F     | 286/297 (96%)   | 267 (93%)  | 19 (7%)  | 15          | 3 |
| All | All   | 1716/1782 (96%) | 1609 (94%) | 107 (6%) | 16          | 4 |

All (107) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | LYS  |
| 1   | A     | 20  | THR  |
| 1   | A     | 33  | ASP  |
| 1   | A     | 63  | LEU  |
| 1   | A     | 74  | VAL  |
| 1   | A     | 100 | LEU  |
| 1   | A     | 133 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 136 | LEU  |
| 1   | A     | 150 | LEU  |
| 1   | A     | 163 | VAL  |
| 1   | A     | 165 | LYS  |
| 1   | A     | 215 | VAL  |
| 1   | A     | 261 | LEU  |
| 1   | A     | 297 | THR  |
| 1   | A     | 313 | VAL  |
| 1   | A     | 316 | VAL  |
| 1   | A     | 319 | GLU  |
| 1   | A     | 354 | LEU  |
| 1   | A     | 364 | LEU  |
| 1   | A     | 373 | ARG  |
| 1   | B     | 9   | LYS  |
| 1   | B     | 52  | LYS  |
| 1   | B     | 63  | LEU  |
| 1   | B     | 74  | VAL  |
| 1   | B     | 100 | LEU  |
| 1   | B     | 133 | ASP  |
| 1   | B     | 136 | LEU  |
| 1   | B     | 150 | LEU  |
| 1   | B     | 163 | VAL  |
| 1   | B     | 165 | LYS  |
| 1   | B     | 203 | GLU  |
| 1   | B     | 215 | VAL  |
| 1   | B     | 261 | LEU  |
| 1   | B     | 297 | THR  |
| 1   | B     | 316 | VAL  |
| 1   | B     | 319 | GLU  |
| 1   | B     | 354 | LEU  |
| 1   | B     | 364 | LEU  |
| 1   | B     | 373 | ARG  |
| 1   | C     | 52  | LYS  |
| 1   | C     | 63  | LEU  |
| 1   | C     | 74  | VAL  |
| 1   | C     | 100 | LEU  |
| 1   | C     | 133 | ASP  |
| 1   | C     | 136 | LEU  |
| 1   | C     | 150 | LEU  |
| 1   | C     | 163 | VAL  |
| 1   | C     | 165 | LYS  |
| 1   | C     | 215 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 261 | LEU  |
| 1   | C     | 297 | THR  |
| 1   | C     | 313 | VAL  |
| 1   | C     | 316 | VAL  |
| 1   | C     | 354 | LEU  |
| 1   | C     | 364 | LEU  |
| 1   | C     | 373 | ARG  |
| 1   | D     | 63  | LEU  |
| 1   | D     | 74  | VAL  |
| 1   | D     | 100 | LEU  |
| 1   | D     | 133 | ASP  |
| 1   | D     | 136 | LEU  |
| 1   | D     | 150 | LEU  |
| 1   | D     | 163 | VAL  |
| 1   | D     | 165 | LYS  |
| 1   | D     | 215 | VAL  |
| 1   | D     | 261 | LEU  |
| 1   | D     | 297 | THR  |
| 1   | D     | 313 | VAL  |
| 1   | D     | 316 | VAL  |
| 1   | D     | 354 | LEU  |
| 1   | D     | 364 | LEU  |
| 1   | D     | 373 | ARG  |
| 1   | E     | 52  | LYS  |
| 1   | E     | 63  | LEU  |
| 1   | E     | 74  | VAL  |
| 1   | E     | 100 | LEU  |
| 1   | E     | 133 | ASP  |
| 1   | E     | 136 | LEU  |
| 1   | E     | 150 | LEU  |
| 1   | E     | 163 | VAL  |
| 1   | E     | 215 | VAL  |
| 1   | E     | 261 | LEU  |
| 1   | E     | 297 | THR  |
| 1   | E     | 316 | VAL  |
| 1   | E     | 317 | ASN  |
| 1   | E     | 354 | LEU  |
| 1   | E     | 364 | LEU  |
| 1   | E     | 373 | ARG  |
| 1   | F     | 9   | LYS  |
| 1   | F     | 52  | LYS  |
| 1   | F     | 63  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 74  | VAL  |
| 1   | F     | 100 | LEU  |
| 1   | F     | 133 | ASP  |
| 1   | F     | 136 | LEU  |
| 1   | F     | 150 | LEU  |
| 1   | F     | 163 | VAL  |
| 1   | F     | 165 | LYS  |
| 1   | F     | 215 | VAL  |
| 1   | F     | 261 | LEU  |
| 1   | F     | 297 | THR  |
| 1   | F     | 313 | VAL  |
| 1   | F     | 316 | VAL  |
| 1   | F     | 319 | GLU  |
| 1   | F     | 354 | LEU  |
| 1   | F     | 364 | LEU  |
| 1   | F     | 373 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 79  | HIS  |
| 1   | A     | 109 | HIS  |
| 1   | A     | 131 | GLN  |
| 1   | A     | 221 | GLN  |
| 1   | A     | 244 | GLN  |
| 1   | A     | 265 | GLN  |
| 1   | A     | 286 | ASN  |
| 1   | A     | 299 | ASN  |
| 1   | A     | 305 | HIS  |
| 1   | A     | 317 | ASN  |
| 1   | A     | 338 | ASN  |
| 1   | B     | 79  | HIS  |
| 1   | B     | 109 | HIS  |
| 1   | B     | 131 | GLN  |
| 1   | B     | 221 | GLN  |
| 1   | B     | 234 | GLN  |
| 1   | B     | 244 | GLN  |
| 1   | B     | 265 | GLN  |
| 1   | B     | 286 | ASN  |
| 1   | B     | 299 | ASN  |
| 1   | B     | 300 | GLN  |
| 1   | B     | 305 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 317 | ASN  |
| 1   | B     | 338 | ASN  |
| 1   | C     | 79  | HIS  |
| 1   | C     | 109 | HIS  |
| 1   | C     | 131 | GLN  |
| 1   | C     | 221 | GLN  |
| 1   | C     | 244 | GLN  |
| 1   | C     | 265 | GLN  |
| 1   | C     | 299 | ASN  |
| 1   | C     | 300 | GLN  |
| 1   | C     | 304 | GLN  |
| 1   | C     | 305 | HIS  |
| 1   | C     | 317 | ASN  |
| 1   | C     | 338 | ASN  |
| 1   | D     | 79  | HIS  |
| 1   | D     | 109 | HIS  |
| 1   | D     | 131 | GLN  |
| 1   | D     | 169 | ASN  |
| 1   | D     | 221 | GLN  |
| 1   | D     | 244 | GLN  |
| 1   | D     | 265 | GLN  |
| 1   | D     | 299 | ASN  |
| 1   | D     | 300 | GLN  |
| 1   | D     | 304 | GLN  |
| 1   | D     | 305 | HIS  |
| 1   | D     | 317 | ASN  |
| 1   | D     | 338 | ASN  |
| 1   | E     | 67  | GLN  |
| 1   | E     | 79  | HIS  |
| 1   | E     | 109 | HIS  |
| 1   | E     | 131 | GLN  |
| 1   | E     | 221 | GLN  |
| 1   | E     | 244 | GLN  |
| 1   | E     | 265 | GLN  |
| 1   | E     | 299 | ASN  |
| 1   | E     | 300 | GLN  |
| 1   | E     | 304 | GLN  |
| 1   | E     | 305 | HIS  |
| 1   | E     | 317 | ASN  |
| 1   | E     | 338 | ASN  |
| 1   | F     | 79  | HIS  |
| 1   | F     | 109 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 131 | GLN  |
| 1   | F     | 221 | GLN  |
| 1   | F     | 244 | GLN  |
| 1   | F     | 265 | GLN  |
| 1   | F     | 299 | ASN  |
| 1   | F     | 300 | GLN  |
| 1   | F     | 304 | GLN  |
| 1   | F     | 305 | HIS  |
| 1   | F     | 317 | ASN  |
| 1   | F     | 338 | ASN  |
| 1   | F     | 361 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

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.