



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:51 AM UTC

PDB ID : 2CAS / pdb\_00002cas  
Title : THE CANINE PARVOVIRUS EMPTY CAPSID STRUCTURE  
Authors : Wu, H.; Rossmann, M.G.  
Deposited on : 1993-08-24  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
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

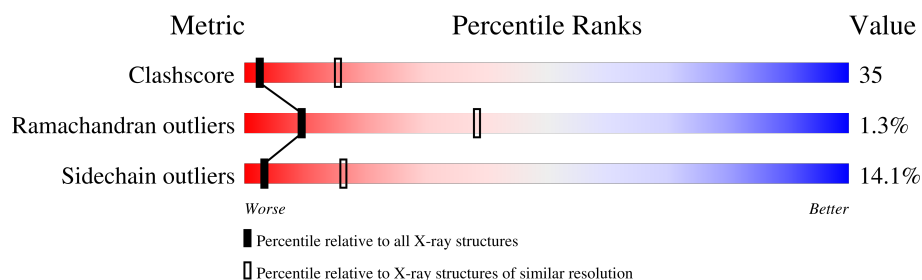
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



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

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     | 548    | <div> <div></div> <div>32%</div> <div>44%</div> <div>18%</div> <div>6%</div> </div> |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4434 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 CANINE PARVOVIRUS EMPTY CAPSID (STRAIN D) VIRAL PROTEIN 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 548      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4347  | 2760 | 742 | 829 | 16 |         |         |       |

- Molecule 2 is water.

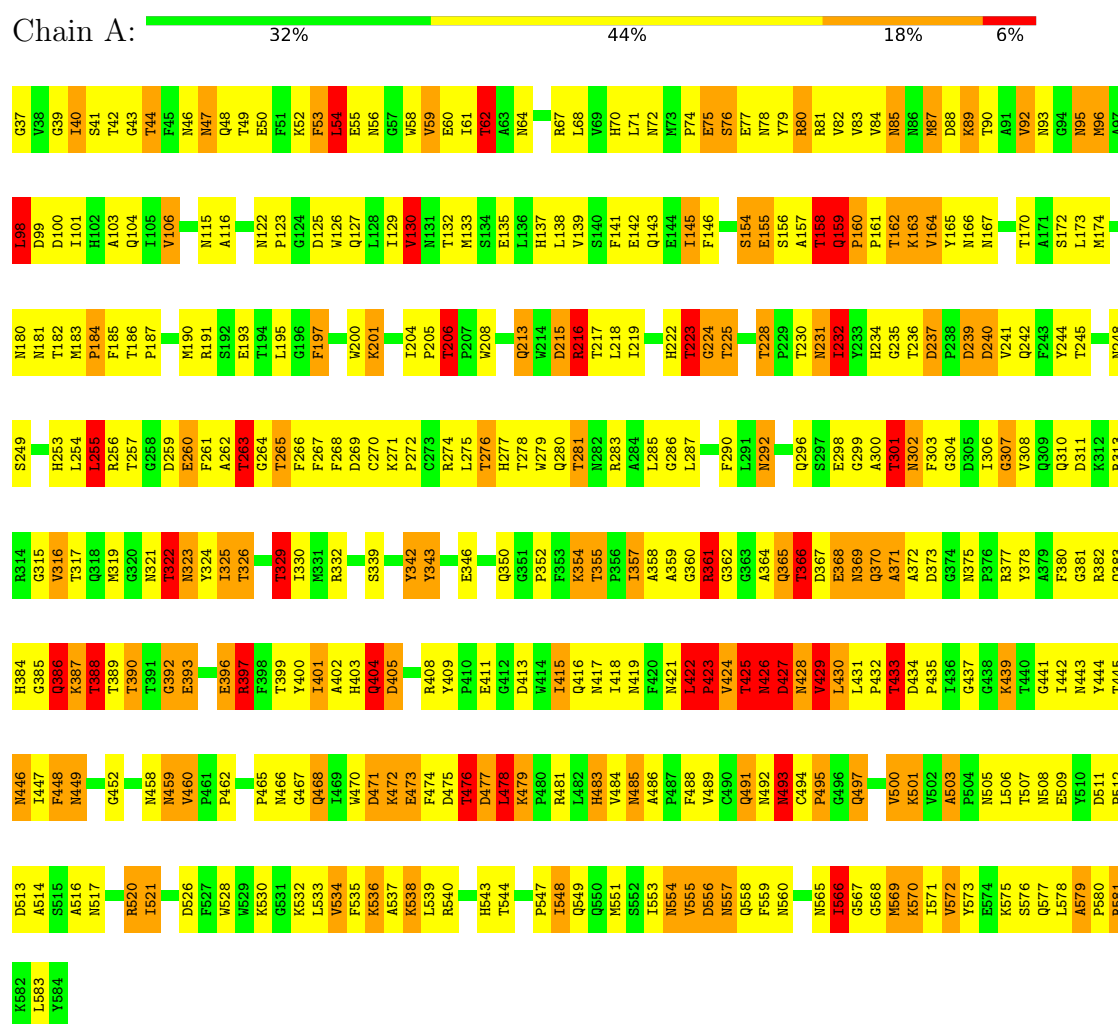
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 87       | Total | O  | 0       | 0       |
|     |       |          | 87    | 87 |         |         |

### 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: CANINE PARVOVIRUS EMPTY CAPSID (STRAIN D) VIRAL PROTEIN 2



## 4 Data and refinement statistics

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

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | P 43 21 2                                       | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 254.50Å 254.50Å 795.00Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | (Not available) – 3.00                          | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) ((Not available)-3.00)          | Depositor |
| $R_{merge}$                                              | (Not available)                                 | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | PROLSQ, X-PLOR                                  | Depositor |
| R, $R_{free}$                                            | 0.211 , (Not available)                         | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 4434                                            | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 14.0                                            | 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     | 1.54         | 27/4476 (0.6%) | 2.74        | 426/6123 (7.0%) |

All (27) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 306 | ILE  | C-O    | 12.45 | 1.36        | 1.24     |
| 1   | A     | 422 | LEU  | C-O    | 11.56 | 1.39        | 1.24     |
| 1   | A     | 263 | THR  | C-O    | 10.77 | 1.37        | 1.23     |
| 1   | A     | 304 | GLY  | N-CA   | 9.37  | 1.53        | 1.44     |
| 1   | A     | 264 | GLY  | N-CA   | 9.01  | 1.58        | 1.45     |
| 1   | A     | 423 | PRO  | N-CA   | 8.67  | 1.58        | 1.47     |
| 1   | A     | 307 | GLY  | N-CA   | 8.65  | 1.57        | 1.45     |
| 1   | A     | 416 | GLN  | N-CA   | 7.13  | 1.54        | 1.46     |
| 1   | A     | 423 | PRO  | CA-CB  | -6.40 | 1.44        | 1.53     |
| 1   | A     | 274 | ARG  | NE-CZ  | 6.23  | 1.40        | 1.33     |
| 1   | A     | 263 | THR  | CA-C   | -6.22 | 1.44        | 1.52     |
| 1   | A     | 423 | PRO  | N-CD   | -6.19 | 1.39        | 1.47     |
| 1   | A     | 405 | ASP  | CG-OD2 | 5.88  | 1.36        | 1.25     |
| 1   | A     | 240 | ASP  | CG-OD2 | 5.79  | 1.36        | 1.25     |
| 1   | A     | 452 | GLY  | N-CA   | 5.77  | 1.52        | 1.44     |
| 1   | A     | 422 | LEU  | CA-CB  | 5.71  | 1.62        | 1.53     |
| 1   | A     | 37  | GLY  | N-CA   | 5.66  | 1.54        | 1.45     |
| 1   | A     | 249 | SER  | C-N    | -5.60 | 1.27        | 1.33     |
| 1   | A     | 270 | CYS  | N-CA   | 5.44  | 1.52        | 1.46     |
| 1   | A     | 509 | GLU  | CD-OE2 | 5.40  | 1.35        | 1.25     |
| 1   | A     | 366 | THR  | CA-CB  | 5.29  | 1.61        | 1.53     |
| 1   | A     | 329 | THR  | CA-CB  | 5.28  | 1.61        | 1.53     |
| 1   | A     | 307 | GLY  | C-O    | 5.17  | 1.30        | 1.23     |
| 1   | A     | 439 | LYS  | N-CA   | 5.12  | 1.52        | 1.46     |
| 1   | A     | 360 | GLY  | N-CA   | 5.06  | 1.52        | 1.45     |
| 1   | A     | 422 | LEU  | CA-C   | -5.06 | 1.46        | 1.52     |
| 1   | A     | 160 | PRO  | CA-CB  | -5.03 | 1.47        | 1.54     |

All (426) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 405 | ASP  | CA-CB-CG   | 23.76  | 136.36      | 112.60   |
| 1   | A     | 403 | HIS  | CA-CB-CG   | 21.23  | 135.03      | 113.80   |
| 1   | A     | 492 | ASN  | CA-CB-CG   | -15.85 | 96.75       | 112.60   |
| 1   | A     | 425 | THR  | CA-CB-OG1  | -13.59 | 89.22       | 109.60   |
| 1   | A     | 274 | ARG  | CD-NE-CZ   | -13.35 | 105.71      | 124.40   |
| 1   | A     | 342 | TYR  | O-C-N      | 12.68  | 138.39      | 123.30   |
| 1   | A     | 421 | ASN  | OD1-CG-ND2 | 12.55  | 135.15      | 122.60   |
| 1   | A     | 365 | GLN  | CA-C-N     | -12.34 | 105.97      | 123.00   |
| 1   | A     | 365 | GLN  | C-N-CA     | -12.34 | 105.97      | 123.00   |
| 1   | A     | 404 | GLN  | CA-C-O     | -12.21 | 106.33      | 120.49   |
| 1   | A     | 115 | ASN  | CA-CB-CG   | 12.17  | 124.77      | 112.60   |
| 1   | A     | 72  | ASN  | OD1-CG-ND2 | 12.11  | 134.71      | 122.60   |
| 1   | A     | 72  | ASN  | CA-CB-CG   | -12.04 | 100.56      | 112.60   |
| 1   | A     | 421 | ASN  | CA-CB-CG   | -11.97 | 100.63      | 112.60   |
| 1   | A     | 547 | PRO  | CA-C-N     | 11.97  | 135.07      | 122.27   |
| 1   | A     | 547 | PRO  | C-N-CA     | 11.97  | 135.07      | 122.27   |
| 1   | A     | 460 | VAL  | N-CA-CB    | -11.78 | 95.84       | 110.33   |
| 1   | A     | 423 | PRO  | CB-CA-C    | 11.63  | 130.75      | 111.56   |
| 1   | A     | 380 | PHE  | CA-C-N     | 11.47  | 133.62      | 122.27   |
| 1   | A     | 380 | PHE  | C-N-CA     | 11.47  | 133.62      | 122.27   |
| 1   | A     | 160 | PRO  | N-CA-C     | -11.44 | 96.75       | 110.70   |
| 1   | A     | 419 | ASN  | CA-CB-CG   | -11.26 | 101.34      | 112.60   |
| 1   | A     | 139 | VAL  | N-CA-C     | 11.04  | 122.16      | 111.67   |
| 1   | A     | 422 | LEU  | CA-C-O     | -10.96 | 105.14      | 120.16   |
| 1   | A     | 422 | LEU  | N-CA-C     | 10.72  | 133.50      | 109.81   |
| 1   | A     | 433 | THR  | CA-CB-OG1  | -10.43 | 93.96       | 109.60   |
| 1   | A     | 263 | THR  | CA-C-O     | -10.41 | 110.21      | 121.56   |
| 1   | A     | 361 | ARG  | CD-NE-CZ   | 10.39  | 138.95      | 124.40   |
| 1   | A     | 240 | ASP  | CB-CG-OD2  | 10.33  | 142.15      | 118.40   |
| 1   | A     | 566 | ILE  | CA-CB-CG2  | 10.28  | 127.97      | 110.50   |
| 1   | A     | 578 | LEU  | CA-C-O     | -10.24 | 109.70      | 120.55   |
| 1   | A     | 548 | ILE  | CA-CB-CG2  | 10.23  | 127.89      | 110.50   |
| 1   | A     | 342 | TYR  | CA-C-N     | 10.11  | 137.19      | 122.63   |
| 1   | A     | 342 | TYR  | C-N-CA     | 10.11  | 137.19      | 122.63   |
| 1   | A     | 191 | ARG  | NE-CZ-NH2  | 10.01  | 128.21      | 119.20   |
| 1   | A     | 240 | ASP  | CA-CB-CG   | 9.92   | 122.52      | 112.60   |
| 1   | A     | 285 | LEU  | CA-C-O     | -9.91  | 109.41      | 120.32   |
| 1   | A     | 477 | ASP  | CA-CB-CG   | -9.83  | 102.77      | 112.60   |
| 1   | A     | 422 | LEU  | O-C-N      | -9.78  | 110.08      | 121.32   |
| 1   | A     | 540 | ARG  | CD-NE-CZ   | -9.71  | 110.81      | 124.40   |
| 1   | A     | 223 | THR  | CA-CB-OG1  | -9.70  | 95.05       | 109.60   |
| 1   | A     | 492 | ASN  | CA-C-O     | -9.69  | 110.28      | 120.55   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 306 | ILE  | O-C-N      | -9.59 | 112.40      | 122.66   |
| 1   | A     | 512 | PRO  | CA-C-N     | -9.49 | 107.46      | 122.65   |
| 1   | A     | 512 | PRO  | C-N-CA     | -9.49 | 107.46      | 122.65   |
| 1   | A     | 263 | THR  | N-CA-CB    | -9.48 | 96.52       | 110.17   |
| 1   | A     | 483 | HIS  | CA-CB-CG   | 9.43  | 123.23      | 113.80   |
| 1   | A     | 81  | ARG  | CD-NE-CZ   | 9.36  | 137.51      | 124.40   |
| 1   | A     | 301 | THR  | O-C-N      | 9.36  | 132.29      | 122.09   |
| 1   | A     | 100 | ASP  | CA-CB-CG   | 9.32  | 121.92      | 112.60   |
| 1   | A     | 237 | ASP  | N-CA-C     | -9.31 | 97.92       | 109.65   |
| 1   | A     | 478 | LEU  | CA-C-O     | -9.29 | 110.31      | 120.43   |
| 1   | A     | 274 | ARG  | NH1-CZ-NH2 | 9.20  | 131.26      | 119.30   |
| 1   | A     | 263 | THR  | CA-C-N     | -9.11 | 111.08      | 122.75   |
| 1   | A     | 263 | THR  | C-N-CA     | -9.11 | 111.08      | 122.75   |
| 1   | A     | 224 | GLY  | CA-C-N     | 9.00  | 136.20      | 123.07   |
| 1   | A     | 224 | GLY  | C-N-CA     | 9.00  | 136.20      | 123.07   |
| 1   | A     | 388 | THR  | CA-CB-OG1  | -8.97 | 96.15       | 109.60   |
| 1   | A     | 429 | VAL  | O-C-N      | 8.89  | 133.14      | 123.00   |
| 1   | A     | 237 | ASP  | N-CA-CB    | 8.82  | 124.39      | 110.01   |
| 1   | A     | 263 | THR  | O-C-N      | -8.73 | 112.56      | 122.86   |
| 1   | A     | 306 | ILE  | CA-C-O     | -8.71 | 110.26      | 120.98   |
| 1   | A     | 559 | PHE  | CA-CB-CG   | -8.66 | 105.14      | 113.80   |
| 1   | A     | 160 | PRO  | CB-CA-C    | 8.65  | 121.47      | 110.92   |
| 1   | A     | 368 | GLU  | CB-CG-CD   | 8.63  | 127.28      | 112.60   |
| 1   | A     | 315 | GLY  | CA-C-O     | -8.61 | 115.10      | 122.16   |
| 1   | A     | 548 | ILE  | CA-CB-CG1  | -8.56 | 95.85       | 110.40   |
| 1   | A     | 517 | ASN  | CA-CB-CG   | -8.46 | 104.14      | 112.60   |
| 1   | A     | 81  | ARG  | NE-CZ-NH1  | 8.44  | 129.94      | 121.50   |
| 1   | A     | 329 | THR  | CA-CB-OG1  | -8.32 | 97.11       | 109.60   |
| 1   | A     | 366 | THR  | CA-C-O     | 8.30  | 129.42      | 120.38   |
| 1   | A     | 78  | ASN  | OD1-CG-ND2 | 8.27  | 130.87      | 122.60   |
| 1   | A     | 405 | ASP  | CB-CG-OD1  | 8.26  | 137.39      | 118.40   |
| 1   | A     | 388 | THR  | CA-CB-CG2  | 8.25  | 124.53      | 110.50   |
| 1   | A     | 369 | ASN  | CA-C-N     | -8.25 | 110.00      | 122.21   |
| 1   | A     | 369 | ASN  | C-N-CA     | -8.25 | 110.00      | 122.21   |
| 1   | A     | 428 | ASN  | OD1-CG-ND2 | 8.15  | 130.75      | 122.60   |
| 1   | A     | 358 | ALA  | CA-C-O     | -8.14 | 111.79      | 120.42   |
| 1   | A     | 195 | LEU  | N-CA-C     | -8.05 | 100.50      | 110.41   |
| 1   | A     | 216 | ARG  | CA-CB-CG   | 8.05  | 130.19      | 114.10   |
| 1   | A     | 166 | ASN  | OD1-CG-ND2 | 8.04  | 130.64      | 122.60   |
| 1   | A     | 257 | THR  | O-C-N      | 8.01  | 130.61      | 122.12   |
| 1   | A     | 268 | PHE  | CA-CB-CG   | 8.00  | 121.80      | 113.80   |
| 1   | A     | 426 | ASN  | CA-C-N     | -7.96 | 111.32      | 123.17   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 426 | ASN  | C-N-CA     | -7.96 | 111.32      | 123.17   |
| 1   | A     | 240 | ASP  | CB-CA-C    | 7.88  | 123.49      | 110.17   |
| 1   | A     | 401 | ILE  | N-CA-CB    | 7.86  | 121.57      | 111.67   |
| 1   | A     | 413 | ASP  | CA-C-O     | -7.86 | 112.43      | 121.47   |
| 1   | A     | 446 | ASN  | OD1-CG-ND2 | 7.85  | 130.45      | 122.60   |
| 1   | A     | 447 | ILE  | CA-C-N     | 7.77  | 131.75      | 120.71   |
| 1   | A     | 447 | ILE  | C-N-CA     | 7.77  | 131.75      | 120.71   |
| 1   | A     | 130 | VAL  | N-CA-CB    | -7.74 | 100.02      | 110.54   |
| 1   | A     | 240 | ASP  | N-CA-C     | -7.73 | 102.94      | 113.30   |
| 1   | A     | 257 | THR  | CA-CB-OG1  | -7.71 | 98.04       | 109.60   |
| 1   | A     | 343 | TYR  | O-C-N      | 7.70  | 132.07      | 122.91   |
| 1   | A     | 281 | THR  | CA-CB-OG1  | -7.69 | 98.07       | 109.60   |
| 1   | A     | 274 | ARG  | NE-CZ-NH2  | -7.65 | 112.31      | 119.20   |
| 1   | A     | 372 | ALA  | N-CA-C     | 7.62  | 119.60      | 108.86   |
| 1   | A     | 350 | GLN  | N-CA-C     | 7.61  | 122.65      | 112.30   |
| 1   | A     | 78  | ASN  | N-CA-C     | 7.58  | 121.83      | 109.85   |
| 1   | A     | 237 | ASP  | CB-CG-OD2  | 7.58  | 135.84      | 118.40   |
| 1   | A     | 206 | THR  | CB-CA-C    | -7.57 | 96.97       | 108.63   |
| 1   | A     | 554 | ASN  | OD1-CG-ND2 | 7.55  | 130.15      | 122.60   |
| 1   | A     | 228 | THR  | O-C-N      | 7.53  | 130.21      | 121.47   |
| 1   | A     | 371 | ALA  | CA-C-N     | 7.53  | 134.65      | 122.53   |
| 1   | A     | 371 | ALA  | C-N-CA     | 7.53  | 134.65      | 122.53   |
| 1   | A     | 528 | TRP  | CA-C-O     | -7.50 | 112.47      | 120.80   |
| 1   | A     | 477 | ASP  | CA-C-O     | -7.47 | 113.16      | 121.00   |
| 1   | A     | 386 | GLN  | CG-CD-OE1  | 7.45  | 135.70      | 120.80   |
| 1   | A     | 566 | ILE  | CA-CB-CG1  | -7.45 | 97.73       | 110.40   |
| 1   | A     | 232 | ILE  | N-CA-C     | 7.44  | 119.19      | 108.48   |
| 1   | A     | 415 | ILE  | CA-C-O     | -7.38 | 112.03      | 121.40   |
| 1   | A     | 399 | THR  | N-CA-CB    | 7.36  | 122.13      | 110.57   |
| 1   | A     | 78  | ASN  | CA-CB-CG   | -7.36 | 105.24      | 112.60   |
| 1   | A     | 170 | THR  | CA-CB-OG1  | -7.35 | 98.57       | 109.60   |
| 1   | A     | 543 | HIS  | CA-CB-CG   | -7.35 | 106.45      | 113.80   |
| 1   | A     | 304 | GLY  | N-CA-C     | -7.34 | 98.75       | 112.10   |
| 1   | A     | 197 | PHE  | CA-C-O     | -7.33 | 110.41      | 119.28   |
| 1   | A     | 567 | GLY  | N-CA-C     | -7.33 | 104.48      | 115.32   |
| 1   | A     | 481 | ARG  | CD-NE-CZ   | -7.32 | 114.15      | 124.40   |
| 1   | A     | 204 | ILE  | O-C-N      | 7.32  | 129.44      | 121.10   |
| 1   | A     | 129 | ILE  | CA-C-O     | 7.30  | 129.10      | 121.29   |
| 1   | A     | 366 | THR  | N-CA-C     | 7.29  | 120.81      | 109.07   |
| 1   | A     | 41  | SER  | N-CA-CB    | 7.29  | 120.68      | 109.97   |
| 1   | A     | 511 | ASP  | O-C-N      | 7.28  | 131.59      | 121.47   |
| 1   | A     | 517 | ASN  | OD1-CG-ND2 | 7.27  | 129.87      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 78  | ASN  | CA-C-O     | -7.27 | 112.96      | 121.46   |
| 1   | A     | 386 | GLN  | CG-CD-NE2  | -7.26 | 105.51      | 116.40   |
| 1   | A     | 67  | ARG  | CD-NE-CZ   | -7.24 | 114.27      | 124.40   |
| 1   | A     | 75  | GLU  | CA-CB-CG   | 7.22  | 128.54      | 114.10   |
| 1   | A     | 236 | THR  | N-CA-C     | 7.21  | 120.68      | 109.07   |
| 1   | A     | 397 | ARG  | CD-NE-CZ   | -7.21 | 114.31      | 124.40   |
| 1   | A     | 290 | PHE  | CA-C-O     | -7.17 | 112.57      | 120.81   |
| 1   | A     | 241 | VAL  | N-CA-C     | 7.12  | 119.07      | 108.54   |
| 1   | A     | 72  | ASN  | N-CA-CB    | -7.06 | 99.55       | 110.56   |
| 1   | A     | 359 | ALA  | CA-C-O     | -7.06 | 112.13      | 120.60   |
| 1   | A     | 555 | VAL  | CA-C-O     | -7.03 | 111.53      | 120.03   |
| 1   | A     | 322 | THR  | O-C-N      | 7.00  | 131.39      | 123.27   |
| 1   | A     | 381 | GLY  | N-CA-C     | 7.00  | 122.90      | 112.41   |
| 1   | A     | 72  | ASN  | CA-C-O     | -6.99 | 113.14      | 121.66   |
| 1   | A     | 430 | LEU  | CB-CA-C    | 6.99  | 121.17      | 110.62   |
| 1   | A     | 125 | ASP  | O-C-N      | 6.98  | 129.52      | 122.12   |
| 1   | A     | 265 | THR  | CA-C-O     | -6.98 | 112.66      | 120.54   |
| 1   | A     | 75  | GLU  | CG-CD-OE1  | 6.95  | 134.39      | 118.40   |
| 1   | A     | 306 | ILE  | CA-C-N     | -6.93 | 107.82      | 121.41   |
| 1   | A     | 306 | ILE  | C-N-CA     | -6.93 | 107.82      | 121.41   |
| 1   | A     | 75  | GLU  | CG-CD-OE2  | -6.92 | 102.49      | 118.40   |
| 1   | A     | 225 | THR  | N-CA-C     | -6.91 | 95.92       | 108.02   |
| 1   | A     | 145 | ILE  | CA-C-O     | 6.90  | 127.80      | 120.48   |
| 1   | A     | 570 | LYS  | CA-C-O     | -6.87 | 113.91      | 121.33   |
| 1   | A     | 82  | VAL  | N-CA-C     | 6.84  | 118.44      | 108.53   |
| 1   | A     | 180 | ASN  | OD1-CG-ND2 | 6.82  | 129.41      | 122.60   |
| 1   | A     | 253 | HIS  | CA-C-O     | -6.79 | 113.02      | 120.43   |
| 1   | A     | 61  | ILE  | CA-C-O     | 6.79  | 128.39      | 120.71   |
| 1   | A     | 460 | VAL  | CB-CA-C    | 6.77  | 117.51      | 110.88   |
| 1   | A     | 560 | ASN  | OD1-CG-ND2 | 6.76  | 129.37      | 122.60   |
| 1   | A     | 481 | ARG  | CA-C-O     | -6.75 | 111.32      | 119.49   |
| 1   | A     | 206 | THR  | N-CA-CB    | 6.73  | 125.84      | 110.56   |
| 1   | A     | 263 | THR  | CA-CB-OG1  | -6.71 | 99.54       | 109.60   |
| 1   | A     | 439 | LYS  | CB-CA-C    | 6.71  | 120.60      | 109.53   |
| 1   | A     | 96  | MET  | CA-CB-CG   | -6.70 | 100.69      | 114.10   |
| 1   | A     | 392 | GLY  | O-C-N      | 6.69  | 131.40      | 122.70   |
| 1   | A     | 231 | ASN  | CA-CB-CG   | 6.68  | 119.28      | 112.60   |
| 1   | A     | 92  | VAL  | CA-C-O     | -6.67 | 112.56      | 120.76   |
| 1   | A     | 303 | PHE  | CA-C-N     | -6.65 | 115.50      | 122.69   |
| 1   | A     | 303 | PHE  | C-N-CA     | -6.65 | 115.50      | 122.69   |
| 1   | A     | 572 | VAL  | N-CA-CB    | -6.64 | 98.98       | 110.13   |
| 1   | A     | 46  | ASN  | OD1-CG-ND2 | -6.63 | 115.97      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 75  | GLU  | CB-CG-CD   | 6.60  | 123.82      | 112.60   |
| 1   | A     | 62  | THR  | CB-CA-C    | 6.60  | 120.59      | 110.62   |
| 1   | A     | 98  | LEU  | CA-C-N     | 6.59  | 130.11      | 120.82   |
| 1   | A     | 98  | LEU  | C-N-CA     | 6.59  | 130.11      | 120.82   |
| 1   | A     | 554 | ASN  | O-C-N      | 6.59  | 130.04      | 122.99   |
| 1   | A     | 423 | PRO  | N-CA-C     | -6.58 | 98.91       | 112.47   |
| 1   | A     | 40  | ILE  | N-CA-C     | 6.56  | 117.30      | 108.11   |
| 1   | A     | 396 | GLU  | CA-C-O     | -6.56 | 113.52      | 120.80   |
| 1   | A     | 285 | LEU  | O-C-N      | 6.56  | 131.01      | 123.27   |
| 1   | A     | 135 | GLU  | CA-C-O     | -6.55 | 113.69      | 120.89   |
| 1   | A     | 511 | ASP  | CA-C-O     | -6.54 | 112.75      | 119.49   |
| 1   | A     | 426 | ASN  | CA-CB-CG   | -6.52 | 106.08      | 112.60   |
| 1   | A     | 219 | ILE  | N-CA-CB    | -6.52 | 102.09      | 111.21   |
| 1   | A     | 405 | ASP  | CB-CA-C    | 6.52  | 122.16      | 111.41   |
| 1   | A     | 534 | VAL  | CA-C-N     | 6.51  | 133.75      | 122.81   |
| 1   | A     | 534 | VAL  | C-N-CA     | 6.51  | 133.75      | 122.81   |
| 1   | A     | 566 | ILE  | CA-C-O     | 6.51  | 126.71      | 119.42   |
| 1   | A     | 139 | VAL  | N-CA-CB    | -6.50 | 101.51      | 110.68   |
| 1   | A     | 375 | ASN  | CA-C-O     | -6.49 | 113.98      | 119.76   |
| 1   | A     | 67  | ARG  | NE-CZ-NH2  | 6.49  | 125.04      | 119.20   |
| 1   | A     | 556 | ASP  | CA-C-O     | -6.45 | 112.13      | 120.00   |
| 1   | A     | 72  | ASN  | CB-CG-OD1  | -6.45 | 107.91      | 120.80   |
| 1   | A     | 422 | LEU  | N-CA-CB    | -6.44 | 98.90       | 110.37   |
| 1   | A     | 47  | ASN  | OD1-CG-ND2 | -6.44 | 116.16      | 122.60   |
| 1   | A     | 421 | ASN  | N-CA-C     | -6.44 | 99.40       | 109.25   |
| 1   | A     | 180 | ASN  | N-CA-C     | -6.44 | 105.30      | 113.02   |
| 1   | A     | 292 | ASN  | OD1-CG-ND2 | 6.42  | 129.02      | 122.60   |
| 1   | A     | 404 | GLN  | O-C-N      | 6.42  | 130.91      | 123.02   |
| 1   | A     | 184 | PRO  | CA-C-N     | 6.41  | 130.48      | 121.24   |
| 1   | A     | 184 | PRO  | C-N-CA     | 6.41  | 130.48      | 121.24   |
| 1   | A     | 89  | LYS  | CA-C-O     | 6.39  | 127.34      | 119.79   |
| 1   | A     | 85  | ASN  | CA-CB-CG   | -6.39 | 106.21      | 112.60   |
| 1   | A     | 232 | ILE  | CB-CA-C    | -6.38 | 101.12      | 110.62   |
| 1   | A     | 424 | VAL  | CA-C-N     | 6.34  | 130.86      | 122.30   |
| 1   | A     | 424 | VAL  | C-N-CA     | 6.34  | 130.86      | 122.30   |
| 1   | A     | 249 | SER  | N-CA-C     | 6.33  | 121.53      | 113.55   |
| 1   | A     | 459 | ASN  | CB-CG-ND2  | 6.28  | 125.82      | 116.40   |
| 1   | A     | 421 | ASN  | CA-C-O     | -6.28 | 113.21      | 120.49   |
| 1   | A     | 263 | THR  | OG1-CB-CG2 | 6.27  | 121.84      | 109.30   |
| 1   | A     | 225 | THR  | N-CA-CB    | 6.27  | 120.55      | 110.65   |
| 1   | A     | 468 | GLN  | CA-C-O     | -6.25 | 114.28      | 121.47   |
| 1   | A     | 416 | GLN  | CB-CA-C    | 6.25  | 122.05      | 109.68   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 332 | ARG  | CA-C-O    | -6.24 | 114.23      | 120.66   |
| 1   | A     | 365 | GLN  | CA-C-O    | -6.23 | 112.52      | 119.81   |
| 1   | A     | 384 | HIS  | N-CA-C    | 6.21  | 118.83      | 110.88   |
| 1   | A     | 573 | TYR  | O-C-N     | 6.21  | 129.93      | 122.85   |
| 1   | A     | 130 | VAL  | CB-CA-C   | 6.21  | 120.52      | 112.14   |
| 1   | A     | 158 | THR  | CA-CB-OG1 | -6.21 | 100.29      | 109.60   |
| 1   | A     | 434 | ASP  | CA-C-O    | -6.19 | 114.26      | 120.64   |
| 1   | A     | 581 | ARG  | NE-CZ-NH1 | -6.19 | 115.31      | 121.50   |
| 1   | A     | 500 | VAL  | N-CA-CB   | -6.18 | 100.49      | 111.93   |
| 1   | A     | 205 | PRO  | CA-C-O    | -6.18 | 113.99      | 122.15   |
| 1   | A     | 495 | PRO  | CB-CA-C   | 6.17  | 119.13      | 111.23   |
| 1   | A     | 83  | VAL  | O-C-N     | 6.16  | 129.42      | 123.14   |
| 1   | A     | 37  | GLY  | CA-C-N    | -6.15 | 112.68      | 120.56   |
| 1   | A     | 37  | GLY  | C-N-CA    | -6.15 | 112.68      | 120.56   |
| 1   | A     | 184 | PRO  | CB-CA-C   | 6.15  | 119.39      | 111.21   |
| 1   | A     | 255 | LEU  | CA-C-O    | -6.12 | 114.22      | 120.71   |
| 1   | A     | 475 | ASP  | CA-C-N    | 6.12  | 132.42      | 122.81   |
| 1   | A     | 475 | ASP  | C-N-CA    | 6.12  | 132.42      | 122.81   |
| 1   | A     | 76  | SER  | CA-CB-OG  | 6.12  | 123.34      | 111.10   |
| 1   | A     | 53  | PHE  | CA-C-N    | 6.10  | 133.20      | 121.54   |
| 1   | A     | 53  | PHE  | C-N-CA    | 6.10  | 133.20      | 121.54   |
| 1   | A     | 262 | ALA  | CA-C-N    | 6.10  | 130.52      | 120.94   |
| 1   | A     | 262 | ALA  | C-N-CA    | 6.10  | 130.52      | 120.94   |
| 1   | A     | 505 | ASN  | CA-CB-CG  | 6.09  | 118.69      | 112.60   |
| 1   | A     | 388 | THR  | N-CA-CB   | -6.07 | 100.89      | 109.94   |
| 1   | A     | 103 | ALA  | N-CA-C    | -6.06 | 100.02      | 109.72   |
| 1   | A     | 419 | ASN  | CB-CA-C   | 6.06  | 121.84      | 110.63   |
| 1   | A     | 173 | LEU  | N-CA-C    | -6.05 | 100.42      | 110.17   |
| 1   | A     | 163 | LYS  | CA-C-N    | 6.04  | 130.54      | 122.93   |
| 1   | A     | 163 | LYS  | C-N-CA    | 6.04  | 130.54      | 122.93   |
| 1   | A     | 369 | ASN  | O-C-N     | 6.04  | 128.61      | 122.09   |
| 1   | A     | 240 | ASP  | O-C-N     | -6.03 | 114.94      | 122.24   |
| 1   | A     | 474 | PHE  | CA-C-O    | -6.02 | 114.18      | 121.05   |
| 1   | A     | 42  | THR  | CA-C-O    | -6.02 | 112.84      | 119.95   |
| 1   | A     | 427 | ASP  | CB-CG-OD2 | -6.01 | 104.57      | 118.40   |
| 1   | A     | 164 | VAL  | CA-C-O    | 5.99  | 126.97      | 120.57   |
| 1   | A     | 332 | ARG  | NE-CZ-NH1 | 5.98  | 127.48      | 121.50   |
| 1   | A     | 132 | THR  | CA-C-O    | -5.98 | 112.47      | 119.05   |
| 1   | A     | 476 | THR  | N-CA-CB   | -5.98 | 100.86      | 111.08   |
| 1   | A     | 437 | GLY  | O-C-N     | 5.95  | 129.09      | 122.31   |
| 1   | A     | 79  | TYR  | N-CA-C    | -5.95 | 99.97       | 109.96   |
| 1   | A     | 569 | MET  | N-CA-CB   | 5.93  | 121.87      | 111.55   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 159 | GLN  | O-C-N      | 5.92  | 128.13      | 121.32   |
| 1   | A     | 215 | ASP  | CA-C-O     | -5.92 | 113.96      | 120.30   |
| 1   | A     | 557 | ASN  | CA-CB-CG   | -5.89 | 106.70      | 112.60   |
| 1   | A     | 400 | TYR  | CA-C-N     | -5.89 | 115.10      | 123.11   |
| 1   | A     | 400 | TYR  | C-N-CA     | -5.89 | 115.10      | 123.11   |
| 1   | A     | 155 | GLU  | CB-CG-CD   | -5.88 | 102.61      | 112.60   |
| 1   | A     | 458 | ASN  | CA-CB-CG   | 5.87  | 118.47      | 112.60   |
| 1   | A     | 492 | ASN  | OD1-CG-ND2 | 5.87  | 128.47      | 122.60   |
| 1   | A     | 549 | GLN  | CB-CG-CD   | -5.87 | 102.62      | 112.60   |
| 1   | A     | 280 | GLN  | OE1-CD-NE2 | -5.86 | 116.74      | 122.60   |
| 1   | A     | 261 | PHE  | CA-CB-CG   | 5.86  | 119.66      | 113.80   |
| 1   | A     | 460 | VAL  | CA-CB-CG1  | 5.86  | 120.36      | 110.40   |
| 1   | A     | 44  | THR  | CA-CB-OG1  | -5.85 | 100.82      | 109.60   |
| 1   | A     | 513 | ASP  | CA-C-O     | -5.84 | 112.72      | 119.56   |
| 1   | A     | 142 | GLU  | CA-CB-CG   | 5.84  | 125.77      | 114.10   |
| 1   | A     | 155 | GLU  | CB-CA-C    | -5.84 | 101.44      | 110.78   |
| 1   | A     | 292 | ASN  | CA-CB-CG   | -5.84 | 106.76      | 112.60   |
| 1   | A     | 408 | ARG  | N-CA-C     | 5.83  | 118.27      | 109.23   |
| 1   | A     | 448 | PHE  | N-CA-C     | 5.83  | 118.69      | 110.23   |
| 1   | A     | 106 | VAL  | CB-CA-C    | 5.82  | 118.95      | 110.98   |
| 1   | A     | 265 | THR  | CA-CB-OG1  | -5.82 | 100.87      | 109.60   |
| 1   | A     | 449 | ASN  | CA-CB-CG   | 5.82  | 118.42      | 112.60   |
| 1   | A     | 534 | VAL  | O-C-N      | 5.82  | 129.54      | 123.26   |
| 1   | A     | 396 | GLU  | CA-CB-CG   | -5.79 | 102.53      | 114.10   |
| 1   | A     | 329 | THR  | N-CA-C     | 5.77  | 120.47      | 112.45   |
| 1   | A     | 104 | GLN  | OE1-CD-NE2 | 5.77  | 128.37      | 122.60   |
| 1   | A     | 186 | THR  | CA-CB-OG1  | -5.75 | 100.97      | 109.60   |
| 1   | A     | 311 | ASP  | CA-CB-CG   | -5.75 | 106.85      | 112.60   |
| 1   | A     | 578 | LEU  | O-C-N      | 5.75  | 128.22      | 122.12   |
| 1   | A     | 92  | VAL  | N-CA-CB    | -5.74 | 104.74      | 111.39   |
| 1   | A     | 242 | GLN  | CB-CA-C    | -5.73 | 103.91      | 111.82   |
| 1   | A     | 428 | ASN  | CA-CB-CG   | -5.73 | 106.87      | 112.60   |
| 1   | A     | 260 | GLU  | O-C-N      | -5.73 | 116.72      | 123.25   |
| 1   | A     | 60  | GLU  | CG-CD-OE2  | -5.72 | 105.24      | 118.40   |
| 1   | A     | 286 | GLY  | N-CA-C     | 5.72  | 122.89      | 112.37   |
| 1   | A     | 87  | MET  | N-CA-CB    | -5.69 | 100.87      | 110.49   |
| 1   | A     | 329 | THR  | N-CA-CB    | -5.68 | 101.80      | 110.26   |
| 1   | A     | 429 | VAL  | CB-CA-C    | -5.67 | 100.56      | 110.71   |
| 1   | A     | 242 | GLN  | OE1-CD-NE2 | 5.66  | 128.26      | 122.60   |
| 1   | A     | 425 | THR  | N-CA-CB    | -5.66 | 100.66      | 110.17   |
| 1   | A     | 231 | ASN  | CB-CG-ND2  | 5.64  | 124.86      | 116.40   |
| 1   | A     | 276 | THR  | O-C-N      | 5.64  | 130.18      | 123.24   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 106 | VAL  | N-CA-CB   | -5.61 | 104.65      | 111.21   |
| 1   | A     | 303 | PHE  | CA-CB-CG  | -5.61 | 108.19      | 113.80   |
| 1   | A     | 274 | ARG  | CA-CB-CG  | -5.60 | 102.89      | 114.10   |
| 1   | A     | 48  | GLN  | CA-C-N    | -5.60 | 115.28      | 123.00   |
| 1   | A     | 48  | GLN  | C-N-CA    | -5.60 | 115.28      | 123.00   |
| 1   | A     | 508 | ASN  | CA-C-O    | -5.59 | 114.62      | 120.55   |
| 1   | A     | 421 | ASN  | CB-CA-C   | 5.57  | 119.43      | 110.29   |
| 1   | A     | 506 | LEU  | N-CA-CB   | -5.57 | 102.29      | 110.26   |
| 1   | A     | 383 | GLN  | CB-CG-CD  | -5.56 | 103.14      | 112.60   |
| 1   | A     | 321 | ASN  | CA-C-O    | -5.55 | 113.83      | 120.55   |
| 1   | A     | 343 | TYR  | N-CA-C    | -5.54 | 103.80      | 111.28   |
| 1   | A     | 44  | THR  | CA-C-O    | -5.54 | 114.29      | 120.66   |
| 1   | A     | 240 | ASP  | CB-CG-OD1 | -5.54 | 105.65      | 118.40   |
| 1   | A     | 186 | THR  | CA-CB-CG2 | 5.54  | 119.91      | 110.50   |
| 1   | A     | 361 | ARG  | NE-CZ-NH1 | 5.53  | 127.03      | 121.50   |
| 1   | A     | 138 | LEU  | CA-C-O    | -5.53 | 114.66      | 120.58   |
| 1   | A     | 50  | GLU  | CG-CD-OE2 | 5.53  | 131.11      | 118.40   |
| 1   | A     | 281 | THR  | CA-C-O    | -5.53 | 114.92      | 121.66   |
| 1   | A     | 71  | LEU  | N-CA-CB   | -5.52 | 101.54      | 110.81   |
| 1   | A     | 477 | ASP  | O-C-N     | 5.52  | 127.77      | 122.03   |
| 1   | A     | 104 | GLN  | CG-CD-NE2 | -5.51 | 108.13      | 116.40   |
| 1   | A     | 357 | ILE  | CB-CA-C   | 5.51  | 118.83      | 110.62   |
| 1   | A     | 493 | ASN  | N-CA-C    | 5.51  | 118.40      | 108.48   |
| 1   | A     | 223 | THR  | CB-CA-C   | 5.51  | 116.58      | 109.80   |
| 1   | A     | 141 | PHE  | CA-CB-CG  | -5.50 | 108.30      | 113.80   |
| 1   | A     | 533 | LEU  | CA-C-O    | 5.49  | 126.37      | 120.38   |
| 1   | A     | 241 | VAL  | CB-CA-C   | -5.49 | 104.65      | 111.08   |
| 1   | A     | 468 | GLN  | CA-CB-CG  | 5.49  | 125.08      | 114.10   |
| 1   | A     | 428 | ASN  | CB-CG-OD1 | -5.48 | 109.83      | 120.80   |
| 1   | A     | 553 | ILE  | CA-C-O    | -5.48 | 115.35      | 121.98   |
| 1   | A     | 278 | THR  | CA-CB-CG2 | 5.48  | 119.82      | 110.50   |
| 1   | A     | 64  | ASN  | CA-C-O    | -5.48 | 114.46      | 120.43   |
| 1   | A     | 89  | LYS  | N-CA-CB   | -5.46 | 101.89      | 110.30   |
| 1   | A     | 560 | ASN  | N-CA-C    | -5.46 | 106.58      | 113.18   |
| 1   | A     | 99  | ASP  | CA-CB-CG  | -5.46 | 107.14      | 112.60   |
| 1   | A     | 491 | GLN  | CA-C-N    | -5.45 | 112.97      | 120.28   |
| 1   | A     | 491 | GLN  | C-N-CA    | -5.45 | 112.97      | 120.28   |
| 1   | A     | 223 | THR  | CA-C-N    | -5.43 | 110.76      | 121.41   |
| 1   | A     | 223 | THR  | C-N-CA    | -5.43 | 110.76      | 121.41   |
| 1   | A     | 90  | THR  | N-CA-C    | -5.42 | 106.51      | 113.23   |
| 1   | A     | 387 | LYS  | CA-C-O    | 5.42  | 127.09      | 120.92   |
| 1   | A     | 68  | LEU  | N-CA-C    | -5.41 | 99.92       | 108.73   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 417 | ASN  | CA-C-O     | -5.40 | 115.21      | 121.15   |
| 1   | A     | 298 | GLU  | CB-CG-CD   | 5.39  | 121.77      | 112.60   |
| 1   | A     | 471 | ASP  | CA-C-N     | 5.39  | 129.21      | 121.50   |
| 1   | A     | 471 | ASP  | C-N-CA     | 5.39  | 129.21      | 121.50   |
| 1   | A     | 162 | THR  | N-CA-C     | 5.39  | 118.43      | 110.46   |
| 1   | A     | 397 | ARG  | CA-C-O     | -5.37 | 115.49      | 121.51   |
| 1   | A     | 421 | ASN  | CB-CG-ND2  | -5.37 | 108.34      | 116.40   |
| 1   | A     | 80  | ARG  | NH1-CZ-NH2 | -5.37 | 112.32      | 119.30   |
| 1   | A     | 361 | ARG  | NE-CZ-NH2  | -5.36 | 114.38      | 119.20   |
| 1   | A     | 554 | ASN  | CA-C-O     | -5.36 | 115.58      | 121.31   |
| 1   | A     | 479 | LYS  | N-CA-C     | 5.36  | 117.42      | 110.40   |
| 1   | A     | 560 | ASN  | CA-C-O     | -5.36 | 112.25      | 119.11   |
| 1   | A     | 572 | VAL  | CB-CA-C    | 5.36  | 120.05      | 111.32   |
| 1   | A     | 256 | ARG  | CA-C-O     | -5.35 | 114.93      | 121.88   |
| 1   | A     | 182 | THR  | O-C-N      | 5.34  | 128.63      | 122.17   |
| 1   | A     | 322 | THR  | CB-CA-C    | -5.34 | 97.71       | 109.56   |
| 1   | A     | 254 | LEU  | CA-C-N     | -5.33 | 115.20      | 122.93   |
| 1   | A     | 254 | LEU  | C-N-CA     | -5.33 | 115.20      | 122.93   |
| 1   | A     | 325 | ILE  | N-CA-CB    | 5.33  | 118.39      | 111.67   |
| 1   | A     | 428 | ASN  | CA-C-N     | 5.33  | 130.47      | 122.58   |
| 1   | A     | 428 | ASN  | C-N-CA     | 5.33  | 130.47      | 122.58   |
| 1   | A     | 88  | ASP  | CA-C-O     | 5.33  | 126.12      | 120.10   |
| 1   | A     | 396 | GLU  | N-CA-C     | -5.32 | 101.04      | 109.76   |
| 1   | A     | 583 | LEU  | N-CA-C     | -5.32 | 104.39      | 112.04   |
| 1   | A     | 272 | PRO  | N-CA-CB    | 5.31  | 108.95      | 103.38   |
| 1   | A     | 422 | LEU  | CA-C-N     | -5.31 | 113.21      | 119.84   |
| 1   | A     | 422 | LEU  | C-N-CA     | -5.31 | 113.21      | 119.84   |
| 1   | A     | 181 | ASN  | CA-CB-CG   | -5.30 | 107.30      | 112.60   |
| 1   | A     | 549 | GLN  | CA-C-O     | -5.30 | 114.50      | 120.43   |
| 1   | A     | 155 | GLU  | N-CA-C     | 5.29  | 117.25      | 108.20   |
| 1   | A     | 509 | GLU  | CA-C-O     | -5.29 | 114.35      | 120.49   |
| 1   | A     | 155 | GLU  | CG-CD-OE1  | -5.29 | 106.24      | 118.40   |
| 1   | A     | 159 | GLN  | N-CA-C     | -5.28 | 98.14       | 109.81   |
| 1   | A     | 213 | GLN  | N-CA-C     | 5.28  | 117.69      | 110.24   |
| 1   | A     | 323 | ASN  | OD1-CG-ND2 | 5.28  | 127.88      | 122.60   |
| 1   | A     | 405 | ASP  | CA-C-N     | 5.27  | 129.82      | 121.18   |
| 1   | A     | 405 | ASP  | C-N-CA     | 5.27  | 129.82      | 121.18   |
| 1   | A     | 280 | GLN  | CA-C-N     | 5.27  | 132.33      | 122.74   |
| 1   | A     | 280 | GLN  | C-N-CA     | 5.27  | 132.33      | 122.74   |
| 1   | A     | 397 | ARG  | NE-CZ-NH1  | -5.25 | 116.25      | 121.50   |
| 1   | A     | 62  | THR  | CA-C-N     | 5.25  | 129.39      | 122.30   |
| 1   | A     | 62  | THR  | C-N-CA     | 5.25  | 129.39      | 122.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 385 | GLY  | CA-C-O     | -5.25 | 111.44      | 120.57   |
| 1   | A     | 521 | ILE  | O-C-N      | -5.24 | 116.96      | 122.67   |
| 1   | A     | 195 | LEU  | CB-CA-C    | 5.23  | 121.59      | 110.19   |
| 1   | A     | 472 | LYS  | CB-CG-CD   | 5.23  | 123.33      | 111.30   |
| 1   | A     | 513 | ASP  | CA-CB-CG   | 5.22  | 117.82      | 112.60   |
| 1   | A     | 204 | ILE  | CA-C-N     | 5.22  | 125.69      | 120.52   |
| 1   | A     | 204 | ILE  | C-N-CA     | 5.22  | 125.69      | 120.52   |
| 1   | A     | 201 | LYS  | CA-CB-CG   | 5.21  | 124.52      | 114.10   |
| 1   | A     | 316 | VAL  | O-C-N      | 5.21  | 128.50      | 123.03   |
| 1   | A     | 244 | TYR  | CB-CA-C    | -5.20 | 100.02      | 109.38   |
| 1   | A     | 473 | GLU  | O-C-N      | -5.18 | 116.89      | 122.79   |
| 1   | A     | 253 | HIS  | CA-CB-CG   | -5.16 | 108.64      | 113.80   |
| 1   | A     | 452 | GLY  | CA-C-O     | -5.16 | 114.14      | 121.52   |
| 1   | A     | 520 | ARG  | N-CA-C     | 5.16  | 117.98      | 109.72   |
| 1   | A     | 355 | THR  | CA-C-O     | -5.16 | 114.38      | 119.49   |
| 1   | A     | 287 | LEU  | O-C-N      | 5.16  | 125.98      | 121.18   |
| 1   | A     | 500 | VAL  | CA-C-O     | -5.16 | 115.30      | 121.28   |
| 1   | A     | 425 | THR  | OG1-CB-CG2 | 5.15  | 119.61      | 109.30   |
| 1   | A     | 579 | ALA  | N-CA-CB    | 5.15  | 116.99      | 110.04   |
| 1   | A     | 269 | ASP  | CA-C-N     | -5.14 | 113.53      | 122.37   |
| 1   | A     | 269 | ASP  | C-N-CA     | -5.14 | 113.53      | 122.37   |
| 1   | A     | 95  | ASN  | N-CA-C     | 5.14  | 118.86      | 112.59   |
| 1   | A     | 172 | SER  | N-CA-C     | 5.13  | 117.60      | 109.50   |
| 1   | A     | 544 | THR  | CA-CB-OG1  | -5.12 | 101.92      | 109.60   |
| 1   | A     | 326 | THR  | CA-CB-OG1  | -5.12 | 101.93      | 109.60   |
| 1   | A     | 503 | ALA  | CA-C-O     | -5.11 | 115.25      | 120.87   |
| 1   | A     | 560 | ASN  | N-CA-CB    | 5.10  | 118.97      | 110.41   |
| 1   | A     | 483 | HIS  | N-CA-C     | -5.09 | 100.15      | 108.76   |
| 1   | A     | 274 | ARG  | NE-CZ-NH1  | -5.08 | 116.42      | 121.50   |
| 1   | A     | 41  | SER  | O-C-N      | 5.08  | 129.08      | 122.89   |
| 1   | A     | 197 | PHE  | N-CA-C     | 5.07  | 119.44      | 113.16   |
| 1   | A     | 540 | ARG  | NE-CZ-NH1  | -5.06 | 116.44      | 121.50   |
| 1   | A     | 433 | THR  | N-CA-CB    | -5.06 | 103.08      | 110.47   |
| 1   | A     | 452 | GLY  | O-C-N      | 5.05  | 126.82      | 121.77   |
| 1   | A     | 269 | ASP  | CA-CB-CG   | 5.05  | 117.65      | 112.60   |
| 1   | A     | 95  | ASN  | CA-C-N     | 5.05  | 127.30      | 120.38   |
| 1   | A     | 95  | ASN  | C-N-CA     | 5.05  | 127.30      | 120.38   |
| 1   | A     | 206 | THR  | O-C-N      | 5.05  | 127.34      | 121.39   |
| 1   | A     | 67  | ARG  | CA-CB-CG   | 5.04  | 124.19      | 114.10   |
| 1   | A     | 357 | ILE  | CA-CB-CG2  | 5.03  | 119.05      | 110.50   |
| 1   | A     | 352 | PRO  | CB-CA-C    | 5.02  | 117.53      | 110.60   |
| 1   | A     | 130 | VAL  | O-C-N      | -5.02 | 117.00      | 121.87   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 54  | LEU  | CA-C-O  | 5.01  | 127.68      | 120.51   |
| 1   | A     | 281 | THR  | N-CA-CB | -5.01 | 102.74      | 110.56   |
| 1   | A     | 416 | GLN  | CA-C-N  | 5.01  | 127.96      | 120.90   |
| 1   | A     | 416 | GLN  | C-N-CA  | 5.01  | 127.96      | 120.90   |
| 1   | A     | 415 | ILE  | CA-C-N  | -5.00 | 113.13      | 121.94   |
| 1   | A     | 415 | ILE  | C-N-CA  | -5.00 | 113.13      | 121.94   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 4347  | 0        | 4143     | 294     | 0            |
| 2   | A     | 87    | 0        | 0        | 8       | 0            |
| All | All   | 4434  | 0        | 4143     | 294     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (294) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:361:ARG:NE   | 1:A:366:THR:CG2  | 1.93                     | 1.32              |
| 1:A:366:THR:HB   | 1:A:370:GLN:O    | 1.28                     | 1.24              |
| 1:A:361:ARG:CZ   | 1:A:366:THR:HG21 | 1.68                     | 1.20              |
| 1:A:366:THR:HG22 | 1:A:370:GLN:CG   | 1.73                     | 1.18              |
| 1:A:159:GLN:O    | 1:A:161:PRO:HD3  | 1.45                     | 1.16              |
| 1:A:361:ARG:NE   | 1:A:366:THR:HG21 | 1.56                     | 1.13              |
| 1:A:366:THR:CG2  | 1:A:370:GLN:HG3  | 1.78                     | 1.12              |
| 1:A:422:LEU:O    | 1:A:424:VAL:N    | 1.84                     | 1.09              |
| 1:A:159:GLN:HB2  | 1:A:160:PRO:HD3  | 1.10                     | 1.08              |
| 1:A:156:SER:HB3  | 1:A:162:THR:HG23 | 1.30                     | 1.08              |
| 1:A:174:MET:HE2  | 1:A:503:ALA:HA   | 1.29                     | 1.08              |
| 1:A:361:ARG:CZ   | 1:A:366:THR:CG2  | 2.29                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:370:GLN:HE21 | 1:A:370:GLN:HA   | 1.13                     | 1.05              |
| 1:A:366:THR:HA   | 1:A:370:GLN:HB3  | 1.09                     | 1.05              |
| 1:A:122:ASN:HB2  | 1:A:123:PRO:HD2  | 1.39                     | 1.02              |
| 1:A:159:GLN:HB2  | 1:A:160:PRO:CD   | 1.89                     | 1.01              |
| 1:A:366:THR:CA   | 1:A:370:GLN:HB3  | 1.90                     | 1.01              |
| 1:A:361:ARG:NE   | 1:A:366:THR:HG23 | 1.78                     | 0.97              |
| 1:A:85:ASN:HA    | 1:A:101:ILE:HG12 | 1.49                     | 0.94              |
| 1:A:361:ARG:NH2  | 1:A:370:GLN:OE1  | 2.00                     | 0.94              |
| 1:A:366:THR:HG22 | 1:A:370:GLN:HG3  | 0.95                     | 0.94              |
| 1:A:389:THR:HG21 | 1:A:566:ILE:HG22 | 1.50                     | 0.94              |
| 1:A:292:ASN:HD22 | 1:A:307:GLY:H    | 1.17                     | 0.90              |
| 1:A:361:ARG:CD   | 1:A:366:THR:CG2  | 2.50                     | 0.89              |
| 1:A:361:ARG:NH2  | 1:A:409:TYR:HE1  | 1.71                     | 0.88              |
| 1:A:158:THR:HG23 | 1:A:159:GLN:H    | 1.39                     | 0.88              |
| 1:A:388:THR:HG22 | 1:A:568:GLY:HA2  | 1.54                     | 0.87              |
| 1:A:93:ASN:HD22  | 1:A:225:THR:HB   | 1.40                     | 0.86              |
| 1:A:185:PHE:CE2  | 1:A:187:PRO:HG3  | 2.10                     | 0.86              |
| 1:A:361:ARG:CD   | 1:A:366:THR:HG23 | 2.05                     | 0.86              |
| 1:A:266:PHE:HZ   | 1:A:493:ASN:O    | 1.58                     | 0.86              |
| 1:A:158:THR:HG22 | 1:A:160:PRO:HD2  | 1.57                     | 0.86              |
| 1:A:361:ARG:HA   | 2:A:784:HOH:O    | 1.74                     | 0.86              |
| 1:A:370:GLN:HA   | 1:A:370:GLN:NE2  | 1.88                     | 0.85              |
| 1:A:193:GLU:OE1  | 1:A:206:THR:HG21 | 1.78                     | 0.84              |
| 1:A:53:PHE:CD1   | 1:A:59:VAL:CG1   | 2.60                     | 0.84              |
| 1:A:365:GLN:O    | 1:A:370:GLN:CB   | 2.25                     | 0.84              |
| 1:A:361:ARG:NH2  | 1:A:409:TYR:CE1  | 2.44                     | 0.84              |
| 1:A:302:ASN:N    | 1:A:302:ASN:HD22 | 1.75                     | 0.83              |
| 1:A:485:ASN:H    | 1:A:485:ASN:HD22 | 1.27                     | 0.82              |
| 1:A:362:GLY:HA2  | 1:A:366:THR:OG1  | 1.80                     | 0.82              |
| 1:A:364:ALA:HB3  | 1:A:365:GLN:NE2  | 1.93                     | 0.81              |
| 1:A:156:SER:HB3  | 1:A:162:THR:CG2  | 2.09                     | 0.81              |
| 1:A:159:GLN:CB   | 1:A:160:PRO:HD3  | 2.02                     | 0.80              |
| 1:A:435:PRO:HB3  | 1:A:439:LYS:O    | 1.81                     | 0.80              |
| 1:A:174:MET:HE2  | 1:A:503:ALA:CA   | 2.10                     | 0.80              |
| 1:A:388:THR:HB   | 1:A:569:MET:H    | 1.46                     | 0.80              |
| 1:A:158:THR:CG2  | 1:A:159:GLN:H    | 1.94                     | 0.80              |
| 1:A:158:THR:CG2  | 1:A:159:GLN:N    | 2.44                     | 0.79              |
| 1:A:324:TYR:O    | 1:A:329:THR:HG21 | 1.82                     | 0.79              |
| 1:A:53:PHE:CD1   | 1:A:59:VAL:HG12  | 2.18                     | 0.78              |
| 1:A:319:MET:HE1  | 1:A:329:THR:OG1  | 1.84                     | 0.78              |
| 1:A:471:ASP:OD2  | 1:A:483:HIS:HD2  | 1.67                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:366:THR:HA   | 1:A:370:GLN:CB   | 2.03                     | 0.77              |
| 1:A:478:LEU:N    | 1:A:478:LEU:HD23 | 2.00                     | 0.76              |
| 1:A:361:ARG:CD   | 1:A:366:THR:HG21 | 2.14                     | 0.76              |
| 1:A:422:LEU:O    | 1:A:423:PRO:C    | 2.20                     | 0.76              |
| 1:A:158:THR:H    | 1:A:161:PRO:HA   | 1.50                     | 0.75              |
| 1:A:393:GLU:OE1  | 1:A:393:GLU:HA   | 1.86                     | 0.74              |
| 1:A:89:LYS:HD2   | 1:A:98:LEU:HD12  | 1.70                     | 0.74              |
| 1:A:382:ARG:NH2  | 1:A:390:THR:O    | 2.19                     | 0.74              |
| 1:A:443:ASN:H    | 1:A:446:ASN:ND2  | 1.85                     | 0.74              |
| 1:A:266:PHE:HZ   | 1:A:493:ASN:C    | 1.96                     | 0.73              |
| 1:A:389:THR:HG23 | 1:A:568:GLY:HA2  | 1.68                     | 0.73              |
| 1:A:292:ASN:HD22 | 1:A:307:GLY:N    | 1.87                     | 0.73              |
| 1:A:156:SER:O    | 1:A:158:THR:N    | 2.21                     | 0.73              |
| 1:A:127:GLN:HG3  | 1:A:551:MET:HG2  | 1.71                     | 0.73              |
| 1:A:174:MET:HE3  | 1:A:501:LYS:HG2  | 1.69                     | 0.73              |
| 1:A:361:ARG:HD2  | 1:A:366:THR:HG23 | 1.72                     | 0.71              |
| 1:A:183:MET:HE3  | 1:A:208:TRP:HH2  | 1.54                     | 0.71              |
| 1:A:266:PHE:CD1  | 1:A:495:PRO:HG3  | 2.26                     | 0.71              |
| 1:A:361:ARG:HH21 | 1:A:409:TYR:HE1  | 1.34                     | 0.71              |
| 1:A:156:SER:N    | 1:A:162:THR:O    | 2.25                     | 0.70              |
| 1:A:74:PRO:HB2   | 1:A:76:SER:O     | 1.91                     | 0.70              |
| 1:A:84:VAL:O     | 1:A:101:ILE:HA   | 1.91                     | 0.70              |
| 1:A:377:ARG:NH2  | 1:A:397:ARG:HD2  | 2.07                     | 0.70              |
| 1:A:322:THR:HG22 | 1:A:324:TYR:H    | 1.56                     | 0.69              |
| 1:A:281:THR:HG22 | 1:A:283:ARG:H    | 1.58                     | 0.69              |
| 1:A:216:ARG:NH2  | 1:A:231:ASN:OD1  | 2.20                     | 0.69              |
| 1:A:424:VAL:HG22 | 1:A:429:VAL:HG22 | 1.74                     | 0.69              |
| 1:A:361:ARG:NH2  | 1:A:370:GLN:CD   | 2.52                     | 0.68              |
| 1:A:361:ARG:HE   | 1:A:366:THR:CG2  | 2.04                     | 0.67              |
| 1:A:389:THR:CG2  | 1:A:566:ILE:HG22 | 2.23                     | 0.67              |
| 1:A:431:LEU:C    | 1:A:433:THR:H    | 2.00                     | 0.67              |
| 1:A:465:PRO:HD2  | 1:A:466:ASN:ND2  | 2.11                     | 0.66              |
| 1:A:401:ILE:O    | 1:A:575:LYS:HE2  | 1.95                     | 0.66              |
| 1:A:507:THR:HG22 | 1:A:521:ILE:HG13 | 1.78                     | 0.65              |
| 1:A:361:ARG:CZ   | 1:A:366:THR:HG22 | 2.26                     | 0.65              |
| 1:A:319:MET:CE   | 1:A:329:THR:OG1  | 2.45                     | 0.65              |
| 1:A:158:THR:CG2  | 1:A:160:PRO:HD2  | 2.27                     | 0.64              |
| 1:A:310:GLN:HA   | 1:A:313:ARG:HD2  | 1.78                     | 0.64              |
| 1:A:459:ASN:ND2  | 1:A:460:VAL:H    | 1.95                     | 0.64              |
| 1:A:346:GLU:OE2  | 1:A:355:THR:OG1  | 2.16                     | 0.64              |
| 1:A:477:ASP:C    | 1:A:478:LEU:HD23 | 2.23                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:362:GLY:CA   | 1:A:366:THR:OG1  | 2.46                     | 0.63              |
| 1:A:386:GLN:HB2  | 1:A:396:GLU:HB2  | 1.79                     | 0.63              |
| 1:A:53:PHE:CE1   | 1:A:59:VAL:HG11  | 2.33                     | 0.63              |
| 1:A:266:PHE:CZ   | 1:A:493:ASN:O    | 2.48                     | 0.62              |
| 1:A:396:GLU:HG3  | 1:A:397:ARG:N    | 2.12                     | 0.62              |
| 1:A:425:THR:O    | 1:A:427:ASP:N    | 2.33                     | 0.62              |
| 1:A:54:LEU:CD1   | 1:A:54:LEU:N     | 2.63                     | 0.61              |
| 1:A:54:LEU:N     | 1:A:54:LEU:HD13  | 2.16                     | 0.61              |
| 1:A:237:ASP:OD1  | 1:A:239:ASP:N    | 2.33                     | 0.61              |
| 1:A:158:THR:HG22 | 1:A:159:GLN:N    | 2.16                     | 0.61              |
| 1:A:361:ARG:NH2  | 1:A:370:GLN:CG   | 2.63                     | 0.61              |
| 1:A:174:MET:CE   | 1:A:501:LYS:NZ   | 2.64                     | 0.60              |
| 1:A:365:GLN:O    | 1:A:370:GLN:HB2  | 2.00                     | 0.60              |
| 1:A:570:LYS:HD3  | 1:A:572:VAL:HG23 | 1.84                     | 0.60              |
| 1:A:276:THR:C    | 1:A:577:GLN:HB3  | 2.26                     | 0.60              |
| 1:A:322:THR:HG22 | 1:A:323:ASN:N    | 2.16                     | 0.60              |
| 1:A:364:ALA:HB3  | 1:A:365:GLN:HE22 | 1.65                     | 0.60              |
| 1:A:74:PRO:O     | 1:A:520:ARG:NH2  | 2.28                     | 0.60              |
| 1:A:156:SER:O    | 1:A:162:THR:HG22 | 2.02                     | 0.59              |
| 1:A:365:GLN:O    | 1:A:370:GLN:HG2  | 2.02                     | 0.59              |
| 1:A:389:THR:HG23 | 1:A:568:GLY:CA   | 2.32                     | 0.59              |
| 1:A:39:GLY:O     | 1:A:40:ILE:HD13  | 2.02                     | 0.59              |
| 1:A:58:TRP:CZ2   | 1:A:538:LYS:HD2  | 2.37                     | 0.59              |
| 1:A:240:ASP:OD2  | 2:A:816:HOH:O    | 2.16                     | 0.59              |
| 1:A:317:THR:HG22 | 1:A:330:ILE:HA   | 1.83                     | 0.59              |
| 1:A:476:THR:CG2  | 1:A:478:LEU:O    | 2.50                     | 0.58              |
| 1:A:299:GLY:C    | 1:A:301:THR:H    | 2.11                     | 0.58              |
| 1:A:159:GLN:O    | 1:A:161:PRO:CD   | 2.35                     | 0.58              |
| 1:A:308:VAL:HG12 | 1:A:313:ARG:HG3  | 1.84                     | 0.58              |
| 1:A:183:MET:HE3  | 1:A:208:TRP:CH2  | 2.38                     | 0.58              |
| 1:A:85:ASN:HA    | 1:A:101:ILE:CG1  | 2.30                     | 0.58              |
| 1:A:143:GLN:O    | 1:A:263:THR:HB   | 2.03                     | 0.58              |
| 1:A:292:ASN:ND2  | 1:A:307:GLY:H    | 1.97                     | 0.58              |
| 1:A:424:VAL:CG2  | 1:A:429:VAL:HG22 | 2.34                     | 0.58              |
| 1:A:93:ASN:ND2   | 1:A:225:THR:HB   | 2.16                     | 0.58              |
| 1:A:223:THR:HG22 | 2:A:820:HOH:O    | 2.03                     | 0.57              |
| 1:A:378:TYR:O    | 1:A:397:ARG:HA   | 2.04                     | 0.57              |
| 1:A:310:GLN:HG2  | 1:A:313:ARG:NH1  | 2.20                     | 0.57              |
| 1:A:59:VAL:HG23  | 1:A:537:ALA:HB3  | 1.86                     | 0.56              |
| 1:A:174:MET:CE   | 1:A:501:LYS:HZ2  | 2.19                     | 0.56              |
| 1:A:361:ARG:CG   | 1:A:366:THR:HG21 | 2.36                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:365:GLN:O    | 1:A:370:GLN:CG   | 2.53                     | 0.56              |
| 1:A:302:ASN:N    | 1:A:302:ASN:ND2  | 2.48                     | 0.56              |
| 1:A:122:ASN:HB2  | 1:A:123:PRO:CD   | 2.25                     | 0.55              |
| 1:A:361:ARG:NH2  | 1:A:370:GLN:HG3  | 2.21                     | 0.55              |
| 1:A:52:LYS:O     | 1:A:52:LYS:HG2   | 2.07                     | 0.55              |
| 1:A:471:ASP:OD2  | 1:A:483:HIS:CD2  | 2.55                     | 0.55              |
| 1:A:361:ARG:HE   | 1:A:366:THR:HG23 | 1.66                     | 0.55              |
| 1:A:462:PRO:HD2  | 1:A:576:SER:OG   | 2.07                     | 0.55              |
| 1:A:388:THR:CG2  | 1:A:569:MET:H    | 2.20                     | 0.54              |
| 1:A:431:LEU:C    | 1:A:433:THR:N    | 2.64                     | 0.54              |
| 1:A:361:ARG:NH2  | 1:A:366:THR:HG22 | 2.23                     | 0.54              |
| 1:A:53:PHE:CE1   | 1:A:59:VAL:CG1   | 2.89                     | 0.54              |
| 1:A:230:THR:HB   | 1:A:232:ILE:HD11 | 1.88                     | 0.54              |
| 1:A:174:MET:HE3  | 1:A:501:LYS:NZ   | 2.23                     | 0.53              |
| 1:A:354:LYS:NZ   | 1:A:373:ASP:OD1  | 2.41                     | 0.53              |
| 1:A:485:ASN:H    | 1:A:485:ASN:ND2  | 2.03                     | 0.53              |
| 1:A:460:VAL:HG21 | 1:A:484:VAL:HA   | 1.91                     | 0.53              |
| 1:A:62:THR:HB    | 1:A:534:VAL:HG22 | 1.90                     | 0.53              |
| 1:A:570:LYS:CD   | 1:A:572:VAL:HG23 | 2.38                     | 0.53              |
| 1:A:377:ARG:HH21 | 1:A:397:ARG:HD2  | 1.72                     | 0.53              |
| 1:A:281:THR:HG22 | 1:A:283:ARG:HB2  | 1.91                     | 0.53              |
| 1:A:393:GLU:OE1  | 1:A:393:GLU:CA   | 2.56                     | 0.53              |
| 1:A:52:LYS:O     | 1:A:54:LEU:HD13  | 2.08                     | 0.52              |
| 1:A:364:ALA:CB   | 1:A:365:GLN:NE2  | 2.71                     | 0.52              |
| 1:A:154:SER:OG   | 1:A:164:VAL:HG13 | 2.09                     | 0.52              |
| 1:A:339:SER:O    | 1:A:449:ASN:HA   | 2.10                     | 0.52              |
| 1:A:365:GLN:C    | 1:A:370:GLN:HG2  | 2.35                     | 0.52              |
| 1:A:443:ASN:H    | 1:A:446:ASN:HD21 | 1.56                     | 0.52              |
| 1:A:322:THR:HG22 | 1:A:323:ASN:H    | 1.75                     | 0.52              |
| 1:A:382:ARG:HG3  | 1:A:386:GLN:HG2  | 1.90                     | 0.52              |
| 1:A:213:GLN:HG3  | 1:A:240:ASP:HB3  | 1.91                     | 0.52              |
| 1:A:215:ASP:N    | 1:A:235:GLY:O    | 2.43                     | 0.52              |
| 1:A:158:THR:N    | 1:A:161:PRO:HA   | 2.23                     | 0.51              |
| 1:A:425:THR:O    | 1:A:426:ASN:C    | 2.53                     | 0.51              |
| 1:A:245:THR:OG1  | 1:A:248:ASN:HB2  | 2.11                     | 0.51              |
| 1:A:361:ARG:NH2  | 1:A:409:TYR:CD1  | 2.77                     | 0.51              |
| 1:A:483:HIS:HB3  | 1:A:485:ASN:ND2  | 2.25                     | 0.51              |
| 1:A:465:PRO:HD2  | 1:A:466:ASN:HD22 | 1.74                     | 0.51              |
| 1:A:232:ILE:HB   | 1:A:234:HIS:CD2  | 2.46                     | 0.51              |
| 1:A:299:GLY:O    | 1:A:301:THR:N    | 2.43                     | 0.51              |
| 1:A:343:TYR:HE1  | 1:A:373:ASP:HB2  | 1.76                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:145:ILE:O    | 1:A:260:GLU:HG2  | 2.11                     | 0.51              |
| 1:A:122:ASN:CB   | 1:A:123:PRO:HD2  | 2.16                     | 0.50              |
| 1:A:579:ALA:HB1  | 1:A:580:PRO:HD2  | 1.93                     | 0.50              |
| 1:A:361:ARG:HG3  | 1:A:362:GLY:N    | 2.26                     | 0.50              |
| 1:A:58:TRP:CE2   | 1:A:538:LYS:HD2  | 2.45                     | 0.50              |
| 1:A:183:MET:HB3  | 1:A:184:PRO:HD2  | 1.94                     | 0.50              |
| 1:A:470:TRP:HA   | 1:A:488:PHE:O    | 2.11                     | 0.50              |
| 1:A:557:ASN:OD1  | 1:A:558:GLN:N    | 2.46                     | 0.49              |
| 1:A:365:GLN:O    | 1:A:370:GLN:HB3  | 2.00                     | 0.49              |
| 1:A:158:THR:HB   | 1:A:162:THR:HG22 | 1.95                     | 0.49              |
| 1:A:435:PRO:CB   | 1:A:439:LYS:O    | 2.57                     | 0.49              |
| 1:A:185:PHE:HA   | 1:A:497:GLN:NE2  | 2.28                     | 0.48              |
| 1:A:266:PHE:CZ   | 1:A:493:ASN:C    | 2.84                     | 0.48              |
| 1:A:476:THR:O    | 1:A:479:LYS:HE2  | 2.12                     | 0.48              |
| 1:A:126:TRP:O    | 1:A:130:VAL:HB   | 2.13                     | 0.48              |
| 1:A:77:GLU:OE1   | 1:A:520:ARG:NH1  | 2.45                     | 0.48              |
| 1:A:183:MET:CE   | 1:A:208:TRP:CH2  | 2.96                     | 0.48              |
| 1:A:361:ARG:HH11 | 1:A:361:ARG:HG2  | 1.79                     | 0.47              |
| 1:A:95:ASN:O     | 1:A:98:LEU:HB2   | 2.13                     | 0.47              |
| 1:A:409:TYR:CE2  | 1:A:411:GLU:HB2  | 2.49                     | 0.47              |
| 1:A:361:ARG:NH1  | 1:A:366:THR:HG21 | 2.24                     | 0.47              |
| 1:A:174:MET:HE1  | 1:A:501:LYS:HZ2  | 1.79                     | 0.47              |
| 1:A:197:PHE:N    | 1:A:197:PHE:CD1  | 2.83                     | 0.47              |
| 1:A:326:THR:H    | 1:A:329:THR:CG2  | 2.26                     | 0.47              |
| 1:A:183:MET:HE3  | 1:A:183:MET:HB3  | 1.75                     | 0.47              |
| 1:A:365:GLN:N    | 1:A:365:GLN:CD   | 2.72                     | 0.47              |
| 1:A:425:THR:O    | 1:A:428:ASN:N    | 2.47                     | 0.47              |
| 1:A:43:GLY:HA3   | 1:A:146:PHE:CD2  | 2.50                     | 0.46              |
| 1:A:441:GLY:O    | 1:A:442:ILE:HD13 | 2.15                     | 0.46              |
| 1:A:302:ASN:HD22 | 1:A:302:ASN:H    | 1.60                     | 0.46              |
| 1:A:80:ARG:HB2   | 1:A:106:VAL:HB   | 1.97                     | 0.46              |
| 1:A:368:GLU:HA   | 2:A:793:HOH:O    | 2.15                     | 0.46              |
| 1:A:299:GLY:C    | 1:A:301:THR:N    | 2.74                     | 0.46              |
| 1:A:536:LYS:HE3  | 1:A:536:LYS:HB2  | 1.41                     | 0.46              |
| 1:A:571:ILE:HA   | 2:A:731:HOH:O    | 2.14                     | 0.46              |
| 1:A:319:MET:HE1  | 1:A:329:THR:HG1  | 1.76                     | 0.46              |
| 1:A:361:ARG:CG   | 1:A:362:GLY:N    | 2.79                     | 0.46              |
| 1:A:158:THR:HG22 | 1:A:160:PRO:CD   | 2.39                     | 0.45              |
| 1:A:92:VAL:O     | 1:A:95:ASN:HB2   | 2.15                     | 0.45              |
| 1:A:370:GLN:OE1  | 1:A:409:TYR:HE1  | 2.00                     | 0.45              |
| 1:A:137:HIS:O    | 1:A:535:PHE:HA   | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:174:MET:HE2  | 1:A:503:ALA:CB   | 2.47                     | 0.45              |
| 1:A:53:PHE:HD1   | 1:A:59:VAL:CG1   | 2.26                     | 0.44              |
| 1:A:429:VAL:HG11 | 1:A:431:LEU:HD21 | 1.99                     | 0.44              |
| 1:A:432:PRO:HA   | 1:A:443:ASN:HD22 | 1.81                     | 0.44              |
| 1:A:133:MET:SD   | 1:A:539:LEU:HD23 | 2.57                     | 0.44              |
| 1:A:430:LEU:HD12 | 1:A:430:LEU:HA   | 1.95                     | 0.44              |
| 1:A:213:GLN:HG3  | 1:A:240:ASP:CB   | 2.47                     | 0.44              |
| 1:A:443:ASN:ND2  | 1:A:445:THR:H    | 2.15                     | 0.44              |
| 1:A:174:MET:CG   | 1:A:503:ALA:HB2  | 2.47                     | 0.44              |
| 1:A:156:SER:CB   | 1:A:162:THR:HG23 | 2.22                     | 0.44              |
| 1:A:326:THR:H    | 1:A:329:THR:HB   | 1.83                     | 0.43              |
| 1:A:222:HIS:CE1  | 1:A:224:GLY:O    | 2.71                     | 0.43              |
| 1:A:388:THR:HB   | 1:A:569:MET:O    | 2.17                     | 0.43              |
| 1:A:411:GLU:OE1  | 1:A:411:GLU:N    | 2.47                     | 0.43              |
| 1:A:468:GLN:HG2  | 1:A:486:ALA:HB2  | 1.99                     | 0.43              |
| 1:A:266:PHE:CZ   | 1:A:494:CYS:CA   | 3.02                     | 0.43              |
| 1:A:354:LYS:CE   | 1:A:355:THR:O    | 2.67                     | 0.43              |
| 1:A:70:HIS:CD2   | 1:A:526:ASP:OD1  | 2.72                     | 0.43              |
| 1:A:55:GLU:O     | 1:A:56:ASN:HB2   | 2.19                     | 0.43              |
| 1:A:565:ASN:C    | 1:A:566:ILE:HD13 | 2.44                     | 0.43              |
| 1:A:222:HIS:O    | 1:A:223:THR:C    | 2.61                     | 0.43              |
| 1:A:325:ILE:HA   | 1:A:329:THR:CG2  | 2.49                     | 0.43              |
| 1:A:59:VAL:CG2   | 1:A:537:ALA:HB3  | 2.48                     | 0.43              |
| 1:A:255:LEU:HB3  | 1:A:259:ASP:HB2  | 2.01                     | 0.43              |
| 1:A:476:THR:HG23 | 1:A:478:LEU:O    | 2.19                     | 0.43              |
| 1:A:554:ASN:OD1  | 1:A:556:ASP:N    | 2.50                     | 0.43              |
| 1:A:277:HIS:O    | 1:A:580:PRO:HA   | 2.19                     | 0.43              |
| 1:A:325:ILE:HA   | 1:A:329:THR:HG22 | 2.01                     | 0.43              |
| 1:A:266:PHE:CZ   | 1:A:494:CYS:HA   | 2.54                     | 0.42              |
| 1:A:369:ASN:O    | 1:A:371:ALA:N    | 2.44                     | 0.42              |
| 1:A:382:ARG:NH2  | 1:A:392:GLY:O    | 2.48                     | 0.42              |
| 1:A:404:GLN:H    | 1:A:404:GLN:HG3  | 1.53                     | 0.42              |
| 1:A:397:ARG:HH11 | 1:A:397:ARG:HD3  | 1.46                     | 0.42              |
| 1:A:74:PRO:HD2   | 1:A:520:ARG:NH1  | 2.34                     | 0.42              |
| 1:A:155:GLU:HA   | 1:A:163:LYS:HA   | 2.00                     | 0.42              |
| 1:A:471:ASP:O    | 1:A:489:VAL:HA   | 2.19                     | 0.42              |
| 1:A:232:ILE:HB   | 1:A:234:HIS:NE2  | 2.35                     | 0.42              |
| 1:A:367:ASP:CG   | 1:A:368:GLU:H    | 2.27                     | 0.42              |
| 1:A:53:PHE:C     | 1:A:54:LEU:HD13  | 2.45                     | 0.42              |
| 1:A:74:PRO:HD2   | 1:A:520:ARG:HH12 | 1.84                     | 0.42              |
| 1:A:126:TRP:NE1  | 1:A:130:VAL:HG21 | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:133:MET:HB2  | 1:A:275:LEU:HD12 | 2.02                     | 0.42              |
| 1:A:43:GLY:HA3   | 1:A:146:PHE:CG   | 2.55                     | 0.42              |
| 1:A:89:LYS:HE2   | 1:A:89:LYS:HB2   | 1.73                     | 0.42              |
| 1:A:366:THR:HG22 | 1:A:370:GLN:HG2  | 1.88                     | 0.42              |
| 1:A:201:LYS:HG2  | 2:A:759:HOH:O    | 2.19                     | 0.42              |
| 1:A:432:PRO:HA   | 1:A:443:ASN:ND2  | 2.35                     | 0.42              |
| 1:A:514:ALA:C    | 1:A:516:ALA:H    | 2.28                     | 0.42              |
| 1:A:557:ASN:OD1  | 1:A:557:ASN:C    | 2.62                     | 0.42              |
| 1:A:122:ASN:OD1  | 1:A:122:ASN:C    | 2.63                     | 0.41              |
| 1:A:265:THR:HG21 | 1:A:267:PHE:CZ   | 2.54                     | 0.41              |
| 1:A:296:GLN:OE1  | 1:A:296:GLN:HA   | 2.11                     | 0.41              |
| 1:A:324:TYR:O    | 1:A:329:THR:CG2  | 2.62                     | 0.41              |
| 1:A:409:TYR:CD2  | 1:A:411:GLU:HB2  | 2.55                     | 0.41              |
| 1:A:580:PRO:HD3  | 2:A:803:HOH:O    | 2.20                     | 0.41              |
| 1:A:163:LYS:HE2  | 1:A:165:TYR:OH   | 2.21                     | 0.41              |
| 1:A:137:HIS:HA   | 2:A:761:HOH:O    | 2.20                     | 0.41              |
| 1:A:322:THR:CG2  | 1:A:324:TYR:H    | 2.29                     | 0.41              |
| 1:A:174:MET:HG2  | 1:A:503:ALA:HB2  | 2.03                     | 0.41              |
| 1:A:217:THR:HB   | 1:A:232:ILE:HD12 | 2.03                     | 0.41              |
| 1:A:485:ASN:HD22 | 1:A:485:ASN:N    | 2.04                     | 0.40              |
| 1:A:566:ILE:HD12 | 1:A:566:ILE:HA   | 1.56                     | 0.40              |
| 1:A:174:MET:CE   | 1:A:501:LYS:HZ3  | 2.33                     | 0.40              |
| 1:A:216:ARG:CZ   | 1:A:218:LEU:HB2  | 2.50                     | 0.40              |
| 1:A:422:LEU:HD23 | 1:A:422:LEU:HA   | 1.75                     | 0.40              |
| 1:A:493:ASN:O    | 1:A:493:ASN:ND2  | 2.50                     | 0.40              |
| 1:A:200:TRP:HZ2  | 1:A:569:MET:HE2  | 1.86                     | 0.40              |
| 1:A:275:LEU:HD23 | 1:A:275:LEU:HA   | 1.88                     | 0.40              |
| 1:A:415:ILE:HG12 | 1:A:444:TYR:CZ   | 2.56                     | 0.40              |
| 1:A:39:GLY:C     | 1:A:40:ILE:HD13  | 2.46                     | 0.40              |
| 1:A:279:TRP:CE3  | 1:A:279:TRP:C    | 2.99                     | 0.40              |
| 1:A:459:ASN:HD22 | 1:A:460:VAL:H    | 1.68                     | 0.40              |
| 1:A:116:ALA:HA   | 1:A:467:GLY:O    | 2.22                     | 0.40              |
| 1:A:193:GLU:HB3  | 1:A:206:THR:CG2  | 2.52                     | 0.40              |
| 1:A:266:PHE:CE1  | 1:A:495:PRO:HD3  | 2.56                     | 0.40              |
| 1:A:326:THR:OG1  | 1:A:329:THR:HB   | 2.21                     | 0.40              |
| 1:A:366:THR:CB   | 1:A:370:GLN:HB3  | 2.50                     | 0.40              |

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|---------|----------|-------------|----|
| 1   | A     | 546/548 (100%) | 509 (93%) | 30 (6%) | 7 (1%)   | 9           | 38 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 157 | ALA  |
| 1   | A     | 300 | ALA  |
| 1   | A     | 426 | ASN  |
| 1   | A     | 402 | ALA  |
| 1   | A     | 87  | MET  |
| 1   | A     | 159 | GLN  |
| 1   | A     | 423 | PRO  |

### 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     | 476/476 (100%) | 409 (86%) | 67 (14%) | 3           | 16 |

All (67) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 44  | THR  |
| 1   | A     | 47  | ASN  |
| 1   | A     | 49  | THR  |
| 1   | A     | 54  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 59  | VAL  |
| 1   | A     | 62  | THR  |
| 1   | A     | 75  | GLU  |
| 1   | A     | 96  | MET  |
| 1   | A     | 98  | LEU  |
| 1   | A     | 130 | VAL  |
| 1   | A     | 154 | SER  |
| 1   | A     | 158 | THR  |
| 1   | A     | 167 | ASN  |
| 1   | A     | 190 | MET  |
| 1   | A     | 206 | THR  |
| 1   | A     | 216 | ARG  |
| 1   | A     | 223 | THR  |
| 1   | A     | 228 | THR  |
| 1   | A     | 232 | ILE  |
| 1   | A     | 239 | ASP  |
| 1   | A     | 255 | LEU  |
| 1   | A     | 263 | THR  |
| 1   | A     | 271 | LYS  |
| 1   | A     | 301 | THR  |
| 1   | A     | 302 | ASN  |
| 1   | A     | 316 | VAL  |
| 1   | A     | 322 | THR  |
| 1   | A     | 329 | THR  |
| 1   | A     | 342 | TYR  |
| 1   | A     | 354 | LYS  |
| 1   | A     | 357 | ILE  |
| 1   | A     | 361 | ARG  |
| 1   | A     | 366 | THR  |
| 1   | A     | 370 | GLN  |
| 1   | A     | 386 | GLN  |
| 1   | A     | 387 | LYS  |
| 1   | A     | 388 | THR  |
| 1   | A     | 390 | THR  |
| 1   | A     | 393 | GLU  |
| 1   | A     | 397 | ARG  |
| 1   | A     | 404 | GLN  |
| 1   | A     | 405 | ASP  |
| 1   | A     | 418 | ILE  |
| 1   | A     | 422 | LEU  |
| 1   | A     | 425 | THR  |
| 1   | A     | 427 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 429 | VAL  |
| 1   | A     | 433 | THR  |
| 1   | A     | 448 | PHE  |
| 1   | A     | 472 | LYS  |
| 1   | A     | 473 | GLU  |
| 1   | A     | 476 | THR  |
| 1   | A     | 478 | LEU  |
| 1   | A     | 485 | ASN  |
| 1   | A     | 491 | GLN  |
| 1   | A     | 493 | ASN  |
| 1   | A     | 497 | GLN  |
| 1   | A     | 500 | VAL  |
| 1   | A     | 501 | LYS  |
| 1   | A     | 530 | LYS  |
| 1   | A     | 532 | LYS  |
| 1   | A     | 536 | LYS  |
| 1   | A     | 538 | LYS  |
| 1   | A     | 548 | ILE  |
| 1   | A     | 555 | VAL  |
| 1   | A     | 566 | ILE  |
| 1   | A     | 581 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 70  | HIS  |
| 1   | A     | 159 | GLN  |
| 1   | A     | 167 | ASN  |
| 1   | A     | 181 | ASN  |
| 1   | A     | 234 | HIS  |
| 1   | A     | 292 | ASN  |
| 1   | A     | 302 | ASN  |
| 1   | A     | 309 | GLN  |
| 1   | A     | 350 | GLN  |
| 1   | A     | 365 | GLN  |
| 1   | A     | 384 | HIS  |
| 1   | A     | 386 | GLN  |
| 1   | A     | 419 | ASN  |
| 1   | A     | 421 | ASN  |
| 1   | A     | 443 | ASN  |
| 1   | A     | 446 | ASN  |
| 1   | A     | 458 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 459 | ASN  |
| 1   | A     | 468 | GLN  |
| 1   | A     | 483 | HIS  |
| 1   | A     | 485 | ASN  |
| 1   | A     | 491 | GLN  |
| 1   | A     | 497 | GLN  |
| 1   | A     | 505 | ASN  |
| 1   | A     | 549 | GLN  |
| 1   | A     | 560 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

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.