



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:32 PM UTC

PDB ID : 1NEL / pdb\_00001nel  
Title : FLUORIDE INHIBITION OF YEAST ENOLASE: CRYSTAL STRUCTURE OF THE ENOLASE-MG2+-F-PI COMPLEX AT 2.6-ANGSTROMS RESOLUTION  
Authors : Lebioda, L.; Zhang, E.; Lewinski, K.; Brewer, M.J.  
Deposited on : 1993-08-20  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

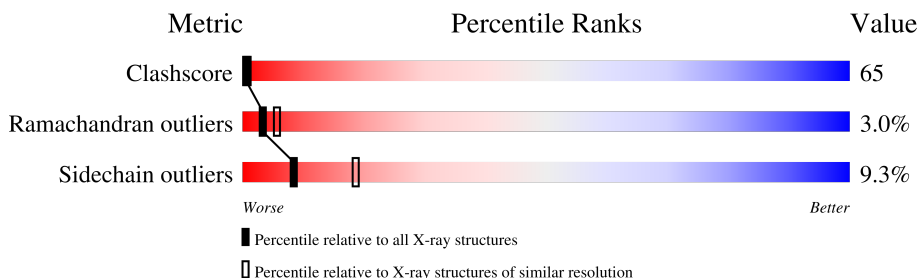
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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                      | 4347 (2.60-2.60)                                      |
| Ramachandran outliers | 187476                      | 4277 (2.60-2.60)                                      |
| Sidechain outliers    | 187428                      | 4277 (2.60-2.60)                                      |

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     | 436    | <div> <div></div> <div>24%</div> <div>43%</div> <div>28%</div> <div>5%</div> </div> |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3570 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 ENOLASE.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 436      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3289  | 2076 | 569 | 638 | 6 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 84      | SER      | LYS    | conflict | UNP P00924 |

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 4 is FLUORIDE ION (CCD ID: F) (formula: F).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 4   | A     | 1        | Total | F | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

- Molecule 5 is water.

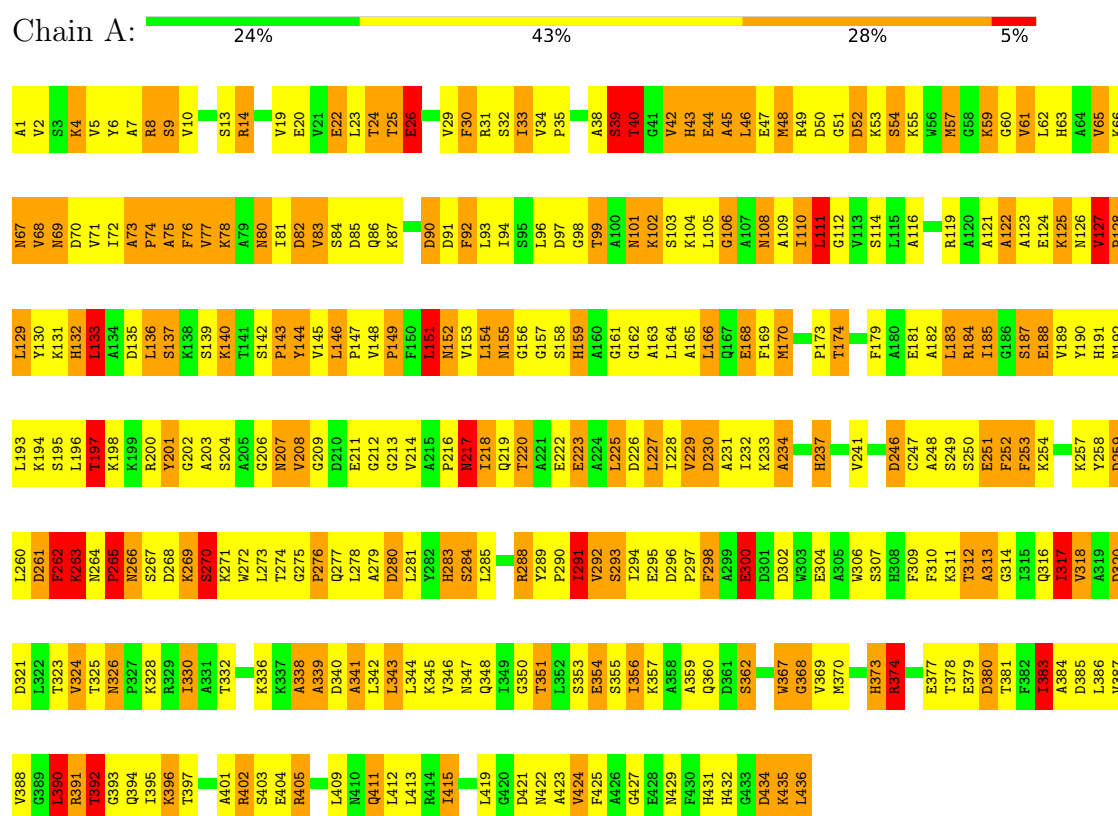
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 5   | A     | 274      | Total | O   | 0       | 0       |
|     |       |          | 274   | 274 |         |         |

### 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: ENOLASE



## 4 Data and refinement statistics

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

| Property                                                 | Value                                          | Source    |
|----------------------------------------------------------|------------------------------------------------|-----------|
| Space group                                              | P 42 21 2                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 122.50Å 122.50Å 67.00Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | (Not available) – 2.60                         | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) ((Not available)-2.60)         | Depositor |
| $R_{merge}$                                              | (Not available)                                | Depositor |
| $R_{sym}$                                                | (Not available)                                | Depositor |
| Refinement program                                       | PROLSQ                                         | Depositor |
| R, $R_{free}$                                            | 0.169 , (Not available)                        | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 3570                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 20.0                                           | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F, PO4, MG

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     | 1.08         | 1/3349 (0.0%) | 2.56        | 273/4531 (6.0%) |

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                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 368 | GLY  | N-CA  | 5.57 | 1.49        | 1.44     |

All (273) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | A     | 278 | LEU  | N-CA-C   | -11.70 | 97.30       | 111.69   |
| 1   | A     | 300 | GLU  | CA-CB-CG | 11.50  | 137.09      | 114.10   |
| 1   | A     | 435 | LYS  | CB-CA-C  | 11.46  | 128.60      | 111.76   |
| 1   | A     | 146 | LEU  | N-CA-C   | -11.30 | 95.83       | 110.07   |
| 1   | A     | 146 | LEU  | CB-CA-C  | 10.98  | 124.35      | 108.87   |
| 1   | A     | 192 | ASN  | CA-CB-CG | -10.87 | 101.73      | 112.60   |
| 1   | A     | 82  | ASP  | CA-CB-CG | -10.77 | 101.83      | 112.60   |
| 1   | A     | 142 | SER  | N-CA-CB  | -10.75 | 94.01       | 110.99   |
| 1   | A     | 110 | ILE  | N-CA-C   | 10.57  | 121.07      | 110.82   |
| 1   | A     | 280 | ASP  | CA-CB-CG | 10.47  | 123.07      | 112.60   |
| 1   | A     | 304 | GLU  | CA-C-O   | -10.26 | 110.05      | 120.82   |
| 1   | A     | 108 | ASN  | CA-CB-CG | 9.99   | 122.59      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 142 | SER  | N-CA-C     | 9.93  | 126.41      | 108.94   |
| 1   | A     | 251 | GLU  | N-CA-C     | 9.77  | 124.30      | 112.38   |
| 1   | A     | 22  | GLU  | CB-CG-CD   | 9.56  | 128.86      | 112.60   |
| 1   | A     | 223 | GLU  | CA-CB-CG   | 9.43  | 132.96      | 114.10   |
| 1   | A     | 155 | ASN  | CA-CB-CG   | 8.98  | 121.58      | 112.60   |
| 1   | A     | 422 | ASN  | CA-CB-CG   | -8.98 | 103.62      | 112.60   |
| 1   | A     | 226 | ASP  | CA-CB-CG   | 8.94  | 121.54      | 112.60   |
| 1   | A     | 262 | PHE  | CA-CB-CG   | 8.75  | 122.55      | 113.80   |
| 1   | A     | 396 | LYS  | CA-CB-CG   | 8.69  | 131.48      | 114.10   |
| 1   | A     | 152 | ASN  | CA-CB-CG   | 8.58  | 121.18      | 112.60   |
| 1   | A     | 69  | ASN  | CA-C-O     | -8.44 | 112.21      | 120.90   |
| 1   | A     | 405 | ARG  | CD-NE-CZ   | 8.43  | 136.21      | 124.40   |
| 1   | A     | 189 | VAL  | O-C-N      | 8.39  | 130.01      | 121.87   |
| 1   | A     | 435 | LYS  | CA-C-O     | 8.39  | 136.11      | 121.09   |
| 1   | A     | 92  | PHE  | CA-CB-CG   | 8.33  | 122.13      | 113.80   |
| 1   | A     | 269 | LYS  | N-CA-C     | -8.33 | 102.22      | 112.38   |
| 1   | A     | 250 | SER  | CA-C-N     | 8.33  | 133.93      | 120.60   |
| 1   | A     | 250 | SER  | C-N-CA     | 8.33  | 133.93      | 120.60   |
| 1   | A     | 46  | LEU  | N-CA-C     | 8.31  | 122.27      | 108.73   |
| 1   | A     | 10  | VAL  | CA-C-O     | -8.29 | 110.41      | 120.78   |
| 1   | A     | 152 | ASN  | CA-C-O     | -8.21 | 108.77      | 120.51   |
| 1   | A     | 368 | GLY  | N-CA-C     | -8.14 | 101.57      | 112.81   |
| 1   | A     | 229 | VAL  | CB-CA-C    | 8.11  | 121.95      | 111.81   |
| 1   | A     | 149 | PRO  | CA-C-O     | -8.11 | 111.48      | 120.97   |
| 1   | A     | 192 | ASN  | OD1-CG-ND2 | 8.11  | 130.71      | 122.60   |
| 1   | A     | 183 | LEU  | CB-CA-C    | 8.09  | 124.60      | 110.85   |
| 1   | A     | 91  | ASP  | CA-C-O     | -8.09 | 112.17      | 121.07   |
| 1   | A     | 76  | PHE  | CA-C-O     | -8.05 | 112.54      | 121.00   |
| 1   | A     | 76  | PHE  | CA-CB-CG   | 8.03  | 121.83      | 113.80   |
| 1   | A     | 33  | ILE  | CA-C-O     | -8.02 | 111.21      | 121.40   |
| 1   | A     | 159 | HIS  | CA-CB-CG   | -7.94 | 105.86      | 113.80   |
| 1   | A     | 261 | ASP  | CA-CB-CG   | -7.83 | 104.77      | 112.60   |
| 1   | A     | 72  | ILE  | O-C-N      | 7.83  | 129.58      | 121.91   |
| 1   | A     | 283 | HIS  | N-CA-C     | -7.78 | 102.75      | 111.07   |
| 1   | A     | 339 | ALA  | N-CA-C     | 7.69  | 118.73      | 107.88   |
| 1   | A     | 25  | THR  | CA-CB-OG1  | -7.69 | 98.07       | 109.60   |
| 1   | A     | 142 | SER  | CA-C-O     | -7.67 | 111.21      | 121.02   |
| 1   | A     | 270 | SER  | N-CA-C     | -7.56 | 103.79      | 112.87   |
| 1   | A     | 137 | SER  | O-C-N      | 7.56  | 131.41      | 122.34   |
| 1   | A     | 340 | ASP  | CA-C-O     | -7.51 | 111.70      | 119.51   |
| 1   | A     | 339 | ALA  | CA-C-O     | 7.51  | 129.43      | 121.25   |
| 1   | A     | 391 | ARG  | N-CA-CB    | -7.48 | 100.83      | 112.13   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 30  | PHE  | CA-CB-CG | -7.46 | 106.34      | 113.80   |
| 1   | A     | 220 | THR  | N-CA-CB  | -7.45 | 99.78       | 110.44   |
| 1   | A     | 26  | GLU  | CB-CG-CD | 7.43  | 125.23      | 112.60   |
| 1   | A     | 435 | LYS  | CA-C-N   | 7.41  | 135.05      | 121.70   |
| 1   | A     | 435 | LYS  | C-N-CA   | 7.41  | 135.05      | 121.70   |
| 1   | A     | 276 | PRO  | CA-C-N   | 7.41  | 133.27      | 120.68   |
| 1   | A     | 276 | PRO  | C-N-CA   | 7.41  | 133.27      | 120.68   |
| 1   | A     | 425 | PHE  | CA-CB-CG | 7.40  | 121.20      | 113.80   |
| 1   | A     | 288 | ARG  | CA-CB-CG | 7.38  | 128.86      | 114.10   |
| 1   | A     | 298 | PHE  | CA-CB-CG | -7.38 | 106.42      | 113.80   |
| 1   | A     | 108 | ASN  | N-CA-CB  | 7.37  | 121.71      | 110.28   |
| 1   | A     | 217 | ASN  | CA-CB-CG | 7.34  | 119.94      | 112.60   |
| 1   | A     | 188 | GLU  | O-C-N    | 7.27  | 129.94      | 122.09   |
| 1   | A     | 4   | LYS  | N-CA-CB  | -7.26 | 98.23       | 110.49   |
| 1   | A     | 47  | GLU  | N-CA-CB  | 7.24  | 122.22      | 110.42   |
| 1   | A     | 207 | ASN  | CA-C-O   | -7.17 | 113.75      | 121.56   |
| 1   | A     | 122 | ALA  | N-CA-C   | -7.12 | 103.21      | 110.97   |
| 1   | A     | 25  | THR  | N-CA-CB  | 7.06  | 121.53      | 110.87   |
| 1   | A     | 225 | LEU  | CB-CA-C  | 7.04  | 122.82      | 110.85   |
| 1   | A     | 77  | VAL  | CA-C-N   | 7.04  | 130.28      | 120.29   |
| 1   | A     | 77  | VAL  | C-N-CA   | 7.04  | 130.28      | 120.29   |
| 1   | A     | 261 | ASP  | O-C-N    | 7.03  | 131.18      | 121.83   |
| 1   | A     | 143 | PRO  | N-CA-C   | 7.01  | 130.33      | 112.10   |
| 1   | A     | 184 | ARG  | CD-NE-CZ | -6.99 | 114.61      | 124.40   |
| 1   | A     | 346 | VAL  | N-CA-CB  | 6.99  | 117.96      | 110.62   |
| 1   | A     | 67  | ASN  | CA-C-O   | -6.92 | 113.21      | 120.55   |
| 1   | A     | 183 | LEU  | N-CA-C   | -6.92 | 103.81      | 111.36   |
| 1   | A     | 350 | GLY  | N-CA-C   | 6.87  | 124.15      | 115.42   |
| 1   | A     | 144 | TYR  | CA-C-O   | -6.87 | 113.71      | 121.81   |
| 1   | A     | 318 | VAL  | CA-C-O   | 6.87  | 127.76      | 120.48   |
| 1   | A     | 166 | LEU  | N-CA-C   | -6.83 | 101.06      | 110.35   |
| 1   | A     | 218 | ILE  | CA-C-O   | -6.83 | 112.24      | 120.78   |
| 1   | A     | 93  | LEU  | CA-C-O   | -6.82 | 113.61      | 120.90   |
| 1   | A     | 68  | VAL  | N-CA-C   | 6.81  | 117.42      | 110.82   |
| 1   | A     | 285 | LEU  | CA-C-N   | 6.77  | 129.36      | 120.28   |
| 1   | A     | 285 | LEU  | C-N-CA   | 6.77  | 129.36      | 120.28   |
| 1   | A     | 411 | GLN  | CA-C-O   | -6.76 | 113.74      | 120.70   |
| 1   | A     | 434 | ASP  | O-C-N    | 6.72  | 129.27      | 122.08   |
| 1   | A     | 266 | ASN  | CB-CA-C  | 6.71  | 122.11      | 111.91   |
| 1   | A     | 411 | GLN  | N-CA-CB  | 6.70  | 119.79      | 110.07   |
| 1   | A     | 144 | TYR  | N-CA-C   | -6.69 | 101.52      | 110.55   |
| 1   | A     | 20  | GLU  | CA-C-O   | -6.68 | 112.97      | 120.32   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 85  | ASP  | CA-CB-CG  | -6.66 | 105.94      | 112.60   |
| 1   | A     | 133 | LEU  | CB-CA-C   | 6.65  | 121.99      | 110.68   |
| 1   | A     | 411 | GLN  | N-CA-C    | -6.63 | 103.98      | 111.14   |
| 1   | A     | 184 | ARG  | NE-CZ-NH1 | -6.57 | 114.93      | 121.50   |
| 1   | A     | 248 | ALA  | CA-C-O    | -6.56 | 114.23      | 121.84   |
| 1   | A     | 110 | ILE  | N-CA-CB   | -6.54 | 101.11      | 110.52   |
| 1   | A     | 392 | THR  | CA-CB-OG1 | -6.53 | 99.81       | 109.60   |
| 1   | A     | 20  | GLU  | CG-CD-OE1 | -6.49 | 103.47      | 118.40   |
| 1   | A     | 248 | ALA  | N-CA-C    | -6.48 | 102.44      | 111.39   |
| 1   | A     | 284 | SER  | CA-C-N    | 6.48  | 128.86      | 120.44   |
| 1   | A     | 284 | SER  | C-N-CA    | 6.48  | 128.86      | 120.44   |
| 1   | A     | 323 | THR  | CA-CB-OG1 | -6.47 | 99.89       | 109.60   |
| 1   | A     | 222 | GLU  | CA-C-N    | 6.47  | 129.25      | 120.38   |
| 1   | A     | 222 | GLU  | C-N-CA    | 6.47  | 129.25      | 120.38   |
| 1   | A     | 356 | ILE  | N-CA-C    | -6.46 | 104.03      | 110.62   |
| 1   | A     | 25  | THR  | N-CA-C    | -6.46 | 100.39      | 109.69   |
| 1   | A     | 40  | THR  | CA-C-O    | 6.46  | 129.74      | 120.51   |
| 1   | A     | 121 | ALA  | CA-C-O    | 6.39  | 127.33      | 120.24   |
| 1   | A     | 338 | ALA  | N-CA-C    | -6.37 | 105.33      | 113.23   |
| 1   | A     | 197 | THR  | CB-CA-C   | 6.37  | 120.82      | 110.95   |
| 1   | A     | 201 | TYR  | N-CA-C    | 6.35  | 121.06      | 113.12   |
| 1   | A     | 99  | THR  | CA-C-O    | -6.33 | 114.25      | 121.40   |
| 1   | A     | 129 | LEU  | CB-CA-C   | 6.31  | 120.68      | 110.96   |
| 1   | A     | 111 | LEU  | CA-C-N    | 6.30  | 127.08      | 120.03   |
| 1   | A     | 111 | LEU  | C-N-CA    | 6.30  | 127.08      | 120.03   |
| 1   | A     | 208 | VAL  | CA-C-O    | 6.28  | 128.63      | 120.78   |
| 1   | A     | 54  | SER  | CA-CB-OG  | -6.24 | 98.61       | 111.10   |
| 1   | A     | 73  | ALA  | CA-C-N    | 6.24  | 126.43      | 119.32   |
| 1   | A     | 73  | ALA  | C-N-CA    | 6.24  | 126.43      | 119.32   |
| 1   | A     | 48  | MET  | N-CA-C    | 6.22  | 118.42      | 108.41   |
| 1   | A     | 330 | ILE  | N-CA-C    | -6.20 | 104.70      | 110.53   |
| 1   | A     | 67  | ASN  | N-CA-C    | -6.18 | 104.54      | 111.28   |
| 1   | A     | 78  | LYS  | N-CA-C    | 6.18  | 118.10      | 111.36   |
| 1   | A     | 402 | ARG  | CG-CD-NE  | 6.18  | 125.59      | 112.00   |
| 1   | A     | 84  | SER  | N-CA-C    | -6.17 | 105.01      | 112.54   |
| 1   | A     | 125 | LYS  | N-CA-C    | -6.10 | 105.69      | 113.01   |
| 1   | A     | 294 | ILE  | N-CA-CB   | 6.08  | 121.27      | 111.23   |
| 1   | A     | 112 | GLY  | CA-C-O    | -6.04 | 114.88      | 120.80   |
| 1   | A     | 234 | ALA  | CA-C-N    | 6.03  | 130.25      | 120.60   |
| 1   | A     | 234 | ALA  | C-N-CA    | 6.03  | 130.25      | 120.60   |
| 1   | A     | 251 | GLU  | CB-CG-CD  | -6.01 | 102.39      | 112.60   |
| 1   | A     | 65  | VAL  | N-CA-C    | -6.00 | 104.66      | 110.72   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 132 | HIS  | N-CA-CB    | 6.00  | 118.67      | 109.91   |
| 1   | A     | 278 | LEU  | CB-CA-C    | 6.00  | 121.67      | 110.70   |
| 1   | A     | 266 | ASN  | OD1-CG-ND2 | -6.00 | 116.61      | 122.60   |
| 1   | A     | 52  | ASP  | CA-CB-CG   | -5.96 | 106.64      | 112.60   |
| 1   | A     | 81  | ILE  | CB-CA-C    | -5.95 | 102.89      | 111.34   |
| 1   | A     | 75  | ALA  | CA-C-N     | 5.94  | 128.49      | 120.65   |
| 1   | A     | 75  | ALA  | C-N-CA     | 5.94  | 128.49      | 120.65   |
| 1   | A     | 252 | PHE  | CA-CB-CG   | 5.93  | 119.73      | 113.80   |
| 1   | A     | 309 | PHE  | N-CA-C     | -5.92 | 104.52      | 110.97   |
| 1   | A     | 30  | PHE  | CB-CA-C    | 5.92  | 119.42      | 109.48   |
| 1   | A     | 132 | HIS  | CA-CB-CG   | -5.91 | 107.89      | 113.80   |
| 1   | A     | 317 | ILE  | O-C-N      | 5.90  | 129.46      | 123.20   |
| 1   | A     | 402 | ARG  | NE-CZ-NH2  | 5.89  | 124.50      | 119.20   |
| 1   | A     | 290 | PRO  | CB-CA-C    | 5.88  | 121.26      | 111.56   |
| 1   | A     | 403 | SER  | N-CA-C     | 5.88  | 119.92      | 112.87   |
| 1   | A     | 343 | LEU  | N-CA-C     | -5.86 | 100.97      | 109.59   |
| 1   | A     | 368 | GLY  | O-C-N      | -5.86 | 116.84      | 123.11   |
| 1   | A     | 266 | ASN  | N-CA-C     | -5.85 | 101.63      | 110.70   |
| 1   | A     | 388 | VAL  | CB-CA-C    | 5.84  | 119.70      | 112.04   |
| 1   | A     | 144 | TYR  | CA-C-N     | -5.81 | 115.37      | 123.10   |
| 1   | A     | 144 | TYR  | C-N-CA     | -5.81 | 115.37      | 123.10   |
| 1   | A     | 404 | GLU  | CA-C-O     | 5.80  | 126.72      | 119.12   |
| 1   | A     | 125 | LYS  | CA-C-N     | 5.79  | 132.60      | 121.54   |
| 1   | A     | 125 | LYS  | C-N-CA     | 5.79  | 132.60      | 121.54   |
| 1   | A     | 111 | LEU  | CA-C-O     | 5.77  | 128.76      | 120.51   |
| 1   | A     | 151 | LEU  | N-CA-CB    | -5.77 | 100.48      | 110.17   |
| 1   | A     | 83  | VAL  | CA-C-O     | -5.75 | 113.59      | 120.78   |
| 1   | A     | 47  | GLU  | CA-CB-CG   | 5.74  | 125.59      | 114.10   |
| 1   | A     | 380 | ASP  | CA-C-O     | -5.72 | 114.76      | 121.16   |
| 1   | A     | 168 | GLU  | CG-CD-OE1  | -5.71 | 105.26      | 118.40   |
| 1   | A     | 397 | THR  | CA-CB-CG2  | 5.71  | 120.22      | 110.50   |
| 1   | A     | 61  | VAL  | O-C-N      | 5.71  | 129.71      | 122.57   |
| 1   | A     | 351 | THR  | O-C-N      | 5.71  | 130.26      | 123.24   |
| 1   | A     | 252 | PHE  | O-C-N      | 5.70  | 129.83      | 122.19   |
| 1   | A     | 8   | ARG  | CA-CB-CG   | 5.70  | 125.50      | 114.10   |
| 1   | A     | 14  | ARG  | NE-CZ-NH2  | -5.70 | 114.07      | 119.20   |
| 1   | A     | 412 | LEU  | CA-C-O     | -5.69 | 114.52      | 120.55   |
| 1   | A     | 373 | HIS  | O-C-N      | 5.68  | 128.45      | 122.20   |
| 1   | A     | 291 | ILE  | N-CA-C     | 5.68  | 116.92      | 108.23   |
| 1   | A     | 265 | PRO  | CA-C-N     | -5.67 | 113.82      | 122.21   |
| 1   | A     | 265 | PRO  | C-N-CA     | -5.67 | 113.82      | 122.21   |
| 1   | A     | 312 | THR  | N-CA-CB    | -5.66 | 101.86      | 110.92   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 192 | ASN  | CA-C-N    | 5.66  | 127.79      | 120.44   |
| 1   | A     | 192 | ASN  | C-N-CA    | 5.66  | 127.79      | 120.44   |
| 1   | A     | 99  | THR  | CB-CA-C   | 5.65  | 122.50      | 110.07   |
| 1   | A     | 19  | VAL  | N-CA-C    | 5.65  | 116.71      | 108.58   |
| 1   | A     | 44  | GLU  | CA-C-O    | -5.62 | 114.46      | 120.92   |
| 1   | A     | 304 | GLU  | O-C-N     | 5.62  | 127.85      | 122.07   |
| 1   | A     | 383 | ILE  | O-C-N     | 5.61  | 127.53      | 121.87   |
| 1   | A     | 38  | ALA  | O-C-N     | 5.60  | 128.66      | 123.50   |
| 1   | A     | 39  | SER  | N-CA-C    | -5.60 | 98.87       | 110.80   |
| 1   | A     | 59  | LYS  | N-CA-CB   | 5.59  | 119.40      | 110.73   |
| 1   | A     | 108 | ASN  | N-CA-C    | -5.57 | 105.36      | 111.82   |
| 1   | A     | 220 | THR  | CA-CB-OG1 | -5.56 | 101.26      | 109.60   |
| 1   | A     | 70  | ASP  | CA-CB-CG  | -5.55 | 107.05      | 112.60   |
| 1   | A     | 161 | GLY  | CA-C-N    | 5.54  | 130.07      | 121.32   |
| 1   | A     | 161 | GLY  | C-N-CA    | 5.54  | 130.07      | 121.32   |
| 1   | A     | 266 | ASN  | O-C-N     | 5.53  | 129.91      | 122.61   |
| 1   | A     | 9   | SER  | CB-CA-C   | 5.52  | 118.83      | 109.50   |
| 1   | A     | 159 | HIS  | N-CA-C    | 5.51  | 118.05      | 111.71   |
| 1   | A     | 86  | GLN  | N-CA-C    | -5.51 | 104.30      | 111.02   |
| 1   | A     | 367 | TRP  | N-CA-CB   | -5.49 | 102.86      | 110.38   |
| 1   | A     | 80  | ASN  | CA-CB-CG  | -5.49 | 107.11      | 112.60   |
| 1   | A     | 170 | MET  | O-C-N     | 5.49  | 129.61      | 123.19   |
| 1   | A     | 354 | GLU  | CA-C-O    | -5.47 | 113.67      | 119.97   |
| 1   | A     | 381 | THR  | CA-C-N    | 5.47  | 127.92      | 120.54   |
| 1   | A     | 381 | THR  | C-N-CA    | 5.47  | 127.92      | 120.54   |
| 1   | A     | 127 | VAL  | O-C-N     | 5.47  | 127.33      | 121.10   |
| 1   | A     | 166 | LEU  | CB-CA-C   | 5.46  | 119.40      | 109.62   |
| 1   | A     | 42  | VAL  | N-CA-C    | 5.46  | 115.90      | 110.23   |
| 1   | A     | 87  | LYS  | CA-C-O    | -5.45 | 114.74      | 120.63   |
| 1   | A     | 145 | VAL  | CB-CA-C   | 5.45  | 118.51      | 110.77   |
| 1   | A     | 152 | ASN  | O-C-N     | 5.44  | 129.82      | 122.59   |
| 1   | A     | 298 | PHE  | CA-C-O    | -5.44 | 114.98      | 121.56   |
| 1   | A     | 99  | THR  | N-CA-CB   | -5.43 | 102.23      | 111.69   |
| 1   | A     | 311 | LYS  | CA-CB-CG  | 5.42  | 124.95      | 114.10   |
| 1   | A     | 125 | LYS  | CA-CB-CG  | 5.42  | 124.95      | 114.10   |
| 1   | A     | 174 | THR  | CA-CB-OG1 | -5.40 | 101.51      | 109.60   |
| 1   | A     | 126 | ASN  | N-CA-CB   | 5.39  | 119.60      | 110.49   |
| 1   | A     | 259 | ASP  | CA-CB-CG  | 5.39  | 117.99      | 112.60   |
| 1   | A     | 390 | LEU  | CA-C-N    | -5.35 | 114.65      | 122.19   |
| 1   | A     | 390 | LEU  | C-N-CA    | -5.35 | 114.65      | 122.19   |
| 1   | A     | 404 | GLU  | N-CA-C    | -5.33 | 106.75      | 113.20   |
| 1   | A     | 424 | VAL  | CA-C-O    | -5.33 | 114.69      | 120.67   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 292 | VAL  | N-CA-CB    | -5.33 | 105.99      | 112.33   |
| 1   | A     | 276 | PRO  | N-CD-CG    | -5.33 | 95.21       | 103.20   |
| 1   | A     | 356 | ILE  | CB-CA-C    | 5.33  | 119.33      | 112.14   |
| 1   | A     | 185 | ILE  | CB-CG1-CD1 | -5.30 | 102.67      | 113.80   |
| 1   | A     | 253 | PHE  | O-C-N      | 5.29  | 129.21      | 123.13   |
| 1   | A     | 434 | ASP  | CA-C-N     | -5.28 | 114.71      | 123.37   |
| 1   | A     | 434 | ASP  | C-N-CA     | -5.28 | 114.71      | 123.37   |
| 1   | A     | 291 | ILE  | N-CA-CB    | -5.28 | 104.98      | 111.00   |
| 1   | A     | 360 | GLN  | CB-CA-C    | 5.28  | 119.09      | 110.96   |
| 1   | A     | 367 | TRP  | CA-C-O     | -5.26 | 116.00      | 121.99   |
| 1   | A     | 154 | LEU  | CB-CA-C    | 5.25  | 119.21      | 109.70   |
| 1   | A     | 230 | ASP  | CA-C-O     | -5.25 | 114.87      | 121.02   |
| 1   | A     | 304 | GLU  | N-CA-CB    | 5.25  | 117.62      | 110.01   |
| 1   | A     | 72  | ILE  | N-CA-CB    | 5.25  | 116.69      | 110.55   |
| 1   | A     | 106 | GLY  | CA-C-N     | 5.24  | 128.03      | 120.38   |
| 1   | A     | 106 | GLY  | C-N-CA     | 5.24  | 128.03      | 120.38   |
| 1   | A     | 325 | THR  | CA-C-O     | -5.24 | 115.76      | 121.84   |
| 1   | A     | 170 | MET  | CA-C-O     | -5.24 | 114.99      | 120.80   |
| 1   | A     | 133 | LEU  | CA-C-O     | -5.23 | 114.98      | 120.63   |
| 1   | A     | 332 | THR  | CA-C-O     | -5.23 | 115.33      | 120.82   |
| 1   | A     | 128 | PRO  | CB-CA-C    | 5.22  | 117.81      | 110.98   |
| 1   | A     | 90  | ASP  | CB-CA-C    | 5.21  | 119.15      | 110.81   |
| 1   | A     | 391 | ARG  | CA-C-O     | -5.20 | 115.09      | 121.28   |
| 1   | A     | 383 | ILE  | N-CA-CB    | 5.20  | 119.54      | 110.65   |
| 1   | A     | 137 | SER  | CA-C-O     | -5.20 | 113.48      | 119.56   |
| 1   | A     | 332 | THR  | N-CA-CB    | 5.20  | 117.55      | 110.01   |
| 1   | A     | 201 | TYR  | CA-C-O     | -5.17 | 113.52      | 119.78   |
| 1   | A     | 283 | HIS  | N-CA-CB    | 5.16  | 117.49      | 110.01   |
| 1   | A     | 40  | THR  | CA-CB-OG1  | -5.15 | 101.88      | 109.60   |
| 1   | A     | 10  | VAL  | O-C-N      | 5.14  | 129.00      | 122.57   |
| 1   | A     | 341 | ALA  | CA-C-O     | -5.14 | 115.24      | 120.99   |
| 1   | A     | 209 | GLY  | N-CA-C     | -5.13 | 105.73      | 112.81   |
| 1   | A     | 237 | HIS  | CA-C-O     | 5.13  | 126.16      | 119.95   |
| 1   | A     | 183 | LEU  | CA-C-O     | -5.13 | 114.99      | 120.42   |
| 1   | A     | 252 | PHE  | N-CA-C     | -5.13 | 104.48      | 111.56   |
| 1   | A     | 368 | GLY  | CA-C-N     | 5.12  | 131.18      | 121.97   |
| 1   | A     | 368 | GLY  | C-N-CA     | 5.12  | 131.18      | 121.97   |
| 1   | A     | 288 | ARG  | CA-C-O     | -5.09 | 113.12      | 119.18   |
| 1   | A     | 314 | GLY  | N-CA-C     | -5.09 | 108.23      | 115.30   |
| 1   | A     | 69  | ASN  | CA-CB-CG   | -5.09 | 107.51      | 112.60   |
| 1   | A     | 320 | ASP  | O-C-N      | 5.07  | 126.31      | 120.58   |
| 1   | A     | 128 | PRO  | N-CA-C     | -5.07 | 103.32      | 111.38   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 74  | PRO  | N-CA-C   | 5.06  | 121.29      | 113.75   |
| 1   | A     | 412 | LEU  | CB-CA-C  | 5.06  | 119.19      | 110.79   |
| 1   | A     | 261 | ASP  | CA-C-O   | -5.05 | 115.37      | 121.89   |
| 1   | A     | 133 | LEU  | N-CA-C   | -5.05 | 105.22      | 111.33   |
| 1   | A     | 246 | ASP  | N-CA-CB  | 5.03  | 120.12      | 110.82   |
| 1   | A     | 409 | LEU  | CB-CA-C  | 5.02  | 118.85      | 110.81   |
| 1   | A     | 132 | HIS  | O-C-N    | 5.02  | 127.25      | 122.03   |
| 1   | A     | 14  | ARG  | CD-NE-CZ | -5.01 | 117.38      | 124.40   |
| 1   | A     | 323 | THR  | N-CA-C   | 5.01  | 120.23      | 113.72   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 374 | ARG  | 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     | 3289  | 0        | 3293     | 427     | 11           |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 5     | 0        | 0        | 0       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 274   | 0        | 0        | 111     | 10           |
| All | All   | 3570  | 0        | 3293     | 427     | 11           |

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 65.

All (427) 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:345:LYS:HD3 | 1:A:374:ARG:NH1 | 1.19                     | 1.47              |
| 1:A:101:ASN:ND2 | 1:A:103:SER:HB3 | 1.52                     | 1.24              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:257:LYS:NZ   | 1:A:269:LYS:HE2  | 1.54                     | 1.22              |
| 1:A:345:LYS:CD   | 1:A:374:ARG:NH1  | 2.03                     | 1.21              |
| 1:A:48:MET:HE3   | 5:A:572:HOH:O    | 1.44                     | 1.18              |
| 1:A:262:PHE:O    | 1:A:263:LYS:HG3  | 1.40                     | 1.17              |
| 1:A:99:THR:HG21  | 1:A:104:LYS:HB2  | 1.23                     | 1.15              |
| 1:A:97:ASP:O     | 1:A:99:THR:HG23  | 1.48                     | 1.10              |
| 1:A:383:ILE:HG23 | 5:A:495:HOH:O    | 1.55                     | 1.07              |
| 1:A:101:ASN:HD21 | 1:A:103:SER:HB3  | 0.94                     | 1.06              |
| 1:A:345:LYS:CD   | 1:A:374:ARG:HH12 | 1.62                     | 1.03              |
| 1:A:125:LYS:HE3  | 1:A:132:HIS:CE1  | 1.94                     | 1.02              |
| 1:A:379:GLU:HG3  | 5:A:504:HOH:O    | 1.57                     | 1.01              |
| 1:A:413:LEU:HD22 | 5:A:490:HOH:O    | 1.58                     | 1.01              |
| 1:A:254:LYS:HA   | 5:A:622:HOH:O    | 1.62                     | 1.00              |
| 1:A:257:LYS:HZ1  | 1:A:269:LYS:HE2  | 1.17                     | 0.99              |
| 1:A:391:ARG:NH1  | 1:A:434:ASP:O    | 1.96                     | 0.98              |
| 1:A:385:ASP:OD1  | 5:A:633:HOH:O    | 1.82                     | 0.98              |
| 1:A:227:LEU:HD13 | 5:A:749:HOH:O    | 1.64                     | 0.96              |
| 1:A:200:ARG:HD2  | 5:A:749:HOH:O    | 1.63                     | 0.96              |
| 1:A:252:PHE:HB3  | 1:A:262:PHE:CD1  | 2.01                     | 0.96              |
| 1:A:300:GLU:HG3  | 5:A:619:HOH:O    | 1.65                     | 0.96              |
| 1:A:261:ASP:OD2  | 1:A:264:ASN:CA   | 2.14                     | 0.94              |
| 1:A:345:LYS:CE   | 1:A:374:ARG:HH12 | 1.80                     | 0.94              |
| 1:A:143:PRO:HB2  | 1:A:424:VAL:HG22 | 1.50                     | 0.93              |
| 1:A:46:LEU:HD22  | 1:A:103:SER:HA   | 1.49                     | 0.93              |
| 1:A:261:ASP:OD2  | 1:A:264:ASN:HA   | 1.69                     | 0.92              |
| 1:A:345:LYS:HD3  | 1:A:374:ARG:HH12 | 1.11                     | 0.91              |
| 1:A:324:VAL:HG13 | 1:A:348:GLN:HG2  | 1.51                     | 0.91              |
| 1:A:257:LYS:CE   | 1:A:269:LYS:HE2  | 2.00                     | 0.91              |
| 1:A:267:SER:HA   | 5:A:581:HOH:O    | 1.69                     | 0.91              |
| 1:A:391:ARG:O    | 1:A:434:ASP:HA   | 1.71                     | 0.91              |
| 1:A:257:LYS:HZ2  | 1:A:269:LYS:HG2  | 1.36                     | 0.90              |
| 1:A:51:GLY:N     | 5:A:689:HOH:O    | 2.04                     | 0.89              |
| 1:A:99:THR:CG2   | 1:A:104:LYS:HB2  | 2.02                     | 0.89              |
| 1:A:345:LYS:HD3  | 1:A:374:ARG:HH11 | 1.37                     | 0.88              |
| 1:A:313:ALA:HB3  | 5:A:482:HOH:O    | 1.72                     | 0.87              |
| 1:A:125:LYS:HE3  | 1:A:132:HIS:HE1  | 1.40                     | 0.87              |
| 1:A:268:ASP:OD2  | 1:A:270:SER:HB2  | 1.76                     | 0.86              |
| 1:A:326:ASN:ND2  | 1:A:328:LYS:HB3  | 1.92                     | 0.85              |
| 1:A:257:LYS:HZ2  | 1:A:269:LYS:CG   | 1.89                     | 0.85              |
| 1:A:261:ASP:HB3  | 1:A:264:ASN:HD22 | 1.42                     | 0.85              |
| 1:A:193:LEU:O    | 1:A:197:THR:HG23 | 1.76                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:168:GLU:OE1  | 1:A:170:MET:HE2  | 1.77                     | 0.84              |
| 1:A:78:LYS:HD2   | 5:A:679:HOH:O    | 1.78                     | 0.83              |
| 1:A:187:SER:HB2  | 5:A:549:HOH:O    | 1.77                     | 0.83              |
| 1:A:268:ASP:CG   | 1:A:270:SER:HB2  | 2.04                     | 0.83              |
| 1:A:25:THR:HG21  | 5:A:721:HOH:O    | 1.78                     | 0.83              |
| 1:A:101:ASN:HD21 | 1:A:103:SER:CB   | 1.88                     | 0.82              |
| 1:A:173:PRO:HG2  | 1:A:182:ALA:HB1  | 1.61                     | 0.82              |
| 1:A:200:ARG:NH1  | 5:A:602:HOH:O    | 2.13                     | 0.82              |
| 1:A:401:ALA:O    | 1:A:402:ARG:HB2  | 1.79                     | 0.79              |
| 1:A:166:LEU:HD22 | 1:A:247:CYS:HA   | 1.65                     | 0.79              |
| 1:A:261:ASP:O    | 1:A:263:LYS:N    | 2.16                     | 0.78              |
| 1:A:262:PHE:O    | 1:A:263:LYS:CG   | 2.27                     | 0.78              |
| 1:A:379:GLU:OE2  | 5:A:508:HOH:O    | 2.02                     | 0.78              |
| 1:A:211:GLU:OE2  | 5:A:529:HOH:O    | 2.02                     | 0.77              |
| 1:A:326:ASN:HD22 | 1:A:328:LYS:H    | 1.28                     | 0.77              |
| 1:A:97:ASP:OD1   | 1:A:105:LEU:N    | 2.16                     | 0.77              |
| 1:A:257:LYS:NZ   | 1:A:269:LYS:CE   | 2.42                     | 0.77              |
| 1:A:33:ILE:HG22  | 1:A:378:THR:HG21 | 1.67                     | 0.77              |
| 1:A:320:ASP:HA   | 5:A:650:HOH:O    | 1.83                     | 0.76              |
| 1:A:391:ARG:HD2  | 5:A:486:HOH:O    | 1.86                     | 0.76              |
| 1:A:73:ALA:HB1   | 5:A:625:HOH:O    | 1.85                     | 0.76              |
| 1:A:163:ALA:H    | 1:A:217:ASN:ND2  | 1.82                     | 0.76              |
| 1:A:344:LEU:C    | 1:A:344:LEU:HD23 | 2.09                     | 0.76              |
| 1:A:50:ASP:OD2   | 1:A:62:LEU:HB2   | 1.86                     | 0.75              |
| 1:A:320:ASP:OD1  | 5:A:650:HOH:O    | 2.04                     | 0.75              |
| 1:A:344:LEU:HD23 | 1:A:344:LEU:O    | 1.87                     | 0.75              |
| 1:A:195:SER:HA   | 5:A:675:HOH:O    | 1.87                     | 0.74              |
| 1:A:144:TYR:HD2  | 1:A:419:LEU:HD13 | 1.52                     | 0.74              |
| 1:A:139:SER:HA   | 5:A:485:HOH:O    | 1.87                     | 0.74              |
| 1:A:131:LYS:HG2  | 5:A:724:HOH:O    | 1.88                     | 0.73              |
| 1:A:59:LYS:HE3   | 5:A:559:HOH:O    | 1.89                     | 0.73              |
| 1:A:4:LYS:O      | 1:A:4:LYS:HG2    | 1.87                     | 0.73              |
| 1:A:257:LYS:NZ   | 1:A:269:LYS:HG2  | 2.03                     | 0.73              |
| 1:A:261:ASP:C    | 1:A:263:LYS:H    | 1.96                     | 0.72              |
| 1:A:143:PRO:HG3  | 1:A:424:VAL:CG1  | 2.20                     | 0.72              |
| 1:A:42:VAL:HG23  | 1:A:43:HIS:N     | 2.04                     | 0.71              |
| 1:A:293:SER:CB   | 5:A:446:HOH:O    | 2.31                     | 0.71              |
| 1:A:50:ASP:OD2   | 1:A:62:LEU:N     | 2.23                     | 0.71              |
| 1:A:436:LEU:O    | 1:A:436:LEU:HG   | 1.90                     | 0.71              |
| 1:A:1:ALA:N      | 5:A:463:HOH:O    | 2.19                     | 0.71              |
| 1:A:9:SER:C      | 5:A:535:HOH:O    | 2.34                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:30:PHE:CE2   | 1:A:123:ALA:HB2  | 2.26                     | 0.71              |
| 1:A:345:LYS:NZ   | 1:A:374:ARG:HH12 | 1.88                     | 0.71              |
| 1:A:30:PHE:HE2   | 1:A:123:ALA:HB2  | 1.56                     | 0.70              |
| 1:A:49:ARG:O     | 5:A:689:HOH:O    | 2.09                     | 0.70              |
| 1:A:268:ASP:O    | 1:A:271:LYS:HB2  | 1.92                     | 0.70              |
| 1:A:228:ILE:O    | 1:A:232:ILE:HG13 | 1.90                     | 0.70              |
| 1:A:9:SER:HB3    | 5:A:695:HOH:O    | 1.90                     | 0.69              |
| 1:A:111:LEU:HB2  | 5:A:761:HOH:O    | 1.90                     | 0.69              |
| 1:A:104:LYS:HG2  | 5:A:683:HOH:O    | 1.92                     | 0.69              |
| 1:A:261:ASP:CB   | 1:A:264:ASN:HD22 | 2.05                     | 0.68              |
| 1:A:362:SER:O    | 1:A:367:TRP:HB2  | 1.93                     | 0.68              |
| 1:A:295:GLU:OE1  | 1:A:396:LYS:NZ   | 2.25                     | 0.68              |
| 1:A:194:LYS:HG2  | 1:A:198:LYS:HE2  | 1.76                     | 0.68              |
| 1:A:227:LEU:CD1  | 5:A:749:HOH:O    | 2.32                     | 0.68              |
| 1:A:208:VAL:HB   | 1:A:213:GLY:O    | 1.94                     | 0.68              |
| 1:A:148:VAL:HG11 | 1:A:174:THR:HG22 | 1.74                     | 0.68              |
| 1:A:300:GLU:HB2  | 1:A:321:ASP:O    | 1.93                     | 0.68              |
| 1:A:196:LEU:HD12 | 1:A:231:ALA:HB2  | 1.74                     | 0.67              |
| 1:A:82:ASP:OD1   | 1:A:82:ASP:C     | 2.35                     | 0.67              |
| 1:A:143:PRO:HG3  | 1:A:424:VAL:HG13 | 1.74                     | 0.67              |
| 1:A:390:LEU:O    | 1:A:391:ARG:HB3  | 1.93                     | 0.67              |
| 1:A:326:ASN:O    | 1:A:330:ILE:HG13 | 1.94                     | 0.67              |
| 1:A:61:VAL:HA    | 5:A:573:HOH:O    | 1.94                     | 0.66              |
| 1:A:155:ASN:OD1  | 5:A:795:HOH:O    | 2.13                     | 0.66              |
| 1:A:63:HIS:O     | 1:A:66:LYS:N     | 2.29                     | 0.66              |
| 1:A:140:LYS:O    | 5:A:486:HOH:O    | 2.13                     | 0.66              |
| 1:A:330:ILE:CD1  | 1:A:342:LEU:HD22 | 2.26                     | 0.65              |
| 1:A:312:THR:HG21 | 5:A:629:HOH:O    | 1.94                     | 0.65              |
| 1:A:262:PHE:C    | 1:A:263:LYS:HG3  | 2.19                     | 0.65              |
| 1:A:181:GLU:OE1  | 5:A:790:HOH:O    | 2.12                     | 0.65              |
| 1:A:262:PHE:HE2  | 5:A:525:HOH:O    | 1.79                     | 0.65              |
| 1:A:373:HIS:H    | 1:A:373:HIS:CD2  | 2.14                     | 0.65              |
| 1:A:97:ASP:OD2   | 1:A:99:THR:OG1   | 2.07                     | 0.64              |
| 1:A:288:ARG:HD2  | 5:A:638:HOH:O    | 1.97                     | 0.64              |
| 1:A:49:ARG:NH2   | 5:A:591:HOH:O    | 2.30                     | 0.64              |
| 1:A:257:LYS:HE3  | 1:A:269:LYS:HE2  | 1.76                     | 0.64              |
| 1:A:317:ILE:HG22 | 1:A:339:ALA:CB   | 2.26                     | 0.64              |
| 1:A:218:ILE:HG23 | 1:A:223:GLU:HG2  | 1.80                     | 0.64              |
| 1:A:22:GLU:OE2   | 1:A:31:ARG:NH2   | 2.31                     | 0.64              |
| 1:A:44:GLU:HA    | 1:A:324:VAL:HG11 | 1.80                     | 0.63              |
| 1:A:144:TYR:CD2  | 1:A:419:LEU:HD13 | 2.33                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:131:LYS:O    | 1:A:131:LYS:HD3  | 1.99                     | 0.63              |
| 1:A:261:ASP:OD2  | 1:A:264:ASN:CB   | 2.45                     | 0.63              |
| 1:A:14:ARG:NH1   | 5:A:553:HOH:O    | 2.32                     | 0.62              |
| 1:A:49:ARG:CZ    | 5:A:591:HOH:O    | 2.46                     | 0.62              |
| 1:A:265:PRO:C    | 1:A:267:SER:H    | 2.07                     | 0.62              |
| 1:A:306:TRP:HE3  | 1:A:338:ALA:O    | 1.82                     | 0.62              |
| 1:A:163:ALA:H    | 1:A:217:ASN:HD22 | 1.45                     | 0.62              |
| 1:A:269:LYS:C    | 1:A:271:LYS:N    | 2.52                     | 0.62              |
| 1:A:42:VAL:CG2   | 1:A:43:HIS:N     | 2.62                     | 0.62              |
| 1:A:156:GLY:O    | 1:A:164:LEU:O    | 2.17                     | 0.62              |
| 1:A:326:ASN:ND2  | 1:A:328:LYS:H    | 1.97                     | 0.62              |
| 1:A:345:LYS:CE   | 1:A:374:ARG:NH1  | 2.52                     | 0.62              |
| 1:A:34:VAL:HG13  | 1:A:35:PRO:HD2   | 1.82                     | 0.62              |
| 1:A:80:ASN:O     | 1:A:80:ASN:ND2   | 2.33                     | 0.62              |
| 1:A:324:VAL:HG12 | 1:A:324:VAL:O    | 1.99                     | 0.62              |
| 1:A:14:ARG:CZ    | 5:A:553:HOH:O    | 2.47                     | 0.62              |
| 1:A:316:GLN:OE1  | 1:A:431:HIS:ND1  | 2.32                     | 0.62              |
| 1:A:249:SER:OG   | 1:A:298:PHE:C    | 2.43                     | 0.61              |
| 1:A:269:LYS:C    | 1:A:271:LYS:H    | 2.07                     | 0.61              |
| 1:A:101:ASN:C    | 1:A:101:ASN:HD22 | 2.08                     | 0.61              |
| 1:A:330:ILE:HD13 | 1:A:342:LEU:HD22 | 1.82                     | 0.61              |
| 1:A:326:ASN:HD22 | 1:A:328:LYS:N    | 1.99                     | 0.61              |
| 1:A:384:ALA:O    | 1:A:387:VAL:HG12 | 1.99                     | 0.61              |
| 1:A:166:LEU:CD2  | 1:A:247:CYS:HA   | 2.29                     | 0.61              |
| 1:A:274:THR:OG1  | 1:A:276:PRO:HD2  | 2.01                     | 0.61              |
| 1:A:25:THR:OG1   | 1:A:26:GLU:N     | 2.29                     | 0.60              |
| 1:A:103:SER:CB   | 5:A:734:HOH:O    | 2.49                     | 0.60              |
| 1:A:143:PRO:CB   | 1:A:424:VAL:HG22 | 2.26                     | 0.60              |
| 1:A:218:ILE:HG23 | 1:A:223:GLU:CG   | 2.32                     | 0.60              |
| 1:A:257:LYS:HZ1  | 1:A:269:LYS:CE   | 2.04                     | 0.60              |
| 1:A:268:ASP:OD1  | 1:A:270:SER:HB2  | 2.01                     | 0.60              |
| 1:A:30:PHE:CE2   | 1:A:123:ALA:CB   | 2.84                     | 0.60              |
| 1:A:34:VAL:HG12  | 1:A:35:PRO:O     | 2.01                     | 0.60              |
| 1:A:44:GLU:HA    | 1:A:324:VAL:CG1  | 2.32                     | 0.60              |
| 1:A:144:TYR:CD2  | 1:A:419:LEU:CD1  | 2.84                     | 0.60              |
| 1:A:271:LYS:O    | 1:A:272:TRP:C    | 2.45                     | 0.60              |
| 1:A:252:PHE:HB2  | 1:A:259:ASP:O    | 2.02                     | 0.59              |
| 1:A:317:ILE:HG22 | 1:A:339:ALA:HB2  | 1.83                     | 0.59              |
| 1:A:343:LEU:HD23 | 1:A:345:LYS:HE3  | 1.83                     | 0.59              |
| 1:A:44:GLU:OE1   | 5:A:470:HOH:O    | 2.15                     | 0.59              |
| 1:A:261:ASP:C    | 1:A:263:LYS:N    | 2.55                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:159:HIS:N    | 1:A:159:HIS:CD2  | 2.70                     | 0.59              |
| 1:A:49:ARG:C     | 5:A:689:HOH:O    | 2.44                     | 0.59              |
| 1:A:262:PHE:C    | 1:A:263:LYS:HE3  | 2.28                     | 0.59              |
| 1:A:129:LEU:O    | 1:A:132:HIS:N    | 2.35                     | 0.59              |
| 1:A:265:PRO:HD2  | 1:A:266:ASN:H    | 1.66                     | 0.59              |
| 1:A:261:ASP:OD2  | 1:A:264:ASN:N    | 2.35                     | 0.58              |
| 1:A:52:ASP:C     | 1:A:52:ASP:OD1   | 2.42                     | 0.58              |
| 1:A:103:SER:HB3  | 5:A:734:HOH:O    | 2.04                     | 0.58              |
| 1:A:33:ILE:CG2   | 1:A:378:THR:HG21 | 2.32                     | 0.57              |
| 1:A:71:VAL:O     | 1:A:74:PRO:HG2   | 2.04                     | 0.57              |
| 1:A:110:ILE:O    | 1:A:111:LEU:C    | 2.47                     | 0.57              |
| 1:A:144:TYR:HD2  | 1:A:419:LEU:CD1  | 2.18                     | 0.57              |
| 1:A:111:LEU:CB   | 5:A:761:HOH:O    | 2.51                     | 0.57              |
| 1:A:211:GLU:CD   | 1:A:373:HIS:HE1  | 2.12                     | 0.57              |
| 1:A:387:VAL:HG21 | 1:A:395:ILE:HB   | 1.86                     | 0.57              |
| 1:A:68:VAL:O     | 1:A:73:ALA:HB2   | 2.04                     | 0.57              |
| 1:A:265:PRO:CD   | 1:A:266:ASN:N    | 2.68                     | 0.57              |
| 1:A:194:LYS:CG   | 1:A:198:LYS:HE2  | 2.35                     | 0.57              |
| 1:A:201:TYR:HD1  | 5:A:593:HOH:O    | 1.87                     | 0.57              |
| 1:A:373:HIS:H    | 1:A:373:HIS:HD2  | 1.53                     | 0.57              |
| 1:A:383:ILE:HG13 | 1:A:395:ILE:HD11 | 1.86                     | 0.57              |
| 1:A:43:HIS:C     | 1:A:324:VAL:HG11 | 2.30                     | 0.56              |
| 1:A:173:PRO:CG   | 1:A:182:ALA:HB1  | 2.34                     | 0.56              |
| 1:A:251:GLU:HA   | 5:A:791:HOH:O    | 2.06                     | 0.56              |
| 1:A:324:VAL:O    | 1:A:324:VAL:CG1  | 2.53                     | 0.56              |
| 1:A:101:ASN:ND2  | 1:A:103:SER:CB   | 2.47                     | 0.56              |
| 1:A:252:PHE:HD2  | 1:A:262:PHE:CE1  | 2.23                     | 0.56              |
| 1:A:343:LEU:CD2  | 1:A:345:LYS:HE3  | 2.35                     | 0.56              |
| 1:A:369:VAL:O    | 1:A:392:THR:HB   | 2.06                     | 0.56              |
| 1:A:4:LYS:O      | 1:A:4:LYS:CG     | 2.51                     | 0.56              |
| 1:A:4:LYS:HE2    | 5:A:605:HOH:O    | 2.06                     | 0.56              |
| 1:A:201:TYR:CA   | 5:A:593:HOH:O    | 2.54                     | 0.56              |
| 1:A:57:MET:HE1   | 5:A:552:HOH:O    | 2.04                     | 0.56              |
| 1:A:140:LYS:HB2  | 1:A:391:ARG:NE   | 2.20                     | 0.56              |
| 1:A:43:HIS:HD2   | 5:A:733:HOH:O    | 1.88                     | 0.55              |
| 1:A:50:ASP:HB2   | 5:A:574:HOH:O    | 2.06                     | 0.55              |
| 1:A:194:LYS:O    | 1:A:198:LYS:HE3  | 2.06                     | 0.55              |
| 1:A:42:VAL:CG2   | 1:A:43:HIS:H     | 2.19                     | 0.55              |
| 1:A:57:MET:CE    | 5:A:552:HOH:O    | 2.54                     | 0.55              |
| 1:A:280:ASP:HB2  | 5:A:637:HOH:O    | 2.06                     | 0.55              |
| 1:A:320:ASP:CA   | 5:A:650:HOH:O    | 2.50                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:101:ASN:HD22 | 1:A:103:SER:H    | 1.55                     | 0.55              |
| 1:A:373:HIS:ND1  | 1:A:405:ARG:NH1  | 2.54                     | 0.55              |
| 1:A:257:LYS:CE   | 1:A:269:LYS:CE   | 2.81                     | 0.55              |
| 1:A:76:PHE:O     | 1:A:77:VAL:C     | 2.50                     | 0.55              |
| 1:A:390:LEU:O    | 1:A:391:ARG:CB   | 2.55                     | 0.55              |
| 1:A:67:ASN:O     | 1:A:71:VAL:HB    | 2.06                     | 0.55              |
| 1:A:185:ILE:HG12 | 1:A:237:HIS:CE1  | 2.42                     | 0.55              |
| 1:A:225:LEU:HD11 | 1:A:291:ILE:HD11 | 1.89                     | 0.55              |
| 1:A:32:SER:OG    | 1:A:116:ALA:HB2  | 2.07                     | 0.55              |
| 1:A:190:TYR:O    | 1:A:193:LEU:HB3  | 2.07                     | 0.54              |
| 1:A:229:VAL:O    | 1:A:232:ILE:N    | 2.40                     | 0.54              |
| 1:A:281:LEU:O    | 1:A:281:LEU:HD12 | 2.07                     | 0.54              |
| 1:A:1:ALA:N      | 1:A:26:GLU:OE2   | 2.36                     | 0.54              |
| 1:A:312:THR:CG2  | 5:A:629:HOH:O    | 2.54                     | 0.54              |
| 1:A:94:ILE:HG23  | 5:A:690:HOH:O    | 2.08                     | 0.54              |
| 1:A:163:ALA:N    | 1:A:217:ASN:ND2  | 2.55                     | 0.54              |
| 1:A:216:PRO:HG2  | 1:A:218:ILE:HG13 | 1.89                     | 0.54              |
| 1:A:273:LEU:HA   | 1:A:277:GLN:OE1  | 2.08                     | 0.54              |
| 1:A:153:VAL:HB   | 1:A:193:LEU:HD23 | 1.88                     | 0.54              |
| 1:A:201:TYR:HE2  | 1:A:227:LEU:CD2  | 2.21                     | 0.54              |
| 1:A:219:GLN:N    | 1:A:223:GLU:OE1  | 2.37                     | 0.54              |
| 1:A:201:TYR:HA   | 5:A:593:HOH:O    | 2.08                     | 0.53              |
| 1:A:2:VAL:HG22   | 1:A:23:LEU:HD21  | 1.90                     | 0.53              |
| 1:A:251:GLU:CD   | 5:A:791:HOH:O    | 2.51                     | 0.53              |
| 1:A:111:LEU:O    | 1:A:114:SER:HB3  | 2.08                     | 0.53              |
| 1:A:69:ASN:HB2   | 5:A:681:HOH:O    | 2.09                     | 0.53              |
| 1:A:146:LEU:HD21 | 1:A:415:ILE:HG22 | 1.91                     | 0.53              |
| 1:A:155:ASN:CG   | 5:A:795:HOH:O    | 2.51                     | 0.52              |
| 1:A:265:PRO:CD   | 1:A:266:ASN:H    | 2.21                     | 0.52              |
| 1:A:104:LYS:CG   | 5:A:683:HOH:O    | 2.53                     | 0.52              |
| 1:A:261:ASP:CB   | 1:A:264:ASN:ND2  | 2.72                     | 0.52              |
| 1:A:166:LEU:HD22 | 1:A:247:CYS:SG   | 2.50                     | 0.52              |
| 1:A:200:ARG:NH1  | 5:A:642:HOH:O    | 2.43                     | 0.52              |
| 1:A:32:SER:HA    | 1:A:380:ASP:OD2  | 2.09                     | 0.52              |
| 1:A:246:ASP:HA   | 1:A:295:GLU:HB3  | 1.91                     | 0.52              |
| 1:A:252:PHE:O    | 1:A:258:TYR:HA   | 2.09                     | 0.52              |
| 1:A:102:LYS:NZ   | 1:A:354:GLU:OE2  | 2.42                     | 0.52              |
| 1:A:257:LYS:HE3  | 1:A:269:LYS:CE   | 2.38                     | 0.52              |
| 1:A:268:ASP:OD2  | 1:A:270:SER:CB   | 2.55                     | 0.52              |
| 1:A:44:GLU:CA    | 1:A:324:VAL:HG11 | 2.39                     | 0.52              |
| 1:A:157:GLY:O    | 1:A:158:SER:C    | 2.53                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:386:LEU:HG   | 1:A:390:LEU:HD12 | 1.91                     | 0.51              |
| 1:A:55:LYS:HE3   | 5:A:697:HOH:O    | 2.10                     | 0.51              |
| 1:A:411:GLN:NE2  | 5:A:487:HOH:O    | 2.42                     | 0.51              |
| 1:A:73:ALA:HB3   | 1:A:74:PRO:CD    | 2.40                     | 0.51              |
| 1:A:265:PRO:C    | 1:A:267:SER:N    | 2.64                     | 0.51              |
| 1:A:165:ALA:HB2  | 1:A:260:LEU:O    | 2.11                     | 0.51              |
| 1:A:211:GLU:CD   | 1:A:373:HIS:CE1  | 2.89                     | 0.51              |
| 1:A:220:THR:HA   | 5:A:555:HOH:O    | 2.10                     | 0.51              |
| 1:A:127:VAL:HG23 | 1:A:128:PRO:O    | 2.11                     | 0.50              |
| 1:A:157:GLY:C    | 1:A:159:HIS:N    | 2.68                     | 0.50              |
| 1:A:292:VAL:O    | 5:A:645:HOH:O    | 2.19                     | 0.50              |
| 1:A:164:LEU:HD21 | 1:A:169:PHE:CE2  | 2.47                     | 0.50              |
| 1:A:165:ALA:N    | 5:A:773:HOH:O    | 2.41                     | 0.50              |
| 1:A:251:GLU:CA   | 5:A:791:HOH:O    | 2.59                     | 0.50              |
| 1:A:268:ASP:C    | 1:A:270:SER:N    | 2.65                     | 0.50              |
| 1:A:298:PHE:HB2  | 1:A:306:TRP:CD1  | 2.46                     | 0.50              |
| 1:A:83:VAL:HG22  | 5:A:722:HOH:O    | 2.12                     | 0.50              |
| 1:A:200:ARG:NH2  | 1:A:230:ASP:OD2  | 2.39                     | 0.50              |
| 1:A:343:LEU:HD11 | 1:A:396:LYS:HD2  | 1.94                     | 0.50              |
| 1:A:257:LYS:HZ2  | 1:A:269:LYS:HE2  | 1.67                     | 0.50              |
| 1:A:279:ALA:O    | 1:A:283:HIS:HD2  | 1.94                     | 0.50              |
| 1:A:139:SER:C    | 1:A:140:LYS:O    | 2.52                     | 0.50              |
| 1:A:24:THR:HG23  | 1:A:29:VAL:HG22  | 1.94                     | 0.49              |
| 1:A:373:HIS:CD2  | 1:A:396:LYS:O    | 2.65                     | 0.49              |
| 1:A:268:ASP:O    | 1:A:271:LYS:N    | 2.37                     | 0.49              |
| 1:A:281:LEU:O    | 1:A:284:SER:HB3  | 2.12                     | 0.49              |
| 1:A:208:VAL:HG21 | 1:A:212:GLY:HA2  | 1.94                     | 0.49              |
| 1:A:257:LYS:HB3  | 1:A:272:TRP:HB3  | 1.94                     | 0.49              |
| 1:A:31:ARG:O     | 1:A:119:ARG:NH1  | 2.45                     | 0.49              |
| 1:A:152:ASN:OD1  | 1:A:155:ASN:ND2  | 2.45                     | 0.49              |
| 1:A:227:LEU:HD22 | 5:A:749:HOH:O    | 2.12                     | 0.49              |
| 1:A:218:ILE:HG23 | 1:A:223:GLU:HB3  | 1.94                     | 0.49              |
| 1:A:4:LYS:CE     | 5:A:471:HOH:O    | 2.59                     | 0.49              |
| 1:A:111:LEU:HD22 | 1:A:347:ASN:HA   | 1.95                     | 0.49              |
| 1:A:429:ASN:HA   | 5:A:630:HOH:O    | 2.12                     | 0.49              |
| 1:A:42:VAL:CG2   | 1:A:43:HIS:CE1   | 2.95                     | 0.49              |
| 1:A:283:HIS:O    | 1:A:284:SER:C    | 2.56                     | 0.49              |
| 1:A:149:PRO:HG2  | 1:A:151:LEU:HD11 | 1.95                     | 0.48              |
| 1:A:233:LYS:O    | 1:A:234:ALA:C    | 2.56                     | 0.48              |
| 1:A:194:LYS:HE3  | 1:A:206:GLY:O    | 2.13                     | 0.48              |
| 1:A:380:ASP:OD2  | 5:A:498:HOH:O    | 2.19                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:263:LYS:N    | 1:A:263:LYS:HE3  | 2.29                     | 0.48              |
| 1:A:154:LEU:HD11 | 1:A:218:ILE:HD12 | 1.95                     | 0.48              |
| 1:A:201:TYR:CB   | 5:A:593:HOH:O    | 2.62                     | 0.48              |
| 1:A:261:ASP:OD2  | 1:A:264:ASN:CG   | 2.57                     | 0.48              |
| 1:A:310:PHE:CD1  | 1:A:310:PHE:C    | 2.92                     | 0.48              |
| 1:A:252:PHE:CD2  | 1:A:262:PHE:CE1  | 3.02                     | 0.48              |
| 1:A:257:LYS:CB   | 1:A:272:TRP:HB3  | 2.43                     | 0.48              |
| 1:A:52:ASP:CB    | 5:A:583:HOH:O    | 2.61                     | 0.48              |
| 1:A:281:LEU:HD12 | 1:A:281:LEU:C    | 2.39                     | 0.48              |
| 1:A:266:ASN:CG   | 5:A:793:HOH:O    | 2.57                     | 0.48              |
| 1:A:265:PRO:HD2  | 1:A:266:ASN:N    | 2.29                     | 0.47              |
| 1:A:30:PHE:CZ    | 1:A:123:ALA:CB   | 2.97                     | 0.47              |
| 1:A:129:LEU:O    | 1:A:130:TYR:C    | 2.57                     | 0.47              |
| 1:A:211:GLU:OE1  | 1:A:373:HIS:HE1  | 1.98                     | 0.47              |
| 1:A:184:ARG:HH11 | 1:A:184:ARG:HD3  | 1.34                     | 0.47              |
| 1:A:75:ALA:HB1   | 1:A:92:PHE:HZ    | 1.80                     | 0.47              |
| 1:A:188:GLU:OE1  | 5:A:702:HOH:O    | 2.19                     | 0.47              |
| 1:A:218:ILE:HG22 | 1:A:219:GLN:N    | 2.29                     | 0.47              |
| 1:A:73:ALA:HB3   | 1:A:74:PRO:HD2   | 1.96                     | 0.47              |
| 1:A:125:LYS:CE   | 1:A:132:HIS:CE1  | 2.84                     | 0.47              |
| 1:A:300:GLU:HB3  | 1:A:321:ASP:HB3  | 1.96                     | 0.47              |
| 1:A:351:THR:OG1  | 1:A:354:GLU:HG3  | 2.15                     | 0.47              |
| 1:A:50:ASP:C     | 5:A:689:HOH:O    | 2.52                     | 0.47              |
| 1:A:14:ARG:HG2   | 5:A:595:HOH:O    | 2.14                     | 0.46              |
| 1:A:97:ASP:O     | 1:A:99:THR:CG2   | 2.41                     | 0.46              |
| 1:A:106:GLY:O    | 1:A:109:ALA:HB3  | 2.15                     | 0.46              |
| 1:A:324:VAL:HG12 | 5:A:467:HOH:O    | 2.14                     | 0.46              |
| 1:A:208:VAL:HA   | 1:A:213:GLY:O    | 2.14                     | 0.46              |
| 1:A:208:VAL:CB   | 1:A:213:GLY:O    | 2.62                     | 0.46              |
| 1:A:368:GLY:CA   | 5:A:587:HOH:O    | 2.62                     | 0.46              |
| 1:A:44:GLU:CD    | 1:A:348:GLN:HG3  | 2.40                     | 0.46              |
| 1:A:159:HIS:N    | 1:A:159:HIS:HD2  | 2.14                     | 0.46              |
| 1:A:262:PHE:C    | 1:A:263:LYS:CE   | 2.88                     | 0.46              |
| 1:A:139:SER:O    | 1:A:140:LYS:O    | 2.34                     | 0.46              |
| 1:A:280:ASP:OD2  | 5:A:753:HOH:O    | 2.21                     | 0.46              |
| 1:A:101:ASN:HD22 | 1:A:103:SER:N    | 2.14                     | 0.46              |
| 1:A:154:LEU:HD11 | 1:A:218:ILE:CD1  | 2.46                     | 0.46              |
| 1:A:143:PRO:HG3  | 1:A:424:VAL:HG11 | 1.95                     | 0.46              |
| 1:A:30:PHE:N     | 1:A:30:PHE:CD1   | 2.84                     | 0.45              |
| 1:A:65:VAL:HG12  | 5:A:681:HOH:O    | 2.15                     | 0.45              |
| 1:A:98:GLY:C     | 1:A:99:THR:CG2   | 2.88                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:90:ASP:OD2   | 1:A:353:SER:HB2  | 2.16                     | 0.45              |
| 1:A:216:PRO:HG2  | 1:A:218:ILE:CD1  | 2.46                     | 0.45              |
| 1:A:46:LEU:HD23  | 1:A:46:LEU:O     | 2.16                     | 0.45              |
| 1:A:122:ALA:C    | 1:A:124:GLU:N    | 2.73                     | 0.45              |
| 1:A:111:LEU:CD2  | 1:A:347:ASN:HA   | 2.46                     | 0.45              |
| 1:A:131:LYS:NZ   | 1:A:135:ASP:OD1  | 2.49                     | 0.45              |
| 1:A:345:LYS:HZ2  | 1:A:374:ARG:HH12 | 1.64                     | 0.45              |
| 1:A:46:LEU:HD13  | 5:A:736:HOH:O    | 2.17                     | 0.45              |
| 1:A:307:SER:OG   | 1:A:336:LYS:O    | 2.30                     | 0.45              |
| 1:A:4:LYS:HD3    | 5:A:471:HOH:O    | 2.17                     | 0.45              |
| 1:A:5:VAL:HB     | 5:A:625:HOH:O    | 2.17                     | 0.45              |
| 1:A:164:LEU:HD21 | 1:A:169:PHE:HE2  | 1.80                     | 0.45              |
| 1:A:392:THR:OG1  | 1:A:393:GLY:N    | 2.50                     | 0.45              |
| 1:A:166:LEU:CD2  | 1:A:247:CYS:SG   | 3.05                     | 0.45              |
| 1:A:266:ASN:HD22 | 1:A:266:ASN:HA   | 1.66                     | 0.45              |
| 1:A:162:GLY:HA2  | 1:A:217:ASN:ND2  | 2.33                     | 0.44              |
| 1:A:201:TYR:HB3  | 5:A:593:HOH:O    | 2.17                     | 0.44              |
| 1:A:90:ASP:CG    | 1:A:351:THR:HB   | 2.41                     | 0.44              |
| 1:A:262:PHE:C    | 1:A:263:LYS:CG   | 2.83                     | 0.44              |
| 1:A:434:ASP:C    | 1:A:435:LYS:CG   | 2.89                     | 0.44              |
| 1:A:133:LEU:HD23 | 1:A:386:LEU:HA   | 1.98                     | 0.44              |
| 1:A:253:PHE:C    | 1:A:254:LYS:HG3  | 2.41                     | 0.44              |
| 1:A:127:VAL:HB   | 1:A:128:PRO:HD2  | 1.99                     | 0.44              |
| 1:A:359:ALA:CB   | 1:A:390:LEU:CD2  | 2.95                     | 0.44              |
| 1:A:318:VAL:HA   | 1:A:341:ALA:HB3  | 1.99                     | 0.44              |
| 1:A:6:TYR:HE1    | 1:A:8:ARG:HB3    | 1.81                     | 0.44              |
| 1:A:13:SER:N     | 1:A:377:GLU:O    | 2.40                     | 0.44              |
| 1:A:39:SER:O     | 1:A:40:THR:O     | 2.36                     | 0.44              |
| 1:A:380:ASP:CG   | 5:A:498:HOH:O    | 2.58                     | 0.44              |
| 1:A:144:TYR:CD2  | 1:A:419:LEU:HD11 | 2.52                     | 0.44              |
| 1:A:391:ARG:CD   | 5:A:486:HOH:O    | 2.55                     | 0.44              |
| 1:A:181:GLU:CD   | 5:A:790:HOH:O    | 2.61                     | 0.44              |
| 1:A:370:MET:HA   | 1:A:394:GLN:O    | 2.18                     | 0.43              |
| 1:A:6:TYR:CD1    | 1:A:7:ALA:N      | 2.86                     | 0.43              |
| 1:A:69:ASN:O     | 1:A:73:ALA:HB3   | 2.18                     | 0.43              |
| 1:A:140:LYS:N    | 5:A:485:HOH:O    | 2.24                     | 0.43              |
| 1:A:42:VAL:HG23  | 1:A:43:HIS:CG    | 2.53                     | 0.43              |
| 1:A:43:HIS:CD2   | 5:A:733:HOH:O    | 2.69                     | 0.43              |
| 1:A:289:TYR:C    | 1:A:291:ILE:H    | 2.25                     | 0.43              |
| 1:A:5:VAL:N      | 5:A:625:HOH:O    | 2.52                     | 0.43              |
| 1:A:269:LYS:HD2  | 5:A:747:HOH:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:330:ILE:HD11 | 1:A:342:LEU:HD22 | 1.97                     | 0.43              |
| 1:A:122:ALA:O    | 1:A:123:ALA:C    | 2.62                     | 0.43              |
| 1:A:202:GLY:O    | 1:A:203:ALA:C    | 2.61                     | 0.43              |
| 1:A:247:CYS:HB2  | 1:A:296:ASP:O    | 2.19                     | 0.43              |
| 1:A:373:HIS:C    | 1:A:374:ARG:CG   | 2.92                     | 0.43              |
| 1:A:220:THR:HG23 | 5:A:707:HOH:O    | 2.17                     | 0.43              |
| 1:A:275:GLY:N    | 1:A:276:PRO:CD   | 2.81                     | 0.43              |
| 1:A:44:GLU:O     | 1:A:45:ALA:C     | 2.62                     | 0.43              |
| 1:A:131:LYS:HD3  | 1:A:131:LYS:C    | 2.44                     | 0.43              |
| 1:A:264:ASN:CG   | 5:A:581:HOH:O    | 2.61                     | 0.43              |
| 1:A:179:PHE:HE1  | 1:A:183:LEU:CD2  | 2.32                     | 0.42              |
| 1:A:46:LEU:CD1   | 5:A:736:HOH:O    | 2.66                     | 0.42              |
| 1:A:57:MET:HE2   | 5:A:550:HOH:O    | 2.18                     | 0.42              |
| 1:A:369:VAL:O    | 1:A:392:THR:CB   | 2.66                     | 0.42              |
| 1:A:184:ARG:NH1  | 5:A:541:HOH:O    | 2.52                     | 0.42              |
| 1:A:9:SER:CB     | 5:A:535:HOH:O    | 2.67                     | 0.42              |
| 1:A:78:LYS:C     | 1:A:80:ASN:H     | 2.26                     | 0.42              |
| 1:A:101:ASN:ND2  | 1:A:101:ASN:C    | 2.76                     | 0.42              |
| 1:A:261:ASP:O    | 1:A:261:ASP:CG   | 2.61                     | 0.42              |
| 1:A:59:LYS:C     | 1:A:60:GLY:O     | 2.60                     | 0.42              |
| 1:A:136:LEU:N    | 1:A:136:LEU:HD23 | 2.34                     | 0.42              |
| 1:A:139:SER:CA   | 5:A:485:HOH:O    | 2.59                     | 0.42              |
| 1:A:174:THR:HB   | 1:A:427:GLY:O    | 2.20                     | 0.42              |
| 1:A:275:GLY:N    | 1:A:276:PRO:HD3  | 2.35                     | 0.42              |
| 1:A:344:LEU:C    | 1:A:344:LEU:CD2  | 2.85                     | 0.42              |
| 1:A:232:ILE:HD13 | 1:A:241:VAL:HG12 | 2.02                     | 0.42              |
| 1:A:261:ASP:CG   | 1:A:264:ASN:N    | 2.78                     | 0.42              |
| 1:A:166:LEU:HD22 | 1:A:247:CYS:CA   | 2.43                     | 0.42              |
| 1:A:345:LYS:HB2  | 1:A:348:GLN:HB2  | 2.01                     | 0.42              |
| 1:A:119:ARG:HA   | 1:A:129:LEU:HD13 | 2.00                     | 0.42              |
| 1:A:153:VAL:O    | 1:A:214:VAL:HG22 | 2.19                     | 0.42              |
| 1:A:279:ALA:O    | 1:A:283:HIS:CD2  | 2.73                     | 0.42              |
| 1:A:357:LYS:CE   | 5:A:799:HOH:O    | 2.68                     | 0.42              |
| 1:A:52:ASP:O     | 1:A:54:SER:N     | 2.53                     | 0.41              |
| 1:A:137:SER:HB3  | 1:A:356:ILE:HG23 | 2.01                     | 0.41              |
| 1:A:326:ASN:ND2  | 1:A:328:LYS:CB   | 2.74                     | 0.41              |
| 1:A:201:TYR:HE2  | 1:A:227:LEU:HD22 | 1.83                     | 0.41              |
| 1:A:146:LEU:CD1  | 1:A:423:ALA:HB1  | 2.50                     | 0.41              |
| 1:A:168:GLU:OE2  | 1:A:396:LYS:CE   | 2.68                     | 0.41              |
| 1:A:188:GLU:OE1  | 1:A:237:HIS:NE2  | 2.26                     | 0.41              |
| 1:A:26:GLU:H     | 1:A:26:GLU:HG2   | 1.46                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:218:ILE:CG2  | 1:A:223:GLU:HB3  | 2.51                     | 0.41              |
| 1:A:75:ALA:HB1   | 1:A:92:PHE:CZ    | 2.56                     | 0.41              |
| 1:A:78:LYS:C     | 1:A:80:ASN:N     | 2.79                     | 0.41              |
| 1:A:227:LEU:CD2  | 5:A:749:HOH:O    | 2.68                     | 0.41              |
| 1:A:14:ARG:HH11  | 1:A:14:ARG:HD3   | 1.67                     | 0.41              |
| 1:A:35:PRO:HG2   | 1:A:347:ASN:HB3  | 2.03                     | 0.41              |
| 1:A:80:ASN:HA    | 5:A:561:HOH:O    | 2.21                     | 0.41              |
| 1:A:424:VAL:HG23 | 1:A:424:VAL:O    | 2.21                     | 0.41              |
| 1:A:436:LEU:O    | 1:A:436:LEU:CG   | 2.65                     | 0.41              |
| 1:A:43:HIS:O     | 1:A:324:VAL:HG11 | 2.21                     | 0.40              |
| 1:A:391:ARG:O    | 1:A:391:ARG:HG2  | 2.21                     | 0.40              |
| 1:A:297:PRO:HD2  | 1:A:306:TRP:CH2  | 2.56                     | 0.40              |
| 1:A:266:ASN:ND2  | 5:A:793:HOH:O    | 2.54                     | 0.40              |
| 1:A:44:GLU:N     | 1:A:324:VAL:HG11 | 2.36                     | 0.40              |
| 1:A:254:LYS:HD3  | 1:A:272:TRP:CH2  | 2.57                     | 0.40              |

All (11) 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:A:98:GLY:C    | 5:A:754:HOH:O[3_644]   | 0.95                     | 1.25              |
| 1:A:99:THR:N    | 5:A:754:HOH:O[3_644]   | 1.02                     | 1.18              |
| 1:A:204:SER:N   | 5:A:449:HOH:O[8_666]   | 1.03                     | 1.17              |
| 1:A:191:HIS:CD2 | 5:A:557:HOH:O[8_666]   | 1.62                     | 0.58              |
| 1:A:207:ASN:ND2 | 5:A:763:HOH:O[8_666]   | 1.72                     | 0.48              |
| 1:A:98:GLY:O    | 5:A:754:HOH:O[3_644]   | 1.86                     | 0.34              |
| 1:A:98:GLY:CA   | 5:A:754:HOH:O[3_644]   | 1.92                     | 0.28              |
| 1:A:203:ALA:C   | 5:A:449:HOH:O[8_666]   | 2.03                     | 0.17              |
| 1:A:204:SER:CA  | 5:A:449:HOH:O[8_666]   | 2.09                     | 0.11              |
| 1:A:302:ASP:OD2 | 1:A:421:ASP:OD2[4_564] | 2.16                     | 0.04              |
| 1:A:99:THR:CA   | 5:A:754:HOH:O[3_644]   | 2.17                     | 0.03              |

## 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     | 434/436 (100%) | 369 (85%) | 52 (12%) | 13 (3%)  | 3 6         |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 40  | THR  |
| 1   | A     | 39  | SER  |
| 1   | A     | 43  | HIS  |
| 1   | A     | 140 | LYS  |
| 1   | A     | 263 | LYS  |
| 1   | A     | 300 | GLU  |
| 1   | A     | 45  | ALA  |
| 1   | A     | 262 | PHE  |
| 1   | A     | 53  | LYS  |
| 1   | A     | 136 | LEU  |
| 1   | A     | 313 | ALA  |
| 1   | A     | 102 | LYS  |
| 1   | A     | 324 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |
|-----|-------|----------------|-----------|----------|-------------|
| 1   | A     | 344/344 (100%) | 312 (91%) | 32 (9%)  | 8 18        |

All (32) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 24  | THR  |
| 1   | A     | 26  | GLU  |
| 1   | A     | 40  | THR  |
| 1   | A     | 57  | MET  |
| 1   | A     | 96  | LEU  |
| 1   | A     | 101 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 108 | ASN  |
| 1   | A     | 111 | LEU  |
| 1   | A     | 127 | VAL  |
| 1   | A     | 133 | LEU  |
| 1   | A     | 147 | PRO  |
| 1   | A     | 151 | LEU  |
| 1   | A     | 187 | SER  |
| 1   | A     | 197 | THR  |
| 1   | A     | 217 | ASN  |
| 1   | A     | 227 | LEU  |
| 1   | A     | 263 | LYS  |
| 1   | A     | 265 | PRO  |
| 1   | A     | 270 | SER  |
| 1   | A     | 291 | ILE  |
| 1   | A     | 293 | SER  |
| 1   | A     | 317 | ILE  |
| 1   | A     | 326 | ASN  |
| 1   | A     | 355 | SER  |
| 1   | A     | 362 | SER  |
| 1   | A     | 374 | ARG  |
| 1   | A     | 383 | ILE  |
| 1   | A     | 390 | LEU  |
| 1   | A     | 392 | THR  |
| 1   | A     | 415 | ILE  |
| 1   | A     | 432 | HIS  |
| 1   | A     | 436 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 43  | HIS  |
| 1   | A     | 101 | ASN  |
| 1   | A     | 207 | ASN  |
| 1   | A     | 217 | ASN  |
| 1   | A     | 264 | ASN  |
| 1   | A     | 266 | ASN  |
| 1   | A     | 283 | HIS  |
| 1   | A     | 326 | ASN  |
| 1   | A     | 411 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | PO4  | A     | 444 | -    | 4,4,4        | 1.33 | 0           | 6,6,6       | 0.63 | 0           |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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.