



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:18 AM UTC

PDB ID : 3X2E / pdb\_00003x2e  
Title : A thermophilic hydrolase  
Authors : Zheng, Y.; Ko, T.P.; Huang, C.H.  
Deposited on : 2014-12-21  
Resolution : 2.85 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) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

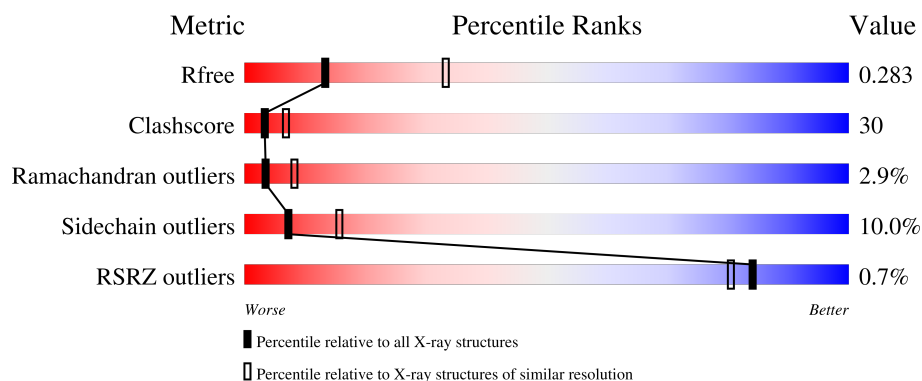
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1407 (2.88-2.84)                                      |
| Clashscore            | 190562                      | 1446 (2.88-2.84)                                      |
| Ramachandran outliers | 187476                      | 1406 (2.88-2.84)                                      |
| Sidechain outliers    | 187428                      | 1407 (2.88-2.84)                                      |
| RSRZ outliers         | 180081                      | 1408 (2.88-2.84)                                      |

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                  |
|-----|-------|--------|---------------------------------------------------|
| 1   | A     | 411    | <div> <div></div> <div>45% 45% 7% ..</div> </div> |
| 1   | B     | 411    | <div> <div></div> <div>43% 45% 9% ..</div> </div> |
| 1   | C     | 411    | <div> <div></div> <div>48% 41% 8% ..</div> </div> |
| 1   | D     | 411    | <div> <div></div> <div>46% 43% 9% .</div> </div>  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12993 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 Adenosylhomocysteinase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 401      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3116  | 1970 | 539 | 593 | 14 |         |         |       |
| 1   | B     | 401      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3116  | 1970 | 539 | 593 | 14 |         |         |       |
| 1   | C     | 401      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3116  | 1970 | 539 | 593 | 14 |         |         |       |
| 1   | D     | 401      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3116  | 1970 | 539 | 593 | 14 |         |         |       |

There are 32 discrepancies between the modelled and reference sequences:

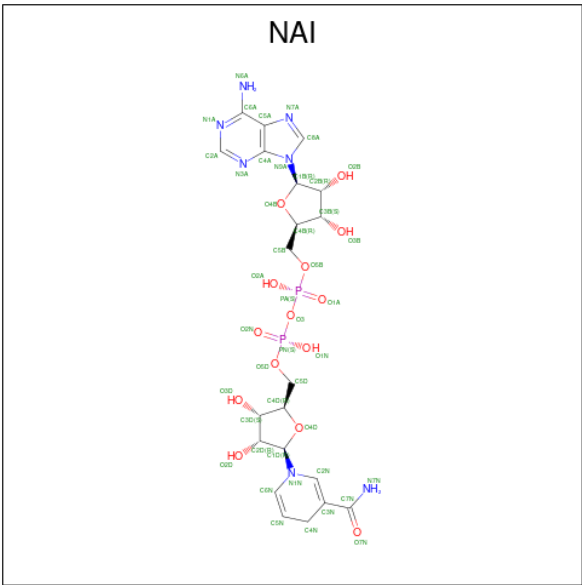
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | MET      | -      | expression tag | UNP O51933 |
| A     | 2       | ALA      | -      | expression tag | UNP O51933 |
| A     | 406     | HIS      | -      | expression tag | UNP O51933 |
| A     | 407     | HIS      | -      | expression tag | UNP O51933 |
| A     | 408     | HIS      | -      | expression tag | UNP O51933 |
| A     | 409     | HIS      | -      | expression tag | UNP O51933 |
| A     | 410     | HIS      | -      | expression tag | UNP O51933 |
| A     | 411     | HIS      | -      | expression tag | UNP O51933 |
| B     | 1       | MET      | -      | expression tag | UNP O51933 |
| B     | 2       | ALA      | -      | expression tag | UNP O51933 |
| B     | 406     | HIS      | -      | expression tag | UNP O51933 |
| B     | 407     | HIS      | -      | expression tag | UNP O51933 |
| B     | 408     | HIS      | -      | expression tag | UNP O51933 |
| B     | 409     | HIS      | -      | expression tag | UNP O51933 |
| B     | 410     | HIS      | -      | expression tag | UNP O51933 |
| B     | 411     | HIS      | -      | expression tag | UNP O51933 |
| C     | 1       | MET      | -      | expression tag | UNP O51933 |
| C     | 2       | ALA      | -      | expression tag | UNP O51933 |
| C     | 406     | HIS      | -      | expression tag | UNP O51933 |
| C     | 407     | HIS      | -      | expression tag | UNP O51933 |
| C     | 408     | HIS      | -      | expression tag | UNP O51933 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 409     | HIS      | -      | expression tag | UNP O51933 |
| C     | 410     | HIS      | -      | expression tag | UNP O51933 |
| C     | 411     | HIS      | -      | expression tag | UNP O51933 |
| D     | 1       | MET      | -      | expression tag | UNP O51933 |
| D     | 2       | ALA      | -      | expression tag | UNP O51933 |
| D     | 406     | HIS      | -      | expression tag | UNP O51933 |
| D     | 407     | HIS      | -      | expression tag | UNP O51933 |
| D     | 408     | HIS      | -      | expression tag | UNP O51933 |
| D     | 409     | HIS      | -      | expression tag | UNP O51933 |
| D     | 410     | HIS      | -      | expression tag | UNP O51933 |
| D     | 411     | HIS      | -      | expression tag | UNP O51933 |

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).

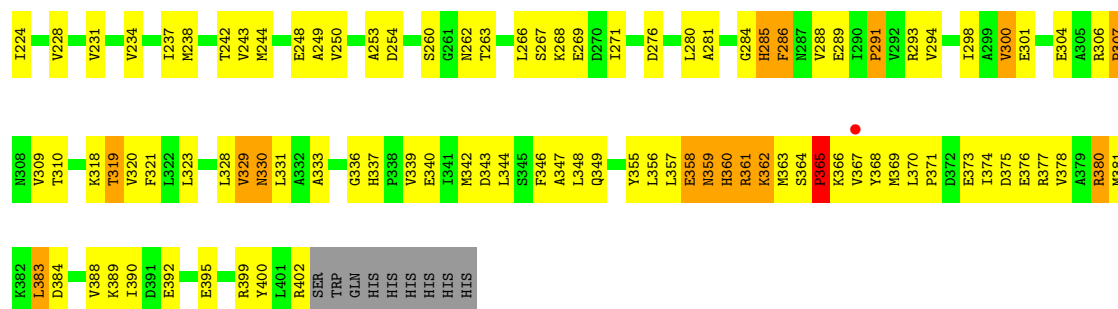


| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |
| 2   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |

- Molecule 3 is water.

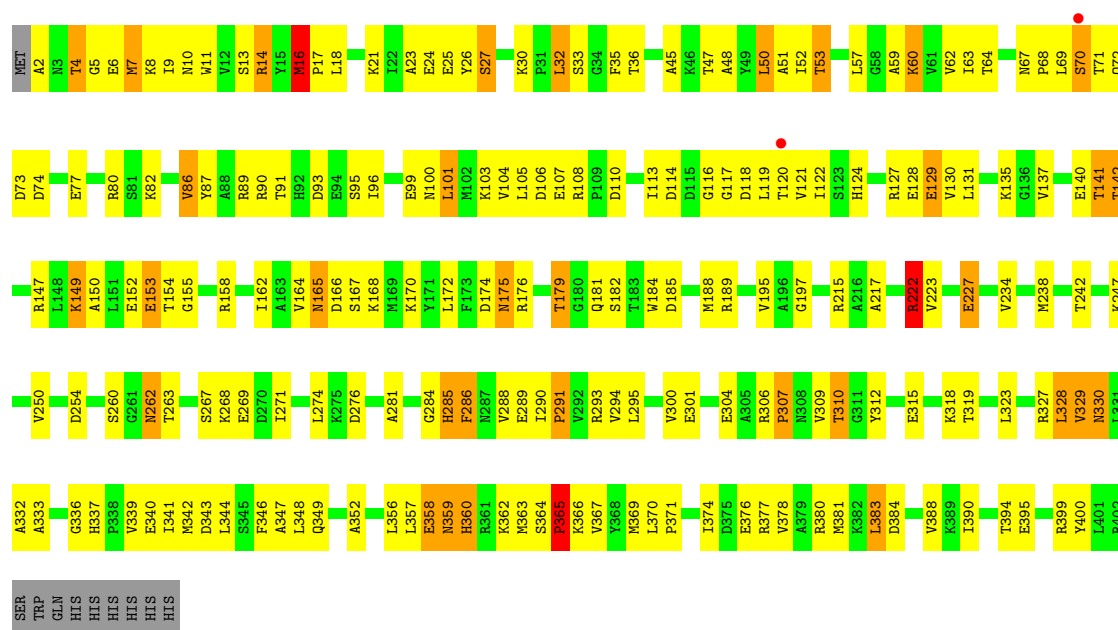
| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | A     | 89       | Total<br>89 | O<br>89 | 0       | 0       |
| 3   | B     | 98       | Total<br>98 | O<br>98 | 0       | 0       |
| 3   | C     | 75       | Total<br>75 | O<br>75 | 0       | 0       |
| 3   | D     | 91       | Total<br>91 | O<br>91 | 0       | 0       |





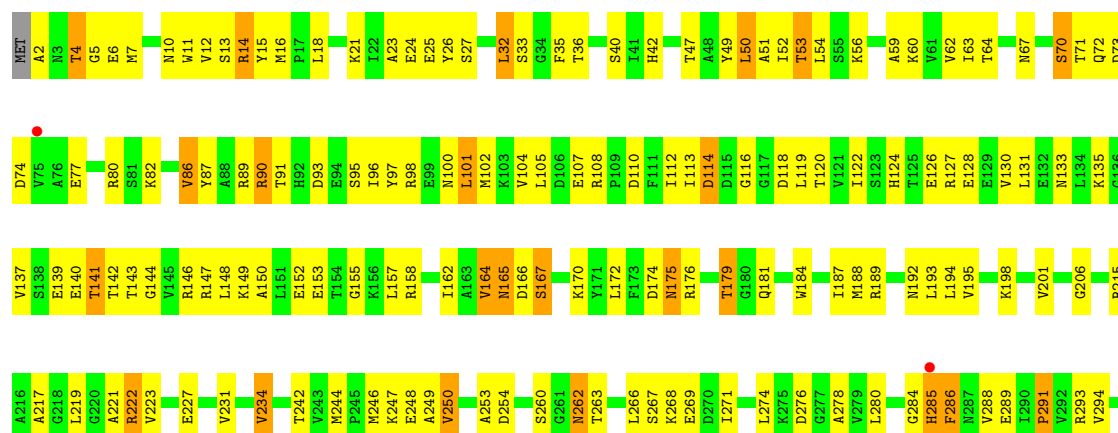
• Molecule 1: Adenosylhomocysteinase

Chain C: 48% 41% 8% ..



• Molecule 1: Adenosylhomocysteinase

Chain D: 46% 43% 9% .





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 106.33Å 112.00Å 164.89Å<br>90.00° 103.50° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 25.00 – 2.85<br>25.00 – 2.85                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (25.00-2.85)<br>93.0 (25.00-2.85)           | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.22 (at 2.84Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.229 , 0.282<br>0.230 , 0.283                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2043 reflections (5.01%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 54.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.856                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 64.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 12993                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 78.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0846e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 1   | A     | 0.55         | 0/3161  | 1.07        | 21/4273 (0.5%)  |
| 1   | B     | 0.61         | 0/3161  | 1.10        | 22/4273 (0.5%)  |
| 1   | C     | 0.55         | 0/3161  | 1.07        | 22/4273 (0.5%)  |
| 1   | D     | 0.60         | 0/3161  | 1.08        | 18/4273 (0.4%)  |
| All | All   | 0.58         | 0/12644 | 1.08        | 83/17092 (0.5%) |

There are no bond length outliers.

All (83) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 329 | VAL  | N-CA-C | 9.25  | 120.06      | 110.62   |
| 1   | C     | 329 | VAL  | N-CA-C | 8.73  | 120.57      | 110.62   |
| 1   | A     | 329 | VAL  | N-CA-C | 8.50  | 120.31      | 110.62   |
| 1   | B     | 329 | VAL  | N-CA-C | 8.29  | 120.07      | 110.62   |
| 1   | B     | 254 | ASP  | N-CA-C | -8.01 | 104.02      | 113.88   |
| 1   | D     | 217 | ALA  | N-CA-C | -7.60 | 103.08      | 111.36   |
| 1   | C     | 222 | ARG  | N-CA-C | -7.22 | 97.48       | 108.96   |
| 1   | C     | 254 | ASP  | N-CA-C | -6.91 | 105.38      | 113.88   |
| 1   | A     | 222 | ARG  | N-CA-C | -6.84 | 98.09       | 108.96   |
| 1   | D     | 222 | ARG  | N-CA-C | -6.82 | 98.12       | 108.96   |
| 1   | D     | 4   | THR  | N-CA-C | -6.79 | 103.65      | 112.68   |
| 1   | B     | 175 | ASN  | N-CA-C | 6.75  | 118.64      | 111.28   |
| 1   | A     | 254 | ASP  | N-CA-C | -6.74 | 105.19      | 113.41   |
| 1   | D     | 254 | ASP  | N-CA-C | -6.73 | 105.20      | 113.41   |
| 1   | B     | 143 | THR  | N-CA-C | -6.71 | 103.89      | 111.07   |
| 1   | C     | 175 | ASN  | N-CA-C | 6.52  | 118.38      | 111.28   |
| 1   | C     | 101 | LEU  | N-CA-C | -6.44 | 104.26      | 111.28   |
| 1   | D     | 175 | ASN  | N-CA-C | 6.40  | 118.25      | 111.28   |
| 1   | B     | 54  | LEU  | N-CA-C | -6.32 | 104.31      | 111.14   |
| 1   | A     | 16  | MET  | CA-C-N | 6.22  | 125.71      | 119.24   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 16  | MET  | C-N-CA | 6.22  | 125.71      | 119.24   |
| 1   | A     | 336 | GLY  | N-CA-C | -6.19 | 101.44      | 112.22   |
| 1   | C     | 4   | THR  | N-CA-C | -6.19 | 104.45      | 112.68   |
| 1   | B     | 217 | ALA  | N-CA-C | -6.17 | 104.61      | 111.71   |
| 1   | A     | 4   | THR  | N-CA-C | -6.11 | 104.55      | 112.68   |
| 1   | D     | 101 | LEU  | N-CA-C | -6.08 | 104.66      | 111.28   |
| 1   | C     | 290 | ILE  | N-CA-C | -6.07 | 100.97      | 107.77   |
| 1   | B     | 339 | VAL  | N-CA-C | 6.05  | 116.72      | 110.36   |
| 1   | B     | 222 | ARG  | N-CA-C | -5.99 | 98.77       | 108.41   |
| 1   | A     | 175 | ASN  | N-CA-C | 5.97  | 117.79      | 111.28   |
| 1   | B     | 4   | THR  | N-CA-C | -5.89 | 104.84      | 112.68   |
| 1   | A     | 149 | LYS  | N-CA-C | -5.89 | 106.13      | 113.55   |
| 1   | B     | 113 | ILE  | N-CA-C | -5.87 | 98.52       | 106.85   |
| 1   | A     | 217 | ALA  | N-CA-C | -5.86 | 104.89      | 111.28   |
| 1   | D     | 142 | THR  | N-CA-C | -5.78 | 105.49      | 113.18   |
| 1   | C     | 142 | THR  | N-CA-C | -5.78 | 105.50      | 113.18   |
| 1   | C     | 336 | GLY  | N-CA-C | -5.77 | 102.18      | 112.22   |
| 1   | B     | 92  | HIS  | N-CA-C | -5.70 | 106.36      | 113.55   |
| 1   | C     | 167 | SER  | N-CA-C | -5.70 | 99.86       | 108.46   |
| 1   | A     | 290 | ILE  | N-CA-C | -5.68 | 102.03      | 107.76   |
| 1   | C     | 114 | ASP  | N-CA-C | 5.68  | 117.86      | 109.69   |
| 1   | C     | 25  | GLU  | N-CA-C | -5.66 | 104.24      | 113.19   |
| 1   | A     | 114 | ASP  | N-CA-C | 5.65  | 118.46      | 109.81   |
| 1   | B     | 150 | ALA  | N-CA-C | -5.65 | 105.21      | 111.71   |
| 1   | C     | 113 | ILE  | N-CA-C | -5.63 | 98.86       | 106.85   |
| 1   | B     | 142 | THR  | N-CA-C | -5.61 | 105.72      | 113.18   |
| 1   | A     | 30  | LYS  | CA-C-N | 5.60  | 125.69      | 119.87   |
| 1   | A     | 30  | LYS  | C-N-CA | 5.60  | 125.69      | 119.87   |
| 1   | D     | 339 | VAL  | N-CA-C | 5.59  | 116.05      | 110.23   |
| 1   | D     | 336 | GLY  | N-CA-C | -5.59 | 102.50      | 112.22   |
| 1   | D     | 50  | LEU  | N-CA-C | -5.56 | 105.14      | 111.14   |
| 1   | A     | 142 | THR  | N-CA-C | -5.55 | 105.80      | 113.18   |
| 1   | D     | 114 | ASP  | N-CA-C | 5.55  | 118.30      | 109.81   |
| 1   | C     | 50  | LEU  | N-CA-C | -5.54 | 105.15      | 111.14   |
| 1   | C     | 339 | VAL  | N-CA-C | 5.54  | 116.17      | 110.36   |
| 1   | B     | 167 | SER  | N-CA-C | -5.52 | 100.13      | 108.46   |
| 1   | A     | 223 | VAL  | N-CA-C | 5.51  | 116.51      | 108.58   |
| 1   | C     | 223 | VAL  | N-CA-C | 5.50  | 116.22      | 108.36   |
| 1   | D     | 113 | ILE  | N-CA-C | -5.49 | 99.06       | 106.85   |
| 1   | A     | 265 | VAL  | N-CA-C | -5.48 | 105.87      | 113.00   |
| 1   | B     | 13  | SER  | N-CA-C | 5.45  | 117.93      | 111.33   |
| 1   | A     | 167 | SER  | N-CA-C | -5.42 | 100.27      | 108.46   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 114 | ASP  | N-CA-C | 5.42  | 117.49      | 109.69   |
| 1   | C     | 16  | MET  | CA-C-N | 5.41  | 124.86      | 119.24   |
| 1   | C     | 16  | MET  | C-N-CA | 5.41  | 124.86      | 119.24   |
| 1   | A     | 143 | THR  | N-CA-C | -5.35 | 105.35      | 111.07   |
| 1   | C     | 149 | LYS  | N-CA-C | -5.34 | 106.44      | 113.12   |
| 1   | D     | 223 | VAL  | N-CA-C | 5.34  | 116.27      | 108.58   |
| 1   | D     | 167 | SER  | N-CA-C | -5.34 | 100.40      | 108.46   |
| 1   | B     | 149 | LYS  | N-CA-C | -5.30 | 106.50      | 113.12   |
| 1   | B     | 101 | LEU  | N-CA-C | -5.29 | 105.51      | 111.28   |
| 1   | C     | 30  | LYS  | CA-C-N | 5.28  | 125.36      | 119.87   |
| 1   | C     | 30  | LYS  | C-N-CA | 5.28  | 125.36      | 119.87   |
| 1   | C     | 217 | ALA  | N-CA-C | -5.27 | 105.53      | 111.28   |
| 1   | D     | 187 | ILE  | N-CA-C | 5.27  | 116.05      | 110.72   |
| 1   | B     | 5   | GLY  | N-CA-C | -5.24 | 107.29      | 113.99   |
| 1   | D     | 54  | LEU  | N-CA-C | -5.11 | 105.71      | 111.28   |
| 1   | B     | 25  | GLU  | N-CA-C | -5.09 | 105.15      | 113.19   |
| 1   | B     | 336 | GLY  | N-CA-C | -5.08 | 101.13      | 113.18   |
| 1   | D     | 25  | GLU  | N-CA-C | -5.07 | 105.17      | 113.19   |
| 1   | A     | 173 | PHE  | N-CA-C | 5.07  | 116.89      | 111.36   |
| 1   | B     | 187 | ILE  | N-CA-C | 5.05  | 115.77      | 110.62   |
| 1   | A     | 54  | LEU  | N-CA-C | -5.02 | 105.89      | 111.36   |

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     | 3116  | 0        | 3190     | 203     | 0            |
| 1   | B     | 3116  | 0        | 3190     | 212     | 0            |
| 1   | C     | 3116  | 0        | 3190     | 191     | 0            |
| 1   | D     | 3116  | 0        | 3190     | 200     | 0            |
| 2   | A     | 44    | 0        | 27       | 2       | 0            |
| 2   | B     | 44    | 0        | 27       | 2       | 0            |
| 2   | C     | 44    | 0        | 27       | 2       | 0            |
| 2   | D     | 44    | 0        | 27       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | A     | 89    | 0        | 0        | 2       | 0            |
| 3   | B     | 98    | 0        | 0        | 4       | 0            |
| 3   | C     | 75    | 0        | 0        | 3       | 0            |
| 3   | D     | 91    | 0        | 0        | 1       | 0            |
| All | All   | 12993 | 0        | 12868    | 772     | 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 30.

All (772) 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:C:67:ASN:HD22  | 1:C:70:SER:HB2   | 1.09                     | 1.10              |
| 1:C:108:ARG:HH21 | 1:C:129:GLU:HB3  | 1.10                     | 1.07              |
| 1:A:245:PRO:HG2  | 1:B:389:LYS:HE3  | 1.36                     | 1.06              |
| 1:A:67:ASN:HD22  | 1:A:70:SER:HB2   | 1.22                     | 1.00              |
| 1:B:361:ARG:HH11 | 1:B:361:ARG:HB3  | 1.25                     | 0.99              |
| 1:D:67:ASN:HD22  | 1:D:70:SER:HB2   | 1.26                     | 0.99              |
| 1:B:135:LYS:HB3  | 1:B:360:HIS:CE1  | 2.02                     | 0.94              |
| 1:C:108:ARG:NH2  | 1:C:129:GLU:HB3  | 1.85                     | 0.91              |
| 1:C:263:THR:HG22 | 1:C:288:VAL:CG2  | 2.00                     | 0.90              |
| 1:C:116:GLY:H    | 1:C:141:THR:HG21 | 1.36                     | 0.90              |
| 1:B:383:LEU:HD12 | 1:B:388:VAL:HB   | 1.52                     | 0.89              |
| 1:A:371:PRO:HB2  | 1:A:373:GLU:CD   | 1.97                     | 0.89              |
| 1:C:87:TYR:HB3   | 1:C:100:ASN:HD22 | 1.37                     | 0.87              |
| 1:A:67:ASN:O     | 1:A:71:THR:HG23  | 1.75                     | 0.86              |
| 1:B:120:THR:HG21 | 1:B:137:VAL:HG11 | 1.56                     | 0.86              |
| 1:C:108:ARG:HG2  | 1:C:130:VAL:HG12 | 1.57                     | 0.86              |
| 1:A:90:ARG:HH11  | 1:A:90:ARG:HB3   | 1.38                     | 0.86              |
| 1:C:165:ASN:HD22 | 1:C:166:ASP:N    | 1.74                     | 0.85              |
| 1:B:165:ASN:HD22 | 1:B:166:ASP:N    | 1.75                     | 0.85              |
| 1:A:348:LEU:HD23 | 1:A:378:VAL:HG21 | 1.57                     | 0.85              |
| 1:A:181:GLN:HE22 | 1:C:195:VAL:H    | 1.24                     | 0.85              |
| 1:D:285:HIS:CG   | 1:D:286:PHE:H    | 1.92                     | 0.85              |
| 1:A:90:ARG:HB3   | 1:A:90:ARG:NH1   | 1.92                     | 0.84              |
| 1:B:116:GLY:H    | 1:B:141:THR:HG21 | 1.40                     | 0.84              |
| 1:B:101:LEU:HD22 | 1:B:119:LEU:HD13 | 1.59                     | 0.84              |
| 1:A:165:ASN:HD22 | 1:A:166:ASP:N    | 1.75                     | 0.83              |
| 1:C:120:THR:HG21 | 1:C:137:VAL:HG11 | 1.57                     | 0.83              |
| 1:A:383:LEU:HD12 | 1:A:388:VAL:HB   | 1.57                     | 0.83              |
| 1:A:152:GLU:OE2  | 1:A:366:LYS:HG3  | 1.79                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:184:TRP:O    | 1:B:188:MET:HG2  | 1.80                     | 0.81              |
| 1:B:268:LYS:NZ   | 1:B:298:ILE:HD11 | 1.95                     | 0.81              |
| 1:C:7:MET:HG3    | 3:C:662:HOH:O    | 1.79                     | 0.81              |
| 1:B:152:GLU:OE2  | 1:B:366:LYS:HG3  | 1.81                     | 0.81              |
| 1:A:120:THR:HG21 | 1:A:137:VAL:HG11 | 1.62                     | 0.81              |
| 1:C:35:PHE:HA    | 1:C:110:ASP:OD2  | 1.81                     | 0.80              |
| 1:D:4:THR:HA     | 1:D:7:MET:HE2    | 1.60                     | 0.80              |
| 1:D:165:ASN:HD22 | 1:D:166:ASP:N    | 1.79                     | 0.80              |
| 1:C:101:LEU:HD22 | 1:C:119:LEU:HD13 | 1.62                     | 0.80              |
| 1:C:276:ASP:OD2  | 1:C:318:LYS:HA   | 1.82                     | 0.79              |
| 1:D:67:ASN:O     | 1:D:71:THR:HG23  | 1.82                     | 0.79              |
| 1:A:102:MET:HG3  | 1:A:127:ARG:HH11 | 1.48                     | 0.78              |
| 1:D:174:ASP:O    | 1:D:179:THR:HG22 | 1.83                     | 0.78              |
| 1:B:300:VAL:HG12 | 1:B:301:GLU:HG3  | 1.64                     | 0.78              |
| 1:A:116:GLY:H    | 1:A:141:THR:HG21 | 1.49                     | 0.78              |
| 1:D:87:TYR:HB3   | 1:D:100:ASN:HD22 | 1.45                     | 0.78              |
| 1:C:140:GLU:HB2  | 1:C:349:GLN:HE21 | 1.47                     | 0.78              |
| 1:A:135:LYS:HB3  | 1:A:360:HIS:NE2  | 1.99                     | 0.78              |
| 1:B:263:THR:HG22 | 1:B:288:VAL:CG2  | 2.13                     | 0.78              |
| 1:D:330:ASN:H    | 1:D:330:ASN:HD22 | 1.30                     | 0.78              |
| 1:A:89:ARG:HH11  | 1:A:89:ARG:HG2   | 1.49                     | 0.77              |
| 1:A:174:ASP:O    | 1:A:179:THR:HG22 | 1.83                     | 0.77              |
| 1:B:181:GLN:HE22 | 1:D:195:VAL:H    | 1.32                     | 0.77              |
| 1:C:348:LEU:HD23 | 1:C:378:VAL:HG21 | 1.65                     | 0.77              |
| 1:C:152:GLU:OE1  | 1:C:367:VAL:HG12 | 1.84                     | 0.77              |
| 1:A:189:ARG:HA   | 1:C:189:ARG:NH2  | 1.99                     | 0.77              |
| 1:C:184:TRP:O    | 1:C:188:MET:HG2  | 1.85                     | 0.77              |
| 1:B:361:ARG:HG2  | 3:B:673:HOH:O    | 1.82                     | 0.77              |
| 1:D:116:GLY:H    | 1:D:141:THR:HG21 | 1.49                     | 0.77              |
| 1:D:263:THR:HG22 | 1:D:288:VAL:CG2  | 2.15                     | 0.77              |
| 1:A:135:LYS:HB3  | 1:A:360:HIS:CE1  | 2.19                     | 0.77              |
| 1:A:67:ASN:HD22  | 1:A:70:SER:CB    | 1.98                     | 0.77              |
| 1:D:139:GLU:OE2  | 1:D:144:GLY:HA3  | 1.85                     | 0.77              |
| 1:D:62:VAL:HG12  | 1:D:104:VAL:HG12 | 1.66                     | 0.76              |
| 1:C:131:LEU:O    | 1:C:131:LEU:HD23 | 1.84                     | 0.76              |
| 1:D:268:LYS:NZ   | 1:D:298:ILE:HD11 | 2.00                     | 0.76              |
| 1:D:348:LEU:HD23 | 1:D:378:VAL:HG21 | 1.67                     | 0.76              |
| 1:B:359:ASN:N    | 1:B:359:ASN:HD22 | 1.84                     | 0.76              |
| 1:B:101:LEU:O    | 1:B:104:VAL:HG22 | 1.84                     | 0.75              |
| 1:A:80:ARG:HE    | 1:A:86:VAL:HG13  | 1.52                     | 0.75              |
| 1:C:36:THR:HG22  | 1:C:60:LYS:HB2   | 1.68                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:195:VAL:H    | 1:C:181:GLN:HE22 | 1.33                     | 0.74              |
| 1:D:108:ARG:HG2  | 1:D:130:VAL:HG12 | 1.69                     | 0.74              |
| 1:D:276:ASP:OD2  | 1:D:318:LYS:HA   | 1.86                     | 0.74              |
| 1:A:101:LEU:HD22 | 1:A:119:LEU:HD13 | 1.70                     | 0.74              |
| 1:C:32:LEU:HD23  | 1:C:59:ALA:HB2   | 1.70                     | 0.74              |
| 1:D:135:LYS:HB3  | 1:D:360:HIS:CE1  | 2.23                     | 0.74              |
| 1:A:285:HIS:CG   | 1:A:286:PHE:H    | 2.05                     | 0.73              |
| 1:C:285:HIS:CG   | 1:C:286:PHE:H    | 2.06                     | 0.73              |
| 1:D:118:ASP:HA   | 1:D:147:ARG:HH22 | 1.54                     | 0.73              |
| 1:D:131:LEU:HD23 | 1:D:131:LEU:O    | 1.87                     | 0.73              |
| 1:C:263:THR:HG22 | 1:C:288:VAL:HG23 | 1.69                     | 0.73              |
| 1:B:285:HIS:CG   | 1:B:286:PHE:H    | 2.06                     | 0.73              |
| 1:C:67:ASN:ND2   | 1:C:70:SER:HB2   | 1.95                     | 0.73              |
| 1:A:101:LEU:O    | 1:A:104:VAL:HG22 | 1.87                     | 0.72              |
| 1:A:87:TYR:HB3   | 1:A:100:ASN:HD22 | 1.53                     | 0.72              |
| 1:C:174:ASP:O    | 1:C:179:THR:HG22 | 1.89                     | 0.72              |
| 1:D:35:PHE:HA    | 1:D:110:ASP:OD2  | 1.87                     | 0.72              |
| 1:D:67:ASN:HD22  | 1:D:70:SER:CB    | 2.01                     | 0.72              |
| 1:C:263:THR:HG22 | 1:C:288:VAL:HG21 | 1.71                     | 0.72              |
| 1:C:67:ASN:O     | 1:C:71:THR:HG23  | 1.89                     | 0.72              |
| 1:C:89:ARG:C     | 1:C:91:THR:H     | 1.98                     | 0.71              |
| 1:D:120:THR:HG21 | 1:D:137:VAL:HG11 | 1.71                     | 0.71              |
| 1:A:195:VAL:H    | 1:C:181:GLN:NE2  | 1.86                     | 0.71              |
| 1:D:89:ARG:C     | 1:D:91:THR:H     | 1.97                     | 0.71              |
| 1:B:281:ALA:HB2  | 1:B:323:LEU:HD12 | 1.72                     | 0.71              |
| 1:C:149:LYS:HG2  | 1:C:367:VAL:HG11 | 1.72                     | 0.71              |
| 1:D:101:LEU:HD22 | 1:D:119:LEU:HD13 | 1.72                     | 0.71              |
| 1:B:402:ARG:O    | 3:B:668:HOH:O    | 2.08                     | 0.70              |
| 1:A:371:PRO:HG2  | 1:A:374:ILE:HG13 | 1.73                     | 0.70              |
| 1:B:121:VAL:HG11 | 1:B:147:ARG:NH2  | 2.06                     | 0.70              |
| 1:A:108:ARG:HG2  | 1:A:130:VAL:HG12 | 1.73                     | 0.70              |
| 1:A:89:ARG:C     | 1:A:91:THR:H     | 1.97                     | 0.70              |
| 1:A:32:LEU:HD23  | 1:A:59:ALA:HB2   | 1.74                     | 0.70              |
| 1:A:73:ASP:OD1   | 1:A:90:ARG:NH2   | 2.25                     | 0.69              |
| 1:B:32:LEU:HD23  | 1:B:59:ALA:HB2   | 1.74                     | 0.69              |
| 1:D:101:LEU:O    | 1:D:104:VAL:HG22 | 1.92                     | 0.69              |
| 1:A:35:PHE:HA    | 1:A:110:ASP:OD2  | 1.92                     | 0.69              |
| 1:B:197:GLY:HA3  | 1:C:238:MET:HE2  | 1.73                     | 0.69              |
| 1:A:90:ARG:HH11  | 1:A:90:ARG:CB    | 2.06                     | 0.69              |
| 1:C:135:LYS:HB3  | 1:C:360:HIS:CE1  | 2.27                     | 0.69              |
| 1:B:135:LYS:HB3  | 1:B:360:HIS:NE2  | 2.08                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:135:LYS:HB3  | 1:D:360:HIS:NE2  | 2.07                     | 0.69              |
| 1:C:371:PRO:HG2  | 1:C:374:ILE:HG13 | 1.74                     | 0.68              |
| 1:D:383:LEU:HD12 | 1:D:388:VAL:HB   | 1.75                     | 0.68              |
| 1:A:181:GLN:HE22 | 1:C:195:VAL:N    | 1.90                     | 0.68              |
| 1:B:361:ARG:HB3  | 1:B:361:ARG:NH1  | 2.05                     | 0.68              |
| 1:C:383:LEU:HD12 | 1:C:388:VAL:HB   | 1.76                     | 0.68              |
| 1:B:318:LYS:HZ2  | 1:B:318:LYS:HB2  | 1.58                     | 0.68              |
| 1:A:359:ASN:N    | 1:A:359:ASN:HD22 | 1.91                     | 0.68              |
| 1:B:165:ASN:ND2  | 1:B:166:ASP:N    | 2.40                     | 0.68              |
| 1:D:149:LYS:HG2  | 1:D:367:VAL:HG11 | 1.76                     | 0.68              |
| 1:B:268:LYS:HZ2  | 1:B:298:ILE:HD11 | 1.56                     | 0.68              |
| 1:B:380:ARG:HD3  | 3:B:675:HOH:O    | 1.93                     | 0.68              |
| 1:C:135:LYS:HB3  | 1:C:360:HIS:NE2  | 2.08                     | 0.68              |
| 1:A:310:THR:HG22 | 3:A:642:HOH:O    | 1.94                     | 0.67              |
| 1:B:34:GLY:H     | 1:B:60:LYS:HZ1   | 1.40                     | 0.67              |
| 1:A:300:VAL:HG12 | 1:A:301:GLU:HG3  | 1.74                     | 0.67              |
| 1:C:158:ARG:NH1  | 1:C:158:ARG:HB2  | 2.10                     | 0.67              |
| 1:A:288:VAL:HG12 | 1:A:293:ARG:HH22 | 1.60                     | 0.67              |
| 1:B:174:ASP:O    | 1:B:179:THR:HG22 | 1.94                     | 0.67              |
| 1:A:67:ASN:ND2   | 1:A:70:SER:HB2   | 2.05                     | 0.67              |
| 1:A:181:GLN:NE2  | 1:C:195:VAL:H    | 1.92                     | 0.67              |
| 1:A:36:THR:HG22  | 1:A:60:LYS:HB2   | 1.76                     | 0.66              |
| 1:D:263:THR:HG22 | 1:D:288:VAL:HG23 | 1.77                     | 0.66              |
| 1:A:194:LEU:O    | 1:A:198:LYS:HD2  | 1.95                     | 0.66              |
| 1:A:185:ASP:O    | 1:A:189:ARG:HG2  | 1.96                     | 0.66              |
| 1:B:276:ASP:OD2  | 1:B:318:LYS:HA   | 1.94                     | 0.66              |
| 1:D:359:ASN:N    | 1:D:359:ASN:HD22 | 1.93                     | 0.66              |
| 1:A:263:THR:HG22 | 1:A:288:VAL:CG2  | 2.26                     | 0.66              |
| 1:A:102:MET:HG3  | 1:A:127:ARG:NH1  | 2.11                     | 0.66              |
| 1:B:364:SER:O    | 1:B:366:LYS:N    | 2.29                     | 0.66              |
| 1:D:371:PRO:HG2  | 1:D:374:ILE:HG13 | 1.76                     | 0.66              |
| 1:B:371:PRO:HG2  | 1:B:374:ILE:HG13 | 1.78                     | 0.66              |
| 1:C:162:ILE:HG13 | 1:C:356:LEU:HD21 | 1.78                     | 0.66              |
| 1:A:330:ASN:H    | 1:A:330:ASN:HD22 | 1.44                     | 0.65              |
| 1:B:356:LEU:CD2  | 1:B:363:MET:HE1  | 2.26                     | 0.65              |
| 1:D:158:ARG:HB2  | 1:D:158:ARG:NH1  | 2.11                     | 0.65              |
| 1:B:162:ILE:HG13 | 1:B:356:LEU:HD21 | 1.79                     | 0.65              |
| 1:A:131:LEU:O    | 1:A:131:LEU:HD23 | 1.96                     | 0.65              |
| 1:B:222:ARG:HH12 | 1:C:222:ARG:NH1  | 1.94                     | 0.65              |
| 1:B:87:TYR:HB3   | 1:B:100:ASN:HD22 | 1.62                     | 0.65              |
| 1:B:101:LEU:HD22 | 1:B:119:LEU:CD1  | 2.27                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:121:VAL:HG11 | 1:C:147:ARG:NH2  | 2.12                     | 0.65              |
| 1:C:359:ASN:HD22 | 1:C:359:ASN:N    | 1.94                     | 0.64              |
| 1:A:16:MET:HB3   | 1:A:343:ASP:OD1  | 1.96                     | 0.64              |
| 1:A:168:LYS:HG2  | 1:A:172:LEU:HD13 | 1.79                     | 0.64              |
| 1:B:195:VAL:H    | 1:D:181:GLN:NE2  | 1.95                     | 0.64              |
| 1:C:165:ASN:ND2  | 1:C:166:ASP:N    | 2.46                     | 0.64              |
| 1:D:50:LEU:HD22  | 1:D:346:PHE:CD1  | 2.33                     | 0.64              |
| 1:D:91:THR:C     | 1:D:93:ASP:H     | 2.05                     | 0.64              |
| 1:A:165:ASN:ND2  | 1:A:166:ASP:N    | 2.46                     | 0.64              |
| 1:B:348:LEU:HD23 | 1:B:378:VAL:HG21 | 1.79                     | 0.64              |
| 1:B:35:PHE:HD1   | 1:B:110:ASP:OD2  | 1.81                     | 0.63              |
| 1:B:165:ASN:HD22 | 1:B:166:ASP:H    | 1.47                     | 0.63              |
| 1:C:300:VAL:HG12 | 1:C:301:GLU:HG3  | 1.81                     | 0.63              |
| 1:B:2:ALA:O      | 1:B:6:GLU:HB2    | 1.99                     | 0.63              |
| 1:A:195:VAL:N    | 1:C:181:GLN:HE22 | 1.97                     | 0.62              |
| 1:B:131:LEU:HD23 | 1:B:131:LEU:O    | 1.99                     | 0.62              |
| 1:D:102:MET:HG3  | 1:D:127:ARG:HH11 | 1.64                     | 0.62              |
| 1:C:101:LEU:O    | 1:C:104:VAL:HG22 | 2.00                     | 0.62              |
| 1:A:168:LYS:O    | 1:A:172:LEU:HD13 | 1.99                     | 0.62              |
| 1:B:359:ASN:O    | 1:B:363:MET:HG3  | 2.00                     | 0.62              |
| 1:C:91:THR:C     | 1:C:93:ASP:H     | 2.07                     | 0.62              |
| 1:D:194:LEU:O    | 1:D:198:LYS:HD2  | 1.99                     | 0.62              |
| 1:B:120:THR:HG21 | 1:B:137:VAL:CG1  | 2.28                     | 0.62              |
| 1:D:32:LEU:HD23  | 1:D:59:ALA:HB2   | 1.82                     | 0.62              |
| 1:B:136:GLY:HA3  | 1:B:356:LEU:HD13 | 1.81                     | 0.62              |
| 1:B:238:MET:HE2  | 1:C:197:GLY:HA3  | 1.82                     | 0.62              |
| 1:D:285:HIS:CD2  | 1:D:286:PHE:H    | 2.17                     | 0.61              |
| 1:D:184:TRP:O    | 1:D:188:MET:HG2  | 2.01                     | 0.61              |
| 1:A:99:GLU:HG3   | 1:A:103:LYS:NZ   | 2.15                     | 0.61              |
| 1:C:364:SER:O    | 1:C:366:LYS:N    | 2.33                     | 0.61              |
| 1:D:40:SER:HG    | 1:D:97:TYR:HH    | 1.48                     | 0.61              |
| 1:B:175:ASN:O    | 1:B:179:THR:CG2  | 2.49                     | 0.61              |
| 1:C:7:MET:HE2    | 1:C:10:ASN:HD22  | 1.65                     | 0.61              |
| 1:D:23:ALA:O     | 1:D:27:SER:HB2   | 2.00                     | 0.61              |
| 1:A:91:THR:C     | 1:A:93:ASP:H     | 2.09                     | 0.61              |
| 1:D:105:LEU:HD22 | 1:D:130:VAL:HG21 | 1.83                     | 0.61              |
| 1:D:364:SER:O    | 1:D:366:LYS:N    | 2.34                     | 0.61              |
| 1:C:16:MET:HE2   | 1:C:343:ASP:CA   | 2.31                     | 0.60              |
| 1:C:185:ASP:O    | 1:C:189:ARG:HG2  | 2.00                     | 0.60              |
| 1:D:374:ILE:O    | 1:D:378:VAL:HG23 | 2.02                     | 0.60              |
| 1:C:327:ARG:NH2  | 1:C:332:ALA:HB1  | 2.16                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:172:LEU:O    | 1:A:176:ARG:HB3  | 2.01                     | 0.60              |
| 1:A:101:LEU:HD22 | 1:A:119:LEU:CD1  | 2.32                     | 0.60              |
| 1:A:23:ALA:O     | 1:A:27:SER:HB2   | 2.02                     | 0.60              |
| 1:C:140:GLU:HB2  | 1:C:349:GLN:NE2  | 2.17                     | 0.60              |
| 1:A:120:THR:HG21 | 1:A:137:VAL:CG1  | 2.29                     | 0.59              |
| 1:B:263:THR:HG22 | 1:B:288:VAL:HG23 | 1.84                     | 0.59              |
| 1:C:175:ASN:O    | 1:C:179:THR:HG23 | 2.02                     | 0.59              |
| 1:D:110:ASP:HB3  | 1:D:135:LYS:HD2  | 1.84                     | 0.59              |
| 1:C:260:SER:O    | 1:C:289:GLU:CD   | 2.45                     | 0.59              |
| 1:A:260:SER:O    | 1:A:289:GLU:CD   | 2.46                     | 0.59              |
| 1:B:175:ASN:O    | 1:B:179:THR:HG23 | 2.01                     | 0.59              |
| 1:B:267:SER:O    | 1:B:271:ILE:HG13 | 2.02                     | 0.59              |
| 1:B:330:ASN:HD22 | 1:B:330:ASN:H    | 1.49                     | 0.59              |
| 1:D:170:LYS:HG2  | 1:D:348:LEU:CD1  | 2.32                     | 0.59              |
| 1:D:36:THR:HG22  | 1:D:60:LYS:HB2   | 1.84                     | 0.59              |
| 1:D:140:GLU:HB2  | 1:D:349:GLN:NE2  | 2.18                     | 0.59              |
| 1:A:118:ASP:O    | 1:A:122:ILE:HG12 | 2.02                     | 0.59              |
| 1:C:120:THR:HG21 | 1:C:137:VAL:CG1  | 2.31                     | 0.59              |
| 1:A:364:SER:O    | 1:A:366:LYS:N    | 2.36                     | 0.59              |
| 1:B:194:LEU:O    | 1:B:198:LYS:HD2  | 2.03                     | 0.59              |
| 1:B:195:VAL:H    | 1:D:181:GLN:HE22 | 1.49                     | 0.59              |
| 1:C:172:LEU:O    | 1:C:176:ARG:HB3  | 2.02                     | 0.58              |
| 1:C:131:LEU:HD11 | 1:C:158:ARG:HH12 | 1.69                     | 0.58              |
| 1:C:394:THR:HG22 | 3:C:648:HOH:O    | 2.04                     | 0.58              |
| 1:C:260:SER:O    | 1:C:289:GLU:OE2  | 2.22                     | 0.58              |
| 1:A:315:GLU:H    | 1:A:315:GLU:CD   | 2.10                     | 0.58              |
| 1:A:62:VAL:HG12  | 1:A:104:VAL:HG12 | 1.86                     | 0.58              |
| 1:C:165:ASN:HD22 | 1:C:166:ASP:H    | 1.52                     | 0.58              |
| 1:A:128:GLU:HA   | 1:A:131:LEU:HB2  | 1.86                     | 0.58              |
| 1:A:288:VAL:HG12 | 1:A:293:ARG:NH2  | 2.18                     | 0.58              |
| 1:B:222:ARG:NH1  | 1:C:222:ARG:NH1  | 2.52                     | 0.58              |
| 1:C:2:ALA:O      | 1:C:6:GLU:HB2    | 2.04                     | 0.58              |
| 1:D:149:LYS:HZ3  | 1:D:367:VAL:HG13 | 1.69                     | 0.58              |
| 1:D:51:ALA:CB    | 1:D:63:ILE:HD11  | 2.33                     | 0.58              |
| 1:D:73:ASP:O     | 1:D:77:GLU:HG2   | 2.03                     | 0.58              |
| 1:A:165:ASN:ND2  | 1:A:165:ASN:C    | 2.61                     | 0.58              |
| 1:B:23:ALA:O     | 1:B:27:SER:HB2   | 2.04                     | 0.58              |
| 1:D:165:ASN:ND2  | 1:D:166:ASP:N    | 2.50                     | 0.58              |
| 1:B:118:ASP:O    | 1:B:122:ILE:HG12 | 2.04                     | 0.58              |
| 1:B:383:LEU:HD12 | 1:B:388:VAL:CB   | 2.31                     | 0.58              |
| 1:B:268:LYS:HZ3  | 1:B:298:ILE:HD11 | 1.67                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:260:SER:O    | 1:A:289:GLU:OE1  | 2.21                     | 0.57              |
| 1:A:80:ARG:NE    | 1:A:86:VAL:HG13  | 2.19                     | 0.57              |
| 1:D:356:LEU:HD23 | 1:D:363:MET:HE1  | 1.85                     | 0.57              |
| 1:C:118:ASP:O    | 1:C:122:ILE:HG12 | 2.04                     | 0.57              |
| 1:C:158:ARG:HB2  | 1:C:158:ARG:HH11 | 1.69                     | 0.57              |
| 1:A:276:ASP:OD2  | 1:A:318:LYS:HA   | 2.05                     | 0.57              |
| 1:B:280:LEU:HD11 | 1:B:320:VAL:HG11 | 1.87                     | 0.57              |
| 1:C:267:SER:OG   | 1:C:269:GLU:HB2  | 2.04                     | 0.57              |
| 1:B:105:LEU:C    | 1:B:107:GLU:H    | 2.13                     | 0.57              |
| 1:D:263:THR:HG22 | 1:D:288:VAL:HG21 | 1.85                     | 0.57              |
| 1:C:135:LYS:HD3  | 1:C:360:HIS:NE2  | 2.20                     | 0.57              |
| 1:A:89:ARG:HG2   | 1:A:89:ARG:NH1   | 2.17                     | 0.56              |
| 1:A:108:ARG:CG   | 1:A:130:VAL:HG12 | 2.34                     | 0.56              |
| 1:A:285:HIS:CG   | 1:A:286:PHE:N    | 2.73                     | 0.56              |
| 1:B:23:ALA:HB2   | 1:B:53:THR:HG22  | 1.85                     | 0.56              |
| 1:C:51:ALA:CB    | 1:C:63:ILE:HD11  | 2.35                     | 0.56              |
| 1:D:285:HIS:CD2  | 1:D:286:PHE:N    | 2.72                     | 0.56              |
| 1:A:165:ASN:HD22 | 1:A:165:ASN:C    | 2.12                     | 0.56              |
| 1:A:184:TRP:O    | 1:A:188:MET:HG2  | 2.04                     | 0.56              |
| 1:C:164:VAL:O    | 1:C:170:LYS:HG3  | 2.05                     | 0.56              |
| 1:A:39:MET:HE2   | 1:A:41:ILE:HG21  | 1.87                     | 0.56              |
| 1:A:105:LEU:C    | 1:A:107:GLU:H    | 2.13                     | 0.56              |
| 1:D:105:LEU:C    | 1:D:107:GLU:H    | 2.13                     | 0.56              |
| 1:D:152:GLU:OE2  | 1:D:366:LYS:HG3  | 2.06                     | 0.56              |
| 1:D:12:VAL:HG13  | 1:D:16:MET:HE2   | 1.87                     | 0.56              |
| 1:D:158:ARG:HB2  | 1:D:158:ARG:HH11 | 1.70                     | 0.56              |
| 1:A:285:HIS:CD2  | 1:A:286:PHE:H    | 2.24                     | 0.56              |
| 1:B:165:ASN:ND2  | 1:B:165:ASN:C    | 2.62                     | 0.56              |
| 1:C:175:ASN:O    | 1:C:179:THR:CG2  | 2.53                     | 0.56              |
| 1:D:285:HIS:CG   | 1:D:286:PHE:N    | 2.63                     | 0.56              |
| 1:A:371:PRO:HB2  | 1:A:373:GLU:OE1  | 2.05                     | 0.56              |
| 1:D:120:THR:HG21 | 1:D:137:VAL:CG1  | 2.36                     | 0.56              |
| 1:A:263:THR:HG23 | 1:B:400:TYR:CE2  | 2.41                     | 0.56              |
| 1:A:348:LEU:CD2  | 1:A:378:VAL:HG21 | 2.32                     | 0.55              |
| 1:C:105:LEU:C    | 1:C:107:GLU:H    | 2.14                     | 0.55              |
| 1:A:73:ASP:CG    | 1:A:90:ARG:NH2   | 2.64                     | 0.55              |
| 1:A:266:LEU:O    | 1:A:291:PRO:HG3  | 2.06                     | 0.55              |
| 1:D:358:GLU:C    | 1:D:360:HIS:H    | 2.14                     | 0.55              |
| 1:B:185:ASP:O    | 1:B:189:ARG:HG2  | 2.06                     | 0.55              |
| 1:B:267:SER:OG   | 1:B:269:GLU:HB2  | 2.07                     | 0.55              |
| 1:A:2:ALA:O      | 1:A:6:GLU:HB2    | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:23:ALA:O     | 1:C:27:SER:HB2   | 2.06                     | 0.55              |
| 1:C:185:ASP:OD2  | 1:C:189:ARG:NH2  | 2.39                     | 0.55              |
| 1:A:358:GLU:C    | 1:A:360:HIS:H    | 2.14                     | 0.55              |
| 1:A:63:ILE:HG22  | 1:A:64:THR:N     | 2.22                     | 0.55              |
| 1:A:162:ILE:HD11 | 1:A:355:TYR:HD2  | 1.72                     | 0.55              |
| 1:D:2:ALA:O      | 1:D:6:GLU:HB2    | 2.06                     | 0.55              |
| 1:B:284:GLY:HA3  | 1:B:289:GLU:OE2  | 2.07                     | 0.55              |
| 1:B:358:GLU:C    | 1:B:360:HIS:H    | 2.15                     | 0.55              |
| 1:C:17:PRO:HG2   | 1:C:18:LEU:H     | 1.72                     | 0.55              |
| 1:D:67:ASN:ND2   | 1:D:70:SER:HB2   | 2.10                     | 0.55              |
| 1:C:168:LYS:O    | 1:C:172:LEU:HD13 | 2.07                     | 0.54              |
| 1:B:108:ARG:HG3  | 1:B:130:VAL:HG12 | 1.89                     | 0.54              |
| 1:C:89:ARG:O     | 1:C:91:THR:HG23  | 2.06                     | 0.54              |
| 1:D:87:TYR:CB    | 1:D:100:ASN:HD22 | 2.18                     | 0.54              |
| 1:D:330:ASN:HD21 | 2:D:500:NAI:H72N | 1.55                     | 0.54              |
| 1:A:52:ILE:O     | 1:A:56:LYS:HG3   | 2.07                     | 0.54              |
| 1:C:165:ASN:ND2  | 1:C:165:ASN:C    | 2.64                     | 0.54              |
| 1:C:285:HIS:CD2  | 1:C:286:PHE:H    | 2.25                     | 0.54              |
| 1:D:260:SER:O    | 1:D:289:GLU:CD   | 2.51                     | 0.54              |
| 1:A:158:ARG:HA   | 1:A:365:PRO:HB3  | 1.90                     | 0.54              |
| 1:C:358:GLU:C    | 1:C:360:HIS:H    | 2.15                     | 0.54              |
| 1:A:400:TYR:CE2  | 1:B:263:THR:HG23 | 2.43                     | 0.54              |
| 1:B:189:ARG:HA   | 1:D:189:ARG:NH2  | 2.23                     | 0.54              |
| 1:D:89:ARG:C     | 1:D:91:THR:N     | 2.66                     | 0.54              |
| 1:D:89:ARG:HD3   | 1:D:90:ARG:NH1   | 2.23                     | 0.54              |
| 1:A:89:ARG:O     | 1:A:91:THR:HG23  | 2.07                     | 0.53              |
| 1:A:319:THR:HG21 | 1:C:14:ARG:NH2   | 2.23                     | 0.53              |
| 1:B:21:LYS:NZ    | 1:B:384:ASP:HB3  | 2.23                     | 0.53              |
| 1:B:128:GLU:HA   | 1:B:131:LEU:HB2  | 1.90                     | 0.53              |
| 1:B:285:HIS:CG   | 1:B:286:PHE:N    | 2.76                     | 0.53              |
| 1:C:165:ASN:HD22 | 1:C:165:ASN:C    | 2.14                     | 0.53              |
| 1:B:356:LEU:HD23 | 1:B:363:MET:HE1  | 1.89                     | 0.53              |
| 1:C:62:VAL:HG12  | 1:C:104:VAL:HG12 | 1.89                     | 0.53              |
| 1:B:263:THR:HG22 | 1:B:288:VAL:HG21 | 1.90                     | 0.53              |
| 1:D:158:ARG:HA   | 1:D:365:PRO:HB3  | 1.90                     | 0.53              |
| 1:D:152:GLU:OE2  | 1:D:367:VAL:HG12 | 2.08                     | 0.53              |
| 1:C:89:ARG:C     | 1:C:91:THR:N     | 2.67                     | 0.53              |
| 1:A:32:LEU:HD12  | 1:A:357:LEU:HD22 | 1.90                     | 0.53              |
| 1:B:160:PRO:HB2  | 1:B:363:MET:HE3  | 1.91                     | 0.53              |
| 1:A:383:LEU:HD12 | 1:A:388:VAL:CB   | 2.33                     | 0.53              |
| 1:B:133:ASN:O    | 1:B:135:LYS:HG3  | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:168:LYS:HG2  | 1:C:172:LEU:HD13 | 1.91                     | 0.53              |
| 1:D:87:TYR:HB3   | 1:D:100:ASN:ND2  | 2.20                     | 0.53              |
| 1:A:80:ARG:HG3   | 1:A:86:VAL:CG1   | 2.39                     | 0.53              |
| 1:B:285:HIS:CD2  | 1:B:286:PHE:H    | 2.26                     | 0.53              |
| 1:B:121:VAL:HG11 | 1:B:147:ARG:HH22 | 1.74                     | 0.52              |
| 1:C:80:ARG:HG3   | 1:C:86:VAL:CG1   | 2.39                     | 0.52              |
| 1:D:42:HIS:O     | 1:D:47:THR:HG21  | 2.08                     | 0.52              |
| 1:B:116:GLY:H    | 1:B:141:THR:CG2  | 2.17                     | 0.52              |
| 1:B:91:THR:HG21  | 1:B:96:ILE:HG12  | 1.92                     | 0.52              |
| 1:B:370:LEU:HD12 | 1:B:371:PRO:HD2  | 1.91                     | 0.52              |
| 1:C:400:TYR:CE2  | 1:D:263:THR:HG23 | 2.44                     | 0.52              |
| 1:A:268:LYS:HE3  | 1:A:298:ILE:CD1  | 2.40                     | 0.52              |
| 1:B:165:ASN:HD22 | 1:B:165:ASN:C    | 2.17                     | 0.52              |
| 1:D:165:ASN:ND2  | 1:D:165:ASN:C    | 2.67                     | 0.52              |
| 1:B:358:GLU:HG3  | 1:B:359:ASN:HD22 | 1.74                     | 0.52              |
| 1:A:285:HIS:CD2  | 1:A:286:PHE:N    | 2.78                     | 0.52              |
| 1:B:158:ARG:HA   | 1:B:365:PRO:HB3  | 1.90                     | 0.52              |
| 1:B:231:VAL:O    | 1:B:234:VAL:HG12 | 2.10                     | 0.52              |
| 1:D:89:ARG:HB3   | 1:D:91:THR:CG2   | 2.40                     | 0.52              |
| 1:D:102:MET:HG3  | 1:D:127:ARG:NH1  | 2.24                     | 0.52              |
| 1:D:165:ASN:HD22 | 1:D:166:ASP:H    | 1.56                     | 0.52              |
| 1:C:158:ARG:HA   | 1:C:365:PRO:HB3  | 1.91                     | 0.52              |
| 1:B:363:MET:HB3  | 1:B:368:TYR:HE2  | 1.74                     | 0.52              |
| 1:C:93:ASP:OD2   | 1:C:95:SER:HB2   | 2.10                     | 0.52              |
| 1:A:164:VAL:O    | 1:A:170:LYS:HG3  | 2.10                     | 0.52              |
| 1:C:128:GLU:HA   | 1:C:131:LEU:HB2  | 1.91                     | 0.52              |
| 1:D:5:GLY:HA3    | 1:D:74:ASP:O     | 2.10                     | 0.52              |
| 1:D:268:LYS:CE   | 1:D:298:ILE:HD11 | 2.41                     | 0.51              |
| 1:A:166:ASP:HB3  | 1:A:369:MET:HE3  | 1.91                     | 0.51              |
| 1:B:35:PHE:HA    | 1:B:110:ASP:OD2  | 2.11                     | 0.51              |
| 1:D:23:ALA:HB2   | 1:D:53:THR:HG22  | 1.91                     | 0.51              |
| 1:D:118:ASP:O    | 1:D:122:ILE:HG12 | 2.10                     | 0.51              |
| 1:B:293:ARG:NH1  | 1:B:293:ARG:HG3  | 2.25                     | 0.51              |
| 1:A:263:THR:HG22 | 1:A:288:VAL:HG23 | 1.91                     | 0.51              |
| 1:A:267:SER:OG   | 1:A:269:GLU:HB2  | 2.10                     | 0.51              |
| 1:A:329:VAL:O    | 1:A:333:ALA:HB3  | 2.09                     | 0.51              |
| 1:C:16:MET:HE2   | 1:C:343:ASP:HA   | 1.92                     | 0.51              |
| 1:C:16:MET:HB3   | 1:C:343:ASP:OD1  | 2.10                     | 0.51              |
| 1:A:67:ASN:ND2   | 1:A:70:SER:C     | 2.69                     | 0.51              |
| 1:D:165:ASN:HD22 | 1:D:165:ASN:C    | 2.17                     | 0.51              |
| 1:A:140:GLU:HA   | 1:A:164:VAL:HG22 | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:376:GLU:OE1  | 1:A:380:ARG:NH1  | 2.44                     | 0.51              |
| 1:B:361:ARG:HH11 | 1:B:361:ARG:CB   | 2.12                     | 0.51              |
| 1:D:293:ARG:HG3  | 1:D:293:ARG:HH11 | 1.76                     | 0.51              |
| 1:B:356:LEU:HD22 | 1:B:363:MET:HE1  | 1.93                     | 0.51              |
| 1:C:68:PRO:HG2   | 1:C:69:LEU:HG    | 1.93                     | 0.51              |
| 1:A:51:ALA:CB    | 1:A:63:ILE:HD11  | 2.41                     | 0.51              |
| 1:A:382:LYS:HE3  | 1:A:386:LEU:HD11 | 1.93                     | 0.51              |
| 1:D:80:ARG:HG3   | 1:D:86:VAL:CG1   | 2.41                     | 0.51              |
| 1:D:309:VAL:HG22 | 1:D:323:LEU:HD23 | 1.93                     | 0.51              |
| 1:D:395:GLU:HA   | 1:D:395:GLU:OE1  | 2.10                     | 0.51              |
| 1:A:110:ASP:HB3  | 1:A:135:LYS:HD2  | 1.93                     | 0.50              |
| 1:C:170:LYS:HG2  | 1:C:348:LEU:CD1  | 2.42                     | 0.50              |
| 1:C:285:HIS:CG   | 1:C:286:PHE:N    | 2.77                     | 0.50              |
| 1:A:203:ALA:HA   | 1:A:226:THR:OG1  | 2.10                     | 0.50              |
| 1:B:304:GLU:OE2  | 1:B:304:GLU:HA   | 2.10                     | 0.50              |
| 1:C:304:GLU:OE2  | 1:C:304:GLU:HA   | 2.11                     | 0.50              |
| 1:D:124:HIS:NE2  | 1:D:157:LEU:HD12 | 2.27                     | 0.50              |
| 1:B:152:GLU:OE1  | 1:B:367:VAL:HG12 | 2.12                     | 0.50              |
| 1:B:164:VAL:O    | 1:B:170:LYS:HG3  | 2.12                     | 0.50              |
| 1:D:21:LYS:HB3   | 1:D:381:MET:HE3  | 1.93                     | 0.50              |
| 1:D:359:ASN:N    | 1:D:359:ASN:ND2  | 2.59                     | 0.50              |
| 1:B:51:ALA:CB    | 1:B:63:ILE:HD11  | 2.41                     | 0.50              |
| 1:B:195:VAL:N    | 1:D:181:GLN:HE22 | 2.09                     | 0.50              |
| 1:B:359:ASN:N    | 1:B:359:ASN:ND2  | 2.54                     | 0.50              |
| 1:D:175:ASN:O    | 1:D:179:THR:HG23 | 2.11                     | 0.50              |
| 1:D:284:GLY:HA3  | 1:D:289:GLU:OE2  | 2.12                     | 0.50              |
| 1:C:281:ALA:HB2  | 1:C:323:LEU:HD12 | 1.92                     | 0.50              |
| 1:B:149:LYS:HG2  | 1:B:367:VAL:HG11 | 1.93                     | 0.50              |
| 1:C:108:ARG:CG   | 1:C:130:VAL:HG12 | 2.36                     | 0.50              |
| 1:D:32:LEU:HD12  | 1:D:357:LEU:HD22 | 1.94                     | 0.50              |
| 1:D:267:SER:OG   | 1:D:269:GLU:HB2  | 2.12                     | 0.50              |
| 1:A:53:THR:O     | 1:A:57:LEU:HG    | 2.12                     | 0.50              |
| 1:C:89:ARG:HB3   | 1:C:91:THR:CG2   | 2.42                     | 0.50              |
| 1:B:34:GLY:N     | 1:B:60:LYS:HZ1   | 2.06                     | 0.50              |
| 1:D:266:LEU:O    | 1:D:291:PRO:HG3  | 2.12                     | 0.49              |
| 1:A:245:PRO:CG   | 1:B:389:LYS:HG3  | 2.42                     | 0.49              |
| 1:A:281:ALA:HB2  | 1:A:323:LEU:HD12 | 1.94                     | 0.49              |
| 1:C:291:PRO:HB2  | 1:C:294:VAL:CG2  | 2.42                     | 0.49              |
| 1:D:356:LEU:O    | 1:D:360:HIS:HA   | 2.11                     | 0.49              |
| 1:A:170:LYS:HG2  | 1:A:348:LEU:CD1  | 2.42                     | 0.49              |
| 1:C:68:PRO:HG2   | 1:C:69:LEU:H     | 1.77                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:172:LEU:O    | 1:D:176:ARG:HB3  | 2.11                     | 0.49              |
| 1:D:313:THR:HA   | 1:D:319:THR:HB   | 1.94                     | 0.49              |
| 1:A:89:ARG:C     | 1:A:91:THR:N     | 2.66                     | 0.49              |
| 1:B:266:LEU:O    | 1:B:291:PRO:HG3  | 2.12                     | 0.49              |
| 1:B:34:GLY:H     | 1:B:60:LYS:NZ    | 2.10                     | 0.49              |
| 1:C:47:THR:O     | 1:C:50:LEU:HB3   | 2.13                     | 0.49              |
| 1:A:139:GLU:HA   | 1:A:139:GLU:OE1  | 2.13                     | 0.49              |
| 1:A:268:LYS:HE3  | 1:A:298:ILE:HD11 | 1.94                     | 0.49              |
| 1:A:175:ASN:O    | 1:A:179:THR:HG23 | 2.12                     | 0.49              |
| 1:C:150:ALA:O    | 1:C:154:THR:HG23 | 2.12                     | 0.49              |
| 1:C:330:ASN:N    | 1:C:330:ASN:HD22 | 2.11                     | 0.49              |
| 1:D:128:GLU:HA   | 1:D:131:LEU:HB2  | 1.93                     | 0.49              |
| 1:A:107:GLU:HA   | 1:A:107:GLU:OE1  | 2.12                     | 0.49              |
| 1:A:224:ILE:HG12 | 1:A:244:MET:HE3  | 1.94                     | 0.49              |
| 1:B:395:GLU:O    | 1:B:399:ARG:HB2  | 2.13                     | 0.49              |
| 1:C:377:ARG:O    | 1:C:381:MET:HG3  | 2.13                     | 0.49              |
| 1:C:140:GLU:HA   | 1:C:164:VAL:HG22 | 1.95                     | 0.48              |
| 1:D:63:ILE:HG22  | 1:D:64:THR:N     | 2.28                     | 0.48              |
| 1:B:90:ARG:HH11  | 1:B:90:ARG:HG2   | 1.78                     | 0.48              |
| 1:B:127:ARG:HA   | 1:B:129:GLU:OE2  | 2.14                     | 0.48              |
| 1:C:318:LYS:HB2  | 1:C:318:LYS:HZ2  | 1.78                     | 0.48              |
| 1:D:47:THR:O     | 1:D:50:LEU:HB3   | 2.13                     | 0.48              |
| 1:D:11:TRP:O     | 1:D:14:ARG:HG2   | 2.13                     | 0.48              |
| 1:D:140:GLU:HA   | 1:D:164:VAL:HG22 | 1.94                     | 0.48              |
| 1:C:9:ILE:O      | 1:C:13:SER:HB3   | 2.13                     | 0.48              |
| 1:D:369:MET:O    | 1:D:370:LEU:C    | 2.56                     | 0.48              |
| 1:A:96:ILE:O     | 1:A:100:ASN:OD1  | 2.32                     | 0.48              |
| 1:B:197:GLY:HA3  | 1:C:238:MET:CE   | 2.42                     | 0.48              |
| 1:A:68:PRO:HG2   | 1:A:69:LEU:H     | 1.79                     | 0.48              |
| 1:A:139:GLU:OE2  | 1:A:144:GLY:HA3  | 2.14                     | 0.48              |
| 1:B:370:LEU:HD11 | 1:B:374:ILE:HD12 | 1.96                     | 0.48              |
| 1:A:4:THR:HA     | 1:A:7:MET:HE2    | 1.96                     | 0.48              |
| 1:D:10:ASN:O     | 1:D:14:ARG:HD2   | 2.13                     | 0.48              |
| 1:D:133:ASN:O    | 1:D:135:LYS:HG3  | 2.13                     | 0.48              |
| 1:C:153:GLU:HG3  | 1:C:154:THR:HG23 | 1.96                     | 0.48              |
| 1:C:250:VAL:HG22 | 1:C:274:LEU:HG   | 1.96                     | 0.48              |
| 1:A:231:VAL:O    | 1:A:234:VAL:HG12 | 2.14                     | 0.48              |
| 1:B:43:LEU:HD23  | 1:B:69:LEU:CD1   | 2.43                     | 0.48              |
| 1:C:32:LEU:HB3   | 1:C:59:ALA:HB2   | 1.95                     | 0.48              |
| 1:C:330:ASN:HD22 | 1:C:330:ASN:H    | 1.61                     | 0.48              |
| 1:B:356:LEU:O    | 1:B:360:HIS:HA   | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:358:GLU:HG3  | 1:B:359:ASN:ND2  | 2.29                     | 0.47              |
| 1:C:369:MET:O    | 1:C:370:LEU:C    | 2.57                     | 0.47              |
| 1:B:16:MET:HB3   | 1:B:343:ASP:OD1  | 2.14                     | 0.47              |
| 1:B:35:PHE:CD1   | 1:B:110:ASP:OD2  | 2.64                     | 0.47              |
| 1:D:91:THR:C     | 1:D:93:ASP:N     | 2.72                     | 0.47              |
| 1:D:268:LYS:HZ2  | 1:D:298:ILE:HD11 | 1.79                     | 0.47              |
| 1:D:330:ASN:H    | 1:D:330:ASN:ND2  | 2.06                     | 0.47              |
| 1:A:42:HIS:HD2   | 1:A:44:GLU:CG    | 2.27                     | 0.47              |
| 1:A:227:GLU:O    | 1:B:390:ILE:HB   | 2.14                     | 0.47              |
| 1:B:52:ILE:O     | 1:B:56:LYS:HG3   | 2.14                     | 0.47              |
| 1:B:260:SER:O    | 1:B:289:GLU:CD   | 2.57                     | 0.47              |
| 1:A:87:TYR:CE2   | 1:A:103:LYS:HB3  | 2.49                     | 0.47              |
| 1:A:244:MET:HG3  | 1:A:249:ALA:HB2  | 1.97                     | 0.47              |
| 1:C:91:THR:HB    | 1:C:96:ILE:HB    | 1.95                     | 0.47              |
| 1:B:189:ARG:HG3  | 1:B:190:ASN:ND2  | 2.29                     | 0.47              |
| 1:B:318:LYS:HB2  | 1:B:318:LYS:NZ   | 2.29                     | 0.47              |
| 1:A:47:THR:O     | 1:A:50:LEU:HB3   | 2.15                     | 0.47              |
| 1:D:329:VAL:O    | 1:D:333:ALA:HB3  | 2.14                     | 0.47              |
| 1:A:165:ASN:HD22 | 1:A:166:ASP:H    | 1.58                     | 0.47              |
| 1:A:356:LEU:O    | 1:A:360:HIS:HA   | 2.15                     | 0.47              |
| 1:A:369:MET:O    | 1:A:370:LEU:C    | 2.57                     | 0.47              |
| 1:B:361:ARG:O    | 1:B:363:MET:N    | 2.48                     | 0.47              |
| 1:C:21:LYS:NZ    | 1:C:384:ASP:HB3  | 2.29                     | 0.47              |
| 1:C:107:GLU:O    | 1:C:108:ARG:C    | 2.57                     | 0.47              |
| 1:C:263:THR:HG23 | 1:D:400:TYR:CE2  | 2.49                     | 0.47              |
| 1:C:359:ASN:O    | 1:C:363:MET:HG3  | 2.14                     | 0.47              |
| 1:D:124:HIS:HA   | 1:D:131:LEU:HD12 | 1.97                     | 0.47              |
| 1:D:188:MET:HE1  | 1:D:219:LEU:HD13 | 1.97                     | 0.47              |
| 1:D:293:ARG:HG3  | 1:D:293:ARG:NH1  | 2.28                     | 0.47              |
| 1:C:104:VAL:HG21 | 1:C:119:LEU:HD21 | 1.96                     | 0.47              |
| 1:C:370:LEU:HD12 | 1:C:371:PRO:HD2  | 1.97                     | 0.47              |
| 1:A:89:ARG:HB3   | 1:A:91:THR:CG2   | 2.45                     | 0.47              |
| 1:B:44:GLU:OE2   | 1:B:46:LYS:HB2   | 2.15                     | 0.47              |
| 1:A:284:GLY:HA3  | 1:A:289:GLU:OE2  | 2.15                     | 0.46              |
| 1:B:71:THR:HG22  | 1:B:90:ARG:HD3   | 1.97                     | 0.46              |
| 1:C:306:ARG:HB2  | 1:C:309:VAL:CG2  | 2.45                     | 0.46              |
| 1:C:395:GLU:OE2  | 1:C:395:GLU:HA   | 2.14                     | 0.46              |
| 1:C:395:GLU:HB3  | 1:C:399:ARG:NH2  | 2.30                     | 0.46              |
| 1:D:89:ARG:O     | 1:D:91:THR:HG23  | 2.15                     | 0.46              |
| 1:A:80:ARG:C     | 1:A:82:LYS:H     | 2.23                     | 0.46              |
| 1:B:110:ASP:OD1  | 1:B:110:ASP:N    | 2.48                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:393:LEU:HD13 | 1:B:228:VAL:HG11 | 1.97                     | 0.46              |
| 1:B:140:GLU:OE2  | 1:B:170:LYS:NZ   | 2.38                     | 0.46              |
| 1:B:189:ARG:NH2  | 1:D:189:ARG:HA   | 2.29                     | 0.46              |
| 1:D:118:ASP:HA   | 1:D:147:ARG:NH2  | 2.28                     | 0.46              |
| 1:D:67:ASN:ND2   | 1:D:70:SER:C     | 2.73                     | 0.46              |
| 1:A:5:GLY:HA3    | 1:A:74:ASP:O     | 2.16                     | 0.46              |
| 1:A:116:GLY:H    | 1:A:141:THR:CG2  | 2.26                     | 0.46              |
| 1:A:124:HIS:NE2  | 1:A:157:LEU:HD12 | 2.31                     | 0.46              |
| 1:A:359:ASN:O    | 1:A:363:MET:HG3  | 2.16                     | 0.46              |
| 1:B:285:HIS:CD2  | 1:B:286:PHE:N    | 2.84                     | 0.46              |
| 1:A:205:TYR:HH   | 1:A:241:PHE:HE2  | 1.63                     | 0.46              |
| 1:A:330:ASN:HD22 | 1:A:330:ASN:N    | 2.11                     | 0.46              |
| 1:B:291:PRO:HB2  | 1:B:294:VAL:CG2  | 2.45                     | 0.46              |
| 1:B:369:MET:O    | 1:B:370:LEU:C    | 2.59                     | 0.46              |
| 1:B:377:ARG:O    | 1:B:381:MET:HG3  | 2.16                     | 0.46              |
| 1:C:63:ILE:HG22  | 1:C:64:THR:N     | 2.31                     | 0.46              |
| 1:D:32:LEU:HB3   | 1:D:59:ALA:HB2   | 1.97                     | 0.46              |
| 1:D:51:ALA:HB2   | 1:D:63:ILE:HD11  | 1.96                     | 0.46              |
| 1:D:98:ARG:NH2   | 1:D:126:GLU:OE1  | 2.46                     | 0.46              |
| 1:D:15:TYR:HB2   | 1:D:339:VAL:HG11 | 1.97                     | 0.46              |
| 1:D:91:THR:HB    | 1:D:96:ILE:HB    | 1.97                     | 0.46              |
| 1:A:42:HIS:CD2   | 1:A:44:GLU:HG2   | 2.50                     | 0.46              |
| 1:B:160:PRO:CB   | 1:B:363:MET:HE3  | 2.45                     | 0.46              |
| 1:B:380:ARG:NH2  | 1:B:392:GLU:OE2  | 2.49                     | 0.46              |
| 1:C:91:THR:C     | 1:C:93:ASP:N     | 2.74                     | 0.46              |
| 1:B:153:GLU:HG3  | 1:B:154:THR:HG23 | 1.97                     | 0.46              |
| 1:B:319:THR:HG21 | 1:D:14:ARG:NH2   | 2.31                     | 0.46              |
| 1:C:16:MET:HE2   | 1:C:343:ASP:HB2  | 1.97                     | 0.46              |
| 1:C:51:ALA:HB2   | 1:C:63:ILE:HD11  | 1.97                     | 0.46              |
| 1:B:188:MET:HE3  | 1:B:195:VAL:HG21 | 1.97                     | 0.46              |
| 1:C:352:ALA:O    | 1:C:356:LEU:HG   | 2.15                     | 0.46              |
| 1:A:29:GLU:OE1   | 1:A:31:PRO:HB3   | 2.16                     | 0.45              |
| 1:A:128:GLU:N    | 1:A:128:GLU:OE1  | 2.49                     | 0.45              |
| 1:A:359:ASN:N    | 1:A:359:ASN:ND2  | 2.60                     | 0.45              |
| 1:A:399:ARG:CG   | 1:A:402:ARG:NH1  | 2.80                     | 0.45              |
| 1:B:171:TYR:O    | 1:B:175:ASN:HB2  | 2.15                     | 0.45              |
| 1:A:42:HIS:O     | 1:A:47:THR:HG21  | 2.16                     | 0.45              |
| 1:B:293:ARG:HG3  | 1:B:293:ARG:HH11 | 1.81                     | 0.45              |
| 1:C:99:GLU:OE2   | 1:C:103:LYS:NZ   | 2.32                     | 0.45              |
| 1:D:268:LYS:HE3  | 1:D:298:ILE:HD11 | 1.98                     | 0.45              |
| 1:A:42:HIS:HD2   | 1:A:44:GLU:HG2   | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:331:LEU:HD13 | 1:A:331:LEU:C    | 2.41                     | 0.45              |
| 1:B:63:ILE:HG22  | 1:B:64:THR:N     | 2.31                     | 0.45              |
| 1:D:67:ASN:HB2   | 1:D:70:SER:OG    | 2.16                     | 0.45              |
| 1:B:76:ALA:O     | 1:B:80:ARG:HG3   | 2.16                     | 0.45              |
| 1:B:105:LEU:C    | 1:B:107:GLU:N    | 2.74                     | 0.45              |
| 1:B:150:ALA:O    | 1:B:154:THR:HG23 | 2.16                     | 0.45              |
| 1:B:158:ARG:HB2  | 1:B:158:ARG:NH1  | 2.30                     | 0.45              |
| 1:C:32:LEU:HD23  | 1:C:59:ALA:CB    | 2.44                     | 0.45              |
| 1:D:162:ILE:HD11 | 1:D:355:TYR:HD2  | 1.81                     | 0.45              |
| 1:D:206:GLY:HA3  | 2:D:500:NAI:O5B  | 2.17                     | 0.45              |
| 1:A:33:SER:C     | 1:A:35:PHE:H     | 2.23                     | 0.45              |
| 1:A:189:ARG:HA   | 1:C:189:ARG:HH21 | 1.77                     | 0.45              |
| 1:B:357:LEU:O    | 1:B:360:HIS:HB2  | 2.16                     | 0.45              |
| 1:C:101:LEU:HD22 | 1:C:119:LEU:CD1  | 2.39                     | 0.45              |
| 1:D:139:GLU:OE1  | 1:D:139:GLU:HA   | 2.17                     | 0.45              |
| 1:D:246:MET:SD   | 1:D:266:LEU:HD21 | 2.56                     | 0.45              |
| 1:B:167:SER:HB2  | 1:B:375:ASP:OD1  | 2.17                     | 0.45              |
| 1:C:5:GLY:HA3    | 1:C:74:ASP:O     | 2.17                     | 0.45              |
| 1:C:284:GLY:O    | 1:C:328:LEU:HD13 | 2.16                     | 0.45              |
| 1:A:91:THR:C     | 1:A:93:ASP:N     | 2.74                     | 0.45              |
| 1:D:346:PHE:O    | 1:D:347:ALA:C    | 2.60                     | 0.45              |
| 1:A:105:LEU:C    | 1:A:107:GLU:N    | 2.75                     | 0.45              |
| 1:A:260:SER:O    | 1:A:289:GLU:OE2  | 2.34                     | 0.45              |
| 1:B:162:ILE:HD11 | 1:B:355:TYR:HD2  | 1.82                     | 0.45              |
| 1:B:237:ILE:HD11 | 1:B:243:VAL:HB   | 1.99                     | 0.45              |
| 1:C:4:THR:HG22   | 1:C:8:LYS:HE3    | 1.97                     | 0.45              |
| 1:C:306:ARG:HB2  | 1:C:309:VAL:HG23 | 1.98                     | 0.45              |
| 1:A:89:ARG:NH1   | 1:A:89:ARG:CG    | 2.80                     | 0.45              |
| 1:A:107:GLU:O    | 1:A:108:ARG:C    | 2.59                     | 0.45              |
| 1:C:23:ALA:HB2   | 1:C:53:THR:HG22  | 1.97                     | 0.45              |
| 1:D:89:ARG:HB3   | 1:D:91:THR:HG23  | 1.98                     | 0.45              |
| 1:D:97:TYR:OH    | 1:D:101:LEU:HD21 | 2.17                     | 0.45              |
| 1:A:68:PRO:HG2   | 1:A:69:LEU:HG    | 1.98                     | 0.44              |
| 1:A:271:ILE:HD11 | 1:A:291:PRO:HG2  | 1.99                     | 0.44              |
| 1:B:80:ARG:C     | 1:B:82:LYS:H     | 2.25                     | 0.44              |
| 1:C:285:HIS:CD2  | 1:C:286:PHE:N    | 2.85                     | 0.44              |
| 1:C:390:ILE:HB   | 1:D:227:GLU:O    | 2.17                     | 0.44              |
| 1:D:192:ASN:CG   | 1:D:192:ASN:O    | 2.59                     | 0.44              |
| 1:A:72:GLN:O     | 1:A:73:ASP:C     | 2.59                     | 0.44              |
| 1:A:87:TYR:CZ    | 1:A:103:LYS:HB3  | 2.53                     | 0.44              |
| 1:B:68:PRO:HA    | 1:B:89:ARG:HG3   | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:371:PRO:HB2  | 1:D:373:GLU:HG2  | 1.99                     | 0.44              |
| 1:B:90:ARG:HG2   | 1:B:90:ARG:NH1   | 2.31                     | 0.44              |
| 1:B:107:GLU:O    | 1:B:108:ARG:C    | 2.60                     | 0.44              |
| 1:C:7:MET:CG     | 3:C:662:HOH:O    | 2.53                     | 0.44              |
| 1:C:47:THR:HA    | 1:C:346:PHE:CZ   | 2.51                     | 0.44              |
| 1:D:26:TYR:OH    | 1:D:377:ARG:NH1  | 2.51                     | 0.44              |
| 1:A:346:PHE:O    | 1:A:349:GLN:N    | 2.51                     | 0.44              |
| 1:B:164:VAL:HG12 | 1:B:370:LEU:HD13 | 2.00                     | 0.44              |
| 1:B:179:THR:HG21 | 1:B:208:CYS:SG   | 2.56                     | 0.44              |
| 1:B:370:LEU:CD1  | 1:B:374:ILE:HD12 | 2.47                     | 0.44              |
| 1:C:116:GLY:H    | 1:C:141:THR:CG2  | 2.18                     | 0.44              |
| 1:D:193:LEU:HB3  | 1:D:198:LYS:NZ   | 2.32                     | 0.44              |
| 1:D:371:PRO:HB2  | 1:D:373:GLU:CD   | 2.42                     | 0.44              |
| 1:A:52:ILE:HG22  | 1:A:56:LYS:HE3   | 1.98                     | 0.44              |
| 1:A:128:GLU:HG3  | 1:A:131:LEU:HD13 | 2.00                     | 0.44              |
| 1:A:346:PHE:O    | 1:A:347:ALA:C    | 2.60                     | 0.44              |
| 1:C:337:HIS:H    | 1:C:342:MET:HE1  | 1.82                     | 0.44              |
| 1:D:36:THR:HG22  | 1:D:60:LYS:HD3   | 2.00                     | 0.44              |
| 1:D:152:GLU:CD   | 1:D:367:VAL:HG12 | 2.42                     | 0.44              |
| 1:D:298:ILE:HD13 | 1:D:298:ILE:HA   | 1.77                     | 0.44              |
| 1:C:80:ARG:C     | 1:C:82:LYS:H     | 2.25                     | 0.44              |
| 1:C:284:GLY:O    | 1:C:328:LEU:CD1  | 2.66                     | 0.44              |
| 1:C:359:ASN:N    | 1:C:359:ASN:ND2  | 2.64                     | 0.44              |
| 1:D:116:GLY:H    | 1:D:141:THR:CG2  | 2.26                     | 0.44              |
| 1:D:170:LYS:HG2  | 1:D:348:LEU:HD12 | 1.99                     | 0.44              |
| 1:A:250:VAL:HG13 | 1:A:273:SER:HB2  | 1.99                     | 0.44              |
| 1:B:185:ASP:OD2  | 1:B:189:ARG:NH2  | 2.46                     | 0.44              |
| 1:D:15:TYR:O     | 1:D:339:VAL:HG12 | 2.18                     | 0.44              |
| 1:D:72:GLN:O     | 1:D:73:ASP:C     | 2.60                     | 0.44              |
| 1:D:164:VAL:O    | 1:D:170:LYS:HG3  | 2.17                     | 0.44              |
| 1:D:291:PRO:HB2  | 1:D:294:VAL:HB   | 2.00                     | 0.44              |
| 1:B:124:HIS:HA   | 1:B:131:LEU:HD12 | 2.00                     | 0.44              |
| 1:B:329:VAL:O    | 1:B:333:ALA:HB3  | 2.18                     | 0.44              |
| 1:D:93:ASP:OD2   | 1:D:95:SER:HB2   | 2.17                     | 0.44              |
| 1:A:32:LEU:HB3   | 1:A:59:ALA:HB2   | 2.00                     | 0.44              |
| 1:A:291:PRO:HB2  | 1:A:294:VAL:HB   | 2.00                     | 0.44              |
| 2:A:500:NAI:H6N  | 2:A:500:NAI:H2D  | 1.88                     | 0.44              |
| 1:B:33:SER:C     | 1:B:35:PHE:H     | 2.26                     | 0.44              |
| 1:C:35:PHE:CA    | 1:C:110:ASP:OD2  | 2.59                     | 0.44              |
| 1:C:346:PHE:O    | 1:C:347:ALA:C    | 2.61                     | 0.44              |
| 1:C:356:LEU:O    | 1:C:360:HIS:HA   | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:201:VAL:CG2  | 1:D:253:ALA:HB2  | 2.48                     | 0.44              |
| 1:D:271:ILE:HD11 | 1:D:291:PRO:HG2  | 1.99                     | 0.44              |
| 1:A:77:GLU:OE2   | 1:A:80:ARG:NH1   | 2.51                     | 0.43              |
| 1:A:338:PRO:HB2  | 1:A:341:ILE:HG12 | 2.00                     | 0.43              |
| 1:B:124:HIS:HA   | 1:B:131:LEU:CD1  | 2.48                     | 0.43              |
| 1:D:98:ARG:HA    | 1:D:101:LEU:HD12 | 1.99                     | 0.43              |
| 1:D:360:HIS:C    | 1:D:360:HIS:HD1  | 2.25                     | 0.43              |
| 1:A:313:THR:HA   | 1:A:319:THR:HB   | 2.00                     | 0.43              |
| 1:D:80:ARG:C     | 1:D:82:LYS:H     | 2.24                     | 0.43              |
| 1:A:153:GLU:HG3  | 1:A:154:THR:HG23 | 1.99                     | 0.43              |
| 1:C:329:VAL:O    | 1:C:333:ALA:HB3  | 2.18                     | 0.43              |
| 1:D:361:ARG:H    | 1:D:361:ARG:HG2  | 1.39                     | 0.43              |
| 1:B:13:SER:HB2   | 1:B:49:TYR:CE1   | 2.52                     | 0.43              |
| 1:B:32:LEU:HD12  | 1:B:357:LEU:HD22 | 1.99                     | 0.43              |
| 1:B:120:THR:CG2  | 1:B:137:VAL:HG21 | 2.48                     | 0.43              |
| 1:D:18:LEU:HD12  | 1:D:344:LEU:HA   | 1.99                     | 0.43              |
| 1:D:21:LYS:NZ    | 1:D:384:ASP:HB3  | 2.33                     | 0.43              |
| 1:D:167:SER:HB2  | 1:D:375:ASP:OD1  | 2.18                     | 0.43              |
| 1:B:244:MET:HG3  | 1:B:249:ALA:HB2  | 1.99                     | 0.43              |
| 1:C:344:LEU:HD23 | 1:C:344:LEU:C    | 2.44                     | 0.43              |
| 1:B:5:GLY:HA3    | 1:B:74:ASP:O     | 2.18                     | 0.43              |
| 1:B:42:HIS:O     | 1:B:47:THR:HG21  | 2.18                     | 0.43              |
| 1:B:330:ASN:HD21 | 2:B:500:NAI:H72N | 1.65                     | 0.43              |
| 1:C:33:SER:C     | 1:C:35:PHE:H     | 2.26                     | 0.43              |
| 1:D:52:ILE:O     | 1:D:56:LYS:HG3   | 2.19                     | 0.43              |
| 1:D:231:VAL:O    | 1:D:234:VAL:HG12 | 2.18                     | 0.43              |
| 1:A:91:THR:HB    | 1:A:96:ILE:HB    | 2.00                     | 0.43              |
| 1:B:69:LEU:HD22  | 1:B:73:ASP:OD1   | 2.19                     | 0.43              |
| 1:B:361:ARG:C    | 1:B:363:MET:N    | 2.76                     | 0.43              |
| 1:C:8:LYS:O      | 1:C:45:ALA:HB1   | 2.19                     | 0.43              |
| 1:C:117:GLY:O    | 1:C:121:VAL:HG23 | 2.18                     | 0.43              |
| 1:D:278:ALA:O    | 1:D:320:VAL:HG13 | 2.19                     | 0.43              |
| 1:D:112:ILE:CG2  | 1:D:114:ASP:HB3  | 2.48                     | 0.43              |
| 1:D:148:LEU:HD23 | 1:D:148:LEU:N    | 2.33                     | 0.43              |
| 1:B:49:TYR:O     | 1:B:53:THR:OG1   | 2.36                     | 0.43              |
| 1:B:102:MET:HG3  | 1:B:127:ARG:NH1  | 2.34                     | 0.43              |
| 1:D:280:LEU:HD11 | 1:D:320:VAL:HG11 | 2.01                     | 0.43              |
| 1:A:399:ARG:HG2  | 1:A:402:ARG:NH1  | 2.34                     | 0.42              |
| 1:C:72:GLN:O     | 1:C:73:ASP:C     | 2.61                     | 0.42              |
| 1:D:383:LEU:HD13 | 1:D:383:LEU:HA   | 1.89                     | 0.42              |
| 1:A:39:MET:HE2   | 1:A:41:ILE:CG2   | 2.48                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:357:LEU:O    | 1:A:360:HIS:HB2  | 2.18                     | 0.42              |
| 1:A:360:HIS:HD1  | 1:A:360:HIS:C    | 2.27                     | 0.42              |
| 1:B:306:ARG:HH11 | 1:B:307:PRO:HD2  | 1.84                     | 0.42              |
| 1:C:337:HIS:HB2  | 1:C:342:MET:CE   | 2.49                     | 0.42              |
| 1:D:398:ARG:O    | 1:D:402:ARG:HG3  | 2.20                     | 0.42              |
| 1:A:104:VAL:HG21 | 1:A:119:LEU:HD21 | 2.01                     | 0.42              |
| 1:A:298:ILE:HG22 | 1:A:314:LEU:HD22 | 2.01                     | 0.42              |
| 1:A:344:LEU:C    | 1:A:344:LEU:HD23 | 2.43                     | 0.42              |
| 1:B:112:ILE:CG2  | 1:B:114:ASP:HB3  | 2.49                     | 0.42              |
| 1:B:135:LYS:HD3  | 1:B:360:HIS:NE2  | 2.34                     | 0.42              |
| 1:B:331:LEU:HD13 | 1:B:331:LEU:C    | 2.43                     | 0.42              |
| 1:C:285:HIS:CE1  | 1:D:400:TYR:OH   | 2.72                     | 0.42              |
| 1:D:260:SER:O    | 1:D:289:GLU:OE1  | 2.37                     | 0.42              |
| 1:D:291:PRO:HB2  | 1:D:294:VAL:CG2  | 2.49                     | 0.42              |
| 1:A:51:ALA:HB2   | 1:A:63:ILE:HD11  | 2.02                     | 0.42              |
| 1:B:44:GLU:C     | 1:B:44:GLU:OE1   | 2.63                     | 0.42              |
| 1:C:16:MET:HE2   | 1:C:343:ASP:CB   | 2.50                     | 0.42              |
| 1:C:310:THR:HG1  | 1:C:312:TYR:HE1  | 1.64                     | 0.42              |
| 1:D:33:SER:C     | 1:D:35:PHE:H     | 2.27                     | 0.42              |
| 1:D:250:VAL:HG22 | 1:D:274:LEU:HG   | 2.01                     | 0.42              |
| 1:B:47:THR:O     | 1:B:50:LEU:HB3   | 2.20                     | 0.42              |
| 1:B:69:LEU:HB3   | 1:B:70:SER:H     | 1.64                     | 0.42              |
| 1:B:94:GLU:O     | 1:B:95:SER:C     | 2.59                     | 0.42              |
| 1:B:201:VAL:CG2  | 1:B:253:ALA:HB2  | 2.48                     | 0.42              |
| 1:B:271:ILE:HD11 | 1:B:291:PRO:HG2  | 2.01                     | 0.42              |
| 1:B:309:VAL:CG1  | 1:B:321:PHE:HB3  | 2.49                     | 0.42              |
| 1:C:67:ASN:O     | 1:C:67:ASN:CG    | 2.63                     | 0.42              |
| 1:C:116:GLY:N    | 1:C:141:THR:HG21 | 2.19                     | 0.42              |
| 1:B:136:GLY:CA   | 1:B:356:LEU:HD13 | 2.49                     | 0.42              |
| 1:D:150:ALA:O    | 1:D:153:GLU:HG2  | 2.19                     | 0.42              |
| 1:D:346:PHE:O    | 1:D:349:GLN:N    | 2.52                     | 0.42              |
| 1:A:98:ARG:HA    | 1:A:101:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:263:THR:HG23 | 1:B:400:TYR:CD2  | 2.55                     | 0.42              |
| 1:B:43:LEU:HD23  | 1:B:69:LEU:HD12  | 2.01                     | 0.42              |
| 1:D:358:GLU:C    | 1:D:360:HIS:N    | 2.77                     | 0.42              |
| 1:A:232:LYS:NZ   | 2:A:500:NAI:O3B  | 2.52                     | 0.42              |
| 1:B:91:THR:OG1   | 1:B:92:HIS:N     | 2.53                     | 0.42              |
| 1:D:149:LYS:NZ   | 1:D:367:VAL:HG13 | 2.34                     | 0.42              |
| 1:A:263:THR:HG22 | 1:A:288:VAL:HG21 | 1.99                     | 0.42              |
| 1:B:62:VAL:HG12  | 1:B:104:VAL:HG12 | 2.02                     | 0.42              |
| 1:B:291:PRO:HB2  | 1:B:294:VAL:HB   | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:227:GLU:OE1  | 2:C:500:NAI:H1B  | 2.19                     | 0.42              |
| 1:A:383:LEU:HD13 | 1:A:383:LEU:HA   | 1.82                     | 0.42              |
| 1:B:26:TYR:HB3   | 1:B:57:LEU:HD22  | 2.02                     | 0.42              |
| 1:B:96:ILE:O     | 1:B:100:ASN:OD1  | 2.38                     | 0.42              |
| 1:B:140:GLU:O    | 1:B:141:THR:O    | 2.38                     | 0.42              |
| 1:D:377:ARG:HG2  | 1:D:377:ARG:NH2  | 2.34                     | 0.42              |
| 1:A:91:THR:HG22  | 1:A:96:ILE:HG21  | 2.02                     | 0.41              |
| 1:A:400:TYR:CZ   | 1:B:263:THR:HG23 | 2.54                     | 0.41              |
| 1:B:319:THR:CG2  | 3:D:657:HOH:O    | 2.67                     | 0.41              |
| 1:C:73:ASP:O     | 1:C:77:GLU:HG2   | 2.19                     | 0.41              |
| 1:C:267:SER:O    | 1:C:271:ILE:HG13 | 2.19                     | 0.41              |
| 1:C:360:HIS:HD1  | 1:C:360:HIS:C    | 2.28                     | 0.41              |
| 1:D:108:ARG:CG   | 1:D:130:VAL:HG12 | 2.47                     | 0.41              |
| 1:D:268:LYS:HZ1  | 1:D:298:ILE:HD11 | 1.81                     | 0.41              |
| 1:D:370:LEU:HD12 | 1:D:371:PRO:HD2  | 2.02                     | 0.41              |
| 1:A:164:VAL:HG12 | 1:A:370:LEU:HD13 | 2.02                     | 0.41              |
| 1:B:285:HIS:O    | 1:B:286:PHE:O    | 2.37                     | 0.41              |
| 1:D:143:THR:O    | 1:D:146:ARG:HB3  | 2.20                     | 0.41              |
| 1:B:174:ASP:OD1  | 1:B:337:HIS:HE1  | 2.03                     | 0.41              |
| 1:B:361:ARG:O    | 1:B:362:LYS:C    | 2.64                     | 0.41              |
| 1:C:227:GLU:O    | 1:D:390:ILE:HB   | 2.19                     | 0.41              |
| 1:A:32:LEU:HD23  | 1:A:59:ALA:CB    | 2.48                     | 0.41              |
| 1:A:344:LEU:HD23 | 1:A:344:LEU:O    | 2.19                     | 0.41              |
| 1:B:140:GLU:HA   | 1:B:164:VAL:HG22 | 2.02                     | 0.41              |
| 1:B:358:GLU:C    | 1:B:360:HIS:N    | 2.77                     | 0.41              |
| 1:C:182:SER:HB2  | 1:C:330:ASN:HB2  | 2.02                     | 0.41              |
| 1:D:330:ASN:HD22 | 1:D:330:ASN:N    | 2.05                     | 0.41              |
| 1:C:17:PRO:HG2   | 1:C:18:LEU:N     | 2.35                     | 0.41              |
| 1:C:105:LEU:C    | 1:C:107:GLU:N    | 2.75                     | 0.41              |
| 1:C:262:ASN:O    | 1:C:289:GLU:HG2  | 2.21                     | 0.41              |
| 1:C:295:LEU:HB3  | 1:C:312:TYR:CD2  | 2.55                     | 0.41              |
| 1:C:356:LEU:HA   | 1:C:363:MET:HE1  | 2.02                     | 0.41              |
| 1:D:195:VAL:HG12 | 1:D:221:ALA:HB2  | 2.03                     | 0.41              |
| 1:B:346:PHE:O    | 1:B:349:GLN:N    | 2.53                     | 0.41              |
| 1:B:361:ARG:HG2  | 1:B:361:ARG:H    | 1.58                     | 0.41              |
| 1:C:11:TRP:O     | 1:C:14:ARG:HG2   | 2.20                     | 0.41              |
| 1:C:295:LEU:HB3  | 1:C:312:TYR:CE2  | 2.55                     | 0.41              |
| 1:C:356:LEU:HD23 | 1:C:363:MET:HE1  | 2.02                     | 0.41              |
| 1:A:64:THR:HG23  | 1:A:100:ASN:HB3  | 2.00                     | 0.41              |
| 1:B:155:GLY:HA2  | 3:B:660:HOH:O    | 2.21                     | 0.41              |
| 1:C:26:TYR:HB3   | 1:C:57:LEU:HD22  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:285:HIS:O    | 1:C:286:PHE:O    | 2.39                     | 0.41              |
| 1:A:63:ILE:CG2   | 1:A:64:THR:N     | 2.83                     | 0.41              |
| 1:C:357:LEU:O    | 1:C:360:HIS:HB2  | 2.21                     | 0.41              |
| 2:C:500:NAI:H6N  | 2:C:500:NAI:H2D  | 1.91                     | 0.41              |
| 1:D:91:THR:O     | 1:D:93:ASP:N     | 2.51                     | 0.41              |
| 1:D:271:ILE:HA   | 1:D:274:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:175:ASN:O    | 1:A:179:THR:CG2  | 2.69                     | 0.41              |
| 1:A:208:CYS:O    | 1:A:212:ILE:HG13 | 2.21                     | 0.41              |
| 1:B:8:LYS:O      | 1:B:45:ALA:HB1   | 2.20                     | 0.41              |
| 1:B:27:SER:O     | 1:B:30:LYS:HG3   | 2.21                     | 0.41              |
| 1:B:319:THR:HG21 | 1:D:14:ARG:HH21  | 1.86                     | 0.41              |
| 1:B:330:ASN:ND2  | 2:B:500:NAI:H72N | 2.19                     | 0.41              |
| 1:B:346:PHE:O    | 1:B:347:ALA:C    | 2.64                     | 0.41              |
| 1:C:106:ASP:OD1  | 1:C:127:ARG:NH1  | 2.54                     | 0.41              |
| 1:C:124:HIS:HA   | 1:C:131:LEU:HD12 | 2.03                     | 0.41              |
| 1:C:346:PHE:O    | 1:C:349:GLN:N    | 2.53                     | 0.41              |
| 1:D:13:SER:HB2   | 1:D:49:TYR:CE1   | 2.56                     | 0.41              |
| 1:D:96:ILE:O     | 1:D:96:ILE:HG22  | 2.20                     | 0.41              |
| 1:D:105:LEU:C    | 1:D:107:GLU:N    | 2.75                     | 0.41              |
| 1:D:162:ILE:HG13 | 1:D:356:LEU:HD21 | 2.03                     | 0.41              |
| 1:D:262:ASN:HD22 | 1:D:262:ASN:HA   | 1.67                     | 0.41              |
| 1:B:222:ARG:NE   | 1:B:224:ILE:HD11 | 2.36                     | 0.41              |
| 1:C:7:MET:CE     | 1:C:10:ASN:HD22  | 2.33                     | 0.41              |
| 1:C:48:ALA:O     | 1:C:52:ILE:HG13  | 2.21                     | 0.41              |
| 1:A:15:TYR:HB2   | 1:A:339:VAL:HG11 | 2.03                     | 0.40              |
| 1:B:4:THR:HG22   | 1:B:8:LYS:HE3    | 2.02                     | 0.40              |
| 1:B:35:PHE:CE2   | 1:B:357:LEU:HD11 | 2.56                     | 0.40              |
| 1:A:205:TYR:CE2  | 1:A:210:ARG:HG2  | 2.56                     | 0.40              |
| 1:B:172:LEU:O    | 1:B:176:ARG:HB3  | 2.20                     | 0.40              |
| 1:B:344:LEU:C    | 1:B:344:LEU:HD23 | 2.47                     | 0.40              |
| 1:D:244:MET:HG3  | 1:D:249:ALA:HB2  | 2.02                     | 0.40              |
| 1:A:133:ASN:O    | 1:A:135:LYS:HG3  | 2.20                     | 0.40              |
| 1:A:356:LEU:HD23 | 1:A:363:MET:HE1  | 2.03                     | 0.40              |
| 1:A:46:LYS:NZ    | 3:A:688:HOH:O    | 2.54                     | 0.40              |
| 1:A:194:LEU:HD13 | 1:C:341:ILE:HG12 | 2.03                     | 0.40              |
| 1:A:250:VAL:HG22 | 1:A:274:LEU:CD2  | 2.52                     | 0.40              |
| 1:B:16:MET:HA    | 1:B:343:ASP:CG   | 2.46                     | 0.40              |
| 1:B:52:ILE:HG22  | 1:B:56:LYS:HE3   | 2.04                     | 0.40              |
| 1:C:104:VAL:O    | 1:C:107:GLU:HB2  | 2.21                     | 0.40              |
| 1:C:121:VAL:HG11 | 1:C:147:ARG:HH21 | 1.84                     | 0.40              |
| 1:D:35:PHE:CA    | 1:D:110:ASP:OD2  | 2.63                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:348:LEU:CD2  | 1:D:378:VAL:HG21 | 2.44                     | 0.40              |
| 1:A:338:PRO:O    | 1:A:339:VAL:C    | 2.64                     | 0.40              |
| 1:C:105:LEU:HD22 | 1:C:130:VAL:HG21 | 2.04                     | 0.40              |
| 1:C:116:GLY:O    | 1:C:147:ARG:HD3  | 2.21                     | 0.40              |
| 1:D:357:LEU:O    | 1:D:360:HIS:HB2  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 399/411 (97%)   | 345 (86%)  | 41 (10%)  | 13 (3%)  | 3           | 7  |
| 1   | B     | 399/411 (97%)   | 350 (88%)  | 39 (10%)  | 10 (2%)  | 4           | 10 |
| 1   | C     | 399/411 (97%)   | 348 (87%)  | 39 (10%)  | 12 (3%)  | 3           | 8  |
| 1   | D     | 399/411 (97%)   | 346 (87%)  | 41 (10%)  | 12 (3%)  | 3           | 8  |
| All | All   | 1596/1644 (97%) | 1389 (87%) | 160 (10%) | 47 (3%)  | 3           | 8  |

All (47) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 141 | THR  |
| 1   | A     | 285 | HIS  |
| 1   | A     | 286 | PHE  |
| 1   | A     | 365 | PRO  |
| 1   | B     | 141 | THR  |
| 1   | B     | 285 | HIS  |
| 1   | B     | 286 | PHE  |
| 1   | B     | 365 | PRO  |
| 1   | C     | 141 | THR  |
| 1   | C     | 285 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 286 | PHE  |
| 1   | C     | 365 | PRO  |
| 1   | D     | 141 | THR  |
| 1   | D     | 285 | HIS  |
| 1   | D     | 286 | PHE  |
| 1   | D     | 365 | PRO  |
| 1   | A     | 328 | LEU  |
| 1   | B     | 362 | LYS  |
| 1   | C     | 328 | LEU  |
| 1   | A     | 360 | HIS  |
| 1   | B     | 155 | GLY  |
| 1   | B     | 328 | LEU  |
| 1   | B     | 360 | HIS  |
| 1   | C     | 358 | GLU  |
| 1   | C     | 360 | HIS  |
| 1   | D     | 328 | LEU  |
| 1   | D     | 358 | GLU  |
| 1   | D     | 360 | HIS  |
| 1   | A     | 155 | GLY  |
| 1   | A     | 358 | GLU  |
| 1   | A     | 362 | LYS  |
| 1   | B     | 358 | GLU  |
| 1   | C     | 155 | GLY  |
| 1   | C     | 362 | LYS  |
| 1   | D     | 362 | LYS  |
| 1   | A     | 73  | ASP  |
| 1   | C     | 90  | ARG  |
| 1   | D     | 90  | ARG  |
| 1   | D     | 291 | PRO  |
| 1   | A     | 90  | ARG  |
| 1   | D     | 155 | GLY  |
| 1   | B     | 291 | PRO  |
| 1   | D     | 307 | PRO  |
| 1   | A     | 291 | PRO  |
| 1   | A     | 307 | PRO  |
| 1   | C     | 307 | PRO  |
| 1   | C     | 291 | 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     | 337/347 (97%)   | 303 (90%)  | 34 (10%)  | 7           | 15 |
| 1   | B     | 337/347 (97%)   | 302 (90%)  | 35 (10%)  | 7           | 14 |
| 1   | C     | 337/347 (97%)   | 302 (90%)  | 35 (10%)  | 7           | 14 |
| 1   | D     | 337/347 (97%)   | 306 (91%)  | 31 (9%)   | 8           | 19 |
| All | All   | 1348/1388 (97%) | 1213 (90%) | 135 (10%) | 7           | 16 |

All (135) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | ARG  |
| 1   | A     | 16  | MET  |
| 1   | A     | 19  | LEU  |
| 1   | A     | 24  | GLU  |
| 1   | A     | 29  | GLU  |
| 1   | A     | 32  | LEU  |
| 1   | A     | 53  | THR  |
| 1   | A     | 60  | LYS  |
| 1   | A     | 70  | SER  |
| 1   | A     | 86  | VAL  |
| 1   | A     | 90  | ARG  |
| 1   | A     | 165 | ASN  |
| 1   | A     | 179 | THR  |
| 1   | A     | 214 | LEU  |
| 1   | A     | 215 | ARG  |
| 1   | A     | 222 | ARG  |
| 1   | A     | 242 | THR  |
| 1   | A     | 247 | LYS  |
| 1   | A     | 248 | GLU  |
| 1   | A     | 250 | VAL  |
| 1   | A     | 262 | ASN  |
| 1   | A     | 293 | ARG  |
| 1   | A     | 307 | PRO  |
| 1   | A     | 310 | THR  |
| 1   | A     | 319 | THR  |
| 1   | A     | 330 | ASN  |
| 1   | A     | 340 | GLU  |
| 1   | A     | 342 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 359 | ASN  |
| 1   | A     | 365 | PRO  |
| 1   | A     | 376 | GLU  |
| 1   | A     | 377 | ARG  |
| 1   | A     | 380 | ARG  |
| 1   | A     | 383 | LEU  |
| 1   | B     | 13  | SER  |
| 1   | B     | 14  | ARG  |
| 1   | B     | 24  | GLU  |
| 1   | B     | 27  | SER  |
| 1   | B     | 29  | GLU  |
| 1   | B     | 32  | LEU  |
| 1   | B     | 53  | THR  |
| 1   | B     | 60  | LYS  |
| 1   | B     | 72  | GLN  |
| 1   | B     | 86  | VAL  |
| 1   | B     | 89  | ARG  |
| 1   | B     | 108 | ARG  |
| 1   | B     | 110 | ASP  |
| 1   | B     | 165 | ASN  |
| 1   | B     | 179 | THR  |
| 1   | B     | 215 | ARG  |
| 1   | B     | 222 | ARG  |
| 1   | B     | 242 | THR  |
| 1   | B     | 248 | GLU  |
| 1   | B     | 250 | VAL  |
| 1   | B     | 262 | ASN  |
| 1   | B     | 300 | VAL  |
| 1   | B     | 307 | PRO  |
| 1   | B     | 310 | THR  |
| 1   | B     | 319 | THR  |
| 1   | B     | 330 | ASN  |
| 1   | B     | 340 | GLU  |
| 1   | B     | 342 | MET  |
| 1   | B     | 359 | ASN  |
| 1   | B     | 361 | ARG  |
| 1   | B     | 365 | PRO  |
| 1   | B     | 373 | GLU  |
| 1   | B     | 376 | GLU  |
| 1   | B     | 380 | ARG  |
| 1   | B     | 383 | LEU  |
| 1   | C     | 7   | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 14  | ARG  |
| 1   | C     | 16  | MET  |
| 1   | C     | 24  | GLU  |
| 1   | C     | 27  | SER  |
| 1   | C     | 32  | LEU  |
| 1   | C     | 53  | THR  |
| 1   | C     | 60  | LYS  |
| 1   | C     | 70  | SER  |
| 1   | C     | 86  | VAL  |
| 1   | C     | 129 | GLU  |
| 1   | C     | 142 | THR  |
| 1   | C     | 153 | GLU  |
| 1   | C     | 165 | ASN  |
| 1   | C     | 179 | THR  |
| 1   | C     | 215 | ARG  |
| 1   | C     | 222 | ARG  |
| 1   | C     | 227 | GLU  |
| 1   | C     | 234 | VAL  |
| 1   | C     | 242 | THR  |
| 1   | C     | 247 | LYS  |
| 1   | C     | 262 | ASN  |
| 1   | C     | 268 | LYS  |
| 1   | C     | 293 | ARG  |
| 1   | C     | 307 | PRO  |
| 1   | C     | 310 | THR  |
| 1   | C     | 315 | GLU  |
| 1   | C     | 319 | THR  |
| 1   | C     | 330 | ASN  |
| 1   | C     | 340 | GLU  |
| 1   | C     | 359 | ASN  |
| 1   | C     | 365 | PRO  |
| 1   | C     | 376 | GLU  |
| 1   | C     | 380 | ARG  |
| 1   | C     | 383 | LEU  |
| 1   | D     | 14  | ARG  |
| 1   | D     | 24  | GLU  |
| 1   | D     | 32  | LEU  |
| 1   | D     | 53  | THR  |
| 1   | D     | 70  | SER  |
| 1   | D     | 86  | VAL  |
| 1   | D     | 164 | VAL  |
| 1   | D     | 165 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 179 | THR  |
| 1   | D     | 215 | ARG  |
| 1   | D     | 222 | ARG  |
| 1   | D     | 234 | VAL  |
| 1   | D     | 242 | THR  |
| 1   | D     | 247 | LYS  |
| 1   | D     | 248 | GLU  |
| 1   | D     | 250 | VAL  |
| 1   | D     | 262 | ASN  |
| 1   | D     | 298 | ILE  |
| 1   | D     | 307 | PRO  |
| 1   | D     | 310 | THR  |
| 1   | D     | 319 | THR  |
| 1   | D     | 330 | ASN  |
| 1   | D     | 340 | GLU  |
| 1   | D     | 342 | MET  |
| 1   | D     | 359 | ASN  |
| 1   | D     | 361 | ARG  |
| 1   | D     | 365 | PRO  |
| 1   | D     | 373 | GLU  |
| 1   | D     | 376 | GLU  |
| 1   | D     | 380 | ARG  |
| 1   | D     | 383 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 42  | HIS  |
| 1   | A     | 72  | GLN  |
| 1   | A     | 100 | ASN  |
| 1   | A     | 165 | ASN  |
| 1   | A     | 181 | GLN  |
| 1   | A     | 190 | ASN  |
| 1   | A     | 330 | ASN  |
| 1   | A     | 337 | HIS  |
| 1   | A     | 349 | GLN  |
| 1   | B     | 10  | ASN  |
| 1   | B     | 100 | ASN  |
| 1   | B     | 165 | ASN  |
| 1   | B     | 181 | GLN  |
| 1   | B     | 190 | ASN  |
| 1   | B     | 262 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 330 | ASN  |
| 1   | B     | 337 | HIS  |
| 1   | B     | 349 | GLN  |
| 1   | B     | 359 | ASN  |
| 1   | C     | 10  | ASN  |
| 1   | C     | 100 | ASN  |
| 1   | C     | 165 | ASN  |
| 1   | C     | 181 | GLN  |
| 1   | C     | 285 | HIS  |
| 1   | C     | 330 | ASN  |
| 1   | C     | 337 | HIS  |
| 1   | C     | 349 | GLN  |
| 1   | C     | 359 | ASN  |
| 1   | D     | 72  | GLN  |
| 1   | D     | 100 | ASN  |
| 1   | D     | 165 | ASN  |
| 1   | D     | 181 | GLN  |
| 1   | D     | 192 | ASN  |
| 1   | D     | 330 | ASN  |
| 1   | D     | 337 | HIS  |
| 1   | D     | 349 | GLN  |
| 1   | D     | 359 | 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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | NAI  | D     | 500 | -    | 47,48,48     | 1.14 | 5 (10%)  | 64,73,73    | 1.63 | 10 (15%) |
| 2   | NAI  | B     | 500 | -    | 47,48,48     | 1.35 | 3 (6%)   | 64,73,73    | 1.62 | 12 (18%) |
| 2   | NAI  | C     | 500 | -    | 47,48,48     | 1.15 | 3 (6%)   | 64,73,73    | 1.67 | 10 (15%) |
| 2   | NAI  | A     | 500 | -    | 47,48,48     | 1.26 | 5 (10%)  | 64,73,73    | 1.60 | 10 (15%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2   | NAI  | D     | 500 | -    | -       | 7/29/72/72  | 0/5/5/5 |
| 2   | NAI  | B     | 500 | -    | -       | 11/29/72/72 | 0/5/5/5 |
| 2   | NAI  | C     | 500 | -    | -       | 6/29/72/72  | 0/5/5/5 |
| 2   | NAI  | A     | 500 | -    | -       | 8/29/72/72  | 0/5/5/5 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 500 | NAI  | PN-O3   | 5.18  | 1.65        | 1.59     |
| 2   | B     | 500 | NAI  | PA-O3   | 3.89  | 1.63        | 1.59     |
| 2   | C     | 500 | NAI  | PN-O3   | 3.84  | 1.63        | 1.59     |
| 2   | A     | 500 | NAI  | PN-O3   | 3.70  | 1.63        | 1.59     |
| 2   | A     | 500 | NAI  | PA-O3   | 3.53  | 1.63        | 1.59     |
| 2   | D     | 500 | NAI  | C7N-C3N | -3.03 | 1.42        | 1.48     |
| 2   | D     | 500 | NAI  | PN-O3   | 2.98  | 1.62        | 1.59     |
| 2   | A     | 500 | NAI  | C7N-C3N | -2.76 | 1.42        | 1.48     |
| 2   | D     | 500 | NAI  | C5A-N7A | -2.50 | 1.34        | 1.39     |
| 2   | A     | 500 | NAI  | C5A-C4A | 2.43  | 1.43        | 1.39     |
| 2   | C     | 500 | NAI  | C6N-N1N | 2.34  | 1.42        | 1.37     |
| 2   | B     | 500 | NAI  | C6N-N1N | 2.28  | 1.42        | 1.37     |
| 2   | C     | 500 | NAI  | C5A-N7A | -2.26 | 1.35        | 1.39     |
| 2   | D     | 500 | NAI  | PA-O3   | 2.23  | 1.61        | 1.59     |
| 2   | A     | 500 | NAI  | C6N-N1N | 2.22  | 1.42        | 1.37     |
| 2   | D     | 500 | NAI  | C6N-N1N | 2.06  | 1.42        | 1.37     |

All (42) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 500 | NAI  | C5A-C4A-N3A | -5.32 | 119.39      | 126.72   |
| 2   | D     | 500 | NAI  | C5A-C4A-N3A | -5.24 | 119.51      | 126.72   |
| 2   | A     | 500 | NAI  | C5A-C4A-N3A | -5.19 | 119.57      | 126.72   |
| 2   | B     | 500 | NAI  | C5A-C4A-N3A | -5.09 | 119.71      | 126.72   |
| 2   | D     | 500 | NAI  | N3A-C2A-N1A | -4.79 | 121.33      | 128.58   |
| 2   | C     | 500 | NAI  | N3A-C2A-N1A | -4.79 | 121.33      | 128.58   |
| 2   | B     | 500 | NAI  | N3A-C2A-N1A | -4.54 | 121.71      | 128.58   |
| 2   | A     | 500 | NAI  | N3A-C2A-N1A | -4.47 | 121.81      | 128.58   |
| 2   | D     | 500 | NAI  | N3A-C4A-N9A | 4.44  | 134.71      | 127.17   |
| 2   | C     | 500 | NAI  | N3A-C4A-N9A | 4.40  | 134.65      | 127.17   |
| 2   | A     | 500 | NAI  | N3A-C4A-N9A | 4.30  | 134.49      | 127.17   |
| 2   | B     | 500 | NAI  | N3A-C4A-N9A | 4.03  | 134.03      | 127.17   |
| 2   | C     | 500 | NAI  | C5A-N7A-C8A | 4.03  | 109.79      | 103.45   |
| 2   | C     | 500 | NAI  | C2A-N3A-C4A | 3.96  | 121.49      | 111.83   |
| 2   | B     | 500 | NAI  | C2A-N3A-C4A | 3.95  | 121.47      | 111.83   |
| 2   | D     | 500 | NAI  | C2A-N3A-C4A | 3.78  | 121.07      | 111.83   |
| 2   | D     | 500 | NAI  | C5A-N7A-C8A | 3.77  | 109.38      | 103.45   |
| 2   | A     | 500 | NAI  | C2A-N3A-C4A | 3.76  | 121.02      | 111.83   |
| 2   | B     | 500 | NAI  | C5A-N7A-C8A | 3.75  | 109.35      | 103.45   |
| 2   | A     | 500 | NAI  | C5A-N7A-C8A | 3.75  | 109.35      | 103.45   |
| 2   | B     | 500 | NAI  | C4A-C5A-N7A | -3.39 | 106.70      | 110.58   |
| 2   | A     | 500 | NAI  | C4A-C5A-N7A | -3.17 | 106.95      | 110.58   |
| 2   | C     | 500 | NAI  | C4A-C5A-N7A | -3.14 | 106.99      | 110.58   |
| 2   | B     | 500 | NAI  | N9A-C8A-N7A | -2.91 | 109.81      | 113.94   |
| 2   | D     | 500 | NAI  | C4A-C5A-N7A | -2.88 | 107.29      | 110.58   |
| 2   | C     | 500 | NAI  | N9A-C8A-N7A | -2.71 | 110.10      | 113.94   |
| 2   | D     | 500 | NAI  | N9A-C8A-N7A | -2.61 | 110.23      | 113.94   |
| 2   | A     | 500 | NAI  | N9A-C8A-N7A | -2.54 | 110.34      | 113.94   |
| 2   | C     | 500 | NAI  | PN-O5D-C5D  | -2.52 | 106.89      | 121.35   |
| 2   | D     | 500 | NAI  | PN-O5D-C5D  | -2.42 | 107.46      | 121.35   |
| 2   | B     | 500 | NAI  | C1D-N1N-C2N | -2.39 | 117.20      | 121.14   |
| 2   | C     | 500 | NAI  | C1D-N1N-C2N | -2.35 | 117.28      | 121.14   |
| 2   | B     | 500 | NAI  | PN-O5D-C5D  | -2.31 | 108.09      | 121.35   |
| 2   | D     | 500 | NAI  | PA-O5B-C5B  | -2.31 | 108.11      | 121.35   |
| 2   | D     | 500 | NAI  | C1D-N1N-C2N | -2.31 | 117.33      | 121.14   |
| 2   | A     | 500 | NAI  | C1D-N1N-C2N | -2.24 | 117.44      | 121.14   |
| 2   | A     | 500 | NAI  | PA-O5B-C5B  | -2.23 | 108.57      | 121.35   |
| 2   | B     | 500 | NAI  | C6A-C5A-N7A | 2.18  | 136.28      | 132.09   |
| 2   | A     | 500 | NAI  | PN-O5D-C5D  | -2.17 | 108.90      | 121.35   |
| 2   | C     | 500 | NAI  | PA-O5B-C5B  | -2.16 | 108.99      | 121.35   |
| 2   | B     | 500 | NAI  | C4A-N9A-C8A | 2.04  | 107.88      | 105.74   |
| 2   | B     | 500 | NAI  | PA-O5B-C5B  | -2.00 | 109.89      | 121.35   |

There are no chirality outliers.

All (32) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 500 | NAI  | C5D-O5D-PN-O2N  |
| 2   | A     | 500 | NAI  | C2N-C3N-C7N-N7N |
| 2   | B     | 500 | NAI  | C5B-O5B-PA-O1A  |
| 2   | B     | 500 | NAI  | C5B-O5B-PA-O3   |
| 2   | B     | 500 | NAI  | O4B-C4B-C5B-O5B |
| 2   | D     | 500 | NAI  | C5D-O5D-PN-O2N  |
| 2   | B     | 500 | NAI  | C3B-C4B-C5B-O5B |
| 2   | A     | 500 | NAI  | C2D-C1D-N1N-C2N |
| 2   | A     | 500 | NAI  | C2D-C1D-N1N-C6N |
| 2   | C     | 500 | NAI  | C2D-C1D-N1N-C6N |
| 2   | B     | 500 | NAI  | C2D-C1D-N1N-C2N |
| 2   | B     | 500 | NAI  | C2D-C1D-N1N-C6N |
| 2   | C     | 500 | NAI  | C2D-C1D-N1N-C2N |
| 2   | A     | 500 | NAI  | O4B-C4B-C5B-O5B |
| 2   | C     | 500 | NAI  | O4B-C4B-C5B-O5B |
| 2   | A     | 500 | NAI  | C3B-C4B-C5B-O5B |
| 2   | C     | 500 | NAI  | C3B-C4B-C5B-O5B |
| 2   | D     | 500 | NAI  | C2D-C1D-N1N-C2N |
| 2   | B     | 500 | NAI  | PN-O3-PA-O5B    |
| 2   | D     | 500 | NAI  | C2D-C1D-N1N-C6N |
| 2   | B     | 500 | NAI  | O4D-C1D-N1N-C2N |
| 2   | B     | 500 | NAI  | O4D-C1D-N1N-C6N |
| 2   | C     | 500 | NAI  | O4D-C1D-N1N-C2N |
| 2   | A     | 500 | NAI  | O4D-C1D-N1N-C2N |
| 2   | C     | 500 | NAI  | O4D-C1D-N1N-C6N |
| 2   | B     | 500 | NAI  | C5B-O5B-PA-O2A  |
| 2   | A     | 500 | NAI  | O4D-C1D-N1N-C6N |
| 2   | D     | 500 | NAI  | O4D-C1D-N1N-C2N |
| 2   | D     | 500 | NAI  | O4B-C4B-C5B-O5B |
| 2   | D     | 500 | NAI  | O4D-C1D-N1N-C6N |
| 2   | D     | 500 | NAI  | C3B-C4B-C5B-O5B |
| 2   | B     | 500 | NAI  | O4D-C4D-C5D-O5D |

There are no ring outliers.

4 monomers are involved in 8 short contacts:

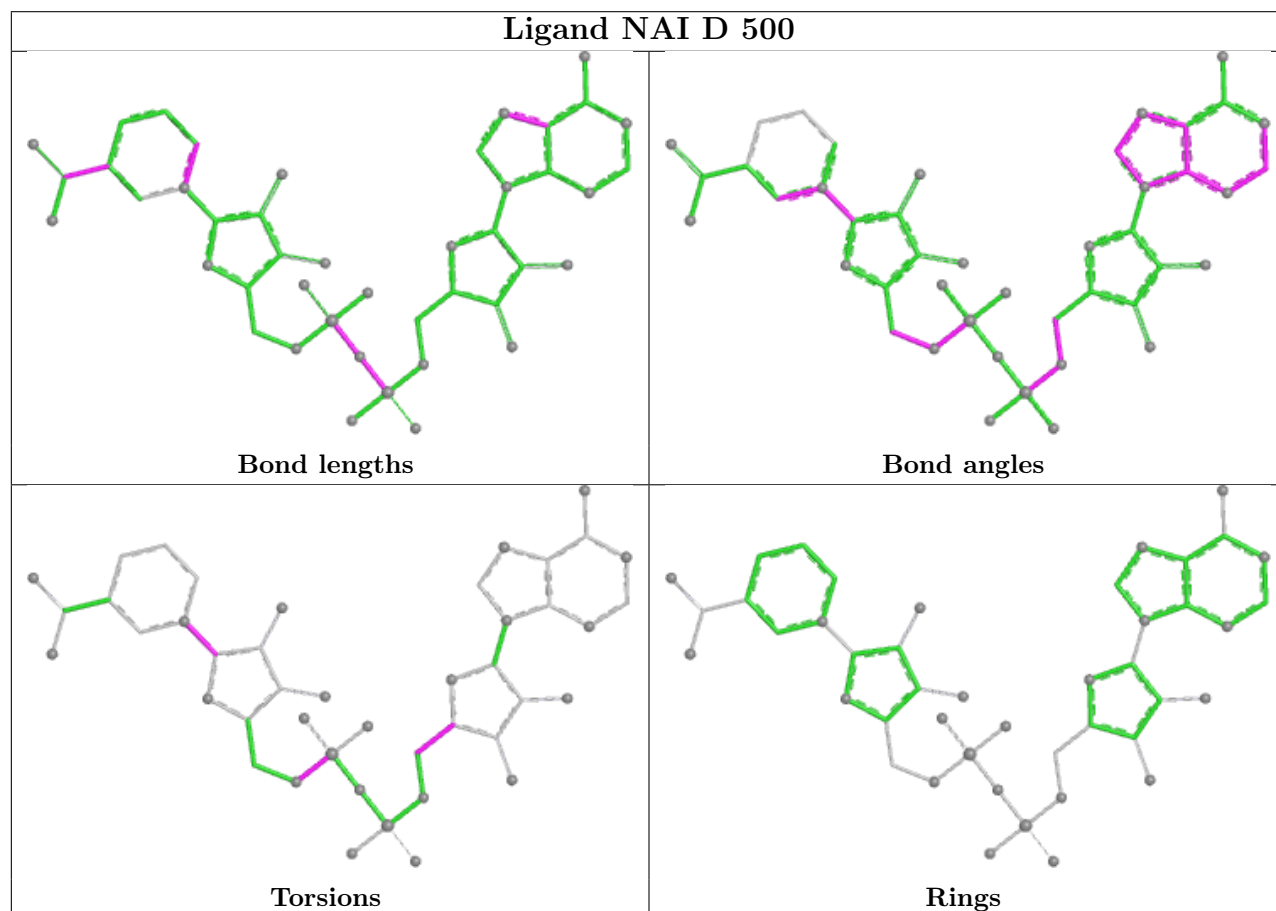
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | D     | 500 | NAI  | 2       | 0            |
| 2   | B     | 500 | NAI  | 2       | 0            |
| 2   | C     | 500 | NAI  | 2       | 0            |

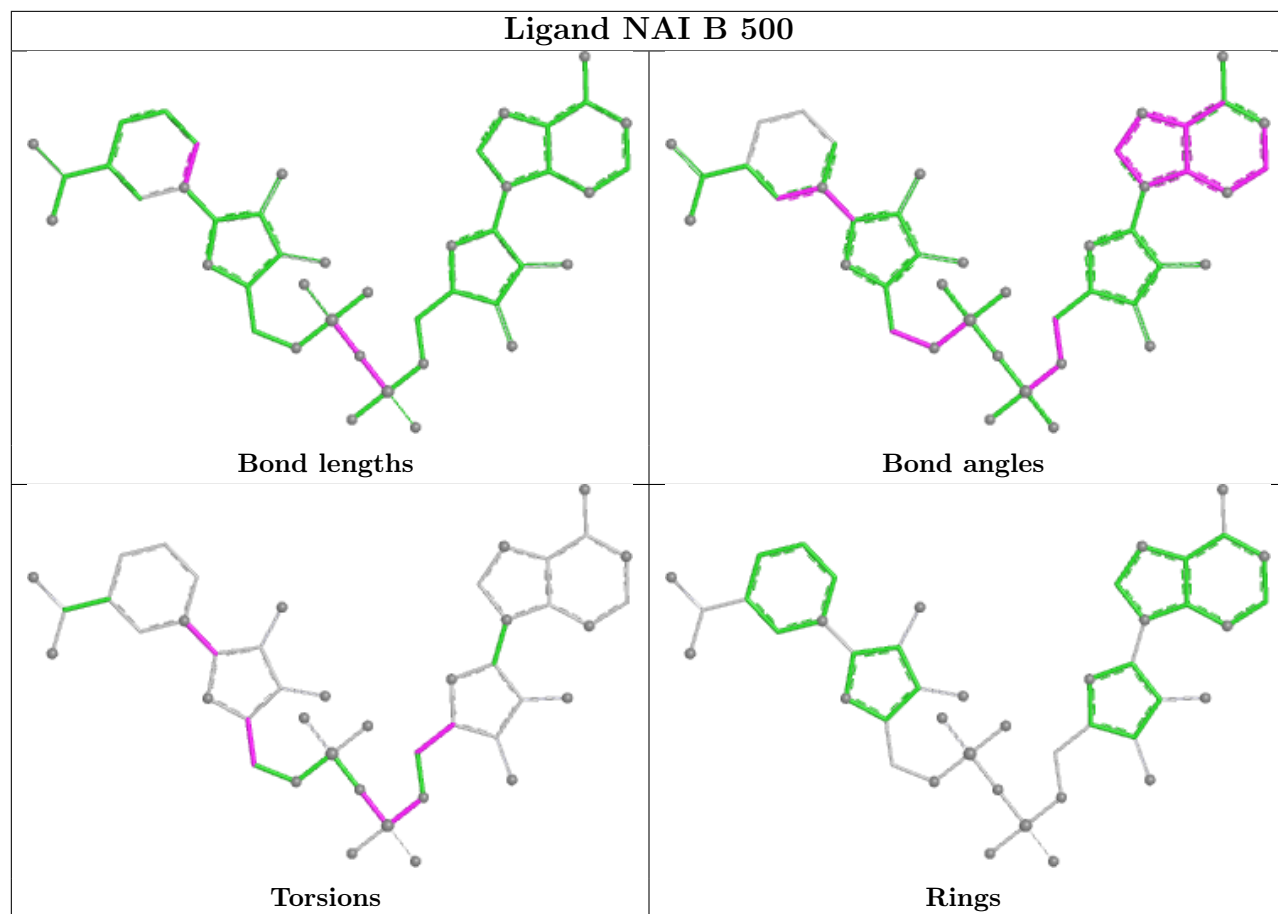
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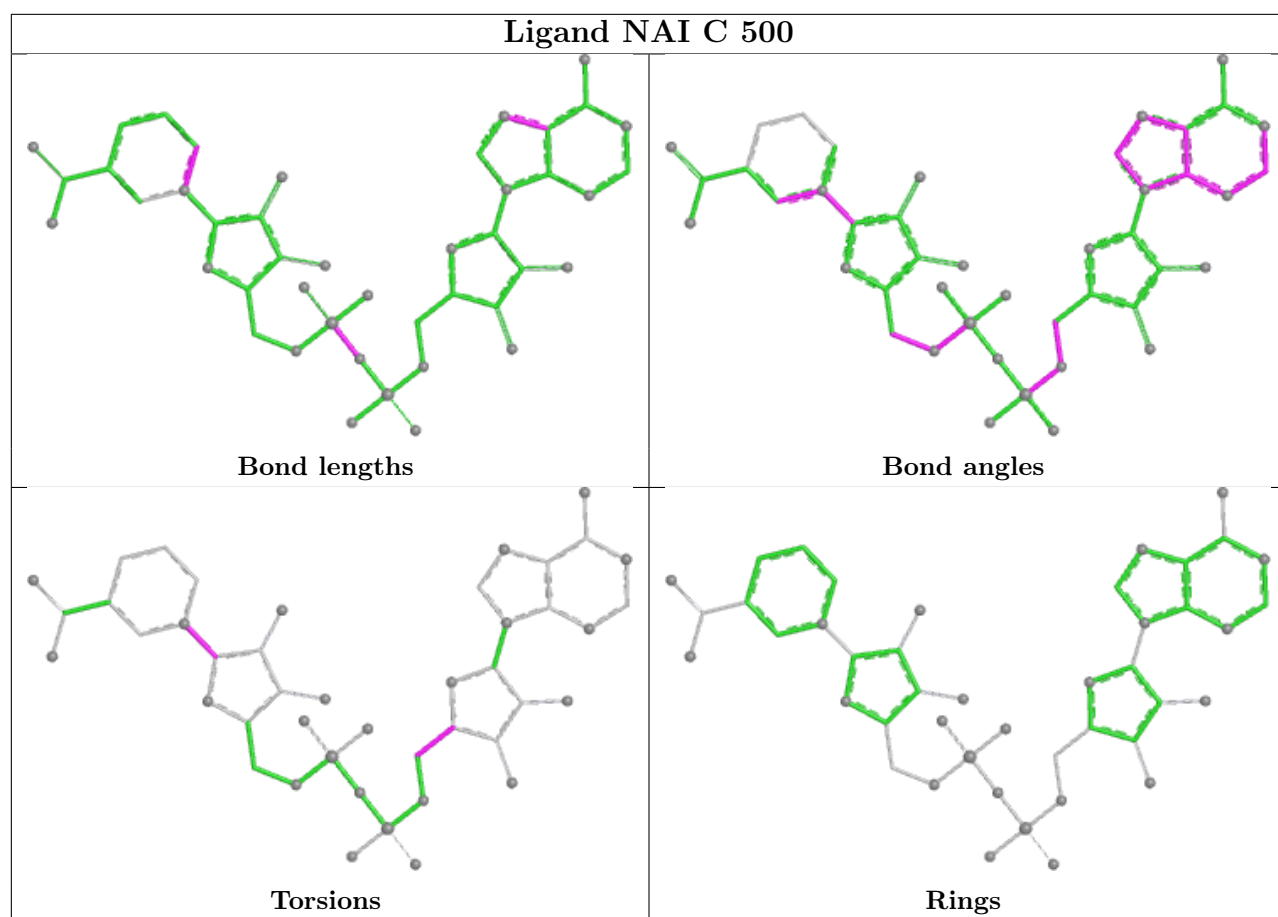
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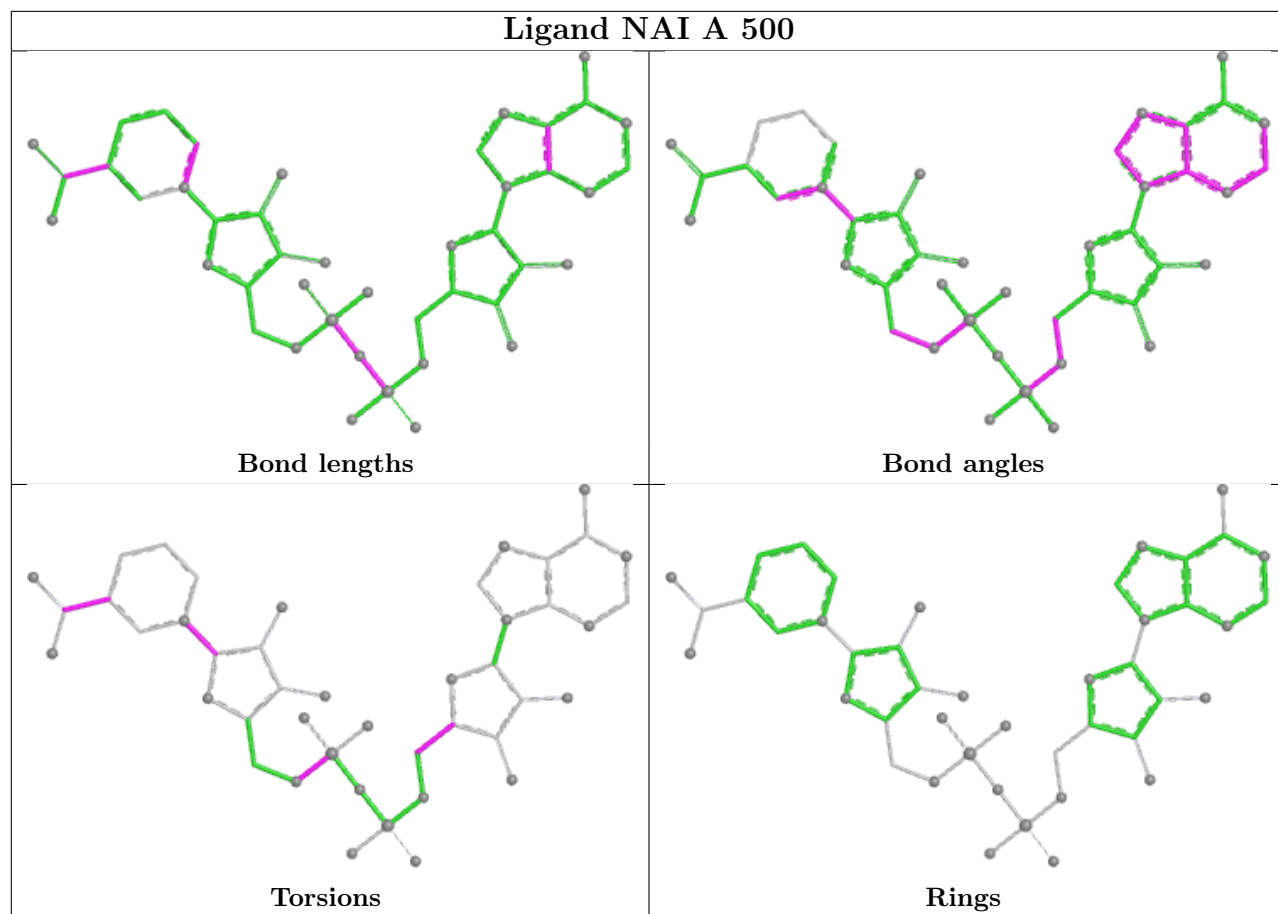
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 500 | NAI  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 401/411 (97%)   | 0.07   | 6 (1%) 72 65  | 29, 83, 127, 140      | 0     |
| 1   | B     | 401/411 (97%)   | -0.11  | 2 (0%) 87 85  | 32, 68, 100, 120      | 0     |
| 1   | C     | 401/411 (97%)   | 0.01   | 2 (0%) 87 85  | 38, 80, 121, 135      | 0     |
| 1   | D     | 401/411 (97%)   | -0.06  | 2 (0%) 87 85  | 35, 74, 112, 121      | 0     |
| All | All   | 1604/1644 (97%) | -0.02  | 12 (0%) 84 80 | 29, 76, 118, 140      | 0     |

All (12) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 2   | ALA  | 3.5  |
| 1   | B     | 367 | VAL  | 3.4  |
| 1   | A     | 96  | ILE  | 3.0  |
| 1   | D     | 285 | HIS  | 2.8  |
| 1   | A     | 88  | ALA  | 2.7  |
| 1   | C     | 70  | SER  | 2.7  |
| 1   | A     | 91  | THR  | 2.4  |
| 1   | C     | 120 | THR  | 2.3  |
| 1   | B     | 130 | VAL  | 2.2  |
| 1   | A     | 145 | VAL  | 2.1  |
| 1   | A     | 26  | TYR  | 2.0  |
| 1   | D     | 75  | VAL  | 2.0  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

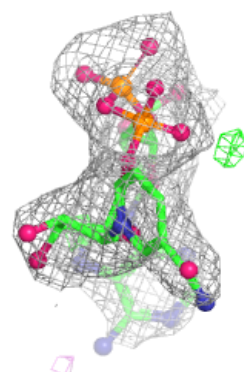
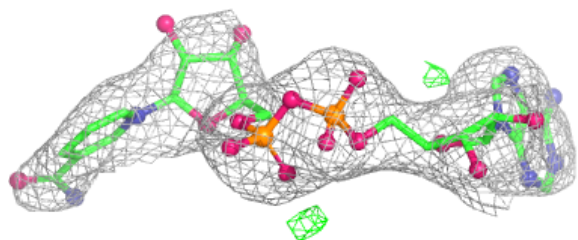
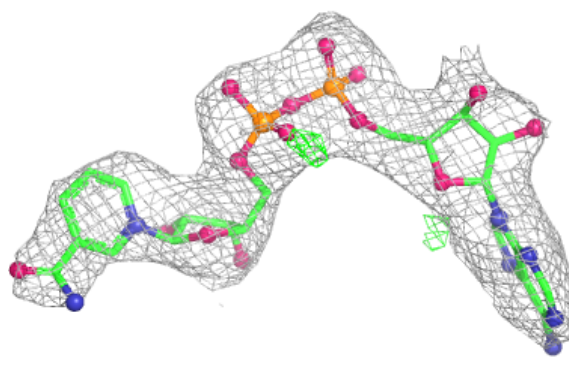
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | NAI  | B     | 500 | 44/44 | 0.93 | 0.09 | 65,72,86,89                | 0     |
| 2   | NAI  | D     | 500 | 44/44 | 0.93 | 0.09 | 58,69,78,81                | 0     |
| 2   | NAI  | C     | 500 | 44/44 | 0.94 | 0.09 | 55,74,88,94                | 0     |
| 2   | NAI  | A     | 500 | 44/44 | 0.94 | 0.08 | 58,75,86,86                | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

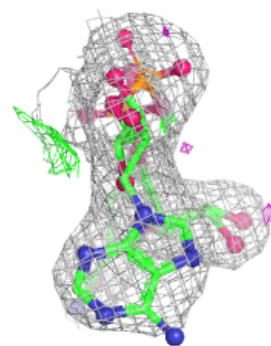
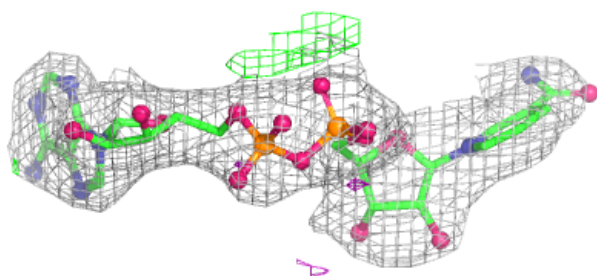
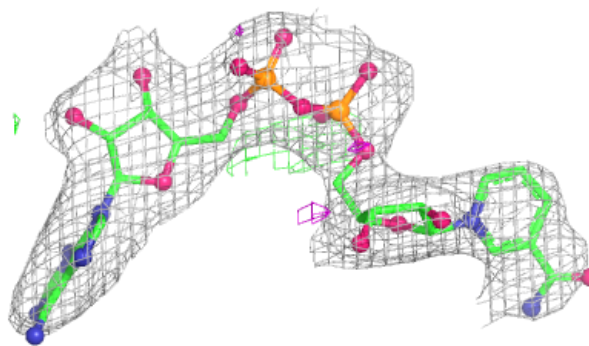
### Electron density around NAI B 500:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

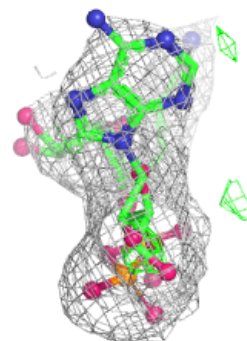
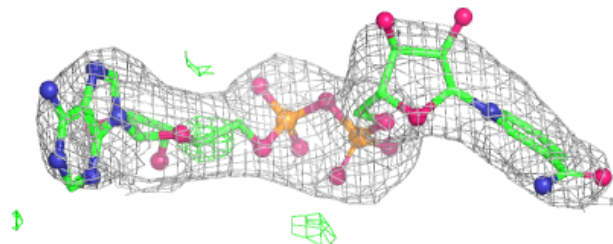
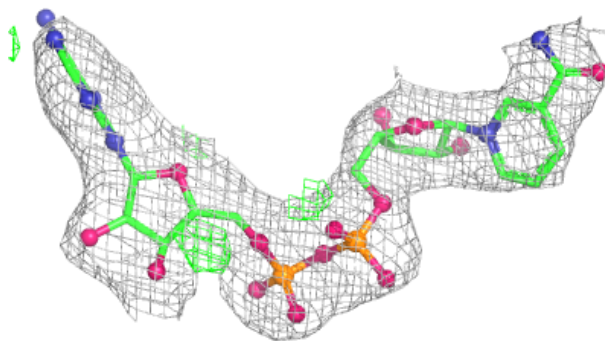


**Electron density around NAI D 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

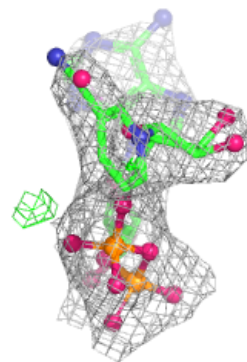
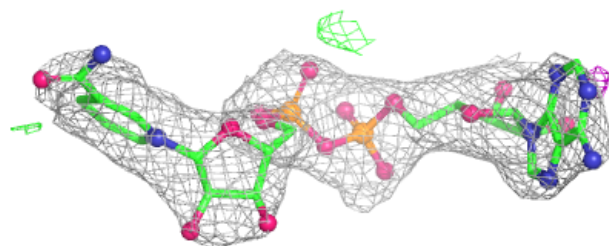
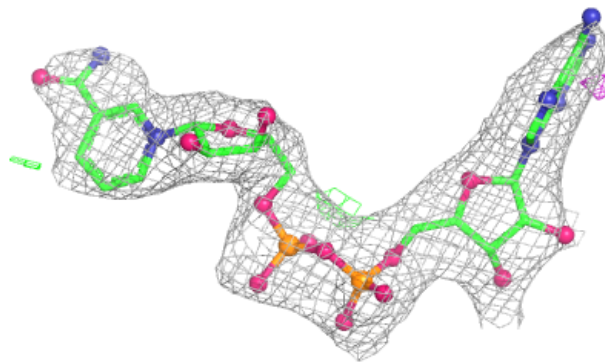
**Electron density around NAI C 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around NAI A 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.