



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:40 AM UTC

PDB ID : 2ZPA / pdb\_00002zpa  
Title : Crystal Structure of tRNA(Met) Cytidine Acetyltransferase  
Authors : Chimnaronk, S.; Manita, T.; Yao, M.; Tanaka, I.  
Deposited on : 2008-07-08  
Resolution : 2.35 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

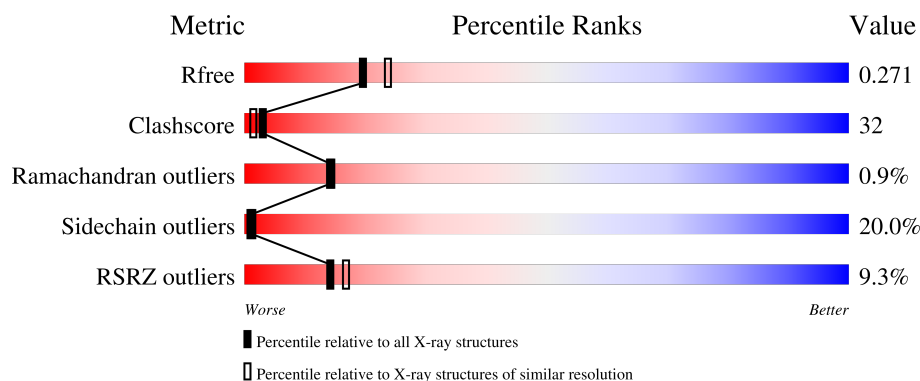
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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                      | 1596 (2.36-2.36)                                      |
| Clashscore            | 190562                      | 1663 (2.36-2.36)                                      |
| Ramachandran outliers | 187476                      | 1646 (2.36-2.36)                                      |
| Sidechain outliers    | 187428                      | 1646 (2.36-2.36)                                      |
| RSRZ outliers         | 180081                      | 1598 (2.36-2.36)                                      |

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     | 671    |                  |
| 1   | B     | 671    |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | ACO  | A     | 700 | X         | -        | -       | -                |
| 2   | ACO  | B     | 701 | X         | -        | -       | -                |

## 2 Entry composition [i](#)

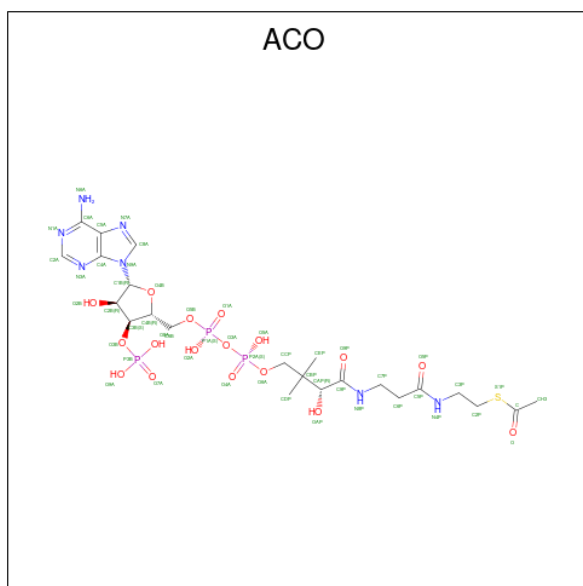
There are 5 unique types of molecules in this entry. The entry contains 10891 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uncharacterized protein ypfl.

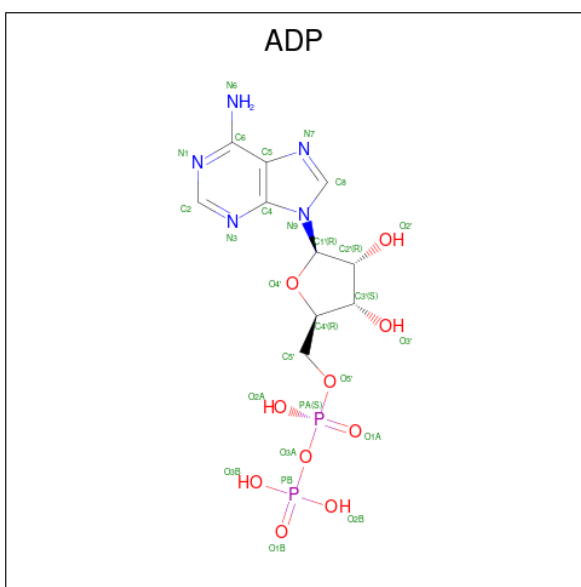
| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 1   | A     | 658      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 5189  | 3291 | 951 | 929 | 8 | 10 |         |         |       |
| 1   | B     | 662      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 5218  | 3309 | 955 | 935 | 8 | 11 |         |         |       |

- Molecule 2 is ACETYL COENZYME \*A (CCD ID: ACO) (formula:  $C_{23}H_{38}N_7O_{17}P_3S$ ).



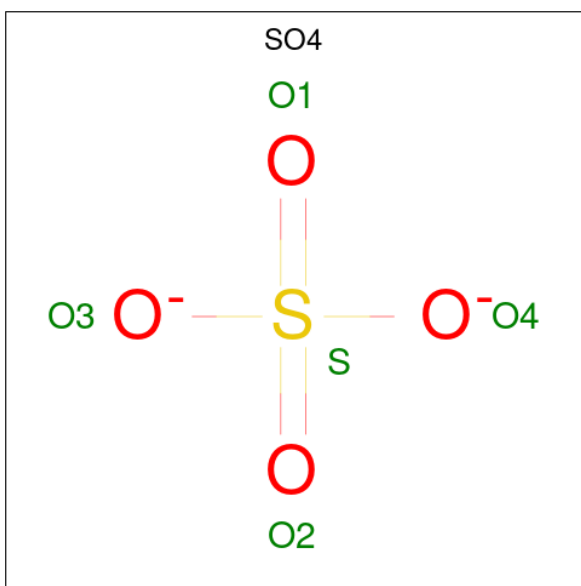
| Mol | Chain | Residues | Atoms |    |   |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 51    | 23 | 7 | 17 | 3 | 1 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 51    | 23 | 7 | 17 | 3 | 1 |         |         |

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula:  $\text{O}_4\text{S}$ ).

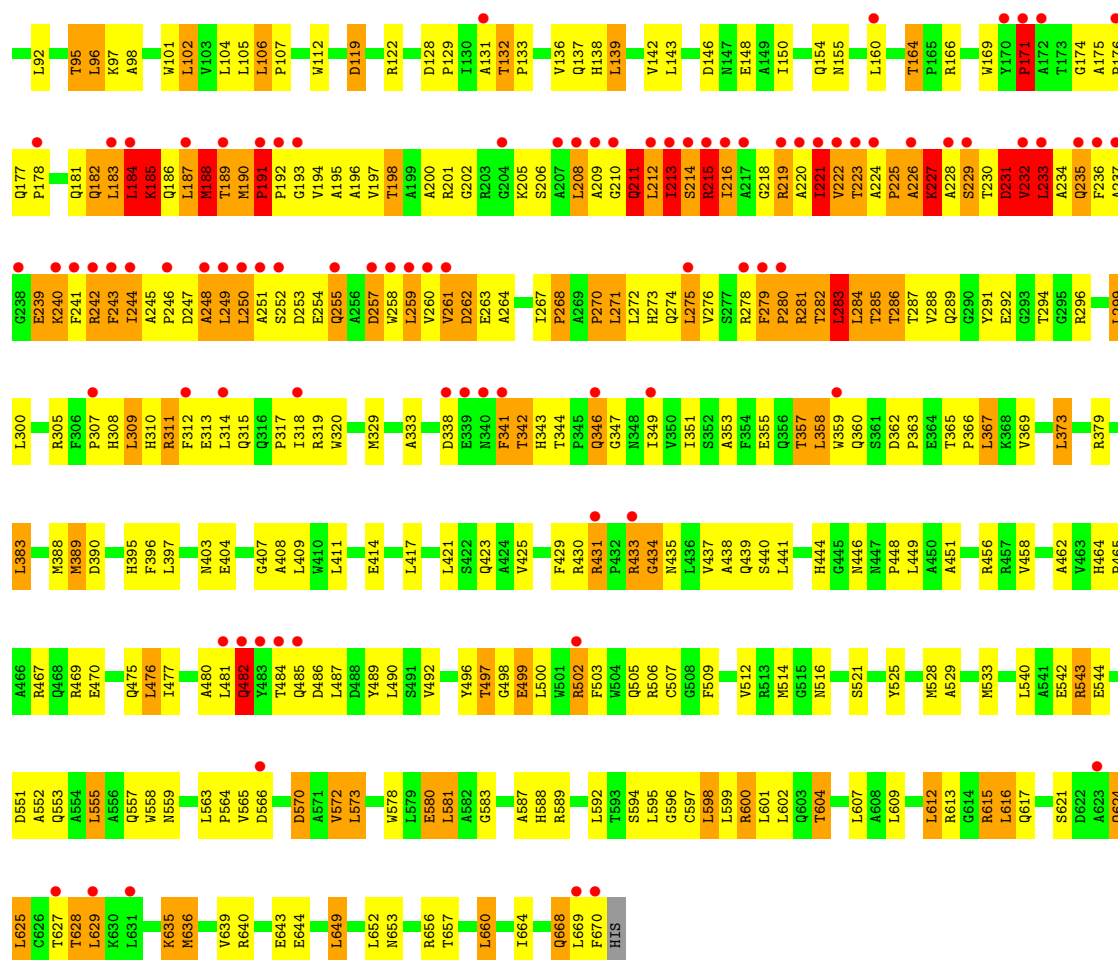


| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | A     | 224      | Total<br>224 | O<br>224 | 0       | 0       |
| 5   | B     | 126      | Total<br>126 | O<br>126 | 0       | 0       |





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 61.30Å 100.99Å 263.12Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 20.00 – 2.35<br>20.00 – 2.35                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.8 (20.00-2.35)<br>96.1 (20.00-2.35)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.06                                                        | Depositor        |
| $R_{sym}$                                                               | 0.06                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.49 (at 2.37Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.235 , 0.274<br>0.233 , 0.271                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5085 reflections (7.68%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 39.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.373                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 46.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 10891                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 47.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: SO4, ACO, ADP

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     | 0.60         | 1/5306 (0.0%)   | 1.13        | 38/7197 (0.5%)   |
| 1   | B     | 0.67         | 12/5335 (0.2%)  | 1.26        | 76/7236 (1.1%)   |
| All | All   | 0.64         | 13/10641 (0.1%) | 1.19        | 114/14433 (0.8%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | B     | 0                   | 2                   |
| All | All   | 0                   | 3                   |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 182 | GLN  | C-N   | 9.56  | 1.47        | 1.33     |
| 1   | B     | 617 | GLN  | N-CA  | 8.73  | 1.57        | 1.46     |
| 1   | B     | 184 | LEU  | C-N   | -7.56 | 1.23        | 1.33     |
| 1   | B     | 185 | LYS  | N-CA  | -7.36 | 1.36        | 1.46     |
| 1   | A     | 51  | SER  | CA-C  | 6.78  | 1.58        | 1.52     |
| 1   | B     | 184 | LEU  | N-CA  | 6.72  | 1.54        | 1.46     |
| 1   | B     | 186 | GLN  | C-N   | -6.33 | 1.24        | 1.34     |
| 1   | B     | 132 | THR  | CA-CB | 5.87  | 1.56        | 1.52     |
| 1   | B     | 231 | ASP  | N-CA  | 5.66  | 1.53        | 1.46     |
| 1   | B     | 188 | MSE  | SE-CE | -5.36 | 1.79        | 1.95     |
| 1   | B     | 190 | MSE  | SE-CE | -5.30 | 1.79        | 1.95     |
| 1   | B     | 215 | ARG  | CA-C  | -5.23 | 1.45        | 1.52     |
| 1   | B     | 270 | PRO  | CA-C  | -5.01 | 1.45        | 1.52     |

All (114) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | B     | 187 | LEU  | N-CA-C     | -18.19 | 87.57       | 112.30   |
| 1   | A     | 66  | GLN  | CA-C-N     | -16.20 | 96.65       | 122.73   |
| 1   | A     | 66  | GLN  | C-N-CA     | -16.20 | 96.65       | 122.73   |
| 1   | A     | 226 | ALA  | N-CA-C     | -14.45 | 89.08       | 110.46   |
| 1   | A     | 201 | ARG  | CD-NE-CZ   | 13.62  | 143.47      | 124.40   |
| 1   | A     | 143 | LEU  | N-CA-C     | -11.44 | 97.62       | 111.69   |
| 1   | B     | 668 | GLN  | OE1-CD-NE2 | -10.65 | 111.95      | 122.60   |
| 1   | B     | 213 | ILE  | CA-C-N     | -10.29 | 103.76      | 122.38   |
| 1   | B     | 213 | ILE  | C-N-CA     | -10.29 | 103.76      | 122.38   |
| 1   | B     | 49  | TRP  | N-CA-CB    | 10.26  | 126.86      | 110.65   |
| 1   | B     | 131 | ALA  | N-CA-C     | 10.23  | 122.51      | 111.36   |
| 1   | B     | 182 | GLN  | OE1-CD-NE2 | -10.21 | 112.39      | 122.60   |
| 1   | A     | 52  | PRO  | N-CA-C     | 10.18  | 127.17      | 111.19   |
| 1   | B     | 255 | GLN  | OE1-CD-NE2 | -10.15 | 112.45      | 122.60   |
| 1   | B     | 48  | LEU  | CA-C-N     | 10.14  | 137.88      | 123.07   |
| 1   | B     | 48  | LEU  | C-N-CA     | 10.14  | 137.88      | 123.07   |
| 1   | A     | 66  | GLN  | OE1-CD-NE2 | -9.79  | 112.81      | 122.60   |
| 1   | A     | 230 | THR  | N-CA-C     | -9.74  | 100.24      | 113.30   |
| 1   | A     | 289 | GLN  | OE1-CD-NE2 | -9.57  | 113.03      | 122.60   |
| 1   | B     | 186 | GLN  | OE1-CD-NE2 | -9.32  | 113.28      | 122.60   |
| 1   | B     | 190 | MSE  | N-CA-C     | 9.19   | 124.15      | 110.10   |
| 1   | B     | 211 | GLN  | OE1-CD-NE2 | -9.01  | 113.59      | 122.60   |
| 1   | B     | 55  | ASP  | N-CA-C     | 8.95   | 123.47      | 109.07   |
| 1   | B     | 360 | GLN  | N-CA-C     | -8.83  | 100.04      | 112.13   |
| 1   | B     | 185 | LYS  | CA-C-N     | -8.78  | 108.12      | 122.08   |
| 1   | B     | 185 | LYS  | C-N-CA     | -8.78  | 108.12      | 122.08   |
| 1   | B     | 191 | PRO  | CB-CA-C    | 8.77   | 121.62      | 110.92   |
| 1   | B     | 434 | GLY  | N-CA-C     | -8.36  | 98.62       | 112.83   |
| 1   | B     | 503 | PHE  | N-CA-C     | -7.96  | 102.55      | 111.14   |
| 1   | A     | 228 | ALA  | N-CA-C     | -7.93  | 99.93       | 110.24   |
| 1   | A     | 2   | ALA  | CA-C-N     | 7.85   | 131.44      | 120.29   |
| 1   | A     | 2   | ALA  | C-N-CA     | 7.85   | 131.44      | 120.29   |
| 1   | B     | 191 | PRO  | CA-C-N     | -7.77  | 111.75      | 119.90   |
| 1   | B     | 191 | PRO  | C-N-CA     | -7.77  | 111.75      | 119.90   |
| 1   | B     | 252 | SER  | N-CA-C     | 7.69   | 121.66      | 111.28   |
| 1   | B     | 191 | PRO  | N-CA-C     | -7.67  | 101.34      | 110.70   |
| 1   | B     | 226 | ALA  | N-CA-C     | -7.66  | 94.48       | 110.80   |
| 1   | B     | 243 | PHE  | N-CA-C     | 7.62   | 121.23      | 108.13   |
| 1   | B     | 54  | PRO  | N-CA-C     | -7.58  | 98.36       | 111.32   |
| 1   | B     | 228 | ALA  | N-CA-C     | -7.55  | 98.81       | 109.69   |
| 1   | B     | 66  | GLN  | N-CA-C     | 7.42   | 121.33      | 109.83   |
| 1   | B     | 164 | THR  | CA-C-N     | 7.38   | 127.83      | 119.93   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 164 | THR  | C-N-CA    | 7.38  | 127.83      | 119.93   |
| 1   | A     | 434 | GLY  | N-CA-C    | -7.13 | 100.70      | 112.83   |
| 1   | B     | 186 | GLN  | N-CA-C    | 7.13  | 123.65      | 113.02   |
| 1   | A     | 52  | PRO  | CA-N-CD   | -7.04 | 102.15      | 112.00   |
| 1   | B     | 668 | GLN  | CG-CD-NE2 | 6.96  | 126.85      | 116.40   |
| 1   | B     | 227 | LYS  | N-CA-C    | 6.93  | 125.57      | 110.80   |
| 1   | B     | 617 | GLN  | N-CA-C    | 6.90  | 122.04      | 112.45   |
| 1   | B     | 255 | GLN  | CG-CD-NE2 | 6.89  | 126.73      | 116.40   |
| 1   | A     | 289 | GLN  | CG-CD-NE2 | 6.83  | 126.64      | 116.40   |
| 1   | A     | 66  | GLN  | CG-CD-NE2 | 6.65  | 126.38      | 116.40   |
| 1   | B     | 231 | ASP  | CB-CA-C   | -6.61 | 100.51      | 110.88   |
| 1   | B     | 182 | GLN  | CG-CD-NE2 | 6.60  | 126.30      | 116.40   |
| 1   | B     | 482 | GLN  | N-CA-C    | 6.59  | 122.18      | 111.37   |
| 1   | A     | 575 | ASP  | N-CA-C    | -6.59 | 104.18      | 111.36   |
| 1   | B     | 343 | HIS  | CA-C-N    | 6.58  | 130.43      | 121.74   |
| 1   | B     | 343 | HIS  | C-N-CA    | 6.58  | 130.43      | 121.74   |
| 1   | A     | 142 | VAL  | CA-C-N    | 6.45  | 131.61      | 120.58   |
| 1   | A     | 142 | VAL  | C-N-CA    | 6.45  | 131.61      | 120.58   |
| 1   | B     | 211 | GLN  | CG-CD-NE2 | 6.37  | 125.96      | 116.40   |
| 1   | B     | 184 | LEU  | CA-C-N    | -6.34 | 109.42      | 121.54   |
| 1   | B     | 184 | LEU  | C-N-CA    | -6.34 | 109.42      | 121.54   |
| 1   | A     | 496 | TYR  | N-CA-C    | 6.32  | 119.80      | 109.76   |
| 1   | B     | 186 | GLN  | CG-CD-NE2 | 6.29  | 125.83      | 116.40   |
| 1   | A     | 483 | TYR  | N-CA-C    | 6.24  | 120.58      | 113.15   |
| 1   | B     | 270 | PRO  | CA-N-CD   | -6.22 | 103.29      | 112.00   |
| 1   | B     | 212 | LEU  | CA-C-N    | -6.19 | 110.82      | 121.97   |
| 1   | B     | 212 | LEU  | C-N-CA    | -6.19 | 110.82      | 121.97   |
| 1   | A     | 401 | GLY  | N-CA-C    | -6.14 | 103.20      | 112.41   |
| 1   | B     | 231 | ASP  | N-CA-C    | 6.11  | 117.61      | 111.07   |
| 1   | B     | 617 | GLN  | N-CA-CB   | -6.11 | 101.16      | 110.26   |
| 1   | B     | 213 | ILE  | CB-CA-C   | 6.10  | 121.29      | 111.29   |
| 1   | A     | 69  | LEU  | N-CA-C    | -6.04 | 97.94       | 110.80   |
| 1   | A     | 361 | SER  | N-CA-C    | 5.91  | 120.77      | 113.50   |
| 1   | B     | 213 | ILE  | O-C-N     | -5.88 | 115.22      | 122.57   |
| 1   | A     | 490 | LEU  | N-CA-C    | -5.85 | 99.87       | 109.40   |
| 1   | B     | 507 | CYS  | N-CA-C    | -5.76 | 106.30      | 113.38   |
| 1   | B     | 189 | THR  | N-CA-C    | -5.75 | 98.34       | 108.23   |
| 1   | B     | 248 | ALA  | N-CA-C    | -5.75 | 106.11      | 113.01   |
| 1   | B     | 273 | HIS  | N-CA-C    | 5.74  | 117.54      | 111.28   |
| 1   | B     | 389 | MSE  | N-CA-C    | 5.73  | 117.33      | 111.14   |
| 1   | A     | 143 | LEU  | N-CA-CB   | 5.72  | 118.73      | 110.20   |
| 1   | A     | 215 | ARG  | N-CA-C    | 5.67  | 120.31      | 113.17   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 52  | PRO  | CB-CA-C | -5.65 | 103.69      | 111.21   |
| 1   | B     | 171 | PRO  | CA-N-CD | -5.61 | 104.14      | 112.00   |
| 1   | B     | 251 | ALA  | N-CA-C  | -5.60 | 106.34      | 112.72   |
| 1   | B     | 102 | LEU  | N-CA-C  | -5.58 | 99.42       | 108.52   |
| 1   | A     | 495 | GLY  | N-CA-C  | -5.56 | 103.24      | 111.03   |
| 1   | A     | 113 | GLU  | N-CA-C  | 5.56  | 118.06      | 111.33   |
| 1   | A     | 433 | ARG  | N-CA-C  | 5.56  | 117.95      | 109.95   |
| 1   | B     | 281 | ARG  | N-CA-C  | 5.55  | 117.68      | 108.13   |
| 1   | B     | 70  | GLY  | N-CA-C  | -5.50 | 107.50      | 114.16   |
| 1   | B     | 230 | THR  | CA-C-N  | 5.44  | 127.52      | 120.44   |
| 1   | B     | 230 | THR  | C-N-CA  | 5.44  | 127.52      | 120.44   |
| 1   | B     | 174 | GLY  | N-CA-C  | -5.44 | 107.70      | 115.64   |
| 1   | A     | 67  | THR  | N-CA-CB | 5.41  | 118.76      | 110.70   |
| 1   | B     | 49  | TRP  | N-CA-C  | -5.38 | 98.61       | 108.02   |
| 1   | B     | 664 | ILE  | N-CA-C  | 5.38  | 115.58      | 110.42   |
| 1   | B     | 96  | LEU  | N-CA-C  | 5.31  | 117.41      | 108.96   |
| 1   | B     | 490 | LEU  | N-CA-C  | -5.31 | 101.22      | 109.72   |
| 1   | B     | 213 | ILE  | CA-C-O  | -5.31 | 114.15      | 120.78   |
| 1   | B     | 215 | ARG  | N-CA-C  | -5.30 | 99.50       | 110.80   |
| 1   | B     | 283 | LEU  | N-CA-C  | -5.25 | 99.96       | 108.52   |
| 1   | A     | 259 | LEU  | N-CA-C  | -5.24 | 99.97       | 108.52   |
| 1   | B     | 344 | THR  | N-CA-CB | 5.21  | 116.79      | 110.17   |
| 1   | A     | 51  | SER  | CA-C-N  | 5.21  | 124.97      | 119.76   |
| 1   | A     | 51  | SER  | C-N-CA  | 5.21  | 124.97      | 119.76   |
| 1   | B     | 270 | PRO  | CA-C-N  | 5.19  | 127.19      | 120.44   |
| 1   | B     | 270 | PRO  | C-N-CA  | 5.19  | 127.19      | 120.44   |
| 1   | A     | 263 | GLU  | N-CA-C  | -5.09 | 104.29      | 111.56   |
| 1   | A     | 261 | VAL  | N-CA-C  | 5.08  | 115.36      | 107.28   |
| 1   | A     | 347 | GLY  | N-CA-C  | 5.03  | 123.03      | 112.17   |
| 1   | B     | 433 | ARG  | N-CA-C  | 5.03  | 116.32      | 109.18   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 359 | TRP  | Mainchain |
| 1   | B     | 48  | LEU  | Peptide   |
| 1   | B     | 656 | ARG  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5189  | 0        | 5151     | 238     | 0            |
| 1   | B     | 5218  | 0        | 5183     | 426     | 0            |
| 2   | A     | 51    | 0        | 30       | 3       | 0            |
| 2   | B     | 51    | 0        | 33       | 7       | 0            |
| 3   | A     | 27    | 0        | 12       | 2       | 0            |
| 4   | B     | 5     | 0        | 0        | 1       | 0            |
| 5   | A     | 224   | 0        | 0        | 13      | 0            |
| 5   | B     | 126   | 0        | 0        | 8       | 0            |
| All | All   | 10891 | 0        | 10409    | 664     | 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 32.

All (664) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:67:THR:CG2   | 1:A:71:ARG:HD3   | 1.36                     | 1.51              |
| 1:B:185:LYS:HG3  | 1:B:215:ARG:NH2  | 1.51                     | 1.25              |
| 1:B:274:GLN:HB3  | 1:B:278:ARG:NH2  | 1.62                     | 1.14              |
| 1:B:221:ILE:HG23 | 1:B:259:LEU:HA   | 1.34                     | 1.08              |
| 1:B:215:ARG:NH1  | 1:B:215:ARG:HG3  | 1.60                     | 1.08              |
| 1:A:506:ARG:NH1  | 1:A:506:ARG:HG3  | 1.52                     | 1.08              |
| 1:A:67:THR:CG2   | 1:A:71:ARG:CD    | 2.31                     | 1.07              |
| 1:B:215:ARG:HG3  | 1:B:215:ARG:HH11 | 1.08                     | 1.07              |
| 1:A:250:LEU:HD13 | 1:A:278:ARG:HH22 | 1.18                     | 1.07              |
| 1:B:185:LYS:CG   | 1:B:215:ARG:HH21 | 1.66                     | 1.06              |
| 1:B:11:THR:HA    | 1:B:14:MSE:HE3   | 1.10                     | 1.05              |
| 1:B:184:LEU:HD11 | 1:B:211:GLN:HG2  | 1.38                     | 1.04              |
| 1:A:506:ARG:HH11 | 1:A:506:ARG:CG   | 1.70                     | 1.04              |
| 1:B:214:SER:HB2  | 1:B:240:LYS:HG3  | 1.38                     | 1.04              |
| 1:A:67:THR:HG21  | 1:A:71:ARG:CD    | 1.89                     | 1.03              |
| 1:B:185:LYS:HB2  | 1:B:215:ARG:HE   | 1.21                     | 1.03              |
| 1:A:506:ARG:HG3  | 1:A:506:ARG:HH11 | 0.89                     | 1.02              |
| 1:B:10:LEU:HG    | 1:B:14:MSE:HE2   | 1.41                     | 1.00              |
| 1:A:11:THR:HA    | 1:A:14:MSE:HE2   | 1.03                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:514:MSE:HE2  | 1:A:525:TYR:HB3  | 1.43                     | 1.00              |
| 1:B:192:PRO:HA   | 1:B:281:ARG:HG2  | 1.43                     | 1.00              |
| 1:B:458:VAL:HB   | 1:B:492:VAL:HG22 | 1.43                     | 0.98              |
| 1:A:67:THR:HG22  | 1:A:67:THR:O     | 1.63                     | 0.98              |
| 1:B:484:THR:HG23 | 1:B:533:MSE:HE1  | 1.44                     | 0.97              |
| 1:B:612:LEU:O    | 1:B:616:LEU:HD12 | 1.64                     | 0.97              |
| 1:B:359:TRP:CZ3  | 1:B:367:LEU:HD13 | 2.00                     | 0.96              |
| 1:A:67:THR:HG21  | 1:A:71:ARG:HD3   | 0.99                     | 0.96              |
| 1:B:497:THR:HG22 | 1:B:500:LEU:H    | 1.27                     | 0.96              |
| 1:B:11:THR:CA    | 1:B:14:MSE:HE3   | 1.95                     | 0.96              |
| 1:B:213:ILE:CG2  | 1:B:237:ALA:HB1  | 1.96                     | 0.95              |
| 1:B:185:LYS:CB   | 1:B:215:ARG:HE   | 1.81                     | 0.94              |
| 1:A:11:THR:HA    | 1:A:14:MSE:CE    | 1.98                     | 0.93              |
| 1:A:514:MSE:HE2  | 1:A:525:TYR:CB   | 1.99                     | 0.93              |
| 1:B:274:GLN:HB3  | 1:B:278:ARG:HH22 | 1.29                     | 0.92              |
| 1:B:264:ALA:CB   | 1:B:284:LEU:HD11 | 1.99                     | 0.91              |
| 1:B:184:LEU:HD11 | 1:B:211:GLN:CG   | 2.01                     | 0.91              |
| 1:B:274:GLN:CB   | 1:B:278:ARG:HH22 | 1.84                     | 0.90              |
| 1:A:250:LEU:HD22 | 1:A:278:ARG:HH21 | 1.36                     | 0.90              |
| 1:B:264:ALA:HB3  | 1:B:284:LEU:HD11 | 1.54                     | 0.89              |
| 1:B:346:GLN:HE21 | 1:B:346:GLN:HA   | 1.38                     | 0.88              |
| 1:B:500:LEU:HD21 | 2:B:701:ACO:H21  | 1.55                     | 0.88              |
| 2:A:700:ACO:H8A  | 2:A:700:ACO:O5B  | 1.73                     | 0.88              |
| 1:B:223:THR:HG23 | 1:B:246:PRO:HD3  | 1.56                     | 0.87              |
| 1:B:359:TRP:HZ3  | 1:B:367:LEU:HD13 | 1.36                     | 0.87              |
| 1:A:11:THR:CA    | 1:A:14:MSE:HE2   | 1.98                     | 0.87              |
| 1:B:274:GLN:CB   | 1:B:278:ARG:NH2  | 2.38                     | 0.87              |
| 1:B:185:LYS:HB2  | 1:B:215:ARG:NE   | 1.90                     | 0.86              |
| 1:A:226:ALA:HA   | 5:A:821:HOH:O    | 1.74                     | 0.86              |
| 1:A:67:THR:HG23  | 1:A:71:ARG:HD3   | 1.55                     | 0.85              |
| 1:B:430:ARG:HH11 | 1:B:670:PHE:HE1  | 1.24                     | 0.85              |
| 1:B:214:SER:CB   | 1:B:240:LYS:HG3  | 2.05                     | 0.85              |
| 1:B:365:THR:HB   | 1:B:366:PRO:HD3  | 1.55                     | 0.85              |
| 1:B:215:ARG:NH1  | 1:B:215:ARG:O    | 2.10                     | 0.85              |
| 1:B:262:ASP:HA   | 1:B:285:THR:HG23 | 1.59                     | 0.84              |
| 1:B:289:GLN:CG   | 1:B:296:ARG:HH11 | 1.91                     | 0.84              |
| 1:B:185:LYS:HG3  | 1:B:215:ARG:HH21 | 0.74                     | 0.84              |
| 1:B:573:LEU:HD22 | 1:B:604:THR:HG21 | 1.60                     | 0.83              |
| 1:B:215:ARG:HH11 | 1:B:215:ARG:C    | 1.87                     | 0.83              |
| 1:B:311:ARG:HH11 | 1:B:311:ARG:HG3  | 1.43                     | 0.83              |
| 1:B:11:THR:HA    | 1:B:14:MSE:CE    | 2.03                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:250:LEU:HD22 | 1:A:278:ARG:NH2  | 1.94                     | 0.83              |
| 1:A:634:ARG:NH1  | 1:A:638:LEU:HB2  | 1.93                     | 0.82              |
| 1:B:214:SER:C    | 1:B:216:ILE:H    | 1.87                     | 0.82              |
| 1:B:178:PRO:O    | 1:B:182:GLN:HG3  | 1.80                     | 0.82              |
| 1:A:621:SER:OG   | 1:A:624:GLN:HG3  | 1.80                     | 0.80              |
| 1:A:289:GLN:HG3  | 1:A:290:GLY:H    | 1.45                     | 0.80              |
| 1:A:198:THR:HG21 | 1:A:311:ARG:HH21 | 1.47                     | 0.80              |
| 1:B:7:LEU:HD13   | 1:B:160:LEU:CD2  | 2.12                     | 0.80              |
| 1:A:471:GLY:O    | 1:A:475:GLN:HG3  | 1.81                     | 0.80              |
| 1:B:244:ILE:HD11 | 1:B:248:ALA:HB3  | 1.64                     | 0.80              |
| 1:A:250:LEU:HA   | 1:A:278:ARG:NH2  | 1.97                     | 0.79              |
| 1:B:68:LEU:HG    | 1:B:71:ARG:HH12  | 1.46                     | 0.79              |
| 1:B:215:ARG:NH1  | 1:B:215:ARG:CG   | 2.40                     | 0.79              |
| 1:B:497:THR:HG23 | 1:B:499:GLU:HG3  | 1.64                     | 0.79              |
| 1:B:262:ASP:HA   | 1:B:285:THR:CG2  | 2.12                     | 0.79              |
| 1:A:67:THR:HG22  | 1:A:71:ARG:HD3   | 1.61                     | 0.79              |
| 1:B:259:LEU:HB3  | 1:B:282:THR:HG23 | 1.65                     | 0.79              |
| 1:A:441:LEU:HD13 | 1:A:528:MSE:HE1  | 1.63                     | 0.78              |
| 1:A:228:ALA:O    | 1:A:229:SER:C    | 2.26                     | 0.78              |
| 1:B:212:LEU:HD12 | 1:B:212:LEU:H    | 1.47                     | 0.78              |
| 1:B:289:GLN:CD   | 1:B:296:ARG:HH11 | 1.91                     | 0.78              |
| 1:B:497:THR:HG22 | 1:B:500:LEU:N    | 1.99                     | 0.78              |
| 1:B:183:LEU:O    | 1:B:183:LEU:HD22 | 1.83                     | 0.77              |
| 1:A:359:TRP:HZ3  | 1:A:367:LEU:HD13 | 1.48                     | 0.77              |
| 1:B:7:LEU:HD13   | 1:B:160:LEU:HD22 | 1.66                     | 0.77              |
| 1:B:190:MSE:HE2  | 1:B:258:TRP:CH2  | 2.19                     | 0.77              |
| 1:B:213:ILE:HB   | 1:B:237:ALA:CB   | 2.14                     | 0.77              |
| 1:B:215:ARG:O    | 1:B:215:ARG:CG   | 2.32                     | 0.77              |
| 1:B:329:MSE:HE2  | 1:B:333:ALA:HB2  | 1.67                     | 0.77              |
| 1:B:185:LYS:CE   | 1:B:189:THR:HA   | 2.15                     | 0.77              |
| 1:A:634:ARG:O    | 1:A:634:ARG:HD3  | 1.85                     | 0.76              |
| 1:B:215:ARG:NH1  | 1:B:216:ILE:HA   | 2.00                     | 0.76              |
| 1:B:213:ILE:CB   | 1:B:237:ALA:HB1  | 2.15                     | 0.76              |
| 1:B:275:LEU:CD2  | 1:B:279:PHE:HE2  | 2.00                     | 0.75              |
| 1:B:213:ILE:HB   | 1:B:237:ALA:HB1  | 1.66                     | 0.75              |
| 1:B:184:LEU:HD11 | 1:B:211:GLN:HB3  | 1.68                     | 0.74              |
| 1:A:250:LEU:HD13 | 1:A:278:ARG:NH2  | 2.00                     | 0.74              |
| 1:A:160:LEU:HD22 | 1:A:161:ALA:O    | 1.87                     | 0.74              |
| 1:A:634:ARG:HD2  | 5:A:913:HOH:O    | 1.88                     | 0.74              |
| 1:B:318:ILE:HD11 | 5:B:1017:HOH:O   | 1.87                     | 0.74              |
| 1:B:215:ARG:HG3  | 1:B:215:ARG:O    | 1.87                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:624:GLN:O    | 1:B:628:THR:HG22 | 1.88                     | 0.73              |
| 1:B:188:MSE:HE1  | 1:B:283:LEU:HG   | 1.71                     | 0.73              |
| 1:B:250:LEU:HD21 | 1:B:271:LEU:HD21 | 1.69                     | 0.73              |
| 1:B:214:SER:HB2  | 1:B:240:LYS:HZ3  | 1.51                     | 0.73              |
| 1:B:309:LEU:HD23 | 1:B:310:HIS:N    | 2.03                     | 0.72              |
| 1:B:184:LEU:HD11 | 1:B:211:GLN:CB   | 2.19                     | 0.72              |
| 1:B:221:ILE:CG2  | 1:B:259:LEU:HA   | 2.18                     | 0.72              |
| 1:B:215:ARG:HH11 | 1:B:215:ARG:CG   | 1.88                     | 0.72              |
| 1:B:213:ILE:O    | 1:B:216:ILE:HG22 | 1.90                     | 0.72              |
| 1:B:209:ALA:CB   | 1:B:233:LEU:HD21 | 2.20                     | 0.72              |
| 1:B:231:ASP:O    | 1:B:235:GLN:HB3  | 1.91                     | 0.71              |
| 1:A:437:VAL:HG13 | 1:A:528:MSE:HE3  | 1.73                     | 0.71              |
| 1:B:636:MSE:HG2  | 5:B:980:HOH:O    | 1.88                     | 0.71              |
| 1:A:402:GLU:C    | 1:A:403:ASN:HD22 | 1.99                     | 0.71              |
| 1:B:240:LYS:HD3  | 1:B:240:LYS:N    | 2.06                     | 0.71              |
| 1:A:227:LYS:HD3  | 1:A:230:THR:HG21 | 1.72                     | 0.71              |
| 1:B:185:LYS:HG3  | 1:B:215:ARG:CZ   | 2.21                     | 0.70              |
| 1:B:268:PRO:HD3  | 1:B:521:SER:O    | 1.90                     | 0.70              |
| 1:A:386:ARG:NH1  | 5:A:957:HOH:O    | 2.23                     | 0.70              |
| 1:A:28:GLU:HG3   | 1:A:154:GLN:OE1  | 1.91                     | 0.70              |
| 1:B:138:HIS:HB2  | 1:B:389:MSE:HE1  | 1.74                     | 0.70              |
| 1:B:581:LEU:HD13 | 1:B:597:CYS:SG   | 2.32                     | 0.69              |
| 1:B:373:LEU:HD13 | 1:B:408:ALA:HB3  | 1.74                     | 0.69              |
| 1:A:67:THR:CG2   | 1:A:67:THR:O     | 2.37                     | 0.69              |
| 1:A:506:ARG:NH1  | 1:A:506:ARG:CG   | 2.35                     | 0.69              |
| 1:B:435:ASN:O    | 1:B:439:GLN:HG2  | 1.92                     | 0.69              |
| 1:B:497:THR:CG2  | 1:B:500:LEU:H    | 2.02                     | 0.69              |
| 1:B:209:ALA:C    | 1:B:233:LEU:HD21 | 2.17                     | 0.69              |
| 1:B:214:SER:C    | 1:B:216:ILE:N    | 2.49                     | 0.69              |
| 1:B:215:ARG:HH12 | 1:B:216:ILE:HA   | 1.57                     | 0.69              |
| 1:B:185:LYS:HE3  | 1:B:189:THR:HA   | 1.73                     | 0.68              |
| 1:B:275:LEU:CD2  | 1:B:279:PHE:CE2  | 2.76                     | 0.68              |
| 1:B:188:MSE:HE3  | 1:B:258:TRP:HZ2  | 1.58                     | 0.68              |
| 1:B:213:ILE:HG21 | 1:B:237:ALA:HB1  | 1.75                     | 0.68              |
| 1:B:221:ILE:O    | 1:B:260:VAL:HG22 | 1.92                     | 0.68              |
| 1:B:222:VAL:HG13 | 1:B:242:ARG:O    | 1.94                     | 0.67              |
| 1:B:244:ILE:HD11 | 1:B:248:ALA:CB   | 2.24                     | 0.67              |
| 1:A:207:ALA:O    | 1:A:211:GLN:HG3  | 1.95                     | 0.67              |
| 1:A:347:GLY:O    | 1:A:467:ARG:NH1  | 2.22                     | 0.67              |
| 1:B:221:ILE:HD13 | 1:B:259:LEU:HG   | 1.74                     | 0.67              |
| 1:B:347:GLY:O    | 1:B:467:ARG:NH1  | 2.28                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:240:LYS:HD3  | 1:B:240:LYS:H    | 1.60                     | 0.67              |
| 1:A:263:GLU:OE2  | 1:A:287:THR:HG23 | 1.95                     | 0.67              |
| 1:B:208:LEU:HD13 | 1:B:208:LEU:C    | 2.20                     | 0.67              |
| 1:B:279:PHE:N    | 1:B:279:PHE:CD2  | 2.63                     | 0.67              |
| 1:B:67:THR:C     | 1:B:68:LEU:HD12  | 2.20                     | 0.66              |
| 1:B:469:ARG:NE   | 2:B:701:ACO:O2B  | 2.28                     | 0.66              |
| 1:B:184:LEU:O    | 1:B:212:LEU:HD21 | 1.93                     | 0.66              |
| 1:B:607:LEU:O    | 1:B:613:ARG:NH1  | 2.27                     | 0.66              |
| 1:B:259:LEU:O    | 1:B:282:THR:HA   | 1.95                     | 0.66              |
| 1:B:484:THR:CG2  | 1:B:533:MSE:HE1  | 2.21                     | 0.66              |
| 1:B:209:ALA:HB3  | 1:B:233:LEU:CD2  | 2.25                     | 0.66              |
| 1:B:184:LEU:CD1  | 1:B:211:GLN:HG2  | 2.21                     | 0.65              |
| 1:A:204:GLY:HA2  | 3:A:800:ADP:O1A  | 1.96                     | 0.65              |
| 1:B:185:LYS:HD3  | 1:B:189:THR:HA   | 1.77                     | 0.65              |
| 1:B:373:LEU:CD1  | 1:B:408:ALA:HB3  | 2.27                     | 0.65              |
| 1:A:286:THR:HG21 | 1:A:299:LEU:HD11 | 1.79                     | 0.65              |
| 1:B:259:LEU:HD23 | 1:B:260:VAL:N    | 2.12                     | 0.65              |
| 1:A:430:ARG:HG3  | 1:A:430:ARG:HH11 | 1.62                     | 0.65              |
| 1:B:249:LEU:HD13 | 1:B:249:LEU:C    | 2.21                     | 0.65              |
| 1:B:349:ILE:HD12 | 1:B:349:ILE:O    | 1.97                     | 0.65              |
| 1:B:213:ILE:HD12 | 1:B:220:ALA:HB3  | 1.78                     | 0.64              |
| 1:B:235:GLN:O    | 1:B:235:GLN:HG2  | 1.96                     | 0.64              |
| 1:B:14:MSE:HE1   | 1:B:101:TRP:CZ2  | 2.32                     | 0.64              |
| 1:B:259:LEU:HD11 | 1:B:275:LEU:HD13 | 1.79                     | 0.64              |
| 1:B:263:GLU:OE1  | 1:B:286:THR:HA   | 1.97                     | 0.64              |
| 1:B:188:MSE:HE1  | 1:B:283:LEU:CD2  | 2.28                     | 0.64              |
| 1:B:14:MSE:HE1   | 1:B:101:TRP:CE2  | 2.33                     | 0.64              |
| 1:B:512:VAL:HG13 | 1:B:544:GLU:HB3  | 1.80                     | 0.64              |
| 1:B:221:ILE:CD1  | 1:B:259:LEU:HG   | 2.29                     | 0.63              |
| 1:B:104:LEU:HG   | 1:B:106:LEU:HD13 | 1.79                     | 0.63              |
| 1:B:214:SER:HB2  | 1:B:240:LYS:CG   | 2.22                     | 0.63              |
| 1:A:199:ALA:HB3  | 1:A:205:LYS:HD3  | 1.80                     | 0.63              |
| 1:A:359:TRP:CZ2  | 1:A:366:PRO:HB2  | 2.34                     | 0.63              |
| 1:A:472:THR:HG23 | 5:A:887:HOH:O    | 1.99                     | 0.63              |
| 1:B:51:SER:O     | 1:B:53:ARG:N     | 2.32                     | 0.63              |
| 1:A:10:LEU:HD22  | 1:A:160:LEU:HD21 | 1.81                     | 0.63              |
| 1:B:128:ASP:HB3  | 1:B:129:PRO:HD2  | 1.78                     | 0.62              |
| 1:A:17:GLU:HB3   | 1:A:166:ARG:HG3  | 1.80                     | 0.62              |
| 1:A:72:GLU:HG2   | 1:A:319:ARG:HH12 | 1.65                     | 0.62              |
| 1:B:670:PHE:CD1  | 1:B:670:PHE:C    | 2.77                     | 0.62              |
| 1:B:28:GLU:HB3   | 5:B:1006:HOH:O   | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:96:LEU:HD21  | 1:A:102:LEU:HD23 | 1.80                     | 0.62              |
| 1:B:264:ALA:HB2  | 1:B:284:LEU:HD11 | 1.79                     | 0.62              |
| 1:B:223:THR:HA   | 1:B:243:PHE:CE1  | 2.34                     | 0.62              |
| 1:A:420:GLN:CD   | 1:A:420:GLN:H    | 2.07                     | 0.62              |
| 1:B:279:PHE:HB3  | 1:B:280:PRO:HD2  | 1.82                     | 0.62              |
| 1:B:196:ALA:CB   | 1:B:309:LEU:HD21 | 2.30                     | 0.62              |
| 1:A:437:VAL:O    | 1:A:441:LEU:HD22 | 2.00                     | 0.61              |
| 1:B:259:LEU:HB3  | 1:B:282:THR:CG2  | 2.30                     | 0.61              |
| 1:B:274:GLN:C    | 1:B:278:ARG:HH21 | 2.07                     | 0.61              |
| 1:B:44:PRO:HA    | 5:B:968:HOH:O    | 2.00                     | 0.61              |
| 1:A:227:LYS:HD3  | 1:A:230:THR:CG2  | 2.29                     | 0.61              |
| 1:B:275:LEU:HD23 | 1:B:279:PHE:HE2  | 1.65                     | 0.61              |
| 1:B:250:LEU:HD21 | 1:B:271:LEU:CD2  | 2.31                     | 0.61              |
| 1:B:311:ARG:HH11 | 1:B:311:ARG:CG   | 2.10                     | 0.61              |
| 1:A:44:PRO:HA    | 5:A:1013:HOH:O   | 1.98                     | 0.61              |
| 1:A:188:MSE:HE1  | 1:A:215:ARG:O    | 2.01                     | 0.61              |
| 1:B:292:GLU:N    | 1:B:292:GLU:OE2  | 2.34                     | 0.61              |
| 1:B:482:GLN:OE1  | 1:B:482:GLN:HA   | 1.99                     | 0.61              |
| 1:A:635:LYS:CD   | 1:A:635:LYS:H    | 2.14                     | 0.60              |
| 1:B:138:HIS:CB   | 1:B:389:MSE:HE1  | 2.31                     | 0.60              |
| 1:B:351:ILE:HD12 | 1:B:476:LEU:HD13 | 1.81                     | 0.60              |
| 1:A:280:PRO:HD3  | 5:A:1004:HOH:O   | 2.01                     | 0.60              |
| 1:B:403:ASN:O    | 1:B:404:GLU:HG2  | 2.01                     | 0.60              |
| 1:A:437:VAL:HG13 | 1:A:528:MSE:CE   | 2.31                     | 0.60              |
| 1:B:48:LEU:HG    | 1:B:49:TRP:N     | 2.08                     | 0.60              |
| 1:B:190:MSE:C    | 1:B:191:PRO:O    | 2.41                     | 0.60              |
| 1:B:296:ARG:NH2  | 1:B:341:PHE:CE2  | 2.68                     | 0.60              |
| 1:B:497:THR:CG2  | 1:B:499:GLU:HG3  | 2.29                     | 0.60              |
| 1:B:621:SER:O    | 1:B:625:LEU:HD22 | 2.01                     | 0.60              |
| 1:A:250:LEU:HA   | 1:A:278:ARG:HH21 | 1.65                     | 0.60              |
| 1:A:372:LEU:HD22 | 1:A:405:ILE:HG22 | 1.83                     | 0.60              |
| 1:A:539:GLN:O    | 1:A:543:ARG:HB2  | 2.01                     | 0.60              |
| 1:B:209:ALA:HB3  | 1:B:233:LEU:HD21 | 1.84                     | 0.60              |
| 1:B:214:SER:HB2  | 1:B:240:LYS:NZ   | 2.16                     | 0.60              |
| 1:B:215:ARG:HH12 | 1:B:216:ILE:CA   | 2.15                     | 0.60              |
| 1:B:359:TRP:HZ3  | 1:B:367:LEU:CD1  | 2.11                     | 0.60              |
| 1:B:506:ARG:HG3  | 1:B:506:ARG:HH11 | 1.67                     | 0.60              |
| 1:B:649:LEU:HB3  | 1:B:657:THR:HG21 | 1.82                     | 0.60              |
| 1:B:430:ARG:NH1  | 1:B:670:PHE:HE1  | 1.95                     | 0.60              |
| 1:B:185:LYS:CD   | 1:B:189:THR:HA   | 2.32                     | 0.60              |
| 1:B:600:ARG:O    | 1:B:604:THR:HG22 | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:373:LEU:CD1  | 1:A:408:ALA:HB3  | 2.32                     | 0.59              |
| 1:B:200:ALA:HA   | 1:B:288:VAL:O    | 2.02                     | 0.59              |
| 1:B:215:ARG:NH1  | 1:B:216:ILE:CA   | 2.65                     | 0.59              |
| 1:B:341:PHE:CD1  | 1:B:342:THR:N    | 2.70                     | 0.59              |
| 1:B:258:TRP:HA   | 1:B:281:ARG:O    | 2.02                     | 0.59              |
| 1:B:264:ALA:HB3  | 1:B:284:LEU:CD1  | 2.30                     | 0.59              |
| 1:A:359:TRP:CZ3  | 1:A:367:LEU:HD13 | 2.35                     | 0.59              |
| 1:A:481:LEU:HD12 | 1:A:533:MSE:HE3  | 1.85                     | 0.59              |
| 1:B:225:PRO:O    | 1:B:227:LYS:N    | 2.35                     | 0.59              |
| 1:B:244:ILE:CG2  | 1:B:249:LEU:HD23 | 2.32                     | 0.59              |
| 1:B:276:VAL:HG12 | 1:B:276:VAL:O    | 2.01                     | 0.59              |
| 1:B:437:VAL:HG13 | 1:B:528:MSE:HE3  | 1.85                     | 0.59              |
| 1:A:67:THR:HG22  | 1:A:71:ARG:HB2   | 1.85                     | 0.59              |
| 1:B:80:ALA:HA    | 1:B:83:GLY:O     | 2.02                     | 0.59              |
| 1:B:639:VAL:O    | 1:B:643:GLU:HG3  | 2.02                     | 0.59              |
| 1:A:635:LYS:HD2  | 5:A:822:HOH:O    | 2.03                     | 0.58              |
| 1:B:222:VAL:HB   | 1:B:260:VAL:CG2  | 2.31                     | 0.58              |
| 1:B:188:MSE:HE1  | 1:B:283:LEU:CG   | 2.33                     | 0.58              |
| 1:A:634:ARG:HD3  | 1:A:634:ARG:C    | 2.28                     | 0.58              |
| 1:B:225:PRO:HG3  | 1:B:267:ILE:HG13 | 1.86                     | 0.58              |
| 1:A:514:MSE:HE2  | 1:A:525:TYR:HB2  | 1.83                     | 0.58              |
| 1:B:184:LEU:HD23 | 1:B:212:LEU:HG   | 1.85                     | 0.58              |
| 1:B:635:LYS:O    | 1:B:639:VAL:HG23 | 2.04                     | 0.58              |
| 1:A:629:LEU:HB3  | 1:A:631:LEU:CD2  | 2.34                     | 0.58              |
| 1:B:261:VAL:HG22 | 1:B:264:ALA:HB2  | 1.85                     | 0.58              |
| 1:B:467:ARG:HD2  | 1:B:470:GLU:OE2  | 2.04                     | 0.58              |
| 1:B:261:VAL:CG2  | 1:B:264:ALA:HB2  | 2.34                     | 0.57              |
| 1:B:296:ARG:NH2  | 1:B:341:PHE:CZ   | 2.71                     | 0.57              |
| 1:B:484:THR:O    | 1:B:485:GLN:HG3  | 2.03                     | 0.57              |
| 1:A:68:LEU:HD12  | 1:A:68:LEU:H     | 1.69                     | 0.57              |
| 1:B:214:SER:O    | 1:B:216:ILE:N    | 2.37                     | 0.57              |
| 1:B:396:PHE:O    | 1:B:397:LEU:HD22 | 2.04                     | 0.57              |
| 1:A:69:LEU:HD11  | 1:A:71:ARG:HD2   | 1.85                     | 0.57              |
| 1:B:195:ALA:HB1  | 1:B:312:PHE:HE2  | 1.68                     | 0.57              |
| 1:B:220:ALA:C    | 1:B:221:ILE:HG22 | 2.29                     | 0.57              |
| 1:B:222:VAL:HA   | 1:B:260:VAL:O    | 2.04                     | 0.57              |
| 1:B:222:VAL:CG1  | 1:B:242:ARG:O    | 2.52                     | 0.57              |
| 1:B:359:TRP:CH2  | 1:B:367:LEU:HD13 | 2.38                     | 0.57              |
| 1:B:194:VAL:HG13 | 1:B:282:THR:OG1  | 2.05                     | 0.56              |
| 1:B:244:ILE:HG23 | 1:B:249:LEU:HD23 | 1.86                     | 0.56              |
| 1:A:14:MSE:HE1   | 1:A:101:TRP:NE1  | 2.20                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:50:ILE:HG21  | 1:A:92:LEU:HD22  | 1.86                     | 0.56              |
| 1:A:176:PRO:HG2  | 1:A:181:GLN:NE2  | 2.20                     | 0.56              |
| 1:B:189:THR:O    | 1:B:189:THR:OG1  | 2.22                     | 0.56              |
| 1:B:209:ALA:C    | 1:B:233:LEU:CD2  | 2.79                     | 0.56              |
| 1:B:259:LEU:HD23 | 1:B:260:VAL:H    | 1.68                     | 0.56              |
| 1:B:594:SER:O    | 1:B:598:LEU:HB2  | 2.05                     | 0.56              |
| 1:A:402:GLU:C    | 1:A:403:ASN:ND2  | 2.63                     | 0.56              |
| 1:B:185:LYS:HA   | 1:B:188:MSE:HB3  | 1.86                     | 0.56              |
| 1:A:345:PRO:HG2  | 1:A:467:ARG:HG3  | 1.88                     | 0.56              |
| 1:A:619:ASN:HB3  | 5:A:990:HOH:O    | 2.05                     | 0.56              |
| 1:A:67:THR:HG21  | 1:A:71:ARG:HH11  | 1.70                     | 0.56              |
| 1:A:634:ARG:HH11 | 1:A:638:LEU:HB2  | 1.67                     | 0.56              |
| 1:B:132:THR:HB   | 1:B:390:ASP:OD2  | 2.06                     | 0.56              |
| 1:A:516:ASN:HD21 | 1:A:555:LEU:HD12 | 1.71                     | 0.56              |
| 1:B:341:PHE:CE1  | 1:B:342:THR:HG23 | 2.41                     | 0.56              |
| 1:B:13:GLN:O     | 1:B:17:GLU:HG3   | 2.05                     | 0.55              |
| 1:B:245:ALA:HB1  | 1:B:246:PRO:HD2  | 1.89                     | 0.55              |
| 1:B:363:PRO:O    | 1:B:367:LEU:HD22 | 2.07                     | 0.55              |
| 1:A:13:GLN:O     | 1:A:17:GLU:HG3   | 2.06                     | 0.55              |
| 1:A:282:THR:HG22 | 1:A:284:LEU:HD13 | 1.89                     | 0.55              |
| 1:A:213:ILE:HG23 | 1:A:220:ALA:HB3  | 1.88                     | 0.55              |
| 1:B:246:PRO:O    | 1:B:249:LEU:HB3  | 2.06                     | 0.55              |
| 1:A:25:LEU:HD12  | 1:A:152:TRP:HB3  | 1.87                     | 0.55              |
| 1:A:309:LEU:HD13 | 1:A:310:HIS:N    | 2.21                     | 0.55              |
| 1:A:318:ILE:HD12 | 1:A:318:ILE:O    | 2.07                     | 0.55              |
| 1:A:430:ARG:HG3  | 1:A:430:ARG:NH1  | 2.21                     | 0.55              |
| 1:B:257:ASP:O    | 1:B:280:PRO:HG2  | 2.07                     | 0.55              |
| 1:B:68:LEU:HD12  | 1:B:68:LEU:N     | 2.22                     | 0.55              |
| 1:B:551:ASP:OD2  | 1:B:596:GLY:HA3  | 2.06                     | 0.54              |
| 1:A:382:PRO:O    | 1:A:386:ARG:HG2  | 2.06                     | 0.54              |
| 1:B:469:ARG:HD3  | 2:B:701:ACO:C8A  | 2.37                     | 0.54              |
| 1:B:190:MSE:SE   | 1:B:310:HIS:HD2  | 2.40                     | 0.54              |
| 1:A:66:GLN:HB3   | 1:A:68:LEU:HD12  | 1.88                     | 0.54              |
| 1:A:223:THR:HG22 | 1:A:261:VAL:HG22 | 1.89                     | 0.54              |
| 1:A:369:VAL:HG12 | 1:A:373:LEU:HD22 | 1.90                     | 0.54              |
| 1:A:629:LEU:HB3  | 1:A:631:LEU:HD21 | 1.89                     | 0.54              |
| 1:B:92:LEU:O     | 1:B:95:THR:HG22  | 2.07                     | 0.54              |
| 1:B:423:GLN:HE21 | 1:B:449:LEU:HD11 | 1.73                     | 0.54              |
| 1:B:506:ARG:NE   | 1:B:506:ARG:HA   | 2.22                     | 0.54              |
| 1:B:274:GLN:CA   | 1:B:278:ARG:NH2  | 2.70                     | 0.54              |
| 1:B:500:LEU:CD2  | 2:B:701:ACO:H21  | 2.35                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:247:ASP:HB2  | 5:A:989:HOH:O    | 2.08                     | 0.54              |
| 1:A:110:GLU:OE2  | 1:A:153:ARG:NH2  | 2.42                     | 0.53              |
| 1:B:14:MSE:HE1   | 1:B:101:TRP:NE1  | 2.24                     | 0.53              |
| 1:B:107:PRO:HB3  | 5:B:927:HOH:O    | 2.08                     | 0.53              |
| 1:B:72:GLU:HB2   | 1:B:97:LYS:HG3   | 1.90                     | 0.53              |
| 1:B:139:LEU:O    | 1:B:143:LEU:HG   | 2.08                     | 0.53              |
| 1:B:467:ARG:NH2  | 1:B:470:GLU:OE1  | 2.41                     | 0.53              |
| 1:A:373:LEU:HD13 | 1:A:408:ALA:HB3  | 1.89                     | 0.53              |
| 1:B:506:ARG:HG3  | 1:B:506:ARG:NH1  | 2.24                     | 0.53              |
| 1:B:213:ILE:HB   | 1:B:237:ALA:HB2  | 1.88                     | 0.53              |
| 1:A:67:THR:HA    | 1:A:69:LEU:HD21  | 1.90                     | 0.53              |
| 1:A:502:ARG:HH22 | 1:B:1:MSE:N      | 2.06                     | 0.53              |
| 1:B:195:ALA:O    | 1:B:284:LEU:N    | 2.38                     | 0.53              |
| 1:A:216:ILE:O    | 1:A:240:LYS:NZ   | 2.42                     | 0.53              |
| 1:A:444:HIS:HD2  | 1:A:593:THR:OG1  | 1.91                     | 0.53              |
| 1:B:259:LEU:CD2  | 1:B:260:VAL:N    | 2.72                     | 0.53              |
| 1:B:299:LEU:HD13 | 1:B:299:LEU:O    | 2.09                     | 0.53              |
| 1:A:68:LEU:HD13  | 1:A:68:LEU:C     | 2.33                     | 0.53              |
| 1:B:72:GLU:HB2   | 1:B:97:LYS:CG    | 2.38                     | 0.53              |
| 1:B:221:ILE:HG12 | 1:B:222:VAL:N    | 2.24                     | 0.53              |
| 1:B:358:LEU:HD13 | 1:B:362:ASP:HB3  | 1.91                     | 0.53              |
| 1:B:294:THR:HG21 | 1:B:299:LEU:HD23 | 1.89                     | 0.53              |
| 1:A:198:THR:HG21 | 1:A:311:ARG:NH2  | 2.21                     | 0.53              |
| 1:A:502:ARG:NH2  | 1:B:1:MSE:N      | 2.57                     | 0.53              |
| 1:B:7:LEU:HD13   | 1:B:160:LEU:HD21 | 1.89                     | 0.53              |
| 1:A:635:LYS:H    | 1:A:635:LYS:HD2  | 1.74                     | 0.52              |
| 1:B:202:GLY:O    | 1:B:317:PRO:HA   | 2.10                     | 0.52              |
| 1:A:250:LEU:CA   | 1:A:278:ARG:NH2  | 2.72                     | 0.52              |
| 1:B:215:ARG:O    | 1:B:215:ARG:CD   | 2.58                     | 0.52              |
| 1:B:649:LEU:HB3  | 1:B:657:THR:CG2  | 2.39                     | 0.52              |
| 1:A:289:GLN:HG3  | 1:A:290:GLY:N    | 2.21                     | 0.52              |
| 1:B:311:ARG:CG   | 1:B:311:ARG:NH1  | 2.72                     | 0.52              |
| 1:A:162:HIS:ND1  | 1:A:162:HIS:N    | 2.56                     | 0.52              |
| 1:B:198:THR:HB   | 1:B:286:THR:HG22 | 1.92                     | 0.52              |
| 1:A:34:GLU:O     | 1:A:38:LYS:HG3   | 2.10                     | 0.52              |
| 1:B:176:PRO:HB3  | 1:B:211:GLN:OE1  | 2.09                     | 0.52              |
| 1:B:249:LEU:CD1  | 1:B:275:LEU:HG   | 2.40                     | 0.52              |
| 1:A:68:LEU:HD13  | 1:A:68:LEU:O     | 2.09                     | 0.51              |
| 1:A:139:LEU:O    | 1:A:143:LEU:HB2  | 2.10                     | 0.51              |
| 1:A:514:MSE:HE3  | 1:A:526:THR:O    | 2.10                     | 0.51              |
| 1:B:16:ARG:HG2   | 1:B:16:ARG:HH21  | 1.75                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:233:LEU:C    | 1:B:233:LEU:HD13 | 2.35                     | 0.51              |
| 1:B:583:GLY:O    | 1:B:587:ALA:HB3  | 2.11                     | 0.51              |
| 1:A:23:LEU:CD1   | 1:A:25:LEU:HD13  | 2.40                     | 0.51              |
| 1:A:67:THR:HG21  | 1:A:71:ARG:NH1   | 2.26                     | 0.51              |
| 1:A:177:GLN:HB3  | 1:A:178:PRO:HD2  | 1.93                     | 0.51              |
| 1:B:395:HIS:NE2  | 1:B:456:ARG:NH2  | 2.58                     | 0.51              |
| 1:A:289:GLN:CG   | 1:A:290:GLY:H    | 2.22                     | 0.51              |
| 1:A:484:THR:HG22 | 1:A:485:GLN:N    | 2.25                     | 0.51              |
| 1:B:175:ALA:HB1  | 1:B:176:PRO:HD2  | 1.93                     | 0.51              |
| 1:B:10:LEU:C     | 1:B:14:MSE:HE2   | 2.36                     | 0.51              |
| 1:B:512:VAL:HG13 | 1:B:544:GLU:CB   | 2.41                     | 0.51              |
| 1:A:328:LYS:O    | 1:A:332:GLU:HG3  | 2.10                     | 0.50              |
| 1:B:196:ALA:HB3  | 1:B:309:LEU:HD21 | 1.94                     | 0.50              |
| 1:B:341:PHE:HD1  | 1:B:342:THR:H    | 1.60                     | 0.50              |
| 1:B:225:PRO:O    | 1:B:226:ALA:C    | 2.52                     | 0.50              |
| 1:B:489:TYR:HA   | 1:B:533:MSE:HG3  | 1.92                     | 0.50              |
| 1:A:513:ARG:NH2  | 5:A:961:HOH:O    | 2.43                     | 0.50              |
| 1:B:205:LYS:O    | 1:B:208:LEU:HB3  | 2.10                     | 0.50              |
| 1:B:222:VAL:HG11 | 1:B:241:PHE:CD1  | 2.46                     | 0.50              |
| 1:A:437:VAL:HG23 | 1:A:457:ARG:HD3  | 1.93                     | 0.50              |
| 1:A:636:MSE:HG3  | 5:A:803:HOH:O    | 2.11                     | 0.50              |
| 1:A:442:ALA:O    | 1:A:589:ARG:NH2  | 2.45                     | 0.50              |
| 1:B:223:THR:HG23 | 1:B:224:ALA:N    | 2.26                     | 0.50              |
| 1:B:621:SER:OG   | 1:B:624:GLN:HB2  | 2.11                     | 0.50              |
| 1:A:23:LEU:HD22  | 1:A:150:ILE:HB   | 1.93                     | 0.50              |
| 1:B:552:ALA:HA   | 1:B:563:LEU:HD22 | 1.93                     | 0.50              |
| 1:B:208:LEU:C    | 1:B:208:LEU:CD1  | 2.85                     | 0.49              |
| 1:B:250:LEU:O    | 1:B:250:LEU:CD1  | 2.60                     | 0.49              |
| 1:B:262:ASP:OD1  | 1:B:285:THR:HG21 | 2.12                     | 0.49              |
| 1:B:485:GLN:O    | 1:B:486:ASP:HB3  | 2.12                     | 0.49              |
| 1:B:486:ASP:OD1  | 1:B:486:ASP:O    | 2.30                     | 0.49              |
| 1:A:252:SER:HB2  | 1:A:254:GLU:OE2  | 2.12                     | 0.49              |
| 1:A:467:ARG:HA   | 1:A:470:GLU:OE2  | 2.12                     | 0.49              |
| 1:B:184:LEU:CD1  | 1:B:211:GLN:HB3  | 2.39                     | 0.49              |
| 1:B:185:LYS:CG   | 1:B:215:ARG:HE   | 2.25                     | 0.49              |
| 1:B:612:LEU:C    | 1:B:616:LEU:HD12 | 2.35                     | 0.49              |
| 1:B:112:TRP:CD2  | 1:B:136:VAL:HG13 | 2.47                     | 0.49              |
| 1:B:222:VAL:HG11 | 1:B:241:PHE:CE1  | 2.46                     | 0.49              |
| 1:A:72:GLU:HG2   | 1:A:319:ARG:NH1  | 2.27                     | 0.49              |
| 1:B:132:THR:HA   | 1:B:390:ASP:CG   | 2.37                     | 0.49              |
| 1:B:119:ASP:OD2  | 1:B:122:ARG:NH1  | 2.45                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:201:ARG:NH1  | 1:B:291:TYR:O    | 2.45                     | 0.49              |
| 1:A:500:LEU:HD21 | 2:A:700:ACO:H22  | 1.94                     | 0.49              |
| 1:B:205:LYS:HE3  | 1:B:287:THR:OG1  | 2.13                     | 0.49              |
| 1:A:119:ASP:OD2  | 1:A:122:ARG:NH1  | 2.46                     | 0.49              |
| 1:A:437:VAL:HG12 | 1:A:441:LEU:HD22 | 1.95                     | 0.49              |
| 1:A:446:ASN:ND2  | 1:A:580:GLU:HG3  | 2.28                     | 0.49              |
| 1:B:169:TRP:CZ3  | 1:B:171:PRO:HD3  | 2.47                     | 0.49              |
| 1:B:525:TYR:CE2  | 1:B:559:ASN:HB3  | 2.48                     | 0.49              |
| 1:A:397:LEU:HB2  | 1:A:409:LEU:HB3  | 1.95                     | 0.48              |
| 1:A:199:ALA:C    | 1:A:288:VAL:HG12 | 2.38                     | 0.48              |
| 1:B:346:GLN:HA   | 1:B:346:GLN:NE2  | 2.18                     | 0.48              |
| 1:A:23:LEU:HD11  | 1:A:25:LEU:HD13  | 1.95                     | 0.48              |
| 1:A:318:ILE:HG12 | 3:A:800:ADP:O4'  | 2.12                     | 0.48              |
| 1:B:206:SER:O    | 1:B:233:LEU:HD22 | 2.13                     | 0.48              |
| 1:A:69:LEU:N     | 1:A:69:LEU:HD23  | 2.28                     | 0.48              |
| 1:A:345:PRO:HG2  | 1:A:467:ARG:CG   | 2.43                     | 0.48              |
| 1:B:188:MSE:CE   | 1:B:258:TRP:HZ2  | 2.25                     | 0.48              |
| 1:B:555:LEU:HD23 | 1:B:563:LEU:HD21 | 1.96                     | 0.48              |
| 1:B:649:LEU:C    | 1:B:657:THR:HG21 | 2.38                     | 0.48              |
| 1:A:179:GLU:OE1  | 1:A:316:GLN:HB2  | 2.13                     | 0.48              |
| 1:A:96:LEU:CD2   | 1:A:102:LEU:HD23 | 2.44                     | 0.48              |
| 1:B:359:TRP:CZ3  | 1:B:367:LEU:CD1  | 2.84                     | 0.48              |
| 1:B:502:ARG:HA   | 1:B:505:GLN:HB3  | 1.96                     | 0.48              |
| 1:A:670:PHE:N    | 1:A:670:PHE:CD2  | 2.79                     | 0.48              |
| 1:A:306:PHE:CB   | 1:A:309:LEU:HD23 | 2.44                     | 0.47              |
| 1:A:353:ALA:HB2  | 1:A:397:LEU:HD13 | 1.95                     | 0.47              |
| 1:B:289:GLN:CD   | 1:B:296:ARG:NH1  | 2.68                     | 0.47              |
| 1:B:132:THR:O    | 1:B:132:THR:OG1  | 2.30                     | 0.47              |
| 1:A:250:LEU:CD1  | 1:A:278:ARG:HH22 | 2.07                     | 0.47              |
| 1:A:50:ILE:CG2   | 1:A:92:LEU:HD22  | 2.45                     | 0.47              |
| 1:A:106:LEU:HB3  | 1:A:107:PRO:HD2  | 1.96                     | 0.47              |
| 1:B:279:PHE:H    | 1:B:279:PHE:HD2  | 1.62                     | 0.47              |
| 1:B:407:GLY:HA2  | 1:B:462:ALA:O    | 2.13                     | 0.47              |
| 1:A:359:TRP:CE2  | 1:A:366:PRO:HB2  | 2.50                     | 0.47              |
| 1:B:196:ALA:HB2  | 1:B:309:LEU:HD21 | 1.97                     | 0.47              |
| 1:B:489:TYR:CD1  | 1:B:489:TYR:C    | 2.92                     | 0.47              |
| 1:B:640:ARG:O    | 1:B:644:GLU:HG3  | 2.14                     | 0.47              |
| 1:B:10:LEU:HD23  | 1:B:160:LEU:HD21 | 1.95                     | 0.47              |
| 1:A:454:ARG:NH2  | 5:A:880:HOH:O    | 2.47                     | 0.47              |
| 1:B:223:THR:CG2  | 1:B:224:ALA:N    | 2.78                     | 0.47              |
| 1:B:18:GLY:HA2   | 1:B:98:ALA:HB1   | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:581:LEU:CD1  | 1:B:597:CYS:SG   | 3.03                     | 0.47              |
| 1:B:215:ARG:O    | 1:B:215:ARG:HD2  | 2.14                     | 0.46              |
| 1:B:222:VAL:HG22 | 1:B:243:PHE:HD1  | 1.79                     | 0.46              |
| 1:A:102:LEU:HD13 | 1:A:102:LEU:C    | 2.41                     | 0.46              |
| 1:B:496:TYR:CD1  | 1:B:514:MSE:HE1  | 2.49                     | 0.46              |
| 1:B:244:ILE:HG23 | 1:B:244:ILE:O    | 2.16                     | 0.46              |
| 1:A:227:LYS:O    | 1:A:228:ALA:C    | 2.58                     | 0.46              |
| 1:A:289:GLN:HG2  | 1:A:336:PHE:O    | 2.14                     | 0.46              |
| 1:B:229:SER:HB3  | 1:B:231:ASP:OD1  | 2.15                     | 0.46              |
| 1:B:184:LEU:HD21 | 1:B:211:GLN:HB3  | 1.97                     | 0.46              |
| 1:B:506:ARG:NH2  | 2:B:701:ACO:O9A  | 2.48                     | 0.46              |
| 1:A:68:LEU:HD12  | 1:A:68:LEU:N     | 2.31                     | 0.46              |
| 1:A:506:ARG:NH1  | 2:A:700:ACO:P3B  | 2.89                     | 0.46              |
| 1:B:310:HIS:HB3  | 1:B:312:PHE:CZ   | 2.51                     | 0.46              |
| 1:A:184:LEU:HD13 | 1:A:208:LEU:HD12 | 1.97                     | 0.46              |
| 1:B:154:GLN:O    | 1:B:155:ASN:HB2  | 2.15                     | 0.46              |
| 1:A:369:VAL:HG13 | 1:A:408:ALA:HB1  | 1.98                     | 0.46              |
| 1:B:222:VAL:HB   | 1:B:260:VAL:HG22 | 1.97                     | 0.46              |
| 1:B:249:LEU:HD11 | 1:B:275:LEU:HG   | 1.98                     | 0.46              |
| 1:A:6:ALA:HB1    | 1:A:160:LEU:HD12 | 1.98                     | 0.46              |
| 1:B:319:ARG:HB2  | 1:B:320:TRP:CE3  | 2.51                     | 0.46              |
| 1:A:259:LEU:HB2  | 1:A:279:PHE:CD2  | 2.51                     | 0.46              |
| 1:B:219:ARG:O    | 1:B:257:ASP:OD1  | 2.34                     | 0.46              |
| 1:B:435:ASN:HB3  | 1:B:438:ALA:HB3  | 1.96                     | 0.46              |
| 1:B:214:SER:CB   | 1:B:240:LYS:HZ3  | 2.26                     | 0.45              |
| 1:A:183:LEU:HD22 | 1:A:314:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:341:PHE:CZ   | 1:A:375:GLY:HA3  | 2.51                     | 0.45              |
| 1:A:634:ARG:HH12 | 1:A:638:LEU:HD13 | 1.81                     | 0.45              |
| 1:B:213:ILE:HG23 | 1:B:240:LYS:HB2  | 1.98                     | 0.45              |
| 1:B:240:LYS:H    | 1:B:240:LYS:CD   | 2.17                     | 0.45              |
| 1:B:279:PHE:HB3  | 1:B:280:PRO:CD   | 2.45                     | 0.45              |
| 1:B:397:LEU:HB2  | 1:B:409:LEU:HB3  | 1.98                     | 0.45              |
| 1:A:660:LEU:HD12 | 1:A:660:LEU:HA   | 1.67                     | 0.45              |
| 1:B:469:ARG:HA   | 1:B:469:ARG:HD2  | 1.71                     | 0.45              |
| 1:B:566:ASP:HB3  | 5:B:997:HOH:O    | 2.16                     | 0.45              |
| 1:B:10:LEU:O     | 1:B:14:MSE:HG3   | 2.16                     | 0.45              |
| 1:B:480:ALA:O    | 1:B:484:THR:CG2  | 2.64                     | 0.45              |
| 1:A:149:ALA:O    | 1:A:151:LEU:HD22 | 2.16                     | 0.45              |
| 1:A:437:VAL:HG12 | 1:A:441:LEU:CD2  | 2.47                     | 0.45              |
| 1:B:193:GLY:O    | 1:B:281:ARG:HA   | 2.17                     | 0.45              |
| 1:A:329:MSE:HE3  | 1:A:329:MSE:HB3  | 1.93                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:122:ARG:NH2  | 1:B:383:LEU:HD11 | 2.31                     | 0.45              |
| 1:B:213:ILE:HG22 | 1:B:237:ALA:HB1  | 1.92                     | 0.45              |
| 1:B:274:GLN:C    | 1:B:278:ARG:NH2  | 2.74                     | 0.45              |
| 1:B:499:GLU:O    | 1:B:500:LEU:C    | 2.55                     | 0.45              |
| 1:B:215:ARG:NH1  | 1:B:215:ARG:C    | 2.63                     | 0.45              |
| 1:B:216:ILE:HD13 | 1:B:218:GLY:H    | 1.82                     | 0.45              |
| 1:B:477:ILE:O    | 1:B:481:LEU:HD23 | 2.17                     | 0.45              |
| 1:B:555:LEU:HD12 | 1:B:595:LEU:HD23 | 1.99                     | 0.45              |
| 1:A:69:LEU:CD1   | 1:A:71:ARG:HD2   | 2.47                     | 0.44              |
| 1:A:306:PHE:HB2  | 1:A:309:LEU:HD23 | 1.99                     | 0.44              |
| 1:B:263:GLU:H    | 1:B:285:THR:HG23 | 1.82                     | 0.44              |
| 1:B:583:GLY:HA3  | 1:B:589:ARG:HD2  | 1.99                     | 0.44              |
| 1:A:262:ASP:HB2  | 1:A:285:THR:OG1  | 2.18                     | 0.44              |
| 1:A:432:PRO:HG2  | 1:A:439:GLN:OE1  | 2.17                     | 0.44              |
| 1:B:17:GLU:HB3   | 1:B:166:ARG:HB2  | 1.99                     | 0.44              |
| 1:B:259:LEU:HD13 | 1:B:282:THR:CG2  | 2.46                     | 0.44              |
| 1:B:464:HIS:ND1  | 1:B:465:PRO:HD2  | 2.32                     | 0.44              |
| 1:B:581:LEU:HG   | 1:B:601:LEU:HD22 | 1.99                     | 0.44              |
| 2:B:701:ACO:N8P  | 2:B:701:ACO:H131 | 2.32                     | 0.44              |
| 1:B:71:ARG:NH2   | 1:B:73:PHE:CZ    | 2.86                     | 0.44              |
| 1:B:213:ILE:CD1  | 1:B:220:ALA:CB   | 2.95                     | 0.44              |
| 1:B:250:LEU:O    | 1:B:250:LEU:HD12 | 2.17                     | 0.44              |
| 1:B:578:TRP:HZ3  | 1:B:657:THR:CG2  | 2.30                     | 0.44              |
| 1:A:228:ALA:O    | 1:A:230:THR:N    | 2.50                     | 0.44              |
| 1:B:446:ASN:HA   | 1:B:580:GLU:OE2  | 2.18                     | 0.44              |
| 1:B:215:ARG:HH12 | 1:B:216:ILE:CB   | 2.31                     | 0.44              |
| 1:B:369:VAL:HG12 | 1:B:373:LEU:HD22 | 2.00                     | 0.44              |
| 1:A:151:LEU:HD22 | 1:A:151:LEU:N    | 2.33                     | 0.44              |
| 1:A:441:LEU:HD13 | 1:A:528:MSE:CE   | 2.41                     | 0.44              |
| 1:B:188:MSE:HE1  | 1:B:283:LEU:HD23 | 1.99                     | 0.44              |
| 1:B:312:PHE:C    | 1:B:313:GLU:HG3  | 2.43                     | 0.44              |
| 1:B:542:GLU:HG3  | 1:B:543:ARG:N    | 2.33                     | 0.44              |
| 1:A:92:LEU:HD23  | 1:A:102:LEU:HD21 | 1.99                     | 0.44              |
| 1:A:143:LEU:HD12 | 1:A:143:LEU:HA   | 1.80                     | 0.44              |
| 1:A:146:ASP:OD2  | 1:A:146:ASP:C    | 2.61                     | 0.44              |
| 1:A:502:ARG:NH2  | 1:B:1:MSE:H2     | 2.14                     | 0.44              |
| 1:A:289:GLN:NE2  | 1:A:374:SER:OG   | 2.49                     | 0.43              |
| 1:B:209:ALA:HB3  | 1:B:233:LEU:HD23 | 1.97                     | 0.43              |
| 1:B:213:ILE:CD1  | 1:B:220:ALA:HB3  | 2.45                     | 0.43              |
| 1:B:216:ILE:HG23 | 1:B:218:GLY:O    | 2.17                     | 0.43              |
| 1:B:264:ALA:CB   | 1:B:284:LEU:CD1  | 2.86                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:481:LEU:HA   | 1:B:484:THR:HG22 | 1.99                     | 0.43              |
| 1:A:74:ARG:O     | 1:A:75:HIS:HB2   | 2.18                     | 0.43              |
| 1:A:250:LEU:CD2  | 1:A:278:ARG:NH2  | 2.75                     | 0.43              |
| 1:A:252:SER:OG   | 1:A:254:GLU:HG2  | 2.18                     | 0.43              |
| 1:A:506:ARG:HA   | 1:A:506:ARG:HD2  | 1.11                     | 0.43              |
| 1:A:553:GLN:CD   | 1:A:569:ASN:ND2  | 2.77                     | 0.43              |
| 1:A:489:TYR:C    | 1:A:489:TYR:CD2  | 2.96                     | 0.43              |
| 1:B:16:ARG:HH21  | 1:B:16:ARG:CG    | 2.32                     | 0.43              |
| 1:B:138:HIS:HB2  | 1:B:389:MSE:CE   | 2.47                     | 0.43              |
| 1:B:177:GLN:HB3  | 1:B:178:PRO:HD2  | 2.01                     | 0.43              |
| 1:B:185:LYS:HD3  | 1:B:189:THR:CA   | 2.48                     | 0.43              |
| 1:A:329:MSE:HE3  | 1:A:330:VAL:HG23 | 2.01                     | 0.43              |
| 1:A:362:ASP:OD1  | 1:A:365:THR:CG2  | 2.66                     | 0.43              |
| 1:B:212:LEU:HD12 | 1:B:212:LEU:N    | 2.23                     | 0.43              |
| 1:B:249:LEU:HD11 | 1:B:275:LEU:CG   | 2.48                     | 0.43              |
| 1:A:92:LEU:O     | 1:A:95:THR:HG22  | 2.19                     | 0.43              |
| 1:B:192:PRO:HB3  | 1:B:280:PRO:HB2  | 2.00                     | 0.43              |
| 1:B:355:GLU:HB2  | 1:B:357:THR:HG23 | 2.01                     | 0.43              |
| 1:A:199:ALA:O    | 1:A:287:THR:HA   | 2.18                     | 0.43              |
| 1:A:314:LEU:HD12 | 1:A:314:LEU:HA   | 1.88                     | 0.43              |
| 1:A:373:LEU:HD11 | 1:A:408:ALA:HB3  | 2.00                     | 0.43              |
| 1:B:185:LYS:HG3  | 1:B:215:ARG:NE   | 2.34                     | 0.43              |
| 1:B:346:GLN:HE21 | 1:B:346:GLN:CA   | 2.12                     | 0.43              |
| 1:A:10:LEU:O     | 1:A:14:MSE:HG3   | 2.19                     | 0.43              |
| 1:A:50:ILE:HD12  | 1:A:51:SER:N     | 2.33                     | 0.43              |
| 1:A:122:ARG:HH21 | 1:A:383:LEU:HD11 | 1.83                     | 0.43              |
| 1:A:161:ALA:C    | 1:A:162:HIS:ND1  | 2.77                     | 0.43              |
| 1:B:190:MSE:O    | 1:B:191:PRO:C    | 2.59                     | 0.43              |
| 1:A:612:LEU:HD22 | 1:A:644:GLU:HB2  | 2.01                     | 0.43              |
| 1:B:485:GLN:O    | 1:B:486:ASP:CB   | 2.66                     | 0.43              |
| 1:A:273:HIS:NE2  | 1:A:305:ARG:HB3  | 2.33                     | 0.43              |
| 1:A:326:LEU:HD12 | 1:A:329:MSE:CE   | 2.49                     | 0.43              |
| 1:A:411:LEU:HD12 | 1:A:458:VAL:HA   | 2.01                     | 0.43              |
| 1:B:181:GLN:HA   | 1:B:181:GLN:OE1  | 2.19                     | 0.43              |
| 1:B:234:ALA:HB2  | 1:B:241:PHE:CD1  | 2.53                     | 0.43              |
| 1:B:509:PHE:HB3  | 1:B:529:ALA:HB1  | 2.00                     | 0.43              |
| 1:B:516:ASN:HB2  | 1:B:592:LEU:HD23 | 2.01                     | 0.43              |
| 1:A:577:ASP:O    | 1:A:581:LEU:HD22 | 2.19                     | 0.43              |
| 1:B:307:PRO:O    | 1:B:308:HIS:HB2  | 2.17                     | 0.43              |
| 1:A:53:ARG:HE    | 1:A:53:ARG:HB3   | 1.45                     | 0.42              |
| 1:A:184:LEU:HD13 | 1:A:208:LEU:CD1  | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:262:ASP:HA   | 1:A:285:THR:OG1  | 2.19                     | 0.42              |
| 1:B:284:LEU:HA   | 1:B:284:LEU:HD13 | 1.64                     | 0.42              |
| 1:A:67:THR:CG2   | 1:A:71:ARG:HH11  | 2.32                     | 0.42              |
| 1:B:210:GLY:N    | 1:B:233:LEU:HD22 | 2.34                     | 0.42              |
| 1:B:245:ALA:O    | 1:B:249:LEU:CB   | 2.67                     | 0.42              |
| 1:B:353:ALA:HB2  | 1:B:397:LEU:HD13 | 2.00                     | 0.42              |
| 1:A:317:PRO:HD2  | 1:A:322:GLN:HB2  | 2.01                     | 0.42              |
| 1:A:339:GLU:O    | 1:A:342:THR:HB   | 2.20                     | 0.42              |
| 1:B:430:ARG:C    | 1:B:431:ARG:HG3  | 2.44                     | 0.42              |
| 1:B:242:ARG:HD3  | 1:B:243:PHE:N    | 2.34                     | 0.42              |
| 1:B:578:TRP:HZ3  | 1:B:657:THR:HG22 | 1.85                     | 0.42              |
| 1:A:276:VAL:HG22 | 1:A:282:THR:HG21 | 2.01                     | 0.42              |
| 1:B:355:GLU:OE1  | 1:B:395:HIS:ND1  | 2.46                     | 0.42              |
| 1:B:497:THR:O    | 1:B:498:GLY:C    | 2.62                     | 0.42              |
| 1:A:92:LEU:CD2   | 1:A:102:LEU:HD21 | 2.49                     | 0.42              |
| 1:B:239:GLU:C    | 1:B:241:PHE:N    | 2.71                     | 0.42              |
| 1:B:496:TYR:OH   | 1:B:564:PRO:HG3  | 2.19                     | 0.42              |
| 1:A:224:ALA:HB1  | 1:A:225:PRO:HD2  | 2.02                     | 0.42              |
| 1:A:490:LEU:HD12 | 1:A:490:LEU:HA   | 1.93                     | 0.42              |
| 1:A:540:LEU:O    | 1:A:544:GLU:HB2  | 2.20                     | 0.42              |
| 1:B:184:LEU:CD1  | 1:B:211:GLN:CG   | 2.87                     | 0.42              |
| 1:B:184:LEU:CG   | 1:B:211:GLN:HB3  | 2.49                     | 0.42              |
| 1:B:355:GLU:O    | 1:B:358:LEU:HB2  | 2.20                     | 0.42              |
| 1:B:395:HIS:CD2  | 1:B:456:ARG:CZ   | 3.02                     | 0.42              |
| 1:B:553:GLN:O    | 1:B:557:GLN:HG3  | 2.19                     | 0.42              |
| 1:A:565:VAL:O    | 1:A:567:PRO:HD3  | 2.20                     | 0.42              |
| 1:B:101:TRP:CH2  | 1:B:150:ILE:HG13 | 2.54                     | 0.42              |
| 1:B:314:LEU:HD23 | 1:B:314:LEU:HA   | 1.93                     | 0.42              |
| 1:B:629:LEU:HD13 | 1:B:629:LEU:HA   | 1.88                     | 0.42              |
| 1:A:323:GLY:O    | 1:A:324:CYS:C    | 2.63                     | 0.42              |
| 1:B:232:VAL:HB   | 1:B:233:LEU:H    | 1.32                     | 0.42              |
| 1:B:421:LEU:O    | 1:B:425:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:441:LEU:HB3  | 1:A:450:ALA:HB1  | 2.02                     | 0.42              |
| 1:B:440:SER:OG   | 1:B:444:HIS:HD2  | 2.02                     | 0.42              |
| 1:B:581:LEU:HD12 | 1:B:581:LEU:HA   | 1.84                     | 0.42              |
| 1:A:13:GLN:HG3   | 1:A:16:ARG:HH21  | 1.84                     | 0.41              |
| 1:A:40:ARG:HG3   | 1:A:41:ASP:N     | 2.35                     | 0.41              |
| 1:B:11:THR:CA    | 1:B:14:MSE:CE    | 2.80                     | 0.41              |
| 1:B:429:PHE:CD1  | 1:B:668:GLN:HA   | 2.54                     | 0.41              |
| 1:B:609:LEU:HD22 | 1:B:644:GLU:HB3  | 2.02                     | 0.41              |
| 1:B:51:SER:CB    | 5:B:1004:HOH:O   | 2.67                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:570:ASP:OD2  | 1:B:572:VAL:HG12 | 2.20                     | 0.41              |
| 1:A:269:ALA:N    | 1:A:270:PRO:HD2  | 2.36                     | 0.41              |
| 1:B:23:LEU:CD1   | 1:B:23:LEU:C     | 2.93                     | 0.41              |
| 1:B:53:ARG:O     | 1:B:55:ASP:OD1   | 2.37                     | 0.41              |
| 1:B:146:ASP:OD2  | 1:B:148:GLU:HB2  | 2.20                     | 0.41              |
| 1:B:148:GLU:OE2  | 1:B:166:ARG:NH2  | 2.54                     | 0.41              |
| 1:B:660:LEU:CD1  | 5:B:1020:HOH:O   | 2.69                     | 0.41              |
| 1:A:106:LEU:HD13 | 1:A:112:TRP:CH2  | 2.54                     | 0.41              |
| 1:B:244:ILE:O    | 1:B:249:LEU:HB2  | 2.20                     | 0.41              |
| 1:B:317:PRO:HG2  | 1:B:320:TRP:O    | 2.20                     | 0.41              |
| 1:B:429:PHE:CE2  | 1:B:588:HIS:HD2  | 2.38                     | 0.41              |
| 1:A:7:LEU:HD12   | 1:A:7:LEU:HA     | 1.91                     | 0.41              |
| 1:A:50:ILE:HD12  | 1:A:50:ILE:C     | 2.45                     | 0.41              |
| 1:A:124:SER:O    | 1:A:125:ASP:HB2  | 2.20                     | 0.41              |
| 1:A:233:LEU:HD23 | 1:A:233:LEU:O    | 2.21                     | 0.41              |
| 1:B:65:LEU:O     | 1:B:66:GLN:HG2   | 2.21                     | 0.41              |
| 1:B:221:ILE:CG1  | 1:B:222:VAL:N    | 2.84                     | 0.41              |
| 1:B:243:PHE:CD2  | 1:B:243:PHE:C    | 2.98                     | 0.41              |
| 1:A:69:LEU:HG    | 1:A:71:ARG:HG3   | 2.02                     | 0.41              |
| 1:B:329:MSE:HE2  | 1:B:333:ALA:CB   | 2.45                     | 0.41              |
| 1:B:434:GLY:O    | 1:B:439:GLN:NE2  | 2.51                     | 0.41              |
| 1:A:294:THR:OG1  | 1:A:299:LEU:CD2  | 2.68                     | 0.41              |
| 1:B:232:VAL:O    | 1:B:233:LEU:C    | 2.63                     | 0.41              |
| 1:B:263:GLU:CD   | 1:B:287:THR:H    | 2.29                     | 0.41              |
| 1:B:388:MSE:HG3  | 1:B:396:PHE:CE1  | 2.56                     | 0.41              |
| 1:B:476:LEU:HD12 | 1:B:476:LEU:HA   | 1.90                     | 0.41              |
| 1:A:23:LEU:C     | 1:A:23:LEU:HD13  | 2.46                     | 0.41              |
| 1:A:362:ASP:O    | 1:A:366:PRO:HD2  | 2.20                     | 0.41              |
| 1:A:578:TRP:CZ3  | 1:A:656:ARG:HG2  | 2.55                     | 0.41              |
| 1:A:629:LEU:CB   | 1:A:631:LEU:CD2  | 2.99                     | 0.41              |
| 1:B:133:PRO:O    | 1:B:137:GLN:HG3  | 2.20                     | 0.41              |
| 1:B:195:ALA:HB3  | 1:B:283:LEU:HD23 | 2.02                     | 0.41              |
| 1:B:202:GLY:N    | 4:B:801:SO4:O2   | 2.54                     | 0.41              |
| 1:A:254:GLU:N    | 1:A:254:GLU:CD   | 2.76                     | 0.41              |
| 1:A:514:MSE:HE3  | 1:A:515:GLY:H    | 1.85                     | 0.41              |
| 1:A:543:ARG:NH1  | 1:A:543:ARG:HG2  | 2.36                     | 0.41              |
| 1:B:10:LEU:HG    | 1:B:14:MSE:CE    | 2.31                     | 0.41              |
| 1:B:15:LYS:HE3   | 1:B:74:ARG:HH11  | 1.85                     | 0.41              |
| 1:B:74:ARG:NH2   | 1:B:74:ARG:HB2   | 2.36                     | 0.41              |
| 1:B:197:VAL:HG12 | 1:B:312:PHE:HB2  | 2.02                     | 0.41              |
| 1:B:208:LEU:O    | 1:B:211:GLN:HB2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:233:LEU:C    | 1:B:233:LEU:CD1  | 2.94                     | 0.41              |
| 1:B:409:LEU:HG   | 1:B:411:LEU:HD22 | 2.02                     | 0.41              |
| 1:B:414:GLU:HG2  | 1:B:435:ASN:HA   | 2.02                     | 0.41              |
| 1:B:417:LEU:HD22 | 1:B:451:ALA:HB1  | 2.01                     | 0.41              |
| 1:B:570:ASP:O    | 1:B:570:ASP:CG   | 2.64                     | 0.41              |
| 1:A:137:GLN:O    | 1:A:141:ARG:HG3  | 2.20                     | 0.41              |
| 1:A:176:PRO:HG2  | 1:A:181:GLN:HE21 | 1.86                     | 0.41              |
| 1:B:363:PRO:O    | 1:B:366:PRO:HD2  | 2.20                     | 0.41              |
| 1:B:365:THR:HB   | 1:B:366:PRO:CD   | 2.39                     | 0.41              |
| 1:A:138:HIS:HA   | 1:A:141:ARG:NH1  | 2.36                     | 0.40              |
| 1:A:205:LYS:CE   | 1:A:287:THR:HG22 | 2.50                     | 0.40              |
| 1:B:274:GLN:CG   | 1:B:278:ARG:HH22 | 2.31                     | 0.40              |
| 1:B:274:GLN:HB3  | 1:B:278:ARG:HH21 | 1.70                     | 0.40              |
| 1:B:309:LEU:HD23 | 1:B:309:LEU:C    | 2.47                     | 0.40              |
| 1:B:653:ASN:O    | 1:B:657:THR:HG23 | 2.20                     | 0.40              |
| 1:A:122:ARG:NH2  | 1:A:383:LEU:HD11 | 2.36                     | 0.40              |
| 1:A:222:VAL:HA   | 1:A:260:VAL:O    | 2.21                     | 0.40              |
| 1:B:7:LEU:CD1    | 1:B:160:LEU:HD22 | 2.44                     | 0.40              |
| 1:B:249:LEU:HD11 | 1:B:275:LEU:HD21 | 2.02                     | 0.40              |
| 1:A:184:LEU:HD12 | 1:A:184:LEU:HA   | 1.88                     | 0.40              |
| 1:A:222:VAL:HG22 | 1:A:243:PHE:HD2  | 1.86                     | 0.40              |
| 1:B:73:PHE:CD1   | 1:B:73:PHE:N     | 2.90                     | 0.40              |
| 1:B:558:TRP:HH2  | 1:B:615:ARG:NH1  | 2.19                     | 0.40              |
| 2:B:701:ACO:H131 | 2:B:701:ACO:HN8  | 1.87                     | 0.40              |
| 1:A:363:PRO:O    | 1:A:367:LEU:HB2  | 2.21                     | 0.40              |
| 1:A:484:THR:CG2  | 1:A:485:GLN:N    | 2.84                     | 0.40              |
| 1:A:547:ARG:HD2  | 5:A:1012:HOH:O   | 2.22                     | 0.40              |
| 1:A:599:LEU:HD11 | 1:A:616:LEU:HB3  | 2.03                     | 0.40              |
| 1:B:211:GLN:C    | 1:B:213:ILE:H    | 2.29                     | 0.40              |
| 1:B:446:ASN:O    | 1:B:448:PRO:HD3  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| 1   | A     | 442/671 (66%)   | 430 (97%)  | 11 (2%) | 1 (0%)   | 43          | 52 |
| 1   | B     | 658/671 (98%)   | 605 (92%)  | 44 (7%) | 9 (1%)   | 9           | 7  |
| All | All   | 1100/1342 (82%) | 1035 (94%) | 55 (5%) | 10 (1%)  | 14          | 14 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 184 | LEU  |
| 1   | B     | 227 | LYS  |
| 1   | B     | 215 | ARG  |
| 1   | B     | 232 | VAL  |
| 1   | B     | 280 | PRO  |
| 1   | A     | 229 | SER  |
| 1   | B     | 213 | ILE  |
| 1   | B     | 225 | PRO  |
| 1   | B     | 221 | ILE  |
| 1   | B     | 233 | LEU  |

### 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     | 525/532 (99%)    | 439 (84%) | 86 (16%)  | 2           | 2 |
| 1   | B     | 535/532 (101%)   | 409 (76%) | 126 (24%) | 1           | 0 |
| All | All   | 1060/1064 (100%) | 848 (80%) | 212 (20%) | 1           | 1 |

All (212) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | THR  |
| 1   | A     | 21  | ARG  |
| 1   | A     | 23  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 25  | LEU  |
| 1   | A     | 29  | GLU  |
| 1   | A     | 37  | LEU  |
| 1   | A     | 43  | LEU  |
| 1   | A     | 49  | TRP  |
| 1   | A     | 50  | ILE  |
| 1   | A     | 52  | PRO  |
| 1   | A     | 53  | ARG  |
| 1   | A     | 68  | LEU  |
| 1   | A     | 69  | LEU  |
| 1   | A     | 72  | GLU  |
| 1   | A     | 95  | THR  |
| 1   | A     | 96  | LEU  |
| 1   | A     | 97  | LYS  |
| 1   | A     | 119 | ASP  |
| 1   | A     | 121 | LEU  |
| 1   | A     | 139 | LEU  |
| 1   | A     | 142 | VAL  |
| 1   | A     | 143 | LEU  |
| 1   | A     | 151 | LEU  |
| 1   | A     | 156 | GLN  |
| 1   | A     | 160 | LEU  |
| 1   | A     | 162 | HIS  |
| 1   | A     | 167 | THR  |
| 1   | A     | 183 | LEU  |
| 1   | A     | 184 | LEU  |
| 1   | A     | 187 | LEU  |
| 1   | A     | 212 | LEU  |
| 1   | A     | 219 | ARG  |
| 1   | A     | 222 | VAL  |
| 1   | A     | 250 | LEU  |
| 1   | A     | 284 | LEU  |
| 1   | A     | 286 | THR  |
| 1   | A     | 299 | LEU  |
| 1   | A     | 300 | LEU  |
| 1   | A     | 301 | LYS  |
| 1   | A     | 309 | LEU  |
| 1   | A     | 314 | LEU  |
| 1   | A     | 316 | GLN  |
| 1   | A     | 318 | ILE  |
| 1   | A     | 334 | LEU  |
| 1   | A     | 365 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 367 | LEU  |
| 1   | A     | 373 | LEU  |
| 1   | A     | 377 | HIS  |
| 1   | A     | 381 | SER  |
| 1   | A     | 411 | LEU  |
| 1   | A     | 420 | GLN  |
| 1   | A     | 430 | ARG  |
| 1   | A     | 431 | ARG  |
| 1   | A     | 441 | LEU  |
| 1   | A     | 449 | LEU  |
| 1   | A     | 453 | LEU  |
| 1   | A     | 472 | THR  |
| 1   | A     | 476 | LEU  |
| 1   | A     | 481 | LEU  |
| 1   | A     | 485 | GLN  |
| 1   | A     | 490 | LEU  |
| 1   | A     | 506 | ARG  |
| 1   | A     | 517 | HIS  |
| 1   | A     | 531 | LEU  |
| 1   | A     | 543 | ARG  |
| 1   | A     | 544 | GLU  |
| 1   | A     | 555 | LEU  |
| 1   | A     | 572 | VAL  |
| 1   | A     | 581 | LEU  |
| 1   | A     | 589 | ARG  |
| 1   | A     | 592 | LEU  |
| 1   | A     | 598 | LEU  |
| 1   | A     | 599 | LEU  |
| 1   | A     | 602 | LEU  |
| 1   | A     | 612 | LEU  |
| 1   | A     | 616 | LEU  |
| 1   | A     | 618 | LYS  |
| 1   | A     | 625 | LEU  |
| 1   | A     | 629 | LEU  |
| 1   | A     | 634 | ARG  |
| 1   | A     | 635 | LYS  |
| 1   | A     | 640 | ARG  |
| 1   | A     | 649 | LEU  |
| 1   | A     | 652 | LEU  |
| 1   | A     | 660 | LEU  |
| 1   | A     | 669 | LEU  |
| 1   | B     | 7   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 16  | ARG  |
| 1   | B     | 22  | LEU  |
| 1   | B     | 23  | LEU  |
| 1   | B     | 25  | LEU  |
| 1   | B     | 37  | LEU  |
| 1   | B     | 39  | LEU  |
| 1   | B     | 40  | ARG  |
| 1   | B     | 43  | LEU  |
| 1   | B     | 48  | LEU  |
| 1   | B     | 53  | ARG  |
| 1   | B     | 67  | THR  |
| 1   | B     | 71  | ARG  |
| 1   | B     | 72  | GLU  |
| 1   | B     | 95  | THR  |
| 1   | B     | 96  | LEU  |
| 1   | B     | 102 | LEU  |
| 1   | B     | 105 | LEU  |
| 1   | B     | 106 | LEU  |
| 1   | B     | 119 | ASP  |
| 1   | B     | 139 | LEU  |
| 1   | B     | 142 | VAL  |
| 1   | B     | 164 | THR  |
| 1   | B     | 171 | PRO  |
| 1   | B     | 183 | LEU  |
| 1   | B     | 184 | LEU  |
| 1   | B     | 185 | LYS  |
| 1   | B     | 187 | LEU  |
| 1   | B     | 188 | MSE  |
| 1   | B     | 191 | PRO  |
| 1   | B     | 198 | THR  |
| 1   | B     | 208 | LEU  |
| 1   | B     | 211 | GLN  |
| 1   | B     | 213 | ILE  |
| 1   | B     | 214 | SER  |
| 1   | B     | 215 | ARG  |
| 1   | B     | 216 | ILE  |
| 1   | B     | 219 | ARG  |
| 1   | B     | 221 | ILE  |
| 1   | B     | 222 | VAL  |
| 1   | B     | 223 | THR  |
| 1   | B     | 229 | SER  |
| 1   | B     | 231 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 232 | VAL  |
| 1   | B     | 233 | LEU  |
| 1   | B     | 235 | GLN  |
| 1   | B     | 236 | PHE  |
| 1   | B     | 239 | GLU  |
| 1   | B     | 240 | LYS  |
| 1   | B     | 242 | ARG  |
| 1   | B     | 244 | ILE  |
| 1   | B     | 247 | ASP  |
| 1   | B     | 249 | LEU  |
| 1   | B     | 250 | LEU  |
| 1   | B     | 253 | ASP  |
| 1   | B     | 254 | GLU  |
| 1   | B     | 255 | GLN  |
| 1   | B     | 257 | ASP  |
| 1   | B     | 259 | LEU  |
| 1   | B     | 261 | VAL  |
| 1   | B     | 262 | ASP  |
| 1   | B     | 268 | PRO  |
| 1   | B     | 270 | PRO  |
| 1   | B     | 271 | LEU  |
| 1   | B     | 272 | LEU  |
| 1   | B     | 275 | LEU  |
| 1   | B     | 279 | PHE  |
| 1   | B     | 282 | THR  |
| 1   | B     | 283 | LEU  |
| 1   | B     | 284 | LEU  |
| 1   | B     | 285 | THR  |
| 1   | B     | 286 | THR  |
| 1   | B     | 299 | LEU  |
| 1   | B     | 300 | LEU  |
| 1   | B     | 305 | ARG  |
| 1   | B     | 309 | LEU  |
| 1   | B     | 311 | ARG  |
| 1   | B     | 315 | GLN  |
| 1   | B     | 338 | ASP  |
| 1   | B     | 341 | PHE  |
| 1   | B     | 342 | THR  |
| 1   | B     | 346 | GLN  |
| 1   | B     | 357 | THR  |
| 1   | B     | 358 | LEU  |
| 1   | B     | 367 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 373 | LEU  |
| 1   | B     | 379 | ARG  |
| 1   | B     | 383 | LEU  |
| 1   | B     | 431 | ARG  |
| 1   | B     | 433 | ARG  |
| 1   | B     | 441 | LEU  |
| 1   | B     | 475 | GLN  |
| 1   | B     | 476 | LEU  |
| 1   | B     | 482 | GLN  |
| 1   | B     | 487 | LEU  |
| 1   | B     | 497 | THR  |
| 1   | B     | 499 | GLU  |
| 1   | B     | 502 | ARG  |
| 1   | B     | 540 | LEU  |
| 1   | B     | 543 | ARG  |
| 1   | B     | 555 | LEU  |
| 1   | B     | 565 | VAL  |
| 1   | B     | 570 | ASP  |
| 1   | B     | 572 | VAL  |
| 1   | B     | 573 | LEU  |
| 1   | B     | 580 | GLU  |
| 1   | B     | 581 | LEU  |
| 1   | B     | 598 | LEU  |
| 1   | B     | 599 | LEU  |
| 1   | B     | 600 | ARG  |
| 1   | B     | 602 | LEU  |
| 1   | B     | 604 | THR  |
| 1   | B     | 612 | LEU  |
| 1   | B     | 615 | ARG  |
| 1   | B     | 616 | LEU  |
| 1   | B     | 624 | GLN  |
| 1   | B     | 625 | LEU  |
| 1   | B     | 627 | THR  |
| 1   | B     | 628 | THR  |
| 1   | B     | 629 | LEU  |
| 1   | B     | 635 | LYS  |
| 1   | B     | 636 | MSE  |
| 1   | B     | 649 | LEU  |
| 1   | B     | 652 | LEU  |
| 1   | B     | 660 | LEU  |
| 1   | B     | 669 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 66  | GLN  |
| 1   | A     | 114 | ASN  |
| 1   | A     | 115 | GLN  |
| 1   | A     | 134 | HIS  |
| 1   | A     | 137 | GLN  |
| 1   | A     | 181 | GLN  |
| 1   | A     | 274 | GLN  |
| 1   | A     | 289 | GLN  |
| 1   | A     | 316 | GLN  |
| 1   | A     | 322 | GLN  |
| 1   | A     | 348 | ASN  |
| 1   | A     | 403 | ASN  |
| 1   | A     | 423 | GLN  |
| 1   | A     | 444 | HIS  |
| 1   | A     | 505 | GLN  |
| 1   | A     | 516 | ASN  |
| 1   | A     | 569 | ASN  |
| 1   | A     | 668 | GLN  |
| 1   | B     | 8   | HIS  |
| 1   | B     | 35  | HIS  |
| 1   | B     | 82  | HIS  |
| 1   | B     | 115 | GLN  |
| 1   | B     | 134 | HIS  |
| 1   | B     | 137 | GLN  |
| 1   | B     | 155 | ASN  |
| 1   | B     | 177 | GLN  |
| 1   | B     | 182 | GLN  |
| 1   | B     | 289 | GLN  |
| 1   | B     | 310 | HIS  |
| 1   | B     | 346 | GLN  |
| 1   | B     | 371 | GLN  |
| 1   | B     | 403 | ASN  |
| 1   | B     | 419 | GLN  |
| 1   | B     | 423 | GLN  |
| 1   | B     | 444 | HIS  |
| 1   | B     | 446 | ASN  |
| 1   | B     | 588 | HIS  |
| 1   | B     | 617 | GLN  |
| 1   | B     | 666 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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   | ACO  | A     | 700 | -    | 51,53,53     | 3.80 | 21 (41%)    | 73,79,79    | 5.05 | 31 (42%)    |
| 3   | ADP  | A     | 800 | -    | 28,29,29     | 1.08 | 1 (3%)      | 43,45,45    | 2.02 | 10 (23%)    |
| 2   | ACO  | B     | 701 | -    | 51,53,53     | 2.96 | 24 (47%)    | 73,79,79    | 4.35 | 31 (42%)    |
| 4   | SO4  | B     | 801 | -    | 4,4,4        | 0.35 | 0           | 6,6,6       | 0.15 | 0           |

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   | ACO  | A     | 700 | -    | 1/1/12/14 | 17/51/67/67 | 0/3/3/3 |
| 3   | ADP  | A     | 800 | -    | -         | 6/16/32/32  | 0/3/3/3 |
| 2   | ACO  | B     | 701 | -    | 1/1/12/14 | 12/51/67/67 | 0/3/3/3 |

All (46) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 700 | ACO  | O5P-C5P | 17.50 | 1.58        | 1.23     |
| 2   | B     | 701 | ACO  | O5P-C5P | 8.20  | 1.39        | 1.23     |
| 2   | A     | 700 | ACO  | O9P-C9P | 7.31  | 1.37        | 1.23     |
| 2   | B     | 701 | ACO  | P1A-O3A | -6.97 | 1.52        | 1.59     |
| 2   | A     | 700 | ACO  | P1A-O3A | -6.38 | 1.52        | 1.59     |
| 2   | A     | 700 | ACO  | CH3-C   | -6.06 | 1.25        | 1.50     |
| 2   | A     | 700 | ACO  | C5A-C4A | 6.00  | 1.49        | 1.39     |
| 2   | A     | 700 | ACO  | C5P-N4P | 5.87  | 1.47        | 1.33     |
| 2   | A     | 700 | ACO  | C2A-N1A | 5.33  | 1.43        | 1.33     |
| 2   | B     | 701 | ACO  | C5P-N4P | 5.17  | 1.45        | 1.33     |
| 2   | B     | 701 | ACO  | C2A-N1A | 5.14  | 1.43        | 1.33     |
| 2   | A     | 700 | ACO  | C5A-C6A | 5.13  | 1.55        | 1.41     |
| 2   | B     | 701 | ACO  | O9P-C9P | 5.05  | 1.33        | 1.23     |
| 2   | B     | 701 | ACO  | CH3-C   | -4.95 | 1.30        | 1.50     |
| 2   | B     | 701 | ACO  | C5A-C6A | 4.64  | 1.53        | 1.41     |
| 2   | B     | 701 | ACO  | P3B-O3B | 4.57  | 1.67        | 1.59     |
| 2   | A     | 700 | ACO  | P3B-O3B | 4.52  | 1.67        | 1.59     |
| 2   | B     | 701 | ACO  | C6P-C5P | 4.45  | 1.60        | 1.51     |
| 2   | A     | 700 | ACO  | C1B-N9A | 4.41  | 1.58        | 1.46     |
| 2   | B     | 701 | ACO  | O4B-C4B | 4.36  | 1.54        | 1.45     |
| 2   | B     | 701 | ACO  | P3B-O7A | 3.99  | 1.62        | 1.50     |
| 2   | A     | 700 | ACO  | P2A-O3A | 3.89  | 1.63        | 1.59     |
| 2   | B     | 701 | ACO  | C5A-C4A | 3.75  | 1.45        | 1.39     |
| 2   | B     | 701 | ACO  | CCP-CBP | -3.62 | 1.46        | 1.52     |
| 2   | A     | 700 | ACO  | C2A-N3A | 3.47  | 1.40        | 1.33     |
| 2   | A     | 700 | ACO  | C4A-N9A | 3.38  | 1.44        | 1.37     |
| 2   | B     | 701 | ACO  | C8A-N7A | 2.97  | 1.37        | 1.31     |
| 2   | B     | 701 | ACO  | OAP-CAP | -2.83 | 1.37        | 1.42     |
| 2   | B     | 701 | ACO  | C1B-N9A | 2.75  | 1.53        | 1.46     |
| 2   | A     | 700 | ACO  | OAP-CAP | 2.74  | 1.47        | 1.42     |
| 2   | A     | 700 | ACO  | O4B-C4B | 2.71  | 1.51        | 1.45     |
| 2   | A     | 700 | ACO  | P3B-O7A | 2.70  | 1.58        | 1.50     |
| 2   | B     | 701 | ACO  | P2A-O3A | 2.59  | 1.62        | 1.59     |
| 2   | A     | 700 | ACO  | C5A-N7A | -2.44 | 1.34        | 1.39     |
| 2   | A     | 700 | ACO  | C8A-N7A | 2.31  | 1.36        | 1.31     |
| 2   | B     | 701 | ACO  | C4A-N3A | 2.31  | 1.38        | 1.34     |
| 2   | A     | 700 | ACO  | O4B-C1B | 2.24  | 1.47        | 1.42     |
| 2   | B     | 701 | ACO  | C6A-N1A | 2.23  | 1.42        | 1.35     |
| 2   | A     | 700 | ACO  | CDP-CBP | 2.22  | 1.58        | 1.53     |
| 2   | B     | 701 | ACO  | C2B-C1B | -2.21 | 1.46        | 1.53     |
| 2   | B     | 701 | ACO  | C8A-N9A | 2.18  | 1.41        | 1.37     |
| 2   | B     | 701 | ACO  | C5A-N7A | -2.17 | 1.35        | 1.39     |
| 3   | A     | 800 | ADP  | C5-N7   | -2.13 | 1.35        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | B     | 701 | ACO  | C2A-N3A | 2.08 | 1.37        | 1.33     |
| 2   | B     | 701 | ACO  | C5B-C4B | 2.06 | 1.57        | 1.51     |
| 2   | A     | 700 | ACO  | C6P-C5P | 2.00 | 1.55        | 1.51     |

All (72) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2   | A     | 700 | ACO  | C2P-C3P-N4P | 16.47  | 146.81      | 112.41   |
| 2   | A     | 700 | ACO  | CEP-CBP-CAP | 15.46  | 135.13      | 108.77   |
| 2   | A     | 700 | ACO  | O5P-C5P-C6P | -15.37 | 94.17       | 122.02   |
| 2   | B     | 701 | ACO  | O5P-C5P-C6P | -15.24 | 94.41       | 122.02   |
| 2   | B     | 701 | ACO  | C2P-C3P-N4P | 14.14  | 141.94      | 112.41   |
| 2   | B     | 701 | ACO  | O5P-C5P-N4P | -13.49 | 96.56       | 123.03   |
| 2   | A     | 700 | ACO  | CEP-CBP-CDP | -12.41 | 84.46       | 109.20   |
| 2   | A     | 700 | ACO  | CAP-C9P-N8P | -11.39 | 94.86       | 116.48   |
| 2   | A     | 700 | ACO  | O5P-C5P-N4P | -10.65 | 102.14      | 123.03   |
| 2   | A     | 700 | ACO  | O2B-C2B-C1B | 10.41  | 145.94      | 110.10   |
| 2   | A     | 700 | ACO  | O6A-CCP-CBP | 10.15  | 126.86      | 110.55   |
| 2   | B     | 701 | ACO  | O2B-C2B-C1B | 8.88   | 140.67      | 110.10   |
| 2   | B     | 701 | ACO  | O6A-CCP-CBP | 8.28   | 123.85      | 110.55   |
| 2   | B     | 701 | ACO  | CAP-C9P-N8P | -7.81  | 101.67      | 116.48   |
| 2   | A     | 700 | ACO  | C3P-N4P-C5P | -7.78  | 108.34      | 122.82   |
| 2   | B     | 701 | ACO  | CEP-CBP-CAP | 7.65   | 121.80      | 108.77   |
| 2   | A     | 700 | ACO  | O9P-C9P-CAP | 7.49   | 141.80      | 120.89   |
| 2   | A     | 700 | ACO  | C2P-S1P-C   | 7.30   | 136.55      | 101.42   |
| 2   | B     | 701 | ACO  | C2P-S1P-C   | 7.28   | 136.45      | 101.42   |
| 2   | B     | 701 | ACO  | C6P-C5P-N4P | 6.44   | 128.08      | 116.34   |
| 2   | A     | 700 | ACO  | CDP-CBP-CAP | -6.33  | 97.97       | 108.77   |
| 2   | B     | 701 | ACO  | C4A-N9A-C1B | -6.09  | 112.38      | 126.63   |
| 2   | B     | 701 | ACO  | C2B-C1B-N9A | -5.81  | 98.87       | 113.30   |
| 2   | B     | 701 | ACO  | C1B-N9A-C8A | 5.69   | 139.72      | 127.09   |
| 2   | A     | 700 | ACO  | CDP-CBP-CCP | 5.42   | 117.17      | 108.22   |
| 2   | B     | 701 | ACO  | O9P-C9P-CAP | 5.36   | 135.87      | 120.89   |
| 2   | B     | 701 | ACO  | CDP-CBP-CAP | -5.36  | 99.64       | 108.77   |
| 2   | A     | 700 | ACO  | C6P-C7P-N8P | -5.34  | 100.64      | 112.00   |
| 2   | B     | 701 | ACO  | CEP-CBP-CCP | -5.32  | 99.44       | 108.22   |
| 3   | A     | 800 | ADP  | C5-C4-N3    | -5.28  | 119.45      | 126.72   |
| 2   | B     | 701 | ACO  | C7P-N8P-C9P | 5.23   | 131.95      | 122.55   |
| 2   | A     | 700 | ACO  | OAP-CAP-CBP | 4.98   | 121.72      | 110.18   |
| 2   | A     | 700 | ACO  | C7P-N8P-C9P | 4.92   | 131.38      | 122.55   |
| 2   | B     | 701 | ACO  | O3B-C3B-C2B | 4.80   | 128.89      | 111.68   |
| 3   | A     | 800 | ADP  | N3-C4-N9    | 4.62   | 135.03      | 127.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 800 | ADP  | N3-C2-N1    | -4.60 | 121.62      | 128.58   |
| 3   | A     | 800 | ADP  | O2A-PA-O3A  | 4.39  | 119.14      | 107.27   |
| 2   | A     | 700 | ACO  | C7P-C6P-C5P | -4.35 | 105.15      | 112.39   |
| 2   | B     | 701 | ACO  | C3P-N4P-C5P | 4.21  | 130.66      | 122.82   |
| 2   | A     | 700 | ACO  | O-C-S1P     | -3.79 | 107.33      | 122.65   |
| 2   | B     | 701 | ACO  | O-C-S1P     | -3.75 | 107.47      | 122.65   |
| 2   | A     | 700 | ACO  | P1A-O5B-C5B | -3.75 | 99.85       | 121.35   |
| 2   | A     | 700 | ACO  | O4B-C4B-C5B | -3.68 | 97.56       | 109.33   |
| 3   | A     | 800 | ADP  | C5-N7-C8    | 3.63  | 109.15      | 103.45   |
| 3   | A     | 800 | ADP  | C2-N3-C4    | 3.62  | 120.67      | 111.83   |
| 2   | B     | 701 | ACO  | C7P-C6P-C5P | -3.58 | 106.44      | 112.39   |
| 2   | B     | 701 | ACO  | O4B-C4B-C5B | 3.47  | 120.47      | 109.33   |
| 2   | A     | 700 | ACO  | OAP-CAP-C9P | 3.34  | 123.32      | 109.38   |
| 2   | B     | 701 | ACO  | P3B-O3B-C3B | 3.11  | 131.75      | 123.43   |
| 2   | B     | 701 | ACO  | O2A-P1A-O3A | -3.09 | 98.93       | 107.27   |
| 2   | B     | 701 | ACO  | O4B-C1B-N9A | -3.08 | 102.17      | 108.09   |
| 2   | A     | 700 | ACO  | CEP-CBP-CCP | -2.95 | 103.35      | 108.22   |
| 2   | A     | 700 | ACO  | C6P-C5P-N4P | 2.86  | 121.56      | 116.34   |
| 3   | A     | 800 | ADP  | C4-C5-N7    | -2.82 | 107.36      | 110.58   |
| 2   | A     | 700 | ACO  | O2A-P1A-O5B | 2.74  | 119.98      | 107.57   |
| 3   | A     | 800 | ADP  | O2A-PA-O1A  | -2.65 | 100.11      | 112.44   |
| 3   | A     | 800 | ADP  | O3A-PA-O1A  | -2.62 | 102.81      | 110.70   |
| 2   | A     | 700 | ACO  | O5B-C5B-C4B | 2.62  | 117.92      | 108.99   |
| 2   | B     | 701 | ACO  | CDP-CBP-CCP | 2.60  | 112.52      | 108.22   |
| 2   | A     | 700 | ACO  | C5B-C4B-C3B | -2.50 | 106.04      | 114.38   |
| 2   | A     | 700 | ACO  | C4A-N9A-C1B | 2.43  | 132.31      | 126.63   |
| 2   | B     | 701 | ACO  | C3B-C2B-C1B | 2.37  | 105.09      | 99.89    |
| 3   | A     | 800 | ADP  | N9-C8-N7    | -2.33 | 110.63      | 113.94   |
| 2   | A     | 700 | ACO  | P2A-O6A-CCP | 2.29  | 133.62      | 121.12   |
| 2   | A     | 700 | ACO  | C3B-C2B-C1B | 2.28  | 104.90      | 99.89    |
| 2   | B     | 701 | ACO  | O3A-P2A-O4A | 2.25  | 117.47      | 110.70   |
| 2   | B     | 701 | ACO  | P2A-O6A-CCP | 2.16  | 132.86      | 121.12   |
| 2   | A     | 700 | ACO  | N3A-C4A-N9A | 2.09  | 130.72      | 127.17   |
| 2   | A     | 700 | ACO  | C5A-C4A-N9A | -2.03 | 103.60      | 105.81   |
| 2   | B     | 701 | ACO  | O3A-P1A-O1A | 2.03  | 116.81      | 110.70   |
| 2   | B     | 701 | ACO  | OAP-CAP-C9P | 2.03  | 117.85      | 109.38   |
| 2   | B     | 701 | ACO  | OAP-CAP-CBP | 2.02  | 114.85      | 110.18   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 2   | A     | 700 | ACO  | C2B  |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 2   | B     | 701 | ACO  | C2B  |

All (35) torsion outliers are listed below:

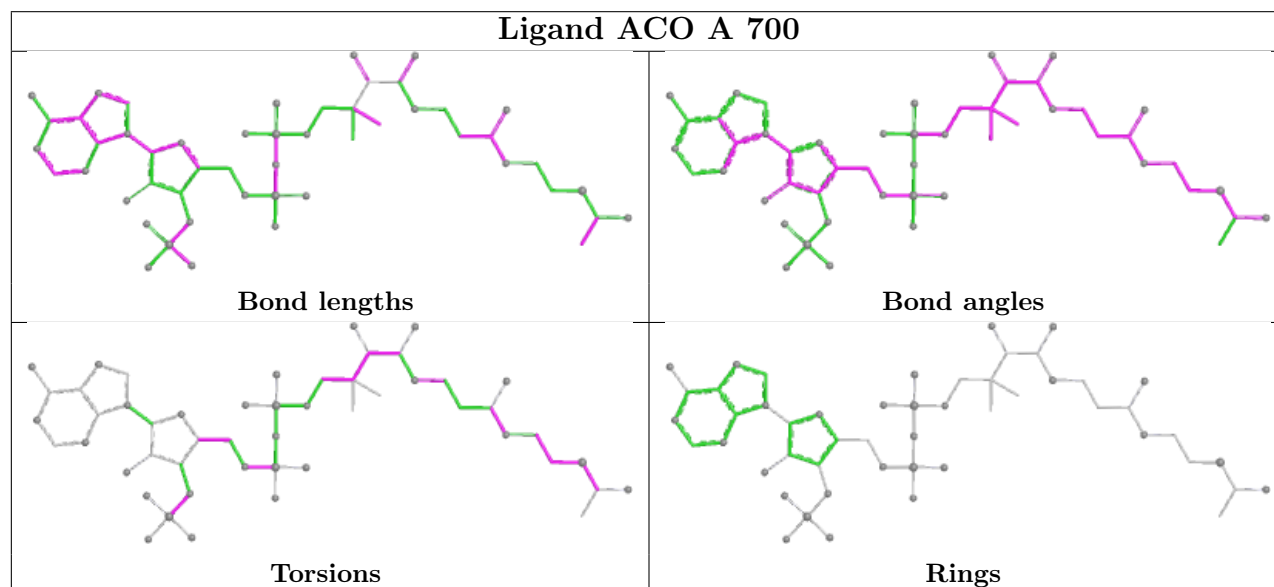
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 700 | ACO  | O4B-C4B-C5B-O5B |
| 2   | A     | 700 | ACO  | C5B-O5B-P1A-O3A |
| 2   | A     | 700 | ACO  | CEP-CBP-CCP-O6A |
| 2   | A     | 700 | ACO  | C9P-CAP-CBP-CCP |
| 2   | A     | 700 | ACO  | C9P-CAP-CBP-CDP |
| 2   | A     | 700 | ACO  | C9P-CAP-CBP-CEP |
| 2   | A     | 700 | ACO  | N8P-C9P-CAP-OAP |
| 2   | A     | 700 | ACO  | S1P-C2P-C3P-N4P |
| 2   | B     | 701 | ACO  | O4B-C4B-C5B-O5B |
| 2   | B     | 701 | ACO  | C5B-O5B-P1A-O1A |
| 2   | B     | 701 | ACO  | C5B-O5B-P1A-O3A |
| 2   | B     | 701 | ACO  | N8P-C9P-CAP-OAP |
| 2   | B     | 701 | ACO  | O5P-C5P-N4P-C3P |
| 2   | B     | 701 | ACO  | C3P-C2P-S1P-C   |
| 2   | B     | 701 | ACO  | CH3-C-S1P-C2P   |
| 3   | A     | 800 | ADP  | C5'-O5'-PA-O1A  |
| 3   | A     | 800 | ADP  | C5'-O5'-PA-O3A  |
| 3   | A     | 800 | ADP  | O4'-C4'-C5'-O5' |
| 2   | A     | 700 | ACO  | O5P-C5P-N4P-C3P |
| 3   | A     | 800 | ADP  | C3'-C4'-C5'-O5' |
| 2   | A     | 700 | ACO  | C6P-C7P-N8P-C9P |
| 2   | A     | 700 | ACO  | C3B-C4B-C5B-O5B |
| 2   | B     | 701 | ACO  | C3B-C4B-C5B-O5B |
| 2   | A     | 700 | ACO  | CH3-C-S1P-C2P   |
| 2   | A     | 700 | ACO  | O9P-C9P-CAP-OAP |
| 2   | B     | 701 | ACO  | O9P-C9P-CAP-OAP |
| 2   | B     | 701 | ACO  | C6P-C7P-N8P-C9P |
| 2   | B     | 701 | ACO  | C9P-CAP-CBP-CEP |
| 3   | A     | 800 | ADP  | PB-O3A-PA-O2A   |
| 2   | B     | 701 | ACO  | C9P-CAP-CBP-CCP |
| 2   | A     | 700 | ACO  | C3P-C2P-S1P-C   |
| 2   | A     | 700 | ACO  | C5B-O5B-P1A-O1A |
| 2   | A     | 700 | ACO  | C3B-O3B-P3B-O8A |
| 2   | A     | 700 | ACO  | C6P-C5P-N4P-C3P |
| 3   | A     | 800 | ADP  | PB-O3A-PA-O1A   |

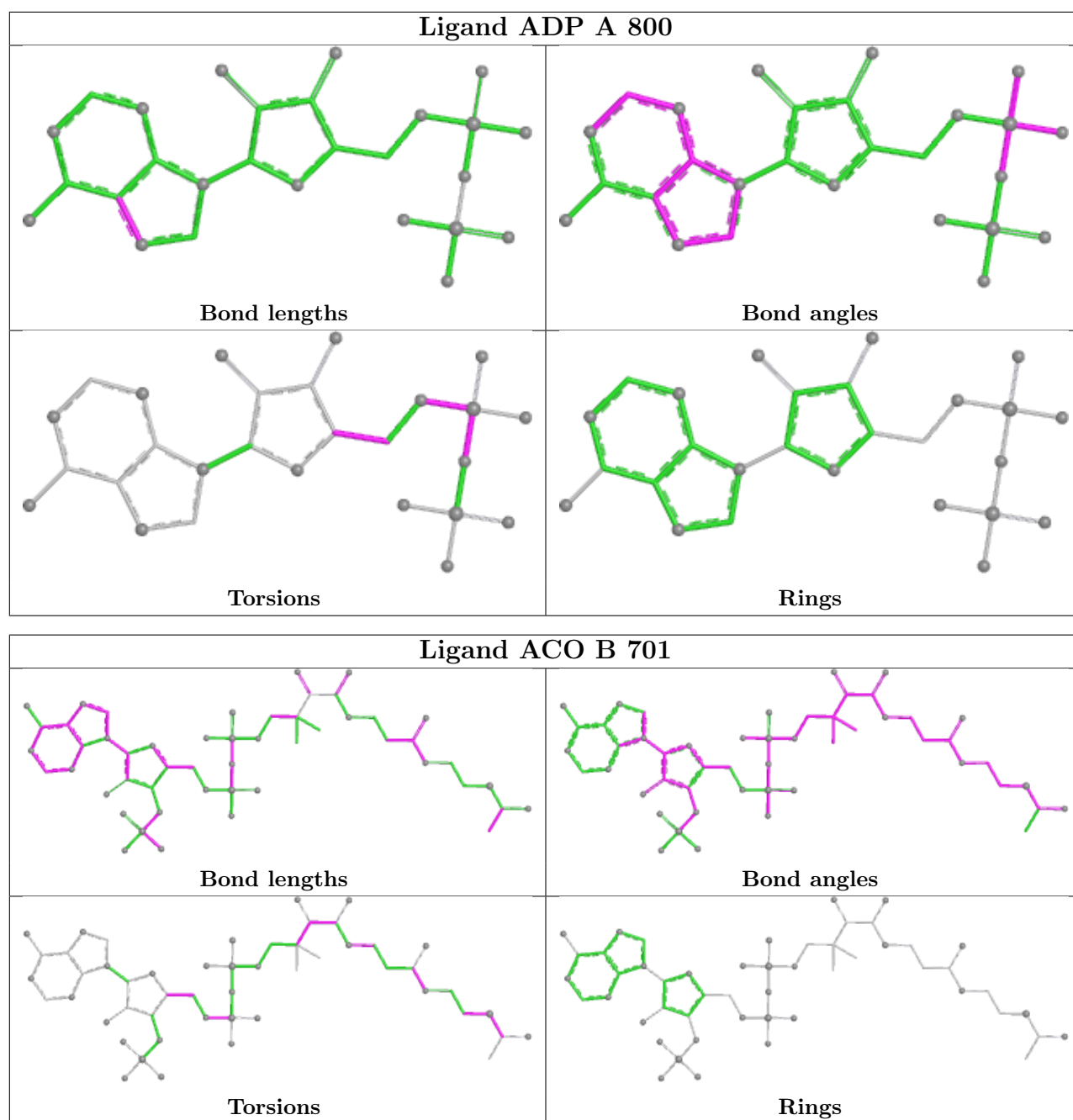
There are no ring outliers.

4 monomers are involved in 13 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 700 | ACO  | 3       | 0            |
| 3   | A     | 800 | ADP  | 2       | 0            |
| 2   | B     | 701 | ACO  | 7       | 0            |
| 4   | B     | 801 | SO4  | 1       | 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

### 6.1 Protein, DNA and RNA chains

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     | 648/671 (96%)   | 0.07   | 24 (3%)  | 45 | 51 | 18, 35, 62, 90        | 0     |
| 1   | B     | 651/671 (97%)   | 0.84   | 97 (14%) | 5  | 6  | 22, 49, 99, 100       | 0     |
| All | All   | 1299/1342 (96%) | 0.46   | 121 (9%) | 14 | 17 | 18, 42, 95, 100       | 0     |

All (121) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 54  | PRO  | 6.4  |
| 1   | B     | 258 | TRP  | 6.0  |
| 1   | A     | 54  | PRO  | 5.5  |
| 1   | B     | 65  | LEU  | 5.3  |
| 1   | B     | 217 | ALA  | 4.9  |
| 1   | B     | 184 | LEU  | 4.8  |
| 1   | B     | 484 | THR  | 4.8  |
| 1   | B     | 187 | LEU  | 4.6  |
| 1   | A     | 228 | ALA  | 4.5  |
| 1   | B     | 56  | ALA  | 4.5  |
| 1   | B     | 221 | ILE  | 4.5  |
| 1   | A     | 2   | ALA  | 4.4  |
| 1   | B     | 216 | ILE  | 4.4  |
| 1   | B     | 212 | LEU  | 4.4  |
| 1   | B     | 226 | ALA  | 4.3  |
| 1   | B     | 482 | GLN  | 4.2  |
| 1   | B     | 232 | VAL  | 4.2  |
| 1   | B     | 251 | ALA  | 4.2  |
| 1   | B     | 483 | TYR  | 4.1  |
| 1   | B     | 241 | PHE  | 4.1  |
| 1   | A     | 52  | PRO  | 4.0  |
| 1   | B     | 209 | ALA  | 4.0  |
| 1   | B     | 244 | ILE  | 4.0  |
| 1   | A     | 226 | ALA  | 4.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 275 | LEU  | 3.9  |
| 1   | B     | 55  | ASP  | 3.9  |
| 1   | B     | 53  | ARG  | 3.8  |
| 1   | B     | 341 | PHE  | 3.6  |
| 1   | B     | 189 | THR  | 3.6  |
| 1   | B     | 318 | ILE  | 3.6  |
| 1   | A     | 66  | GLN  | 3.5  |
| 1   | B     | 312 | PHE  | 3.5  |
| 1   | B     | 191 | PRO  | 3.5  |
| 1   | A     | 670 | PHE  | 3.5  |
| 1   | A     | 70  | GLY  | 3.5  |
| 1   | B     | 69  | LEU  | 3.5  |
| 1   | B     | 237 | ALA  | 3.4  |
| 1   | B     | 502 | ARG  | 3.3  |
| 1   | B     | 243 | PHE  | 3.3  |
| 1   | B     | 183 | LEU  | 3.2  |
| 1   | B     | 670 | PHE  | 3.2  |
| 1   | A     | 668 | GLN  | 3.2  |
| 1   | A     | 67  | THR  | 3.2  |
| 1   | B     | 238 | GLY  | 3.2  |
| 1   | B     | 208 | LEU  | 3.2  |
| 1   | B     | 229 | SER  | 3.1  |
| 1   | B     | 220 | ALA  | 3.1  |
| 1   | B     | 340 | ASN  | 3.1  |
| 1   | B     | 215 | ARG  | 3.1  |
| 1   | B     | 192 | PRO  | 3.1  |
| 1   | A     | 291 | TYR  | 3.0  |
| 1   | B     | 349 | ILE  | 3.0  |
| 1   | A     | 517 | HIS  | 3.0  |
| 1   | B     | 236 | PHE  | 3.0  |
| 1   | B     | 52  | PRO  | 3.0  |
| 1   | A     | 634 | ARG  | 3.0  |
| 1   | B     | 279 | PHE  | 3.0  |
| 1   | B     | 246 | PRO  | 3.0  |
| 1   | B     | 214 | SER  | 2.9  |
| 1   | B     | 249 | LEU  | 2.9  |
| 1   | B     | 250 | LEU  | 2.9  |
| 1   | B     | 623 | ALA  | 2.9  |
| 1   | B     | 170 | TYR  | 2.9  |
| 1   | B     | 219 | ARG  | 2.9  |
| 1   | B     | 233 | LEU  | 2.8  |
| 1   | B     | 314 | LEU  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 669 | LEU  | 2.8  |
| 1   | B     | 228 | ALA  | 2.8  |
| 1   | B     | 255 | GLN  | 2.7  |
| 1   | B     | 223 | THR  | 2.7  |
| 1   | B     | 252 | SER  | 2.7  |
| 1   | B     | 257 | ASP  | 2.6  |
| 1   | B     | 566 | ASP  | 2.6  |
| 1   | B     | 307 | PRO  | 2.6  |
| 1   | A     | 68  | LEU  | 2.5  |
| 1   | A     | 254 | GLU  | 2.5  |
| 1   | B     | 68  | LEU  | 2.5  |
| 1   | B     | 431 | ARG  | 2.5  |
| 1   | B     | 171 | PRO  | 2.5  |
| 1   | B     | 160 | LEU  | 2.5  |
| 1   | B     | 248 | ALA  | 2.5  |
| 1   | A     | 162 | HIS  | 2.5  |
| 1   | B     | 224 | ALA  | 2.4  |
| 1   | A     | 51  | SER  | 2.4  |
| 1   | B     | 259 | LEU  | 2.4  |
| 1   | A     | 485 | GLN  | 2.4  |
| 1   | B     | 278 | ARG  | 2.4  |
| 1   | B     | 178 | PRO  | 2.4  |
| 1   | B     | 261 | VAL  | 2.3  |
| 1   | B     | 338 | ASP  | 2.3  |
| 1   | B     | 346 | GLN  | 2.3  |
| 1   | B     | 485 | GLN  | 2.3  |
| 1   | A     | 69  | LEU  | 2.3  |
| 1   | B     | 172 | ALA  | 2.3  |
| 1   | A     | 569 | ASN  | 2.2  |
| 1   | B     | 193 | GLY  | 2.2  |
| 1   | B     | 210 | GLY  | 2.2  |
| 1   | B     | 629 | LEU  | 2.2  |
| 1   | B     | 631 | LEU  | 2.2  |
| 1   | B     | 67  | THR  | 2.2  |
| 1   | B     | 242 | ARG  | 2.2  |
| 1   | B     | 176 | PRO  | 2.2  |
| 1   | A     | 669 | LEU  | 2.2  |
| 1   | B     | 204 | GLY  | 2.2  |
| 1   | A     | 53  | ARG  | 2.1  |
| 1   | B     | 433 | ARG  | 2.1  |
| 1   | B     | 359 | TRP  | 2.1  |
| 1   | B     | 260 | VAL  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 227 | LYS  | 2.1  |
| 1   | B     | 280 | PRO  | 2.1  |
| 1   | B     | 213 | ILE  | 2.1  |
| 1   | B     | 627 | THR  | 2.1  |
| 1   | B     | 131 | ALA  | 2.1  |
| 1   | B     | 235 | GLN  | 2.1  |
| 1   | B     | 240 | LYS  | 2.0  |
| 1   | B     | 207 | ALA  | 2.0  |
| 1   | B     | 339 | GLU  | 2.0  |
| 1   | B     | 66  | GLN  | 2.0  |
| 1   | B     | 481 | LEU  | 2.0  |
| 1   | A     | 572 | VAL  | 2.0  |
| 1   | B     | 222 | 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](#)

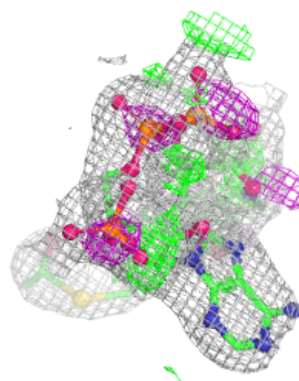
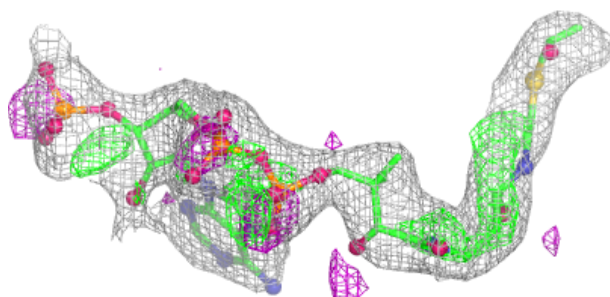
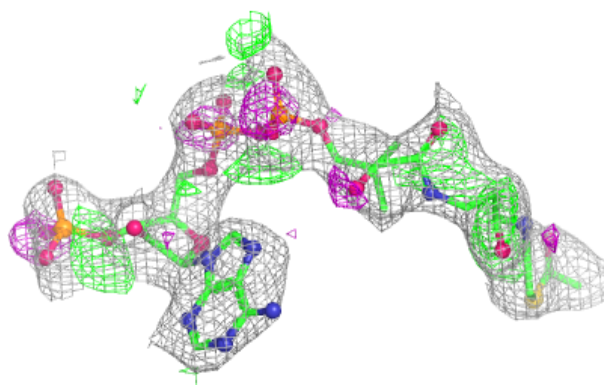
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | SO4  | B     | 801 | 5/5   | 0.76 | 0.12 | 77,78,78,79                 | 0     |
| 2   | ACO  | B     | 701 | 51/51 | 0.87 | 0.18 | 24,50,93,95                 | 0     |
| 2   | ACO  | A     | 700 | 51/51 | 0.88 | 0.19 | 18,66,88,89                 | 0     |
| 3   | ADP  | A     | 800 | 27/27 | 0.94 | 0.09 | 29,38,39,43                 | 0     |

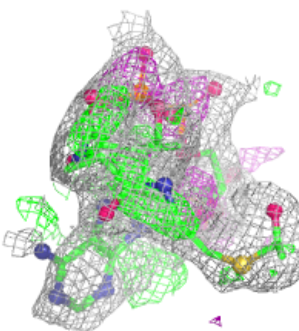
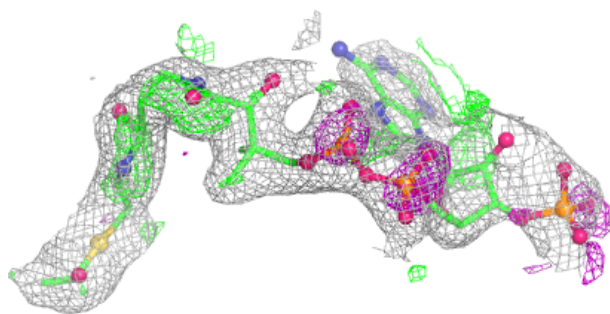
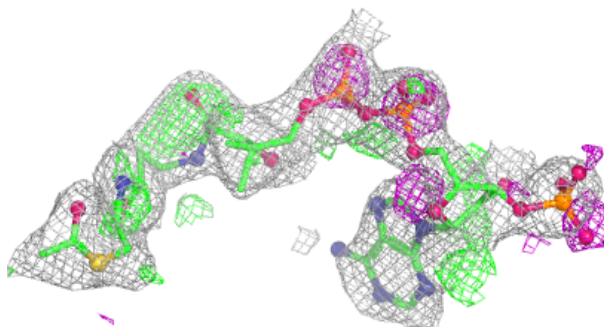
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ACO B 701:**

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

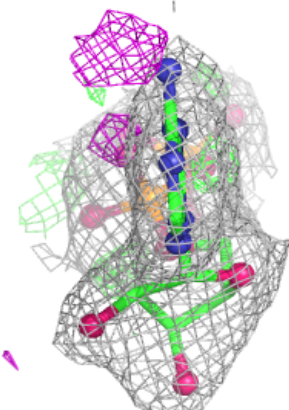
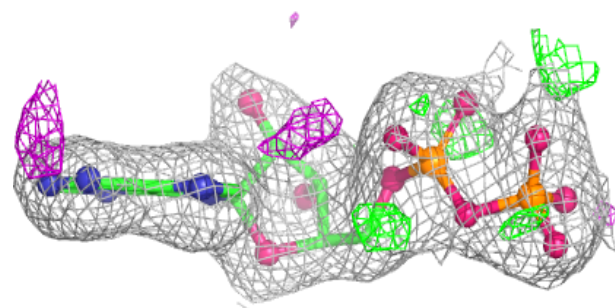
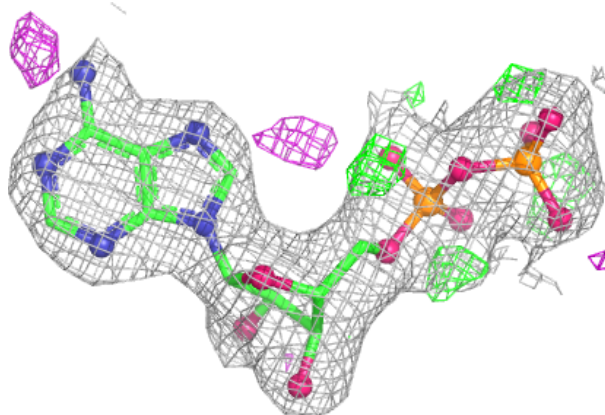
**Electron density around ACO A 700:**

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



**Electron density around ADP A 800:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.