



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:25 PM UTC

PDB ID : 3E74 / pdb\_00003e74  
Title : Crystal structure of E. coli allantoinase with iron ions at the metal center  
Authors : Kim, K.  
Deposited on : 2008-08-17  
Resolution : 2.10 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                                                              |
| 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                                                             |

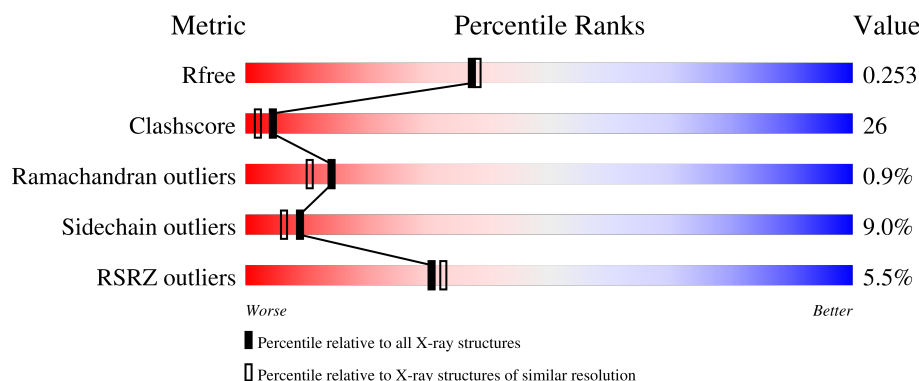
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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                      | 6658 (2.10-2.10)                                      |
| Clashscore            | 190562                      | 7164 (2.10-2.10)                                      |
| Ramachandran outliers | 187476                      | 7099 (2.10-2.10)                                      |
| Sidechain outliers    | 187428                      | 7100 (2.10-2.10)                                      |
| RSRZ outliers         | 180081                      | 6662 (2.10-2.10)                                      |

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     | 473    | <div> <div>5%</div> <div> <div></div> <div>51%</div> <div>31%</div> <div>7%</div> <div>9%</div> </div> </div>  |
| 1   | B     | 473    | <div> <div>5%</div> <div> <div></div> <div>57%</div> <div>28%</div> <div>5%</div> <div>8%</div> </div> </div>  |
| 1   | C     | 473    | <div> <div>3%</div> <div> <div></div> <div>57%</div> <div>26%</div> <div>7%</div> <div>10%</div> </div> </div> |
| 1   | D     | 473    | <div> <div>7%</div> <div> <div></div> <div>53%</div> <div>32%</div> <div>6%</div> <div>9%</div> </div> </div>  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14068 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 Allantoinase.

| Mol | Chain | Residues | Atoms |      |     |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|----|---------|---------|-------|
| 1   | A     | 429      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 3290  | 2073 | 569 | 625 | 11 | 12 |         |         |       |
| 1   | B     | 433      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 3329  | 2098 | 576 | 632 | 11 | 12 |         |         |       |
| 1   | C     | 428      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 3286  | 2071 | 568 | 624 | 11 | 12 |         |         |       |
| 1   | D     | 429      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 3290  | 2073 | 569 | 625 | 11 | 12 |         |         |       |

There are 84 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | -19     | MSE      | -      | expression tag      | UNP P77671 |
| A     | -18     | GLY      | -      | expression tag      | UNP P77671 |
| A     | -17     | SER      | -      | expression tag      | UNP P77671 |
| A     | -16     | SER      | -      | expression tag      | UNP P77671 |
| A     | -15     | HIS      | -      | expression tag      | UNP P77671 |
| A     | -14     | HIS      | -      | expression tag      | UNP P77671 |
| A     | -13     | HIS      | -      | expression tag      | UNP P77671 |
| A     | -12     | HIS      | -      | expression tag      | UNP P77671 |
| A     | -11     | HIS      | -      | expression tag      | UNP P77671 |
| A     | -10     | SER      | -      | expression tag      | UNP P77671 |
| A     | -9      | SER      | -      | expression tag      | UNP P77671 |
| A     | -8      | GLY      | -      | expression tag      | UNP P77671 |
| A     | -7      | GLU      | -      | expression tag      | UNP P77671 |
| A     | -6      | ASN      | -      | expression tag      | UNP P77671 |
| A     | -5      | LEU      | -      | expression tag      | UNP P77671 |
| A     | -4      | TYR      | -      | expression tag      | UNP P77671 |
| A     | -3      | PHE      | -      | expression tag      | UNP P77671 |
| A     | -2      | GLN      | -      | expression tag      | UNP P77671 |
| A     | -1      | GLY      | -      | expression tag      | UNP P77671 |
| A     | 0       | HIS      | -      | expression tag      | UNP P77671 |
| A     | 262     | ILE      | VAL    | engineered mutation | UNP P77671 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | -19     | MSE      | -      | expression tag      | UNP P77671 |
| B     | -18     | GLY      | -      | expression tag      | UNP P77671 |
| B     | -17     | SER      | -      | expression tag      | UNP P77671 |
| B     | -16     | SER      | -      | expression tag      | UNP P77671 |
| B     | -15     | HIS      | -      | expression tag      | UNP P77671 |
| B     | -14     | HIS      | -      | expression tag      | UNP P77671 |
| B     | -13     | HIS      | -      | expression tag      | UNP P77671 |
| B     | -12     | HIS      | -      | expression tag      | UNP P77671 |
| B     | -11     | HIS      | -      | expression tag      | UNP P77671 |
| B     | -10     | SER      | -      | expression tag      | UNP P77671 |
| B     | -9      | SER      | -      | expression tag      | UNP P77671 |
| B     | -8      | GLY      | -      | expression tag      | UNP P77671 |
| B     | -7      | GLU      | -      | expression tag      | UNP P77671 |
| B     | -6      | ASN      | -      | expression tag      | UNP P77671 |
| B     | -5      | LEU      | -      | expression tag      | UNP P77671 |
| B     | -4      | TYR      | -      | expression tag      | UNP P77671 |
| B     | -3      | PHE      | -      | expression tag      | UNP P77671 |
| B     | -2      | GLN      | -      | expression tag      | UNP P77671 |
| B     | -1      | GLY      | -      | expression tag      | UNP P77671 |
| B     | 0       | HIS      | -      | expression tag      | UNP P77671 |
| B     | 262     | ILE      | VAL    | engineered mutation | UNP P77671 |
| C     | -19     | MSE      | -      | expression tag      | UNP P77671 |
| C     | -18     | GLY      | -      | expression tag      | UNP P77671 |
| C     | -17     | SER      | -      | expression tag      | UNP P77671 |
| C     | -16     | SER      | -      | expression tag      | UNP P77671 |
| C     | -15     | HIS      | -      | expression tag      | UNP P77671 |
| C     | -14     | HIS      | -      | expression tag      | UNP P77671 |
| C     | -13     | HIS      | -      | expression tag      | UNP P77671 |
| C     | -12     | HIS      | -      | expression tag      | UNP P77671 |
| C     | -11     | HIS      | -      | expression tag      | UNP P77671 |
| C     | -10     | SER      | -      | expression tag      | UNP P77671 |
| C     | -9      | SER      | -      | expression tag      | UNP P77671 |
| C     | -8      | GLY      | -      | expression tag      | UNP P77671 |
| C     | -7      | GLU      | -      | expression tag      | UNP P77671 |
| C     | -6      | ASN      | -      | expression tag      | UNP P77671 |
| C     | -5      | LEU      | -      | expression tag      | UNP P77671 |
| C     | -4      | TYR      | -      | expression tag      | UNP P77671 |
| C     | -3      | PHE      | -      | expression tag      | UNP P77671 |
| C     | -2      | GLN      | -      | expression tag      | UNP P77671 |
| C     | -1      | GLY      | -      | expression tag      | UNP P77671 |
| C     | 0       | HIS      | -      | expression tag      | UNP P77671 |
| C     | 262     | ILE      | VAL    | engineered mutation | UNP P77671 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| D     | -19     | MSE      | -      | expression tag      | UNP P77671 |
| D     | -18     | GLY      | -      | expression tag      | UNP P77671 |
| D     | -17     | SER      | -      | expression tag      | UNP P77671 |
| D     | -16     | SER      | -      | expression tag      | UNP P77671 |
| D     | -15     | HIS      | -      | expression tag      | UNP P77671 |
| D     | -14     | HIS      | -      | expression tag      | UNP P77671 |
| D     | -13     | HIS      | -      | expression tag      | UNP P77671 |
| D     | -12     | HIS      | -      | expression tag      | UNP P77671 |
| D     | -11     | HIS      | -      | expression tag      | UNP P77671 |
| D     | -10     | SER      | -      | expression tag      | UNP P77671 |
| D     | -9      | SER      | -      | expression tag      | UNP P77671 |
| D     | -8      | GLY      | -      | expression tag      | UNP P77671 |
| D     | -7      | GLU      | -      | expression tag      | UNP P77671 |
| D     | -6      | ASN      | -      | expression tag      | UNP P77671 |
| D     | -5      | LEU      | -      | expression tag      | UNP P77671 |
| D     | -4      | TYR      | -      | expression tag      | UNP P77671 |
| D     | -3      | PHE      | -      | expression tag      | UNP P77671 |
| D     | -2      | GLN      | -      | expression tag      | UNP P77671 |
| D     | -1      | GLY      | -      | expression tag      | UNP P77671 |
| D     | 0       | HIS      | -      | expression tag      | UNP P77671 |
| D     | 262     | ILE      | VAL    | engineered mutation | UNP P77671 |

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | A     | 2        | Total Fe<br>2 2 | 0       | 0       |
| 2   | B     | 2        | Total Fe<br>2 2 | 0       | 0       |
| 2   | C     | 2        | Total Fe<br>2 2 | 0       | 0       |
| 2   | D     | 2        | Total Fe<br>2 2 | 0       | 0       |

- Molecule 3 is water.

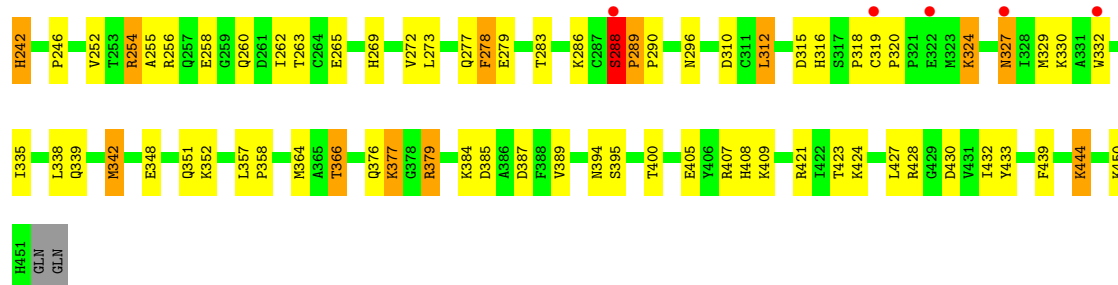
| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 3   | A     | 232      | Total O<br>232 232 | 0       | 0       |
| 3   | B     | 255      | Total O<br>255 255 | 0       | 0       |
| 3   | C     | 219      | Total O<br>219 219 | 0       | 0       |

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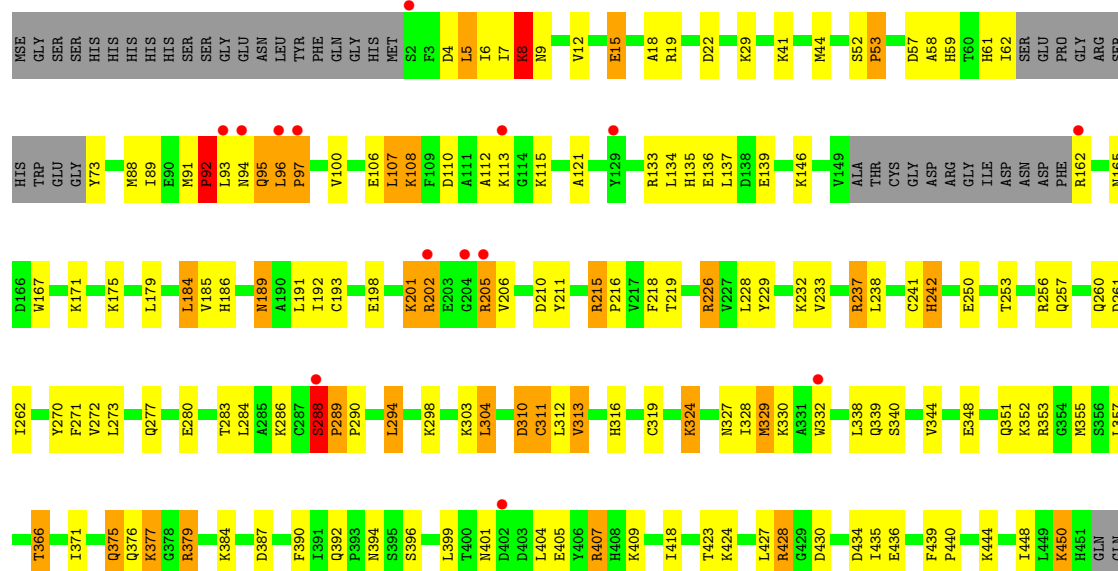
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| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | D     | 159      | Total | O   | 0       | 0       |
|     |       |          | 159   | 159 |         |         |

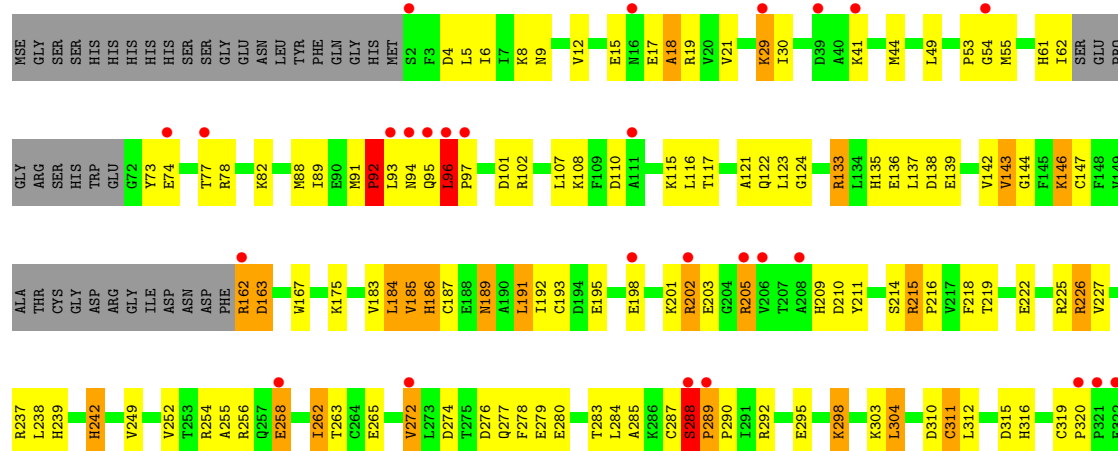




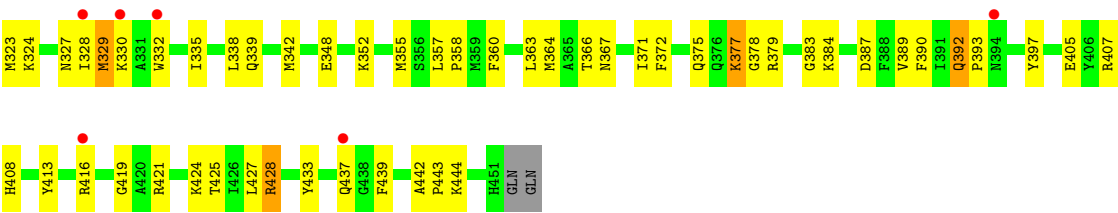
• Molecule 1: Allantoinase



• Molecule 1: Allantoinase







## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 83.68Å 92.45Å 168.43Å<br>90.00° 93.30° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 50.00 – 2.10<br>50.00 – 2.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 79.3 (50.00-2.10)<br>97.2 (50.00-2.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.11                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.44 (at 2.10Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.199 , 0.240<br>0.216 , 0.253                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 14820 reflections (9.99%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 27.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.140                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.39 , 56.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 14068                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 30.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: FE, KCX

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.55         | 0/3323      | 1.12        | 20/4467 (0.4%)  |
| 1   | B     | 0.56         | 0/3365      | 1.12        | 24/4525 (0.5%)  |
| 1   | C     | 0.54         | 0/3319      | 1.11        | 25/4462 (0.6%)  |
| 1   | D     | 0.51         | 0/3323      | 1.08        | 23/4467 (0.5%)  |
| All | All   | 0.54         | 0/13330     | 1.11        | 92/17921 (0.5%) |

There are no bond length outliers.

All (92) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | C     | 288 | SER  | CA-C-N | -12.62 | 107.38      | 120.38   |
| 1   | C     | 288 | SER  | C-N-CA | -12.62 | 107.38      | 120.38   |
| 1   | B     | 288 | SER  | CA-C-N | -12.09 | 107.93      | 120.38   |
| 1   | B     | 288 | SER  | C-N-CA | -12.09 | 107.93      | 120.38   |
| 1   | A     | 96  | LEU  | CA-C-N | -11.12 | 108.35      | 120.14   |
| 1   | A     | 96  | LEU  | C-N-CA | -11.12 | 108.35      | 120.14   |
| 1   | A     | 288 | SER  | CA-C-N | -10.85 | 109.20      | 120.38   |
| 1   | A     | 288 | SER  | C-N-CA | -10.85 | 109.20      | 120.38   |
| 1   | A     | 289 | PRO  | N-CA-C | -10.64 | 97.72       | 110.70   |
| 1   | D     | 288 | SER  | CA-C-N | -9.61  | 110.48      | 120.38   |
| 1   | D     | 288 | SER  | C-N-CA | -9.61  | 110.48      | 120.38   |
| 1   | C     | 289 | PRO  | N-CA-C | -9.35  | 99.29       | 110.70   |
| 1   | A     | 202 | ARG  | N-CA-C | -9.01  | 101.20      | 113.18   |
| 1   | B     | 289 | PRO  | N-CA-C | -8.63  | 100.17      | 110.70   |
| 1   | B     | 439 | PHE  | CA-C-N | 8.47   | 128.45      | 119.05   |
| 1   | B     | 439 | PHE  | C-N-CA | 8.47   | 128.45      | 119.05   |
| 1   | D     | 289 | PRO  | N-CA-C | -8.08  | 100.84      | 110.70   |
| 1   | D     | 96  | LEU  | CA-C-N | -7.87  | 110.00      | 119.84   |
| 1   | D     | 96  | LEU  | C-N-CA | -7.87  | 110.00      | 119.84   |
| 1   | D     | 9   | ASN  | N-CA-C | 7.79   | 122.49      | 113.38   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 96  | LEU  | CA-C-N | -7.54 | 110.42      | 119.84   |
| 1   | B     | 96  | LEU  | C-N-CA | -7.54 | 110.42      | 119.84   |
| 1   | A     | 121 | ALA  | N-CA-C | -7.45 | 100.92      | 110.53   |
| 1   | D     | 439 | PHE  | CA-C-N | 7.02  | 128.62      | 119.84   |
| 1   | D     | 439 | PHE  | C-N-CA | 7.02  | 128.62      | 119.84   |
| 1   | C     | 53  | PRO  | N-CA-C | -6.99 | 100.27      | 111.38   |
| 1   | B     | 185 | VAL  | N-CA-C | 6.95  | 118.12      | 108.12   |
| 1   | D     | 187 | CYS  | N-CA-C | 6.85  | 121.25      | 107.41   |
| 1   | C     | 8   | LYS  | N-CA-C | 6.61  | 120.46      | 109.95   |
| 1   | D     | 258 | GLU  | N-CA-C | -6.59 | 104.98      | 113.16   |
| 1   | A     | 187 | CYS  | N-CA-C | 6.59  | 120.35      | 107.57   |
| 1   | B     | 377 | LYS  | N-CA-C | 6.56  | 119.85      | 109.81   |
| 1   | A     | 116 | LEU  | N-CA-C | 6.48  | 118.72      | 108.67   |
| 1   | B     | 258 | GLU  | N-CA-C | -6.47 | 105.14      | 113.16   |
| 1   | C     | 15  | GLU  | N-CA-C | 6.45  | 117.97      | 111.07   |
| 1   | A     | 281 | ILE  | N-CA-C | 6.45  | 117.20      | 110.62   |
| 1   | B     | 9   | ASN  | N-CA-C | 6.42  | 120.89      | 113.38   |
| 1   | B     | 93  | LEU  | N-CA-C | 6.38  | 120.08      | 112.93   |
| 1   | A     | 440 | PRO  | N-CA-C | 6.31  | 122.30      | 113.53   |
| 1   | B     | 53  | PRO  | N-CA-C | -6.30 | 101.36      | 111.38   |
| 1   | C     | 366 | THR  | N-CA-C | 6.22  | 117.73      | 111.07   |
| 1   | D     | 419 | GLY  | N-CA-C | 6.19  | 122.98      | 115.31   |
| 1   | A     | 91  | MSE  | CA-C-N | 6.18  | 127.56      | 119.84   |
| 1   | A     | 91  | MSE  | C-N-CA | 6.18  | 127.56      | 119.84   |
| 1   | C     | 377 | LYS  | N-CA-C | 6.18  | 119.22      | 110.14   |
| 1   | A     | 185 | VAL  | N-CA-C | 6.15  | 117.62      | 108.46   |
| 1   | B     | 121 | ALA  | N-CA-C | -6.07 | 102.70      | 110.53   |
| 1   | C     | 185 | VAL  | N-CA-C | 5.97  | 117.36      | 108.46   |
| 1   | A     | 377 | LYS  | N-CA-C | 5.95  | 118.89      | 110.14   |
| 1   | D     | 121 | ALA  | N-CA-C | -5.94 | 101.73      | 110.52   |
| 1   | B     | 315 | ASP  | N-CA-C | -5.88 | 103.80      | 111.74   |
| 1   | C     | 439 | PHE  | CA-C-N | 5.84  | 125.71      | 119.28   |
| 1   | C     | 439 | PHE  | C-N-CA | 5.84  | 125.71      | 119.28   |
| 1   | C     | 121 | ALA  | N-CA-C | -5.83 | 102.13      | 110.59   |
| 1   | D     | 377 | LYS  | N-CA-C | 5.81  | 118.69      | 110.14   |
| 1   | B     | 90  | GLU  | N-CA-C | 5.79  | 118.64      | 109.96   |
| 1   | D     | 315 | ASP  | N-CA-C | -5.77 | 103.95      | 111.74   |
| 1   | C     | 97  | PRO  | N-CA-C | -5.76 | 101.45      | 110.50   |
| 1   | D     | 310 | ASP  | N-CA-C | 5.75  | 117.55      | 111.28   |
| 1   | C     | 9   | ASN  | N-CA-C | 5.70  | 119.53      | 112.47   |
| 1   | C     | 96  | LEU  | CA-C-N | -5.63 | 113.30      | 120.23   |
| 1   | C     | 96  | LEU  | C-N-CA | -5.63 | 113.30      | 120.23   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 366 | THR  | N-CA-C  | 5.60  | 117.06      | 111.07   |
| 1   | C     | 353 | ARG  | N-CA-C  | 5.57  | 120.06      | 112.88   |
| 1   | D     | 18  | ALA  | N-CA-C  | -5.57 | 100.11      | 109.07   |
| 1   | C     | 310 | ASP  | N-CA-C  | 5.51  | 116.96      | 111.07   |
| 1   | B     | 15  | GLU  | N-CA-C  | 5.50  | 117.27      | 111.28   |
| 1   | D     | 378 | GLY  | N-CA-C  | 5.44  | 122.59      | 115.36   |
| 1   | A     | 272 | VAL  | N-CA-CB | -5.43 | 106.24      | 112.21   |
| 1   | B     | 366 | THR  | N-CA-C  | 5.34  | 116.78      | 111.07   |
| 1   | D     | 366 | THR  | N-CA-C  | 5.32  | 116.77      | 111.07   |
| 1   | C     | 186 | HIS  | N-CA-C  | -5.32 | 100.43      | 108.67   |
| 1   | C     | 404 | LEU  | N-CA-C  | 5.30  | 118.13      | 110.28   |
| 1   | B     | 116 | LEU  | N-CA-C  | 5.26  | 117.30      | 109.25   |
| 1   | D     | 311 | CYS  | N-CA-C  | 5.25  | 117.05      | 109.07   |
| 1   | D     | 185 | VAL  | N-CA-C  | 5.24  | 116.27      | 108.46   |
| 1   | A     | 310 | ASP  | N-CA-C  | 5.23  | 116.66      | 111.07   |
| 1   | A     | 122 | GLN  | N-CA-C  | 5.22  | 117.75      | 109.50   |
| 1   | C     | 311 | CYS  | N-CA-C  | 5.22  | 117.00      | 109.07   |
| 1   | B     | 187 | CYS  | N-CA-C  | 5.16  | 117.34      | 107.75   |
| 1   | C     | 440 | PRO  | N-CA-C  | 5.15  | 120.61      | 113.65   |
| 1   | B     | 200 | ALA  | N-CA-C  | -5.15 | 105.75      | 111.36   |
| 1   | D     | 186 | HIS  | N-CA-C  | -5.15 | 100.77      | 108.96   |
| 1   | D     | 116 | LEU  | N-CA-C  | 5.14  | 116.64      | 108.67   |
| 1   | D     | 138 | ASP  | N-CA-C  | -5.10 | 105.80      | 111.36   |
| 1   | C     | 12  | VAL  | N-CA-C  | 5.09  | 115.91      | 108.58   |
| 1   | B     | 310 | ASP  | N-CA-C  | 5.08  | 116.81      | 111.28   |
| 1   | B     | 129 | TYR  | N-CA-C  | 5.07  | 119.16      | 112.92   |
| 1   | C     | 289 | PRO  | CA-C-N  | 5.07  | 125.35      | 119.92   |
| 1   | C     | 289 | PRO  | C-N-CA  | 5.07  | 125.35      | 119.92   |
| 1   | A     | 129 | TYR  | N-CA-C  | 5.07  | 118.29      | 112.57   |
| 1   | B     | 342 | MSE  | N-CA-C  | 5.06  | 116.48      | 110.97   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3290  | 0        | 3272     | 218     | 0            |
| 1   | B     | 3329  | 0        | 3299     | 157     | 0            |
| 1   | C     | 3286  | 0        | 3268     | 138     | 0            |
| 1   | D     | 3290  | 0        | 3271     | 196     | 0            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| 2   | C     | 2     | 0        | 0        | 0       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 3   | A     | 232   | 0        | 0        | 12      | 0            |
| 3   | B     | 255   | 0        | 0        | 5       | 0            |
| 3   | C     | 219   | 0        | 0        | 5       | 0            |
| 3   | D     | 159   | 0        | 0        | 10      | 0            |
| All | All   | 14068 | 0        | 13110    | 691     | 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 26.

All (691) 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:D:320:PRO:HG2  | 1:D:323:MSE:HG3  | 1.33                     | 1.09              |
| 1:A:77:THR:HG22  | 1:A:117:THR:HB   | 1.34                     | 1.06              |
| 1:B:102:ARG:HB2  | 1:B:102:ARG:HH11 | 1.18                     | 1.01              |
| 1:D:272:VAL:HG22 | 1:D:416:ARG:HH22 | 1.23                     | 1.00              |
| 1:D:320:PRO:HD2  | 1:D:323:MSE:HE2  | 1.41                     | 0.98              |
| 1:A:77:THR:HG21  | 1:A:117:THR:H    | 1.28                     | 0.97              |
| 1:B:77:THR:HG23  | 1:B:117:THR:HB   | 1.46                     | 0.96              |
| 1:D:216:PRO:O    | 1:D:219:THR:HG22 | 1.64                     | 0.96              |
| 1:A:205:ARG:HH11 | 1:A:205:ARG:HB2  | 1.30                     | 0.96              |
| 1:C:95:GLN:H     | 1:C:95:GLN:HE21  | 1.03                     | 0.95              |
| 1:D:108:LYS:NZ   | 1:D:122:GLN:HE22 | 1.65                     | 0.95              |
| 1:D:238:LEU:HB3  | 1:D:262:ILE:HG22 | 1.49                     | 0.94              |
| 1:D:108:LYS:HZ1  | 1:D:122:GLN:HE22 | 1.04                     | 0.94              |
| 1:C:250:GLU:HG3  | 1:C:303:LYS:HZ1  | 1.32                     | 0.94              |
| 1:C:351:GLN:HE22 | 1:C:394:ASN:H    | 1.13                     | 0.94              |
| 1:A:312:LEU:HD21 | 1:A:345:MSE:HE2  | 1.49                     | 0.92              |
| 1:C:95:GLN:H     | 1:C:95:GLN:NE2   | 1.67                     | 0.92              |
| 1:D:215:ARG:HG3  | 1:D:215:ARG:HH11 | 1.33                     | 0.92              |
| 1:B:351:GLN:HE22 | 1:B:394:ASN:H    | 1.15                     | 0.90              |
| 1:D:203:GLU:HB2  | 1:D:205:ARG:HD3  | 1.53                     | 0.90              |
| 1:B:77:THR:HG21  | 1:B:117:THR:H    | 1.37                     | 0.88              |
| 1:A:205:ARG:HH11 | 1:A:205:ARG:CB   | 1.86                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:423:THR:O    | 1:B:424:LYS:HD2  | 1.73                     | 0.88              |
| 1:C:44:MSE:HE3   | 1:C:424:LYS:NZ   | 1.88                     | 0.87              |
| 1:A:77:THR:HG23  | 1:A:118:ILE:HG12 | 1.54                     | 0.87              |
| 1:A:77:THR:HG21  | 1:A:117:THR:N    | 1.88                     | 0.87              |
| 1:A:288:SER:HB3  | 1:A:289:PRO:HD3  | 1.57                     | 0.86              |
| 1:D:91:MSE:SE    | 1:D:146:KCX:HG2  | 2.25                     | 0.85              |
| 1:D:201:LYS:HE2  | 1:D:330:LYS:HE2  | 1.57                     | 0.84              |
| 1:A:339:GLN:HE22 | 1:A:405:GLU:H    | 1.22                     | 0.84              |
| 1:B:288:SER:HB3  | 1:B:289:PRO:HD3  | 1.59                     | 0.82              |
| 1:C:5:LEU:HD22   | 1:C:6:ILE:N      | 1.95                     | 0.81              |
| 1:B:324:LYS:HE3  | 1:B:332:TRP:O    | 1.79                     | 0.81              |
| 1:C:198:GLU:O    | 1:C:202:ARG:HD3  | 1.80                     | 0.81              |
| 1:D:342:MSE:HE2  | 1:D:342:MSE:HA   | 1.61                     | 0.81              |
| 1:A:162:ARG:N    | 1:A:162:ARG:NE   | 2.28                     | 0.81              |
| 1:A:400:THR:HG22 | 1:A:402:ASP:H    | 1.45                     | 0.80              |
| 1:A:15:GLU:CD    | 1:A:379:ARG:HD3  | 2.06                     | 0.80              |
| 1:B:77:THR:CG2   | 1:B:117:THR:H    | 1.95                     | 0.80              |
| 1:B:71:GLU:HG3   | 1:B:318:PRO:HG3  | 1.63                     | 0.80              |
| 1:B:215:ARG:HH11 | 1:B:215:ARG:HG3  | 1.45                     | 0.79              |
| 1:A:4:ASP:HA     | 1:A:41:LYS:HD3   | 1.65                     | 0.79              |
| 1:A:165:ASN:ND2  | 1:A:168:GLN:H    | 1.80                     | 0.79              |
| 1:A:327:ASN:H    | 1:A:330:LYS:CE   | 1.95                     | 0.79              |
| 1:D:342:MSE:HE1  | 1:D:364:MSE:CG   | 2.13                     | 0.79              |
| 1:A:113:LYS:HD2  | 3:A:680:HOH:O    | 1.81                     | 0.78              |
| 1:B:70:TRP:HB2   | 1:B:320:PRO:HG3  | 1.65                     | 0.78              |
| 1:C:407:ARG:HH11 | 1:C:407:ARG:HB2  | 1.48                     | 0.78              |
| 1:A:91:MSE:SE    | 1:A:146:KCX:HG2  | 2.33                     | 0.78              |
| 1:A:226:ARG:HE   | 1:D:226:ARG:HE   | 1.29                     | 0.78              |
| 1:B:207:THR:HB   | 1:B:210:ASP:OD2  | 1.84                     | 0.78              |
| 1:D:295:GLU:O    | 1:D:298:LYS:HG3  | 1.84                     | 0.78              |
| 1:A:342:MSE:HE1  | 1:A:364:MSE:CG   | 2.14                     | 0.78              |
| 1:B:206:VAL:HG23 | 1:B:329:MSE:HG2  | 1.64                     | 0.78              |
| 1:C:29:LYS:HE2   | 1:C:376:GLN:NE2  | 1.99                     | 0.77              |
| 1:D:133:ARG:HG2  | 1:D:133:ARG:HH11 | 1.47                     | 0.77              |
| 1:A:326:GLY:HA3  | 1:A:330:LYS:HE3  | 1.66                     | 0.77              |
| 1:A:377:LYS:HE3  | 1:A:385:ASP:OD2  | 1.84                     | 0.77              |
| 1:C:226:ARG:HG2  | 1:C:226:ARG:HH11 | 1.49                     | 0.77              |
| 1:C:19:ARG:HG2   | 1:C:19:ARG:HH11  | 1.49                     | 0.77              |
| 1:C:324:LYS:HE3  | 1:C:332:TRP:O    | 1.85                     | 0.77              |
| 1:A:312:LEU:HD22 | 1:A:364:MSE:HE1  | 1.66                     | 0.77              |
| 1:B:377:LYS:HE3  | 1:B:385:ASP:OD2  | 1.85                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:201:LYS:HD2  | 1:C:329:MSE:HG2  | 1.68                     | 0.76              |
| 1:A:62:ILE:HG12  | 1:A:88:MSE:HE1   | 1.68                     | 0.76              |
| 1:D:288:SER:HB2  | 1:D:289:PRO:HD3  | 1.66                     | 0.76              |
| 1:C:44:MSE:HE3   | 1:C:424:LYS:HZ3  | 1.51                     | 0.76              |
| 1:D:96:LEU:HB2   | 1:D:97:PRO:CD    | 2.16                     | 0.75              |
| 1:A:135:HIS:O    | 1:A:139:GLU:HG3  | 1.87                     | 0.75              |
| 1:A:72:GLY:HA3   | 3:A:678:HOH:O    | 1.86                     | 0.74              |
| 1:B:88:MSE:HE2   | 1:B:118:ILE:HD11 | 1.68                     | 0.74              |
| 1:A:228:LEU:HD22 | 1:A:262:ILE:HD13 | 1.68                     | 0.74              |
| 1:B:206:VAL:HG21 | 1:B:327:ASN:CG   | 2.12                     | 0.74              |
| 1:D:237:ARG:NH2  | 1:D:371:ILE:O    | 2.21                     | 0.74              |
| 1:B:430:ASP:HB2  | 1:B:444:LYS:NZ   | 2.02                     | 0.73              |
| 1:D:342:MSE:HE1  | 1:D:364:MSE:SE   | 2.38                     | 0.73              |
| 1:D:17:GLU:OE2   | 1:D:19:ARG:HD2   | 1.88                     | 0.73              |
| 1:A:162:ARG:N    | 1:A:162:ARG:HE   | 1.86                     | 0.73              |
| 1:A:205:ARG:HB3  | 1:A:210:ASP:CG   | 2.13                     | 0.73              |
| 1:D:226:ARG:HG2  | 1:D:226:ARG:HH11 | 1.52                     | 0.73              |
| 1:B:339:GLN:HE22 | 1:B:405:GLU:H    | 1.37                     | 0.73              |
| 1:A:273:LEU:HA   | 1:A:277:GLN:NE2  | 2.04                     | 0.73              |
| 1:D:215:ARG:HH11 | 1:D:215:ARG:CG   | 2.02                     | 0.73              |
| 1:A:232:LYS:HD3  | 1:A:260:GLN:HG2  | 1.71                     | 0.73              |
| 1:A:327:ASN:H    | 1:A:330:LYS:HE3  | 1.52                     | 0.73              |
| 1:A:326:GLY:CA   | 1:A:330:LYS:HE3  | 2.19                     | 0.73              |
| 1:A:250:GLU:HG3  | 1:A:303:LYS:NZ   | 2.03                     | 0.72              |
| 1:B:288:SER:O    | 1:B:289:PRO:C    | 2.30                     | 0.72              |
| 1:A:60:THR:HG21  | 1:A:88:MSE:HB2   | 1.72                     | 0.72              |
| 1:D:73:TYR:O     | 1:D:77:THR:HG22  | 1.90                     | 0.72              |
| 1:A:274:ASP:H    | 1:A:277:GLN:HE21 | 1.37                     | 0.72              |
| 1:A:342:MSE:HA   | 1:A:342:MSE:HE2  | 1.70                     | 0.72              |
| 1:A:312:LEU:CD2  | 1:A:345:MSE:HE2  | 2.20                     | 0.72              |
| 1:B:102:ARG:HH12 | 1:B:136:GLU:HG2  | 1.55                     | 0.72              |
| 1:C:5:LEU:HD22   | 1:C:6:ILE:H      | 1.55                     | 0.71              |
| 1:A:284:LEU:HD11 | 1:A:410:VAL:HG22 | 1.71                     | 0.71              |
| 1:C:201:LYS:HD2  | 1:C:329:MSE:CG   | 2.21                     | 0.71              |
| 1:C:288:SER:HB3  | 1:C:289:PRO:CD   | 2.20                     | 0.71              |
| 1:A:423:THR:HG22 | 1:A:424:LYS:HD3  | 1.72                     | 0.71              |
| 1:D:272:VAL:CG2  | 1:D:416:ARG:HH22 | 2.02                     | 0.71              |
| 1:A:96:LEU:HB2   | 1:A:97:PRO:HD2   | 1.70                     | 0.71              |
| 1:C:95:GLN:HE21  | 1:C:95:GLN:N     | 1.84                     | 0.71              |
| 1:A:77:THR:CG2   | 1:A:117:THR:HB   | 2.19                     | 0.70              |
| 1:D:312:LEU:HD23 | 1:D:363:LEU:HB3  | 1.72                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:226:ARG:HH11 | 1:B:226:ARG:HG2  | 1.56                     | 0.70              |
| 1:D:5:LEU:CD1    | 1:D:44:MSE:HE3   | 2.22                     | 0.69              |
| 1:D:324:LYS:HE3  | 1:D:332:TRP:O    | 1.92                     | 0.69              |
| 1:B:61:HIS:HD1   | 1:B:94:ASN:ND2   | 1.91                     | 0.69              |
| 1:A:165:ASN:C    | 1:A:165:ASN:HD22 | 2.01                     | 0.69              |
| 1:D:82:LYS:HD2   | 1:D:433:TYR:CE1  | 2.28                     | 0.69              |
| 1:B:207:THR:HG23 | 1:B:279:GLU:OE1  | 1.93                     | 0.69              |
| 1:B:342:MSE:HE2  | 1:B:389:VAL:HG11 | 1.75                     | 0.68              |
| 1:A:324:LYS:HE2  | 1:A:332:TRP:O    | 1.91                     | 0.68              |
| 1:B:77:THR:HG23  | 1:B:117:THR:CB   | 2.20                     | 0.68              |
| 1:A:207:THR:HG22 | 1:A:209:HIS:N    | 2.08                     | 0.68              |
| 1:C:238:LEU:HB3  | 1:C:262:ILE:HD12 | 1.76                     | 0.68              |
| 1:D:115:LYS:HD2  | 1:D:115:LYS:N    | 2.09                     | 0.68              |
| 1:D:444:LYS:HE3  | 3:D:532:HOH:O    | 1.94                     | 0.68              |
| 1:A:207:THR:HG23 | 1:A:279:GLU:OE1  | 1.94                     | 0.68              |
| 1:A:327:ASN:N    | 1:A:330:LYS:HE3  | 2.09                     | 0.68              |
| 1:D:146:KCX:HZ   | 1:D:186:HIS:HB2  | 1.58                     | 0.68              |
| 1:D:272:VAL:HG22 | 1:D:416:ARG:NH2  | 2.04                     | 0.67              |
| 1:A:288:SER:HB3  | 1:A:289:PRO:CD   | 2.25                     | 0.67              |
| 1:D:108:LYS:HZ1  | 1:D:122:GLN:NE2  | 1.87                     | 0.67              |
| 1:A:377:LYS:HE2  | 1:A:387:ASP:OD2  | 1.93                     | 0.67              |
| 1:B:73:TYR:O     | 1:B:77:THR:HB    | 1.94                     | 0.67              |
| 1:B:206:VAL:HG23 | 1:B:329:MSE:CG   | 2.25                     | 0.67              |
| 1:C:189:ASN:HD22 | 1:C:192:ILE:H    | 1.43                     | 0.67              |
| 1:B:102:ARG:O    | 1:B:106:GLU:HG3  | 1.95                     | 0.67              |
| 1:B:288:SER:HB3  | 1:B:289:PRO:CD   | 2.25                     | 0.67              |
| 1:A:207:THR:HG22 | 1:A:209:HIS:H    | 1.60                     | 0.66              |
| 1:D:189:ASN:HD22 | 1:D:192:ILE:H    | 1.40                     | 0.66              |
| 1:B:342:MSE:CE   | 1:B:389:VAL:HG11 | 2.26                     | 0.66              |
| 1:D:5:LEU:HD11   | 1:D:44:MSE:HE3   | 1.76                     | 0.66              |
| 1:D:108:LYS:NZ   | 1:D:122:GLN:NE2  | 2.42                     | 0.66              |
| 1:C:44:MSE:HE2   | 1:C:390:PHE:CE2  | 2.31                     | 0.66              |
| 1:C:407:ARG:HD2  | 3:C:687:HOH:O    | 1.96                     | 0.66              |
| 1:C:57:ASP:OD1   | 1:C:313:VAL:HG22 | 1.96                     | 0.66              |
| 1:D:276:ASP:O    | 1:D:280:GLU:HG3  | 1.96                     | 0.66              |
| 1:D:252:VAL:O    | 1:D:256:ARG:HG3  | 1.95                     | 0.66              |
| 1:A:238:LEU:HD13 | 1:A:238:LEU:C    | 2.22                     | 0.65              |
| 1:D:55:MSE:SE    | 1:D:342:MSE:HE3  | 2.47                     | 0.65              |
| 1:A:96:LEU:HB2   | 1:A:97:PRO:CD    | 2.26                     | 0.65              |
| 1:A:102:ARG:HD2  | 1:A:106:GLU:OE2  | 1.95                     | 0.65              |
| 1:A:423:THR:O    | 1:A:424:LYS:HD2  | 1.97                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:63:SER:HB2   | 1:B:71:GLU:N     | 2.10                     | 0.65              |
| 1:C:250:GLU:HG3  | 1:C:303:LYS:NZ   | 2.07                     | 0.65              |
| 1:B:377:LYS:HE2  | 1:B:387:ASP:OD2  | 1.97                     | 0.65              |
| 1:B:254:ARG:HG3  | 1:B:255:ALA:N    | 2.09                     | 0.65              |
| 1:C:96:LEU:HB2   | 1:C:97:PRO:HD3   | 1.77                     | 0.65              |
| 1:C:270:TYR:OH   | 1:C:289:PRO:HG2  | 1.96                     | 0.65              |
| 1:A:339:GLN:HE22 | 1:A:405:GLU:N    | 1.95                     | 0.65              |
| 1:C:304:LEU:HD13 | 1:C:355:MSE:HE1  | 1.79                     | 0.65              |
| 1:D:54:GLY:HA2   | 1:D:389:VAL:HG23 | 1.78                     | 0.64              |
| 1:C:272:VAL:HG12 | 1:C:348:GLU:HG2  | 1.80                     | 0.64              |
| 1:B:15:GLU:CD    | 1:B:379:ARG:HE   | 2.05                     | 0.64              |
| 1:A:370:ASP:OD1  | 1:A:379:ARG:NH2  | 2.28                     | 0.64              |
| 1:A:55:MSE:SE    | 1:A:342:MSE:HE3  | 2.47                     | 0.64              |
| 1:B:102:ARG:HH11 | 1:B:102:ARG:CB   | 2.02                     | 0.64              |
| 1:C:226:ARG:HG2  | 1:C:226:ARG:NH1  | 2.12                     | 0.64              |
| 1:B:430:ASP:HB2  | 1:B:444:LYS:HZ1  | 1.61                     | 0.64              |
| 1:A:250:GLU:HG3  | 1:A:303:LYS:HZ3  | 1.63                     | 0.63              |
| 1:C:193:CYS:SG   | 1:C:215:ARG:NH1  | 2.71                     | 0.63              |
| 1:D:96:LEU:HB2   | 1:D:97:PRO:HD2   | 1.81                     | 0.63              |
| 1:D:201:LYS:HE2  | 1:D:330:LYS:CE   | 2.29                     | 0.63              |
| 1:A:85:ILE:HD12  | 1:A:338:LEU:CD2  | 2.28                     | 0.63              |
| 1:A:272:VAL:CG2  | 1:A:348:GLU:HG3  | 2.29                     | 0.63              |
| 1:B:283:THR:O    | 1:B:324:LYS:HE2  | 1.99                     | 0.63              |
| 1:D:189:ASN:ND2  | 1:D:192:ILE:H    | 1.97                     | 0.63              |
| 1:A:274:ASP:N    | 1:A:277:GLN:HE21 | 1.97                     | 0.63              |
| 1:A:316:HIS:CG   | 1:A:338:LEU:HB2  | 2.34                     | 0.63              |
| 1:B:444:LYS:NZ   | 3:B:878:HOH:O    | 2.32                     | 0.63              |
| 1:C:4:ASP:HA     | 1:C:41:LYS:HD3   | 1.80                     | 0.63              |
| 1:C:288:SER:O    | 1:C:289:PRO:C    | 2.38                     | 0.63              |
| 1:A:102:ARG:NH1  | 1:A:140:VAL:HG23 | 2.14                     | 0.62              |
| 1:A:239:HIS:HE1  | 1:A:265:GLU:OE1  | 1.82                     | 0.62              |
| 1:B:61:HIS:HB2   | 1:B:316:HIS:O    | 1.99                     | 0.62              |
| 1:B:319:CYS:HB2  | 1:B:332:TRP:CZ3  | 2.34                     | 0.62              |
| 1:B:145:PHE:CE1  | 1:B:181:GLN:HG2  | 2.34                     | 0.62              |
| 1:D:288:SER:HB2  | 1:D:289:PRO:CD   | 2.29                     | 0.62              |
| 1:A:105:ILE:O    | 1:A:108:LYS:HB3  | 1.99                     | 0.62              |
| 1:C:215:ARG:HG3  | 1:C:215:ARG:HH11 | 1.65                     | 0.62              |
| 1:D:328:ILE:HD12 | 1:D:328:ILE:H    | 1.63                     | 0.62              |
| 1:B:102:ARG:HB2  | 1:B:102:ARG:NH1  | 2.03                     | 0.62              |
| 1:D:226:ARG:HG2  | 1:D:226:ARG:NH1  | 2.15                     | 0.62              |
| 1:D:205:ARG:HB3  | 1:D:210:ASP:CG   | 2.24                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:228:LEU:CD2  | 1:A:262:ILE:HD13 | 2.29                     | 0.62              |
| 1:D:19:ARG:HG3   | 1:D:21:VAL:HG13  | 1.82                     | 0.62              |
| 1:A:339:GLN:NE2  | 1:A:405:GLU:H    | 1.96                     | 0.61              |
| 1:A:29:LYS:HE2   | 1:A:385:ASP:OD1  | 2.00                     | 0.61              |
| 1:A:400:THR:HG22 | 1:A:402:ASP:N    | 2.15                     | 0.61              |
| 1:B:102:ARG:HB3  | 3:B:899:HOH:O    | 1.99                     | 0.61              |
| 1:D:142:VAL:HG12 | 1:D:144:GLY:H    | 1.65                     | 0.61              |
| 1:A:423:THR:HG22 | 1:A:424:LYS:CD   | 2.31                     | 0.60              |
| 1:D:203:GLU:HB2  | 1:D:205:ARG:CD   | 2.29                     | 0.60              |
| 1:D:427:LEU:HD13 | 1:D:428:ARG:HB2  | 1.81                     | 0.60              |
| 1:B:252:VAL:O    | 1:B:256:ARG:HG3  | 2.00                     | 0.60              |
| 1:D:4:ASP:HA     | 1:D:41:LYS:HD3   | 1.83                     | 0.60              |
| 1:A:312:LEU:HD23 | 1:A:345:MSE:HG3  | 1.82                     | 0.60              |
| 1:C:29:LYS:HE2   | 1:C:376:GLN:HE21 | 1.65                     | 0.60              |
| 1:C:423:THR:O    | 1:C:424:LYS:HD2  | 2.01                     | 0.60              |
| 1:A:165:ASN:HD21 | 1:A:168:GLN:H    | 1.50                     | 0.60              |
| 1:D:198:GLU:O    | 1:D:202:ARG:HD3  | 2.00                     | 0.60              |
| 1:A:59:HIS:CG    | 1:A:91:MSE:HE3   | 2.36                     | 0.60              |
| 1:A:342:MSE:HE1  | 1:A:364:MSE:SE   | 2.51                     | 0.60              |
| 1:D:272:VAL:HG23 | 1:D:348:GLU:HG3  | 1.84                     | 0.60              |
| 1:D:375:GLN:O    | 1:D:384:LYS:HE2  | 2.01                     | 0.60              |
| 1:A:450:LYS:HE2  | 3:A:620:HOH:O    | 2.01                     | 0.60              |
| 1:C:351:GLN:HE22 | 1:C:394:ASN:N    | 1.93                     | 0.60              |
| 1:D:183:VAL:HG13 | 1:D:238:LEU:HD23 | 1.84                     | 0.59              |
| 1:C:238:LEU:HB3  | 1:C:262:ILE:CD1  | 2.31                     | 0.59              |
| 1:B:239:HIS:HD2  | 1:B:263:THR:OG1  | 1.85                     | 0.59              |
| 1:C:288:SER:O    | 1:C:290:PRO:N    | 2.36                     | 0.59              |
| 1:B:366:THR:HG23 | 1:B:379:ARG:HD3  | 1.85                     | 0.59              |
| 1:C:189:ASN:ND2  | 1:C:192:ILE:HG13 | 2.16                     | 0.59              |
| 1:D:162:ARG:HG2  | 1:D:162:ARG:HH11 | 1.67                     | 0.59              |
| 1:D:437:GLN:O    | 1:D:437:GLN:HG2  | 2.03                     | 0.59              |
| 1:B:182:PRO:HB3  | 1:B:237:ARG:HG2  | 1.84                     | 0.59              |
| 1:D:239:HIS:HD2  | 1:D:263:THR:OG1  | 1.86                     | 0.59              |
| 1:C:351:GLN:NE2  | 1:C:394:ASN:H    | 1.94                     | 0.59              |
| 1:A:77:THR:CG2   | 1:A:117:THR:H    | 2.09                     | 0.59              |
| 1:A:95:GLN:O     | 1:A:96:LEU:O     | 2.20                     | 0.59              |
| 1:D:255:ALA:HB3  | 1:D:262:ILE:HD11 | 1.83                     | 0.59              |
| 1:A:88:MSE:HE2   | 1:A:90:GLU:HB2   | 1.85                     | 0.58              |
| 1:A:288:SER:O    | 1:A:289:PRO:C    | 2.43                     | 0.58              |
| 1:A:19:ARG:HD3   | 1:A:21:VAL:HG13  | 1.86                     | 0.58              |
| 1:A:342:MSE:HE1  | 1:A:364:MSE:HG3  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:53:PRO:O     | 1:D:387:ASP:O    | 2.21                     | 0.58              |
| 1:A:77:THR:HG22  | 1:A:117:THR:CB   | 2.23                     | 0.58              |
| 1:A:206:VAL:HA   | 1:A:329:MSE:HG2  | 1.86                     | 0.58              |
| 1:A:96:LEU:HA    | 3:A:682:HOH:O    | 2.04                     | 0.58              |
| 1:A:233:VAL:HG11 | 1:D:218:PHE:CD2  | 2.39                     | 0.58              |
| 1:A:260:GLN:OE1  | 1:A:262:ILE:HD11 | 2.03                     | 0.58              |
| 1:B:73:TYR:CE2   | 1:B:112:ALA:HB2  | 2.39                     | 0.58              |
| 1:C:62:ILE:HD11  | 1:C:88:MSE:SE    | 2.54                     | 0.58              |
| 1:B:91:MSE:SE    | 1:B:146:KCX:HE3  | 2.53                     | 0.57              |
| 1:D:328:ILE:HD12 | 1:D:328:ILE:N    | 2.19                     | 0.57              |
| 1:A:85:ILE:HD12  | 1:A:338:LEU:HD23 | 1.86                     | 0.57              |
| 1:A:274:ASP:OD1  | 1:A:277:GLN:HG3  | 2.05                     | 0.57              |
| 1:A:427:LEU:HD23 | 1:A:444:LYS:HD2  | 1.85                     | 0.57              |
| 1:A:207:THR:CG2  | 1:A:209:HIS:H    | 2.18                     | 0.57              |
| 1:D:133:ARG:HG2  | 1:D:133:ARG:NH1  | 2.15                     | 0.57              |
| 1:A:62:ILE:CG1   | 1:A:88:MSE:HE1   | 2.35                     | 0.57              |
| 1:B:237:ARG:HG3  | 1:B:238:LEU:N    | 2.20                     | 0.57              |
| 1:D:49:LEU:HD13  | 1:D:390:PHE:HB3  | 1.87                     | 0.57              |
| 1:A:211:TYR:CE1  | 1:A:286:LYS:HE3  | 2.39                     | 0.57              |
| 1:A:283:THR:HG22 | 1:A:328:ILE:HD13 | 1.86                     | 0.57              |
| 1:B:133:ARG:HG2  | 1:B:133:ARG:HH11 | 1.69                     | 0.57              |
| 1:A:312:LEU:CD2  | 1:A:364:MSE:HE1  | 2.35                     | 0.57              |
| 1:B:198:GLU:O    | 1:B:202:ARG:HD3  | 2.05                     | 0.57              |
| 1:B:206:VAL:CG2  | 1:B:327:ASN:HB2  | 2.34                     | 0.57              |
| 1:D:407:ARG:HB3  | 3:D:557:HOH:O    | 2.04                     | 0.57              |
| 1:B:272:VAL:CG1  | 1:B:348:GLU:HG3  | 2.35                     | 0.56              |
| 1:D:288:SER:CB   | 1:D:289:PRO:HD3  | 2.35                     | 0.56              |
| 1:C:277:GLN:HA   | 1:C:280:GLU:HG2  | 1.87                     | 0.56              |
| 1:C:428:ARG:HG2  | 1:C:428:ARG:HH11 | 1.70                     | 0.56              |
| 1:D:342:MSE:HE1  | 1:D:364:MSE:HG3  | 1.87                     | 0.56              |
| 1:A:19:ARG:HD3   | 1:A:21:VAL:CG1   | 2.35                     | 0.56              |
| 1:D:288:SER:O    | 1:D:289:PRO:C    | 2.43                     | 0.56              |
| 1:A:92:PRO:HG2   | 1:A:93:LEU:H     | 1.70                     | 0.56              |
| 1:D:29:LYS:HD2   | 1:D:30:ILE:O     | 2.05                     | 0.56              |
| 1:C:19:ARG:HG2   | 1:C:19:ARG:NH1   | 2.15                     | 0.56              |
| 1:D:97:PRO:HG3   | 1:D:107:LEU:HD12 | 1.86                     | 0.56              |
| 1:D:249:VAL:HG11 | 1:D:303:LYS:HG3  | 1.87                     | 0.56              |
| 1:A:232:LYS:HD3  | 1:A:260:GLN:CG   | 2.36                     | 0.56              |
| 1:B:432:ILE:CG2  | 1:B:444:LYS:HE2  | 2.36                     | 0.56              |
| 1:C:260:GLN:HG2  | 1:C:262:ILE:HG12 | 1.86                     | 0.56              |
| 1:D:397:TYR:HB3  | 1:D:421:ARG:NH1  | 2.21                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:207:THR:HG22 | 1:B:210:ASP:H    | 1.71                     | 0.56              |
| 1:C:58:ALA:HA    | 1:C:89:ILE:HB    | 1.88                     | 0.56              |
| 1:A:327:ASN:H    | 1:A:330:LYS:HE2  | 1.67                     | 0.56              |
| 1:C:189:ASN:ND2  | 1:C:192:ILE:H    | 2.03                     | 0.56              |
| 1:C:5:LEU:HD11   | 1:C:7:ILE:HG13   | 1.88                     | 0.55              |
| 1:A:428:ARG:HH11 | 1:A:428:ARG:HG2  | 1.71                     | 0.55              |
| 1:C:206:VAL:HB   | 1:C:327:ASN:HD22 | 1.71                     | 0.55              |
| 1:D:162:ARG:HD2  | 1:D:162:ARG:N    | 2.21                     | 0.55              |
| 1:A:327:ASN:N    | 1:A:330:LYS:CE   | 2.67                     | 0.55              |
| 1:D:249:VAL:HG11 | 1:D:303:LYS:CG   | 2.37                     | 0.55              |
| 1:D:339:GLN:HE22 | 1:D:405:GLU:N    | 2.05                     | 0.55              |
| 1:A:60:THR:CG2   | 1:A:88:MSE:HB2   | 2.36                     | 0.55              |
| 1:A:205:ARG:HB2  | 1:A:205:ARG:NH1  | 2.12                     | 0.55              |
| 1:D:242:HIS:ND1  | 1:D:289:PRO:HG2  | 2.22                     | 0.55              |
| 1:D:272:VAL:CG2  | 1:D:348:GLU:HG3  | 2.37                     | 0.55              |
| 1:D:407:ARG:HH11 | 1:D:407:ARG:HG2  | 1.69                     | 0.55              |
| 1:C:316:HIS:CG   | 1:C:338:LEU:HB2  | 2.41                     | 0.55              |
| 1:A:238:LEU:HD12 | 1:A:262:ILE:HG23 | 1.89                     | 0.55              |
| 1:B:316:HIS:CG   | 1:B:338:LEU:HB2  | 2.41                     | 0.55              |
| 1:C:256:ARG:NH2  | 1:C:310:ASP:OD2  | 2.39                     | 0.55              |
| 1:D:82:LYS:HD2   | 1:D:433:TYR:CZ   | 2.41                     | 0.55              |
| 1:B:207:THR:HG22 | 1:B:209:HIS:N    | 2.22                     | 0.55              |
| 1:C:167:TRP:CZ2  | 1:C:171:LYS:HD3  | 2.42                     | 0.54              |
| 1:D:201:LYS:CE   | 1:D:330:LYS:HE2  | 2.31                     | 0.54              |
| 1:C:135:HIS:HD2  | 1:C:139:GLU:OE2  | 1.90                     | 0.54              |
| 1:C:366:THR:HG23 | 1:C:379:ARG:HD3  | 1.88                     | 0.54              |
| 1:A:377:LYS:NZ   | 1:A:448:ILE:HD11 | 2.21                     | 0.54              |
| 1:C:430:ASP:HB2  | 1:C:444:LYS:HE2  | 1.90                     | 0.54              |
| 1:A:89:ILE:HG22  | 1:A:123:LEU:HG   | 1.89                     | 0.54              |
| 1:A:190:ALA:HB3  | 3:A:635:HOH:O    | 2.07                     | 0.54              |
| 1:B:206:VAL:HG21 | 1:B:327:ASN:CB   | 2.38                     | 0.54              |
| 1:C:44:MSE:HE2   | 1:C:390:PHE:HE2  | 1.71                     | 0.54              |
| 1:A:226:ARG:NE   | 1:D:226:ARG:HE   | 2.03                     | 0.54              |
| 1:B:82:LYS:HG3   | 1:B:433:TYR:CZ   | 2.42                     | 0.54              |
| 1:A:324:LYS:CE   | 1:A:332:TRP:O    | 2.54                     | 0.54              |
| 1:B:239:HIS:HE1  | 1:B:265:GLU:OE1  | 1.91                     | 0.54              |
| 1:D:225:ARG:NH1  | 3:D:520:HOH:O    | 2.36                     | 0.54              |
| 1:B:206:VAL:HG21 | 1:B:327:ASN:HB2  | 1.89                     | 0.54              |
| 1:D:107:LEU:HD13 | 1:D:107:LEU:C    | 2.32                     | 0.54              |
| 1:D:254:ARG:O    | 1:D:258:GLU:HG3  | 2.08                     | 0.54              |
| 1:B:319:CYS:HB2  | 1:B:332:TRP:CE3  | 2.44                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:413:TYR:O    | 1:D:416:ARG:HB3  | 2.09                     | 0.53              |
| 1:D:319:CYS:HB2  | 1:D:323:MSE:CE   | 2.38                     | 0.53              |
| 1:A:5:LEU:HD22   | 1:A:6:ILE:N      | 2.24                     | 0.53              |
| 1:B:195:GLU:HG3  | 1:C:167:TRP:CG   | 2.44                     | 0.53              |
| 1:B:206:VAL:O    | 1:B:206:VAL:HG22 | 2.08                     | 0.53              |
| 1:C:423:THR:HA   | 1:C:435:ILE:HB   | 1.89                     | 0.53              |
| 1:A:167:TRP:HB2  | 1:D:191:LEU:HD13 | 1.91                     | 0.53              |
| 1:B:376:GLN:C    | 1:B:377:LYS:HD2  | 2.33                     | 0.53              |
| 1:D:327:ASN:HD21 | 1:D:330:LYS:HD3  | 1.74                     | 0.53              |
| 1:A:342:MSE:HE1  | 1:A:364:MSE:HB3  | 1.90                     | 0.53              |
| 1:C:94:ASN:HB3   | 1:C:95:GLN:NE2   | 2.24                     | 0.53              |
| 1:A:207:THR:HB   | 1:A:210:ASP:OD2  | 2.09                     | 0.52              |
| 1:A:397:TYR:CG   | 1:A:421:ARG:NH1  | 2.77                     | 0.52              |
| 1:C:237:ARG:NH2  | 1:C:371:ILE:O    | 2.38                     | 0.52              |
| 1:D:256:ARG:HG2  | 1:D:262:ILE:HG13 | 1.92                     | 0.52              |
| 1:A:16:ASN:HB3   | 1:B:15:GLU:OE2   | 2.09                     | 0.52              |
| 1:B:288:SER:O    | 1:B:290:PRO:N    | 2.41                     | 0.52              |
| 1:A:77:THR:CG2   | 1:A:118:ILE:H    | 2.23                     | 0.52              |
| 1:A:238:LEU:HD13 | 1:A:239:HIS:N    | 2.23                     | 0.52              |
| 1:A:284:LEU:HD11 | 1:A:410:VAL:CG2  | 2.39                     | 0.52              |
| 1:A:102:ARG:NE   | 3:A:679:HOH:O    | 2.43                     | 0.52              |
| 1:A:133:ARG:HG2  | 1:A:133:ARG:HH11 | 1.74                     | 0.52              |
| 1:C:107:LEU:C    | 1:C:107:LEU:HD13 | 2.35                     | 0.52              |
| 1:D:54:GLY:HA2   | 1:D:389:VAL:CG2  | 2.39                     | 0.52              |
| 1:D:239:HIS:HE1  | 1:D:265:GLU:OE1  | 1.93                     | 0.52              |
| 1:C:133:ARG:O    | 1:C:136:GLU:HB2  | 2.09                     | 0.52              |
| 1:C:303:LYS:HE2  | 3:C:689:HOH:O    | 2.10                     | 0.52              |
| 1:B:63:SER:CB    | 1:B:71:GLU:N     | 2.72                     | 0.52              |
| 1:B:430:ASP:HB2  | 1:B:444:LYS:HZ3  | 1.74                     | 0.52              |
| 1:A:202:ARG:HH11 | 1:A:202:ARG:HG2  | 1.75                     | 0.52              |
| 1:B:423:THR:C    | 1:B:424:LYS:HD2  | 2.35                     | 0.52              |
| 1:A:102:ARG:CZ   | 3:A:579:HOH:O    | 2.57                     | 0.52              |
| 1:B:327:ASN:ND2  | 1:B:330:LYS:H    | 2.08                     | 0.52              |
| 1:A:202:ARG:HG2  | 1:A:202:ARG:NH1  | 2.24                     | 0.52              |
| 1:B:189:ASN:ND2  | 1:B:192:ILE:H    | 2.08                     | 0.51              |
| 1:A:59:HIS:CD2   | 1:A:91:MSE:HE3   | 2.45                     | 0.51              |
| 1:A:75:THR:HG22  | 1:A:76:GLY:N     | 2.23                     | 0.51              |
| 1:A:110:ASP:HA   | 1:A:113:LYS:HD3  | 1.92                     | 0.51              |
| 1:C:401:ASN:ND2  | 3:C:598:HOH:O    | 2.42                     | 0.51              |
| 1:D:342:MSE:HE1  | 1:D:364:MSE:HB3  | 1.93                     | 0.51              |
| 1:D:215:ARG:CG   | 1:D:215:ARG:NH1  | 2.67                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:80:ALA:HA    | 1:A:338:LEU:HD22 | 1.91                     | 0.51              |
| 1:B:215:ARG:HH11 | 1:B:215:ARG:CG   | 2.18                     | 0.51              |
| 1:D:29:LYS:HD2   | 1:D:30:ILE:C     | 2.36                     | 0.51              |
| 1:D:316:HIS:CG   | 1:D:338:LEU:HB2  | 2.46                     | 0.51              |
| 1:C:327:ASN:OD1  | 1:C:330:LYS:HD3  | 2.11                     | 0.51              |
| 1:D:202:ARG:HD3  | 1:D:202:ARG:H    | 1.75                     | 0.51              |
| 1:A:134:LEU:HD12 | 1:A:175:LYS:HG2  | 1.92                     | 0.51              |
| 1:A:421:ARG:NH2  | 1:A:435:ILE:HD11 | 2.26                     | 0.51              |
| 1:A:129:TYR:HE1  | 1:A:162:ARG:HD2  | 1.74                     | 0.51              |
| 1:C:59:HIS:CG    | 1:C:91:MSE:HE3   | 2.46                     | 0.51              |
| 1:A:384:LYS:HE3  | 1:B:17:GLU:OE2   | 2.11                     | 0.51              |
| 1:C:44:MSE:HE3   | 1:C:424:LYS:HZ2  | 1.69                     | 0.51              |
| 1:C:96:LEU:CB    | 1:C:97:PRO:HD3   | 2.40                     | 0.51              |
| 1:C:434:ASP:OD1  | 1:C:436:GLU:HB2  | 2.10                     | 0.51              |
| 1:D:209:HIS:HD2  | 1:D:279:GLU:OE1  | 1.94                     | 0.51              |
| 1:D:428:ARG:HG2  | 3:D:576:HOH:O    | 2.10                     | 0.50              |
| 1:A:342:MSE:HE1  | 1:A:364:MSE:CB   | 2.42                     | 0.50              |
| 1:D:283:THR:O    | 1:D:324:LYS:HE2  | 2.12                     | 0.50              |
| 1:D:339:GLN:HE22 | 1:D:405:GLU:H    | 1.58                     | 0.50              |
| 1:A:126:LEU:HB3  | 1:A:147:CYS:HB3  | 1.94                     | 0.50              |
| 1:B:162:ARG:NE   | 1:B:162:ARG:HA   | 2.26                     | 0.50              |
| 1:D:82:LYS:HG2   | 1:D:339:GLN:CD   | 2.36                     | 0.50              |
| 1:D:304:LEU:HD21 | 1:D:363:LEU:HD13 | 1.94                     | 0.50              |
| 1:D:428:ARG:HG2  | 1:D:428:ARG:HH11 | 1.76                     | 0.50              |
| 1:B:189:ASN:HD22 | 1:B:192:ILE:H    | 1.59                     | 0.50              |
| 1:B:395:SER:OG   | 1:B:421:ARG:HD2  | 2.10                     | 0.50              |
| 1:C:284:LEU:HD23 | 1:C:324:LYS:HG2  | 1.93                     | 0.50              |
| 1:D:135:HIS:O    | 1:D:139:GLU:HG3  | 2.11                     | 0.50              |
| 1:A:195:GLU:HG3  | 1:D:167:TRP:CG   | 2.47                     | 0.50              |
| 1:C:110:ASP:O    | 1:C:113:LYS:HB2  | 2.11                     | 0.50              |
| 1:D:319:CYS:HB3  | 1:D:332:TRP:CZ3  | 2.46                     | 0.50              |
| 1:A:294:LEU:HD22 | 1:A:298:LYS:CD   | 2.42                     | 0.50              |
| 1:A:428:ARG:HG2  | 3:A:571:HOH:O    | 2.12                     | 0.50              |
| 1:C:6:ILE:HG22   | 1:C:8:LYS:HD2    | 1.93                     | 0.50              |
| 1:D:298:LYS:HD2  | 1:D:298:LYS:C    | 2.37                     | 0.50              |
| 1:D:427:LEU:HD13 | 1:D:427:LEU:C    | 2.36                     | 0.50              |
| 1:B:256:ARG:HG2  | 1:B:262:ILE:HG12 | 1.94                     | 0.50              |
| 1:B:71:GLU:HG3   | 1:B:318:PRO:CG   | 2.36                     | 0.49              |
| 1:B:357:LEU:N    | 1:B:358:PRO:HD2  | 2.27                     | 0.49              |
| 1:C:377:LYS:NZ   | 1:C:448:ILE:HD11 | 2.27                     | 0.49              |
| 1:B:269:HIS:CG   | 1:B:335:ILE:HD12 | 2.47                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:272:VAL:HG12 | 1:B:348:GLU:HG3  | 1.93                     | 0.49              |
| 1:C:184:LEU:N    | 1:C:184:LEU:HD23 | 2.27                     | 0.49              |
| 1:C:201:LYS:HD2  | 1:C:329:MSE:HG3  | 1.94                     | 0.49              |
| 1:D:407:ARG:HG2  | 1:D:407:ARG:NH1  | 2.27                     | 0.49              |
| 1:A:107:LEU:C    | 1:A:107:LEU:HD13 | 2.37                     | 0.49              |
| 1:A:124:GLY:O    | 1:A:145:PHE:HA   | 2.12                     | 0.49              |
| 1:A:198:GLU:O    | 1:A:202:ARG:HB2  | 2.11                     | 0.49              |
| 1:B:59:HIS:CG    | 1:B:91:MSE:HE3   | 2.47                     | 0.49              |
| 1:B:226:ARG:HG2  | 1:B:226:ARG:NH1  | 2.26                     | 0.49              |
| 1:A:131:ILE:HD12 | 1:A:131:ILE:O    | 2.12                     | 0.49              |
| 1:A:209:HIS:HD2  | 1:A:279:GLU:OE1  | 1.95                     | 0.49              |
| 1:B:278:PHE:CD1  | 1:B:278:PHE:C    | 2.89                     | 0.49              |
| 1:D:143:VAL:CG2  | 1:D:372:PHE:O    | 2.60                     | 0.49              |
| 1:B:77:THR:HG21  | 1:B:117:THR:N    | 2.16                     | 0.49              |
| 1:B:82:LYS:HG3   | 1:B:433:TYR:CE1  | 2.47                     | 0.49              |
| 1:B:273:LEU:HA   | 1:B:277:GLN:OE1  | 2.12                     | 0.49              |
| 1:C:409:LYS:HD2  | 1:C:409:LYS:N    | 2.26                     | 0.49              |
| 1:D:320:PRO:CD   | 1:D:323:MSE:HE2  | 2.29                     | 0.49              |
| 1:A:269:HIS:HD2  | 3:A:472:HOH:O    | 1.94                     | 0.49              |
| 1:C:175:LYS:HE2  | 1:C:179:LEU:HD11 | 1.95                     | 0.49              |
| 1:C:407:ARG:HB2  | 1:C:407:ARG:NH1  | 2.21                     | 0.49              |
| 1:A:92:PRO:HG2   | 1:A:93:LEU:HD13  | 1.95                     | 0.49              |
| 1:D:328:ILE:H    | 1:D:328:ILE:CD1  | 2.25                     | 0.49              |
| 1:D:330:LYS:HD2  | 1:D:330:LYS:N    | 2.28                     | 0.49              |
| 1:A:102:ARG:NH1  | 1:A:102:ARG:HB2  | 2.28                     | 0.49              |
| 1:D:146:KCX:HD2  | 1:D:147:CYS:N    | 2.27                     | 0.49              |
| 1:D:288:SER:CB   | 1:D:289:PRO:CD   | 2.91                     | 0.49              |
| 1:B:162:ARG:HA   | 1:B:162:ARG:HE   | 1.77                     | 0.48              |
| 1:C:211:TYR:CE1  | 1:C:286:LYS:HE3  | 2.47                     | 0.48              |
| 1:C:229:TYR:O    | 1:C:233:VAL:HG23 | 2.13                     | 0.48              |
| 1:D:96:LEU:CB    | 1:D:97:PRO:CD    | 2.89                     | 0.48              |
| 1:A:5:LEU:CD2    | 1:A:6:ILE:N      | 2.75                     | 0.48              |
| 1:D:185:VAL:HG11 | 1:D:227:VAL:HG21 | 1.95                     | 0.48              |
| 1:D:319:CYS:SG   | 1:D:324:LYS:HD3  | 2.52                     | 0.48              |
| 1:D:392:GLN:NE2  | 1:D:393:PRO:O    | 2.46                     | 0.48              |
| 1:A:376:GLN:NE2  | 3:A:548:HOH:O    | 2.45                     | 0.48              |
| 1:B:77:THR:CG2   | 1:B:117:THR:HB   | 2.32                     | 0.48              |
| 1:B:96:LEU:O     | 1:B:98:ALA:N     | 2.47                     | 0.48              |
| 1:C:339:GLN:HE22 | 1:C:405:GLU:H    | 1.62                     | 0.48              |
| 1:D:162:ARG:HG2  | 1:D:162:ARG:NH1  | 2.29                     | 0.48              |
| 1:D:342:MSE:HE1  | 1:D:364:MSE:CB   | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:15:GLU:CD    | 1:B:379:ARG:NE   | 2.71                     | 0.48              |
| 1:B:70:TRP:HA    | 1:B:70:TRP:CE3   | 2.48                     | 0.48              |
| 1:C:201:LYS:CE   | 1:C:329:MSE:HG3  | 2.44                     | 0.48              |
| 1:C:206:VAL:HB   | 1:C:327:ASN:ND2  | 2.28                     | 0.48              |
| 1:D:205:ARG:HG2  | 1:D:205:ARG:HH11 | 1.78                     | 0.48              |
| 1:A:96:LEU:CB    | 1:A:97:PRO:CD    | 2.92                     | 0.48              |
| 1:A:286:LYS:NZ   | 1:A:331:ALA:O    | 2.47                     | 0.48              |
| 1:D:397:TYR:CG   | 1:D:421:ARG:NH1  | 2.82                     | 0.48              |
| 1:A:416:ARG:HG2  | 1:A:416:ARG:HH11 | 1.78                     | 0.48              |
| 1:A:382:PRO:O    | 1:B:19:ARG:NH1   | 2.47                     | 0.47              |
| 1:B:89:ILE:HG22  | 1:B:123:LEU:HG   | 1.95                     | 0.47              |
| 1:A:143:VAL:HG22 | 1:A:372:PHE:O    | 2.14                     | 0.47              |
| 1:A:102:ARG:O    | 1:A:106:GLU:HB2  | 2.14                     | 0.47              |
| 1:B:132:ASP:OD2  | 1:B:133:ARG:HD3  | 2.14                     | 0.47              |
| 1:B:145:PHE:HE1  | 1:B:181:GLN:HG2  | 1.76                     | 0.47              |
| 1:B:233:VAL:HG11 | 1:C:218:PHE:CD2  | 2.50                     | 0.47              |
| 1:D:62:ILE:CD1   | 1:D:88:MSE:HE1   | 2.44                     | 0.47              |
| 1:D:392:GLN:HE21 | 1:D:392:GLN:C    | 2.22                     | 0.47              |
| 1:A:283:THR:CG2  | 1:A:328:ILE:HD13 | 2.44                     | 0.47              |
| 1:B:143:VAL:C    | 1:B:181:GLN:NE2  | 2.73                     | 0.47              |
| 1:C:328:ILE:HG12 | 3:C:640:HOH:O    | 2.14                     | 0.47              |
| 1:D:215:ARG:HB3  | 1:D:290:PRO:HG3  | 1.96                     | 0.47              |
| 1:A:284:LEU:CD1  | 1:A:410:VAL:HG22 | 2.41                     | 0.47              |
| 1:B:2:SER:HB3    | 3:B:829:HOH:O    | 2.14                     | 0.47              |
| 1:A:77:THR:HG21  | 1:A:118:ILE:H    | 1.79                     | 0.47              |
| 1:A:370:ASP:CG   | 1:A:379:ARG:HH22 | 2.21                     | 0.47              |
| 1:A:427:LEU:O    | 1:A:444:LYS:HE3  | 2.14                     | 0.47              |
| 1:B:94:ASN:OD1   | 1:B:95:GLN:NE2   | 2.48                     | 0.47              |
| 1:B:133:ARG:HG2  | 1:B:133:ARG:NH1  | 2.29                     | 0.47              |
| 1:B:260:GLN:HG2  | 1:B:262:ILE:HG23 | 1.96                     | 0.47              |
| 1:C:61:HIS:HB2   | 1:C:316:HIS:O    | 2.15                     | 0.47              |
| 1:D:74:GLU:HA    | 3:D:546:HOH:O    | 2.14                     | 0.47              |
| 1:B:63:SER:HB2   | 1:B:71:GLU:C     | 2.39                     | 0.47              |
| 1:A:15:GLU:OE2   | 1:A:379:ARG:HD3  | 2.14                     | 0.47              |
| 1:A:133:ARG:HG2  | 1:A:133:ARG:NH1  | 2.30                     | 0.47              |
| 1:A:304:LEU:HD13 | 1:A:355:MSE:HE1  | 1.96                     | 0.47              |
| 1:A:319:CYS:HB3  | 1:A:332:TRP:CZ3  | 2.50                     | 0.46              |
| 1:D:5:LEU:HG     | 1:D:6:ILE:N      | 2.30                     | 0.46              |
| 1:D:407:ARG:HG3  | 1:D:408:HIS:CD2  | 2.51                     | 0.46              |
| 1:D:425:THR:HB   | 1:D:433:TYR:HB3  | 1.95                     | 0.46              |
| 1:A:13:ILE:HD12  | 1:A:52:SER:HB2   | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:211:TYR:CE1  | 1:B:286:LYS:HE3  | 2.50                     | 0.46              |
| 1:A:165:ASN:ND2  | 1:A:165:ASN:C    | 2.72                     | 0.46              |
| 1:A:250:GLU:HG3  | 1:A:303:LYS:HZ1  | 1.79                     | 0.46              |
| 1:A:294:LEU:HD22 | 1:A:298:LYS:HD3  | 1.97                     | 0.46              |
| 1:B:165:ASN:CG   | 1:C:191:LEU:HD21 | 2.40                     | 0.46              |
| 1:B:339:GLN:HE22 | 1:B:405:GLU:N    | 2.09                     | 0.46              |
| 1:A:73:TYR:CE2   | 1:A:112:ALA:HB2  | 2.51                     | 0.46              |
| 1:A:183:VAL:HG13 | 1:A:238:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:199:GLU:HG2  | 1:A:203:GLU:OE2  | 2.15                     | 0.46              |
| 1:D:339:GLN:NE2  | 1:D:405:GLU:H    | 2.14                     | 0.46              |
| 1:A:435:ILE:HG23 | 1:A:436:GLU:HG3  | 1.98                     | 0.46              |
| 1:D:93:LEU:O     | 1:D:94:ASN:HB2   | 2.16                     | 0.46              |
| 1:D:252:VAL:HG12 | 1:D:256:ARG:HD2  | 1.98                     | 0.46              |
| 1:A:167:TRP:CZ2  | 1:A:171:LYS:HD3  | 2.51                     | 0.46              |
| 1:A:195:GLU:HG3  | 1:D:167:TRP:CD1  | 2.51                     | 0.46              |
| 1:B:278:PHE:HD1  | 1:B:278:PHE:O    | 1.99                     | 0.46              |
| 1:C:215:ARG:HB3  | 1:C:290:PRO:HG3  | 1.97                     | 0.46              |
| 1:C:253:THR:O    | 1:C:257:GLN:HG3  | 2.16                     | 0.46              |
| 1:D:442:ALA:HB1  | 1:D:443:PRO:HD2  | 1.97                     | 0.46              |
| 1:A:252:VAL:O    | 1:A:256:ARG:HG3  | 2.16                     | 0.46              |
| 1:B:226:ARG:HE   | 1:C:226:ARG:HH21 | 1.64                     | 0.46              |
| 1:D:201:LYS:HD2  | 1:D:329:MSE:HG3  | 1.98                     | 0.46              |
| 1:D:367:ASN:O    | 1:D:371:ILE:HG13 | 2.16                     | 0.46              |
| 1:B:207:THR:CG2  | 1:B:208:ALA:N    | 2.79                     | 0.45              |
| 1:A:77:THR:CG2   | 1:A:118:ILE:N    | 2.80                     | 0.45              |
| 1:B:105:ILE:HG13 | 1:B:108:LYS:NZ   | 2.30                     | 0.45              |
| 1:B:206:VAL:HG21 | 1:B:327:ASN:ND2  | 2.30                     | 0.45              |
| 1:D:89:ILE:HG22  | 1:D:123:LEU:HG   | 1.97                     | 0.45              |
| 1:D:312:LEU:HG   | 1:D:364:MSE:HE1  | 1.98                     | 0.45              |
| 1:B:379:ARG:HB3  | 1:B:384:LYS:HG3  | 1.97                     | 0.45              |
| 1:D:77:THR:HG23  | 1:D:117:THR:HB   | 1.98                     | 0.45              |
| 1:A:241:CYS:O    | 1:A:242:HIS:C    | 2.60                     | 0.45              |
| 1:C:57:ASP:OD1   | 1:C:313:VAL:CG2  | 2.65                     | 0.45              |
| 1:A:357:LEU:N    | 1:A:358:PRO:HD2  | 2.31                     | 0.45              |
| 1:B:255:ALA:HB3  | 1:B:262:ILE:CD1  | 2.46                     | 0.45              |
| 1:D:319:CYS:HB2  | 1:D:323:MSE:HE3  | 1.99                     | 0.45              |
| 1:D:74:GLU:O     | 1:D:78:ARG:HB2   | 2.16                     | 0.45              |
| 1:A:226:ARG:HG2  | 1:A:226:ARG:HH11 | 1.80                     | 0.45              |
| 1:B:246:PRO:HD2  | 1:B:296:ASN:ND2  | 2.31                     | 0.45              |
| 1:C:273:LEU:HA   | 1:C:277:GLN:OE1  | 2.17                     | 0.45              |
| 1:C:327:ASN:HD21 | 1:C:329:MSE:CB   | 2.30                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:102:ARG:HB2  | 1:A:102:ARG:HH11 | 1.81                     | 0.45              |
| 1:C:201:LYS:HE3  | 1:C:329:MSE:HG3  | 1.99                     | 0.45              |
| 1:C:216:PRO:HG2  | 1:C:219:THR:HG23 | 1.99                     | 0.45              |
| 1:D:95:GLN:O     | 1:D:96:LEU:C     | 2.59                     | 0.45              |
| 1:A:206:VAL:HA   | 1:A:329:MSE:CG   | 2.47                     | 0.45              |
| 1:B:269:HIS:CD2  | 1:B:335:ILE:HD12 | 2.52                     | 0.45              |
| 1:D:107:LEU:HD13 | 1:D:107:LEU:O    | 2.17                     | 0.45              |
| 1:D:304:LEU:HD13 | 1:D:355:MSE:HE1  | 1.98                     | 0.45              |
| 1:B:432:ILE:HG21 | 1:B:444:LYS:HE2  | 1.98                     | 0.44              |
| 1:C:134:LEU:HD12 | 1:C:175:LYS:HG2  | 1.98                     | 0.44              |
| 1:A:400:THR:CG2  | 3:A:460:HOH:O    | 2.65                     | 0.44              |
| 1:C:59:HIS:N     | 1:C:313:VAL:CG2  | 2.81                     | 0.44              |
| 1:C:288:SER:HB3  | 1:C:289:PRO:HD2  | 1.99                     | 0.44              |
| 1:C:215:ARG:HG2  | 1:C:290:PRO:HD3  | 1.98                     | 0.44              |
| 1:D:201:LYS:HD2  | 1:D:329:MSE:CG   | 2.47                     | 0.44              |
| 1:A:246:PRO:HD2  | 1:A:296:ASN:ND2  | 2.32                     | 0.44              |
| 1:B:74:GLU:HG3   | 1:B:115:LYS:HG3  | 1.99                     | 0.44              |
| 1:D:214:SER:C    | 1:D:216:PRO:HD3  | 2.43                     | 0.44              |
| 1:D:312:LEU:CD2  | 1:D:363:LEU:HB3  | 2.44                     | 0.44              |
| 1:B:77:THR:CG2   | 1:B:117:THR:CB   | 2.92                     | 0.44              |
| 1:D:77:THR:HG21  | 1:D:117:THR:H    | 1.82                     | 0.44              |
| 1:D:357:LEU:N    | 1:D:358:PRO:HD2  | 2.33                     | 0.44              |
| 1:B:312:LEU:HD12 | 1:B:312:LEU:HA   | 1.82                     | 0.44              |
| 1:D:189:ASN:HD21 | 1:D:191:LEU:HB3  | 1.83                     | 0.44              |
| 1:B:145:PHE:CD1  | 1:B:181:GLN:HG2  | 2.53                     | 0.44              |
| 1:C:202:ARG:NH1  | 1:C:202:ARG:HG2  | 2.33                     | 0.44              |
| 1:D:427:LEU:HD11 | 1:D:428:ARG:NH2  | 2.33                     | 0.44              |
| 1:A:277:GLN:O    | 1:A:281:ILE:HG13 | 2.18                     | 0.44              |
| 1:B:63:SER:HB2   | 1:B:71:GLU:H     | 1.80                     | 0.44              |
| 1:B:70:TRP:HB3   | 1:B:408:HIS:HE1  | 1.82                     | 0.44              |
| 1:B:272:VAL:HG11 | 1:B:348:GLU:HG3  | 1.99                     | 0.44              |
| 1:B:427:LEU:HD23 | 1:B:444:LYS:HD2  | 1.99                     | 0.44              |
| 1:C:93:LEU:HB3   | 1:C:162:ARG:HD2  | 1.99                     | 0.44              |
| 1:D:284:LEU:HD12 | 1:D:324:LYS:HG2  | 2.00                     | 0.44              |
| 1:B:191:LEU:HD21 | 1:C:165:ASN:CG   | 2.43                     | 0.44              |
| 1:C:52:SER:OG    | 1:C:53:PRO:HD2   | 2.18                     | 0.44              |
| 1:C:211:TYR:CZ   | 1:C:286:LYS:HE3  | 2.52                     | 0.44              |
| 1:C:384:LYS:HD2  | 1:C:384:LYS:N    | 2.32                     | 0.44              |
| 1:A:321:PRO:HG2  | 1:A:322:GLU:OE2  | 2.18                     | 0.43              |
| 1:B:96:LEU:HB3   | 1:B:97:PRO:CD    | 2.48                     | 0.43              |
| 1:C:327:ASN:ND2  | 1:C:329:MSE:HB2  | 2.32                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:162:ARG:HB2  | 1:D:163:ASP:H    | 1.53                     | 0.43              |
| 1:A:92:PRO:HG2   | 1:A:93:LEU:CD1   | 2.48                     | 0.43              |
| 1:A:102:ARG:NH1  | 1:A:140:VAL:CG2  | 2.81                     | 0.43              |
| 1:A:200:ALA:C    | 1:A:202:ARG:H    | 2.26                     | 0.43              |
| 1:A:205:ARG:HH11 | 1:A:205:ARG:CG   | 2.30                     | 0.43              |
| 1:D:5:LEU:HD13   | 1:D:44:MSE:HE3   | 1.97                     | 0.43              |
| 1:C:8:LYS:HG3    | 1:C:22:ASP:CG    | 2.43                     | 0.43              |
| 1:A:92:PRO:HG2   | 1:A:93:LEU:N     | 2.33                     | 0.43              |
| 1:B:126:LEU:HB3  | 1:B:147:CYS:HB3  | 2.01                     | 0.43              |
| 1:B:215:ARG:HB3  | 1:B:290:PRO:HG3  | 2.00                     | 0.43              |
| 1:D:397:TYR:CB   | 1:D:421:ARG:NH1  | 2.81                     | 0.43              |
| 1:A:428:ARG:HH11 | 1:A:428:ARG:CG   | 2.31                     | 0.43              |
| 1:C:256:ARG:HH22 | 1:C:310:ASP:CG   | 2.26                     | 0.43              |
| 1:C:283:THR:O    | 1:C:286:LYS:HB3  | 2.18                     | 0.43              |
| 1:D:29:LYS:HD3   | 1:D:383:GLY:HA2  | 2.01                     | 0.43              |
| 1:D:184:LEU:N    | 1:D:184:LEU:HD23 | 2.34                     | 0.43              |
| 1:D:292:ARG:HG3  | 3:D:621:HOH:O    | 2.18                     | 0.43              |
| 1:A:41:LYS:H     | 1:A:41:LYS:HD2   | 1.82                     | 0.43              |
| 1:C:250:GLU:CG   | 1:C:303:LYS:HZ1  | 2.16                     | 0.43              |
| 1:A:83:GLY:C     | 1:A:422:ILE:HD13 | 2.44                     | 0.43              |
| 1:A:288:SER:O    | 1:A:290:PRO:N    | 2.51                     | 0.43              |
| 1:D:287:CYS:HB3  | 1:D:335:ILE:HG13 | 1.99                     | 0.43              |
| 1:A:229:TYR:O    | 1:A:232:LYS:HB3  | 2.19                     | 0.43              |
| 1:B:113:LYS:HD2  | 1:B:114:GLY:N    | 2.33                     | 0.43              |
| 1:B:175:LYS:HE2  | 1:B:179:LEU:HG   | 2.01                     | 0.43              |
| 1:B:96:LEU:O     | 1:B:97:PRO:C     | 2.59                     | 0.43              |
| 1:B:424:LYS:HD3  | 3:B:708:HOH:O    | 2.18                     | 0.43              |
| 1:C:428:ARG:HH11 | 1:C:428:ARG:CG   | 2.32                     | 0.43              |
| 1:A:128:SER:HB2  | 1:A:168:GLN:NE2  | 2.34                     | 0.42              |
| 1:A:167:TRP:CG   | 1:D:195:GLU:HG3  | 2.54                     | 0.42              |
| 1:A:198:GLU:O    | 1:A:202:ARG:HD3  | 2.19                     | 0.42              |
| 1:A:273:LEU:HA   | 1:A:277:GLN:HE22 | 1.78                     | 0.42              |
| 1:B:55:MSE:HG3   | 1:B:364:MSE:O    | 2.19                     | 0.42              |
| 1:B:61:HIS:HD1   | 1:B:94:ASN:HD22  | 1.65                     | 0.42              |
| 1:D:61:HIS:HB2   | 1:D:316:HIS:O    | 2.19                     | 0.42              |
| 1:A:261:ASP:C    | 1:A:262:ILE:HG13 | 2.44                     | 0.42              |
| 1:A:304:LEU:HD21 | 1:A:363:LEU:HD13 | 2.01                     | 0.42              |
| 1:A:425:THR:HB   | 1:A:433:TYR:HB3  | 2.00                     | 0.42              |
| 1:B:195:GLU:HG3  | 1:C:167:TRP:CD1  | 2.54                     | 0.42              |
| 1:D:15:GLU:OE2   | 1:D:379:ARG:NE   | 2.45                     | 0.42              |
| 1:D:428:ARG:HH11 | 1:D:428:ARG:CG   | 2.32                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:112:ALA:O    | 1:A:115:LYS:HB2  | 2.19                     | 0.42              |
| 1:A:238:LEU:C    | 1:A:238:LEU:CD1  | 2.92                     | 0.42              |
| 1:B:228:LEU:HD23 | 1:B:238:LEU:HD23 | 2.02                     | 0.42              |
| 1:D:205:ARG:HB3  | 1:D:210:ASP:OD2  | 2.19                     | 0.42              |
| 1:A:203:GLU:HB2  | 1:A:205:ARG:HD3  | 2.02                     | 0.42              |
| 1:B:63:SER:HB2   | 1:B:71:GLU:CA    | 2.48                     | 0.42              |
| 1:B:215:ARG:HG3  | 1:B:215:ARG:NH1  | 2.22                     | 0.42              |
| 1:B:218:PHE:CD2  | 1:C:233:VAL:HG11 | 2.55                     | 0.42              |
| 1:C:73:TYR:N     | 3:C:554:HOH:O    | 2.52                     | 0.42              |
| 1:C:241:CYS:O    | 1:C:242:HIS:C    | 2.63                     | 0.42              |
| 1:D:137:LEU:HD23 | 1:D:137:LEU:HA   | 1.81                     | 0.42              |
| 1:A:75:THR:CG2   | 1:A:76:GLY:N     | 2.82                     | 0.42              |
| 1:A:278:PHE:CD1  | 1:A:278:PHE:C    | 2.96                     | 0.42              |
| 1:B:61:HIS:ND1   | 1:B:94:ASN:ND2   | 2.64                     | 0.42              |
| 1:C:100:VAL:C    | 1:C:137:LEU:HD11 | 2.44                     | 0.42              |
| 1:D:15:GLU:CD    | 1:D:379:ARG:HE   | 2.27                     | 0.42              |
| 1:C:377:LYS:CE   | 1:C:387:ASP:OD2  | 2.67                     | 0.42              |
| 1:D:184:LEU:HD22 | 1:D:239:HIS:HB3  | 2.01                     | 0.42              |
| 1:D:211:TYR:HD1  | 1:D:329:MSE:HE1  | 1.84                     | 0.42              |
| 1:B:77:THR:CG2   | 1:B:117:THR:N    | 2.74                     | 0.42              |
| 1:C:261:ASP:O    | 1:C:262:ILE:HD13 | 2.19                     | 0.42              |
| 1:D:73:TYR:O     | 1:D:77:THR:CG2   | 2.66                     | 0.42              |
| 1:A:142:VAL:HG13 | 1:A:144:GLY:H    | 1.84                     | 0.42              |
| 1:A:269:HIS:CD2  | 1:A:269:HIS:H    | 2.37                     | 0.42              |
| 1:B:241:CYS:O    | 1:B:242:HIS:C    | 2.63                     | 0.42              |
| 1:C:277:GLN:HA   | 1:C:280:GLU:CG   | 2.49                     | 0.42              |
| 1:D:29:LYS:HD2   | 1:D:29:LYS:C     | 2.44                     | 0.42              |
| 1:D:124:GLY:N    | 1:D:142:VAL:HG11 | 2.35                     | 0.42              |
| 1:A:327:ASN:OD1  | 1:A:330:LYS:HG3  | 2.20                     | 0.41              |
| 1:B:255:ALA:HB3  | 1:B:262:ILE:HD11 | 2.02                     | 0.41              |
| 1:C:18:ALA:HB2   | 1:C:357:LEU:HB2  | 2.02                     | 0.41              |
| 1:A:142:VAL:CG1  | 1:A:144:GLY:H    | 2.33                     | 0.41              |
| 1:A:207:THR:CG2  | 1:A:208:ALA:N    | 2.83                     | 0.41              |
| 1:B:69:HIS:N     | 1:B:320:PRO:HD3  | 2.34                     | 0.41              |
| 1:C:59:HIS:N     | 1:C:313:VAL:HG21 | 2.35                     | 0.41              |
| 1:C:319:CYS:SG   | 1:C:324:LYS:HD3  | 2.60                     | 0.41              |
| 1:D:225:ARG:NH1  | 3:D:480:HOH:O    | 2.47                     | 0.41              |
| 1:A:286:LYS:HD3  | 1:A:328:ILE:HG23 | 2.03                     | 0.41              |
| 1:B:206:VAL:CG2  | 1:B:329:MSE:HG2  | 2.42                     | 0.41              |
| 1:C:424:LYS:HE2  | 1:C:434:ASP:OD2  | 2.19                     | 0.41              |
| 1:D:255:ALA:HB3  | 1:D:262:ILE:CD1  | 2.49                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:237:ARG:HD3  | 3:A:569:HOH:O    | 2.20                     | 0.41              |
| 1:B:278:PHE:CD1  | 1:B:278:PHE:O    | 2.73                     | 0.41              |
| 1:D:360:PHE:O    | 1:D:364:MSE:HG2  | 2.21                     | 0.41              |
| 1:D:377:LYS:HD2  | 1:D:377:LYS:N    | 2.36                     | 0.41              |
| 1:A:82:LYS:HG3   | 1:A:433:TYR:CZ   | 2.55                     | 0.41              |
| 1:A:242:HIS:ND1  | 1:A:289:PRO:HG2  | 2.35                     | 0.41              |
| 1:A:316:HIS:CD2  | 1:A:338:LEU:HD12 | 2.56                     | 0.41              |
| 1:A:360:PHE:O    | 1:A:364:MSE:HG2  | 2.20                     | 0.41              |
| 1:B:71:GLU:CG    | 1:B:318:PRO:HG3  | 2.42                     | 0.41              |
| 1:C:427:LEU:O    | 1:C:444:LYS:HE3  | 2.21                     | 0.41              |
| 1:D:143:VAL:HG22 | 1:D:372:PHE:O    | 2.20                     | 0.41              |
| 1:D:324:LYS:NZ   | 3:D:577:HOH:O    | 2.51                     | 0.41              |
| 1:B:12:VAL:O     | 1:B:18:ALA:HA    | 2.20                     | 0.41              |
| 1:B:92:PRO:HB3   | 1:B:123:LEU:O    | 2.20                     | 0.41              |
| 1:D:92:PRO:HG2   | 1:D:93:LEU:H     | 1.86                     | 0.41              |
| 1:D:274:ASP:OD1  | 1:D:277:GLN:HG3  | 2.21                     | 0.41              |
| 1:D:278:PHE:CD1  | 1:D:285:ALA:HB3  | 2.56                     | 0.41              |
| 1:C:434:ASP:OD1  | 1:C:436:GLU:N    | 2.48                     | 0.41              |
| 1:D:133:ARG:NH1  | 1:D:133:ARG:CG   | 2.82                     | 0.41              |
| 1:D:284:LEU:HB2  | 3:D:573:HOH:O    | 2.20                     | 0.41              |
| 1:B:205:ARG:HH11 | 1:B:205:ARG:HG2  | 1.85                     | 0.41              |
| 1:B:377:LYS:HG3  | 3:B:689:HOH:O    | 2.21                     | 0.41              |
| 1:C:294:LEU:HD22 | 1:C:298:LYS:HD3  | 2.02                     | 0.41              |
| 1:C:340:SER:O    | 1:C:344:VAL:HB   | 2.21                     | 0.41              |
| 1:C:396:SER:HA   | 1:C:418:ILE:O    | 2.20                     | 0.41              |
| 1:D:142:VAL:HG12 | 1:D:143:VAL:N    | 2.36                     | 0.41              |
| 1:D:193:CYS:SG   | 1:D:219:THR:HG21 | 2.60                     | 0.41              |
| 1:D:278:PHE:CD1  | 1:D:278:PHE:C    | 2.98                     | 0.41              |
| 1:D:288:SER:O    | 1:D:290:PRO:N    | 2.54                     | 0.41              |
| 1:A:326:GLY:C    | 1:A:330:LYS:HE3  | 2.46                     | 0.41              |
| 1:B:124:GLY:O    | 1:B:145:PHE:HA   | 2.21                     | 0.40              |
| 1:C:6:ILE:CG2    | 1:C:8:LYS:HD2    | 2.51                     | 0.40              |
| 1:C:112:ALA:O    | 1:C:113:LYS:C    | 2.63                     | 0.40              |
| 1:C:228:LEU:HD23 | 1:C:238:LEU:HD23 | 2.04                     | 0.40              |
| 1:C:271:PHE:CE2  | 1:C:304:LEU:HG   | 2.56                     | 0.40              |
| 1:D:101:ASP:HB2  | 1:D:136:GLU:OE1  | 2.21                     | 0.40              |
| 1:D:102:ARG:NH2  | 1:D:139:GLU:OE1  | 2.54                     | 0.40              |
| 1:C:375:GLN:NE2  | 1:C:450:LYS:NZ   | 2.69                     | 0.40              |
| 1:D:62:ILE:HD11  | 1:D:88:MSE:SE    | 2.72                     | 0.40              |
| 1:D:312:LEU:N    | 1:D:312:LEU:HD22 | 2.36                     | 0.40              |
| 1:A:107:LEU:HD13 | 1:A:107:LEU:O    | 2.21                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:135:HIS:HD2 | 1:B:139:GLU:OE2  | 2.04                     | 0.40              |
| 1:C:205:ARG:HB3 | 1:C:210:ASP:CG   | 2.46                     | 0.40              |
| 1:D:428:ARG:NH1 | 1:D:444:LYS:HE2  | 2.37                     | 0.40              |
| 1:A:272:VAL:O   | 1:A:272:VAL:HG13 | 2.21                     | 0.40              |
| 1:A:287:CYS:HB3 | 1:A:335:ILE:HG12 | 2.03                     | 0.40              |
| 1:A:397:TYR:HB3 | 1:A:421:ARG:NH1  | 2.37                     | 0.40              |
| 1:B:28:GLY:C    | 1:B:29:LYS:HD2   | 2.46                     | 0.40              |
| 1:B:226:ARG:NE  | 1:C:226:ARG:HH21 | 2.19                     | 0.40              |
| 1:C:73:TYR:OH   | 1:C:108:LYS:HE2  | 2.21                     | 0.40              |
| 1:C:92:PRO:HG2  | 1:C:93:LEU:HG    | 2.04                     | 0.40              |
| 1:C:377:LYS:HZ1 | 1:C:448:ILE:HD11 | 1.85                     | 0.40              |
| 1:D:8:LYS:NZ    | 3:D:622:HOH:O    | 2.54                     | 0.40              |
| 1:D:12:VAL:O    | 1:D:18:ALA:HA    | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| 1   | A     | 422/473 (89%)   | 405 (96%)  | 13 (3%) | 4 (1%)   | 14          | 10 |
| 1   | B     | 426/473 (90%)   | 410 (96%)  | 11 (3%) | 5 (1%)   | 10          | 7  |
| 1   | C     | 421/473 (89%)   | 405 (96%)  | 13 (3%) | 3 (1%)   | 18          | 15 |
| 1   | D     | 422/473 (89%)   | 402 (95%)  | 16 (4%) | 4 (1%)   | 14          | 10 |
| All | All   | 1691/1892 (89%) | 1622 (96%) | 53 (3%) | 16 (1%)  | 14          | 10 |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 96  | LEU  |
| 1   | A     | 288 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 288 | SER  |
| 1   | C     | 288 | SER  |
| 1   | D     | 96  | LEU  |
| 1   | D     | 288 | SER  |
| 1   | A     | 242 | HIS  |
| 1   | B     | 242 | HIS  |
| 1   | C     | 242 | HIS  |
| 1   | D     | 242 | HIS  |
| 1   | B     | 95  | GLN  |
| 1   | A     | 92  | PRO  |
| 1   | B     | 71  | GLU  |
| 1   | B     | 92  | PRO  |
| 1   | C     | 92  | PRO  |
| 1   | D     | 92  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 350/374 (94%)   | 315 (90%)  | 35 (10%) | 7           | 5  |
| 1   | B     | 354/374 (95%)   | 322 (91%)  | 32 (9%)  | 9           | 6  |
| 1   | C     | 350/374 (94%)   | 317 (91%)  | 33 (9%)  | 8           | 6  |
| 1   | D     | 350/374 (94%)   | 324 (93%)  | 26 (7%)  | 13          | 10 |
| All | All   | 1404/1496 (94%) | 1278 (91%) | 126 (9%) | 9           | 6  |

All (126) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | LEU  |
| 1   | A     | 19  | ARG  |
| 1   | A     | 60  | THR  |
| 1   | A     | 75  | THR  |
| 1   | A     | 92  | PRO  |
| 1   | A     | 102 | ARG  |
| 1   | A     | 106 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 108 | LYS  |
| 1   | A     | 131 | ILE  |
| 1   | A     | 142 | VAL  |
| 1   | A     | 143 | VAL  |
| 1   | A     | 162 | ARG  |
| 1   | A     | 165 | ASN  |
| 1   | A     | 174 | GLN  |
| 1   | A     | 201 | LYS  |
| 1   | A     | 202 | ARG  |
| 1   | A     | 205 | ARG  |
| 1   | A     | 207 | THR  |
| 1   | A     | 226 | ARG  |
| 1   | A     | 272 | VAL  |
| 1   | A     | 286 | LYS  |
| 1   | A     | 294 | LEU  |
| 1   | A     | 304 | LEU  |
| 1   | A     | 306 | ASN  |
| 1   | A     | 311 | CYS  |
| 1   | A     | 312 | LEU  |
| 1   | A     | 322 | GLU  |
| 1   | A     | 324 | LYS  |
| 1   | A     | 330 | LYS  |
| 1   | A     | 338 | LEU  |
| 1   | A     | 375 | GLN  |
| 1   | A     | 384 | LYS  |
| 1   | A     | 428 | ARG  |
| 1   | A     | 444 | LYS  |
| 1   | A     | 450 | LYS  |
| 1   | B     | 41  | LYS  |
| 1   | B     | 70  | TRP  |
| 1   | B     | 71  | GLU  |
| 1   | B     | 77  | THR  |
| 1   | B     | 92  | PRO  |
| 1   | B     | 95  | GLN  |
| 1   | B     | 96  | LEU  |
| 1   | B     | 102 | ARG  |
| 1   | B     | 108 | LYS  |
| 1   | B     | 115 | LYS  |
| 1   | B     | 163 | ASP  |
| 1   | B     | 189 | ASN  |
| 1   | B     | 198 | GLU  |
| 1   | B     | 201 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 202 | ARG  |
| 1   | B     | 205 | ARG  |
| 1   | B     | 207 | THR  |
| 1   | B     | 215 | ARG  |
| 1   | B     | 226 | ARG  |
| 1   | B     | 254 | ARG  |
| 1   | B     | 278 | PHE  |
| 1   | B     | 312 | LEU  |
| 1   | B     | 324 | LYS  |
| 1   | B     | 327 | ASN  |
| 1   | B     | 352 | LYS  |
| 1   | B     | 379 | ARG  |
| 1   | B     | 400 | THR  |
| 1   | B     | 407 | ARG  |
| 1   | B     | 409 | LYS  |
| 1   | B     | 428 | ARG  |
| 1   | B     | 444 | LYS  |
| 1   | B     | 450 | LYS  |
| 1   | C     | 5   | LEU  |
| 1   | C     | 8   | LYS  |
| 1   | C     | 15  | GLU  |
| 1   | C     | 92  | PRO  |
| 1   | C     | 95  | GLN  |
| 1   | C     | 106 | GLU  |
| 1   | C     | 107 | LEU  |
| 1   | C     | 108 | LYS  |
| 1   | C     | 115 | LYS  |
| 1   | C     | 184 | LEU  |
| 1   | C     | 189 | ASN  |
| 1   | C     | 201 | LYS  |
| 1   | C     | 202 | ARG  |
| 1   | C     | 205 | ARG  |
| 1   | C     | 215 | ARG  |
| 1   | C     | 226 | ARG  |
| 1   | C     | 232 | LYS  |
| 1   | C     | 237 | ARG  |
| 1   | C     | 294 | LEU  |
| 1   | C     | 304 | LEU  |
| 1   | C     | 311 | CYS  |
| 1   | C     | 312 | LEU  |
| 1   | C     | 313 | VAL  |
| 1   | C     | 324 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 329 | MSE  |
| 1   | C     | 352 | LYS  |
| 1   | C     | 375 | GLN  |
| 1   | C     | 379 | ARG  |
| 1   | C     | 392 | GLN  |
| 1   | C     | 399 | LEU  |
| 1   | C     | 407 | ARG  |
| 1   | C     | 428 | ARG  |
| 1   | C     | 450 | LYS  |
| 1   | D     | 29  | LYS  |
| 1   | D     | 92  | PRO  |
| 1   | D     | 110 | ASP  |
| 1   | D     | 133 | ARG  |
| 1   | D     | 143 | VAL  |
| 1   | D     | 162 | ARG  |
| 1   | D     | 163 | ASP  |
| 1   | D     | 175 | LYS  |
| 1   | D     | 184 | LEU  |
| 1   | D     | 189 | ASN  |
| 1   | D     | 191 | LEU  |
| 1   | D     | 202 | ARG  |
| 1   | D     | 205 | ARG  |
| 1   | D     | 215 | ARG  |
| 1   | D     | 222 | GLU  |
| 1   | D     | 226 | ARG  |
| 1   | D     | 262 | ILE  |
| 1   | D     | 272 | VAL  |
| 1   | D     | 298 | LYS  |
| 1   | D     | 304 | LEU  |
| 1   | D     | 311 | CYS  |
| 1   | D     | 329 | MSE  |
| 1   | D     | 352 | LYS  |
| 1   | D     | 392 | GLN  |
| 1   | D     | 424 | LYS  |
| 1   | D     | 428 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 135 | HIS  |
| 1   | A     | 165 | ASN  |
| 1   | A     | 174 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 209 | HIS  |
| 1   | A     | 239 | HIS  |
| 1   | A     | 269 | HIS  |
| 1   | A     | 277 | GLN  |
| 1   | A     | 296 | ASN  |
| 1   | A     | 297 | GLN  |
| 1   | A     | 339 | GLN  |
| 1   | A     | 367 | ASN  |
| 1   | A     | 375 | GLN  |
| 1   | A     | 408 | HIS  |
| 1   | B     | 16  | ASN  |
| 1   | B     | 95  | GLN  |
| 1   | B     | 135 | HIS  |
| 1   | B     | 181 | GLN  |
| 1   | B     | 189 | ASN  |
| 1   | B     | 239 | HIS  |
| 1   | B     | 260 | GLN  |
| 1   | B     | 296 | ASN  |
| 1   | B     | 306 | ASN  |
| 1   | B     | 327 | ASN  |
| 1   | B     | 339 | GLN  |
| 1   | B     | 351 | GLN  |
| 1   | B     | 392 | GLN  |
| 1   | B     | 401 | ASN  |
| 1   | B     | 408 | HIS  |
| 1   | B     | 437 | GLN  |
| 1   | C     | 16  | ASN  |
| 1   | C     | 35  | GLN  |
| 1   | C     | 94  | ASN  |
| 1   | C     | 95  | GLN  |
| 1   | C     | 135 | HIS  |
| 1   | C     | 189 | ASN  |
| 1   | C     | 327 | ASN  |
| 1   | C     | 339 | GLN  |
| 1   | C     | 351 | GLN  |
| 1   | C     | 375 | GLN  |
| 1   | C     | 401 | ASN  |
| 1   | D     | 122 | GLN  |
| 1   | D     | 181 | GLN  |
| 1   | D     | 189 | ASN  |
| 1   | D     | 209 | HIS  |
| 1   | D     | 239 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 277 | GLN  |
| 1   | D     | 339 | GLN  |
| 1   | D     | 375 | GLN  |
| 1   | D     | 392 | GLN  |
| 1   | D     | 401 | ASN  |
| 1   | D     | 437 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$ |
| 1   | KCX  | D     | 146 | 1,2  | 10,11,12     | 0.89 | 1 (10%)     | 6,12,14     | 1.79 | 1 (16%)     |
| 1   | KCX  | A     | 146 | 1,2  | 10,11,12     | 0.96 | 1 (10%)     | 6,12,14     | 1.77 | 1 (16%)     |
| 1   | KCX  | B     | 146 | 1,2  | 10,11,12     | 0.95 | 0           | 6,12,14     | 2.39 | 1 (16%)     |
| 1   | KCX  | C     | 146 | 1,2  | 10,11,12     | 0.90 | 0           | 6,12,14     | 1.73 | 1 (16%)     |

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 |
|-----|------|-------|-----|------|---------|-----------|-------|
| 1   | KCX  | D     | 146 | 1,2  | -       | 4/9/10/12 | -     |
| 1   | KCX  | A     | 146 | 1,2  | -       | 3/9/10/12 | -     |
| 1   | KCX  | B     | 146 | 1,2  | -       | 5/9/10/12 | -     |
| 1   | KCX  | C     | 146 | 1,2  | -       | 0/9/10/12 | -     |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | A     | 146 | KCX  | OQ1-CX | 2.27 | 1.25        | 1.21     |
| 1   | D     | 146 | KCX  | OQ1-CX | 2.05 | 1.25        | 1.21     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 146 | KCX  | OQ1-CX-NZ | -5.54 | 116.50      | 124.92   |
| 1   | A     | 146 | KCX  | OQ1-CX-NZ | -4.09 | 118.70      | 124.92   |
| 1   | C     | 146 | KCX  | OQ1-CX-NZ | -4.07 | 118.73      | 124.92   |
| 1   | D     | 146 | KCX  | OQ1-CX-NZ | -3.65 | 119.37      | 124.92   |

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | A     | 146 | KCX  | N-CA-CB-CG  |
| 1   | A     | 146 | KCX  | C-CA-CB-CG  |
| 1   | A     | 146 | KCX  | O-C-CA-CB   |
| 1   | B     | 146 | KCX  | C-CA-CB-CG  |
| 1   | B     | 146 | KCX  | O-C-CA-CB   |
| 1   | D     | 146 | KCX  | N-CA-CB-CG  |
| 1   | D     | 146 | KCX  | C-CA-CB-CG  |
| 1   | D     | 146 | KCX  | O-C-CA-CB   |
| 1   | D     | 146 | KCX  | CG-CD-CE-NZ |
| 1   | B     | 146 | KCX  | CE-CD-CG-CB |
| 1   | B     | 146 | KCX  | N-CA-CB-CG  |
| 1   | B     | 146 | KCX  | CA-CB-CG-CD |

There are no ring outliers.

3 monomers are involved in 5 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | D     | 146 | KCX  | 3       | 0            |
| 1   | A     | 146 | KCX  | 1       | 0            |
| 1   | B     | 146 | KCX  | 1       | 0            |

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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     | 416/473 (87%)   | 0.28   | 22 (5%) 32 34 | 14, 27, 48, 63        | 0     |
| 1   | B     | 420/473 (88%)   | 0.15   | 23 (5%) 30 32 | 14, 24, 45, 69        | 0     |
| 1   | C     | 415/473 (87%)   | 0.19   | 14 (3%) 48 50 | 15, 26, 48, 59        | 0     |
| 1   | D     | 416/473 (87%)   | 0.54   | 33 (7%) 18 20 | 18, 31, 54, 67        | 0     |
| All | All   | 1667/1892 (88%) | 0.29   | 92 (5%) 30 32 | 14, 27, 49, 69        | 0     |

All (92) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 96  | LEU  | 8.5  |
| 1   | A     | 288 | SER  | 7.1  |
| 1   | A     | 96  | LEU  | 7.0  |
| 1   | D     | 288 | SER  | 6.6  |
| 1   | B     | 96  | LEU  | 6.4  |
| 1   | B     | 288 | SER  | 5.7  |
| 1   | C     | 96  | LEU  | 5.5  |
| 1   | B     | 70  | TRP  | 5.4  |
| 1   | C     | 288 | SER  | 5.1  |
| 1   | D     | 94  | ASN  | 4.8  |
| 1   | B     | 69  | HIS  | 4.6  |
| 1   | C     | 97  | PRO  | 4.5  |
| 1   | B     | 94  | ASN  | 4.2  |
| 1   | D     | 332 | TRP  | 4.0  |
| 1   | C     | 94  | ASN  | 3.9  |
| 1   | A     | 94  | ASN  | 3.6  |
| 1   | D     | 95  | GLN  | 3.6  |
| 1   | B     | 201 | LYS  | 3.5  |
| 1   | A     | 332 | TRP  | 3.4  |
| 1   | D     | 206 | VAL  | 3.4  |
| 1   | B     | 2   | SER  | 3.4  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | D            | 202        | ARG         | 3.4         |
| 1          | A            | 95         | GLN         | 3.3         |
| 1          | A            | 97         | PRO         | 3.2         |
| 1          | A            | 104        | SER         | 3.2         |
| 1          | B            | 71         | GLU         | 3.1         |
| 1          | A            | 204        | GLY         | 3.1         |
| 1          | A            | 162        | ARG         | 3.1         |
| 1          | D            | 93         | LEU         | 3.0         |
| 1          | D            | 330        | LYS         | 3.0         |
| 1          | A            | 202        | ARG         | 2.9         |
| 1          | D            | 16         | ASN         | 2.9         |
| 1          | D            | 289        | PRO         | 2.9         |
| 1          | B            | 110        | ASP         | 2.9         |
| 1          | B            | 319        | CYS         | 2.8         |
| 1          | C            | 332        | TRP         | 2.8         |
| 1          | C            | 202        | ARG         | 2.8         |
| 1          | B            | 93         | LEU         | 2.8         |
| 1          | A            | 201        | LYS         | 2.8         |
| 1          | B            | 207        | THR         | 2.8         |
| 1          | D            | 2          | SER         | 2.7         |
| 1          | D            | 111        | ALA         | 2.7         |
| 1          | D            | 394        | ASN         | 2.7         |
| 1          | D            | 162        | ARG         | 2.7         |
| 1          | D            | 321        | PRO         | 2.6         |
| 1          | B            | 63         | SER         | 2.6         |
| 1          | C            | 2          | SER         | 2.6         |
| 1          | A            | 325        | ALA         | 2.6         |
| 1          | A            | 207        | THR         | 2.6         |
| 1          | C            | 93         | LEU         | 2.6         |
| 1          | D            | 29         | LYS         | 2.6         |
| 1          | D            | 437        | GLN         | 2.6         |
| 1          | A            | 131        | ILE         | 2.5         |
| 1          | D            | 198        | GLU         | 2.5         |
| 1          | D            | 208        | ALA         | 2.5         |
| 1          | B            | 95         | GLN         | 2.4         |
| 1          | B            | 332        | TRP         | 2.4         |
| 1          | B            | 202        | ARG         | 2.4         |
| 1          | A            | 149        | VAL         | 2.4         |
| 1          | B            | 97         | PRO         | 2.4         |
| 1          | A            | 175        | LYS         | 2.4         |
| 1          | C            | 113        | LYS         | 2.4         |
| 1          | D            | 205        | ARG         | 2.4         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 77  | THR  | 2.4  |
| 1   | D     | 97  | PRO  | 2.4  |
| 1   | D     | 322 | GLU  | 2.3  |
| 1   | A     | 132 | ASP  | 2.3  |
| 1   | A     | 102 | ARG  | 2.3  |
| 1   | D     | 74  | GLU  | 2.3  |
| 1   | B     | 162 | ARG  | 2.2  |
| 1   | D     | 39  | ASP  | 2.2  |
| 1   | C     | 204 | GLY  | 2.2  |
| 1   | D     | 258 | GLU  | 2.2  |
| 1   | D     | 416 | ARG  | 2.2  |
| 1   | D     | 41  | LYS  | 2.2  |
| 1   | D     | 320 | PRO  | 2.2  |
| 1   | B     | 200 | ALA  | 2.2  |
| 1   | B     | 205 | ARG  | 2.2  |
| 1   | D     | 328 | ILE  | 2.1  |
| 1   | D     | 54  | GLY  | 2.1  |
| 1   | A     | 93  | LEU  | 2.1  |
| 1   | C     | 129 | TYR  | 2.1  |
| 1   | C     | 162 | ARG  | 2.1  |
| 1   | A     | 39  | ASP  | 2.1  |
| 1   | A     | 163 | ASP  | 2.1  |
| 1   | C     | 205 | ARG  | 2.1  |
| 1   | D     | 272 | VAL  | 2.1  |
| 1   | B     | 322 | GLU  | 2.1  |
| 1   | C     | 402 | ASP  | 2.1  |
| 1   | B     | 132 | ASP  | 2.0  |
| 1   | A     | 289 | PRO  | 2.0  |
| 1   | B     | 327 | ASN  | 2.0  |

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

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 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 1   | KCX  | B     | 146 | 12/13 | 0.89 | 0.12 | 24,28,38,38                 | 0     |
| 1   | KCX  | A     | 146 | 12/13 | 0.91 | 0.12 | 24,28,32,32                 | 0     |
| 1   | KCX  | D     | 146 | 12/13 | 0.91 | 0.14 | 24,31,41,46                 | 0     |
| 1   | KCX  | C     | 146 | 12/13 | 0.95 | 0.08 | 20,23,29,29                 | 0     |

### 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 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | FE   | D     | 455 | 1/1   | 0.95 | 0.06 | 44,44,44,44                 | 0     |
| 2   | FE   | C     | 455 | 1/1   | 0.98 | 0.03 | 36,36,36,36                 | 0     |
| 2   | FE   | B     | 454 | 1/1   | 0.99 | 0.03 | 37,37,37,37                 | 0     |
| 2   | FE   | B     | 455 | 1/1   | 0.99 | 0.03 | 35,35,35,35                 | 0     |
| 2   | FE   | C     | 454 | 1/1   | 0.99 | 0.02 | 32,32,32,32                 | 0     |
| 2   | FE   | A     | 454 | 1/1   | 0.99 | 0.03 | 35,35,35,35                 | 0     |
| 2   | FE   | D     | 454 | 1/1   | 0.99 | 0.03 | 43,43,43,43                 | 0     |
| 2   | FE   | A     | 455 | 1/1   | 0.99 | 0.06 | 34,34,34,34                 | 0     |

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

There are no such residues in this entry.