



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2019 – 10:45 PM EDT

PDB ID : 3MC2  
Title : Crystal Structure of the Murine Inhibitor of Carbonic Anhydrase  
Authors : Eckenroth, B.E.; Mason, A.B.; Everse, S.J.  
Deposited on : 2010-03-26  
Resolution : 2.40 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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.3.2  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

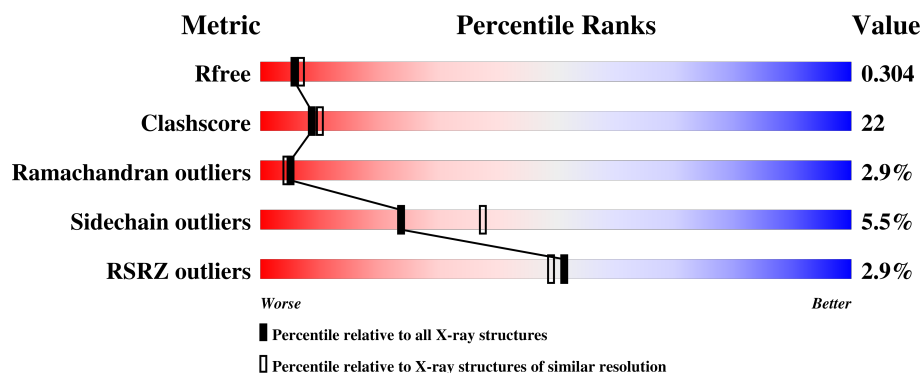
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 111664                      | 3481 (2.40-2.40)                                      |
| Clashscore            | 122126                      | 3956 (2.40-2.40)                                      |
| Ramachandran outliers | 120053                      | 3897 (2.40-2.40)                                      |
| Sidechain outliers    | 120020                      | 3898 (2.40-2.40)                                      |
| RSRZ outliers         | 108989                      | 3386 (2.40-2.40)                                      |

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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     | 687    | <div> <div>3%</div> <div>56%</div> <div>38%</div> <div>• •</div> </div> |
| 1   | B     | 687    | <div> <div>2%</div> <div>58%</div> <div>37%</div> <div>• •</div> </div> |
| 1   | C     | 687    | <div> <div>2%</div> <div>59%</div> <div>35%</div> <div>• •</div> </div> |
| 1   | D     | 687    | <div> <div>4%</div> <div>59%</div> <div>34%</div> <div>• •</div> </div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20772 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 Inhibitor of Carbonic Anhydrase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 675      | Total | C    | N   | O   | S  | 51      | 0       | 0     |
|     |       |          | 5193  | 3257 | 902 | 986 | 48 |         |         |       |
| 1   | B     | 675      | Total | C    | N   | O   | S  | 79      | 0       | 0     |
|     |       |          | 5193  | 3257 | 902 | 986 | 48 |         |         |       |
| 1   | C     | 675      | Total | C    | N   | O   | S  | 45      | 0       | 0     |
|     |       |          | 5193  | 3257 | 902 | 986 | 48 |         |         |       |
| 1   | D     | 675      | Total | C    | N   | O   | S  | 57      | 0       | 0     |
|     |       |          | 5193  | 3257 | 902 | 986 | 48 |         |         |       |

There are 32 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -5      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| A     | -4      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| A     | -3      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| A     | -2      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| A     | -1      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| A     | 0       | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| A     | 470     | ASP      | ASN    | ENGINEERED     | UNP Q9DBD0 |
| A     | 645     | ASP      | ASN    | ENGINEERED     | UNP Q9DBD0 |
| B     | -5      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| B     | -4      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| B     | -3      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| B     | -2      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| B     | -1      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| B     | 0       | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| B     | 470     | ASP      | ASN    | ENGINEERED     | UNP Q9DBD0 |
| B     | 645     | ASP      | ASN    | ENGINEERED     | UNP Q9DBD0 |
| C     | -5      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| C     | -4      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| C     | -3      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| C     | -2      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| C     | -1      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |

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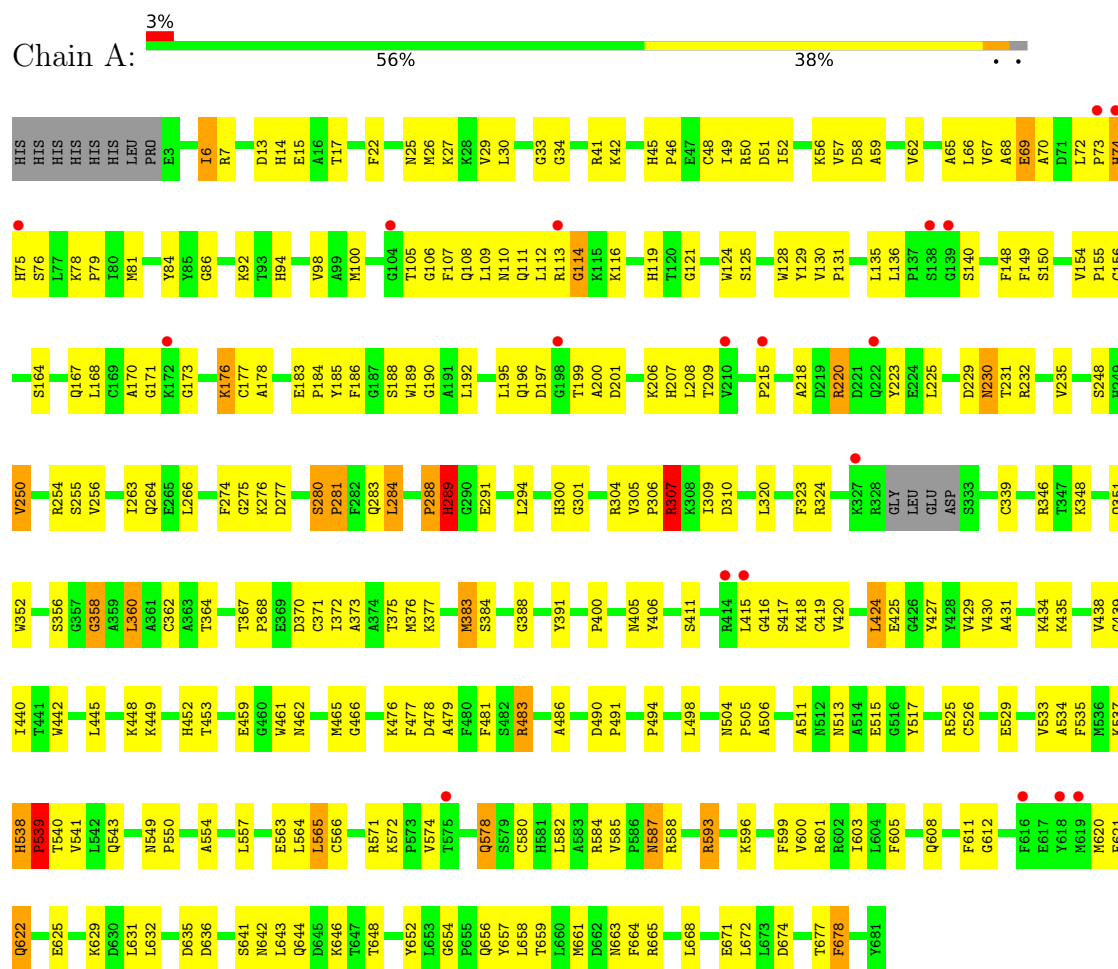
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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 0       | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| C     | 470     | ASP      | ASN    | ENGINEERED     | UNP Q9DBD0 |
| C     | 645     | ASP      | ASN    | ENGINEERED     | UNP Q9DBD0 |
| D     | -5      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| D     | -4      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| D     | -3      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| D     | -2      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| D     | -1      | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| D     | 0       | HIS      | -      | EXPRESSION TAG | UNP Q9DBD0 |
| D     | 470     | ASP      | ASN    | ENGINEERED     | UNP Q9DBD0 |
| D     | 645     | ASP      | ASN    | ENGINEERED     | UNP Q9DBD0 |

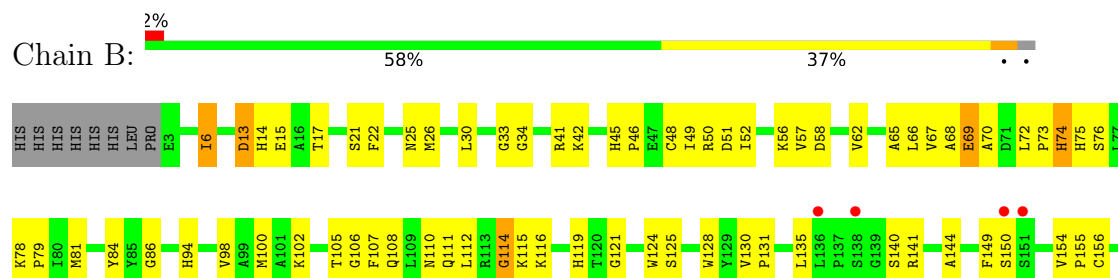
### 3 Residue-property plots

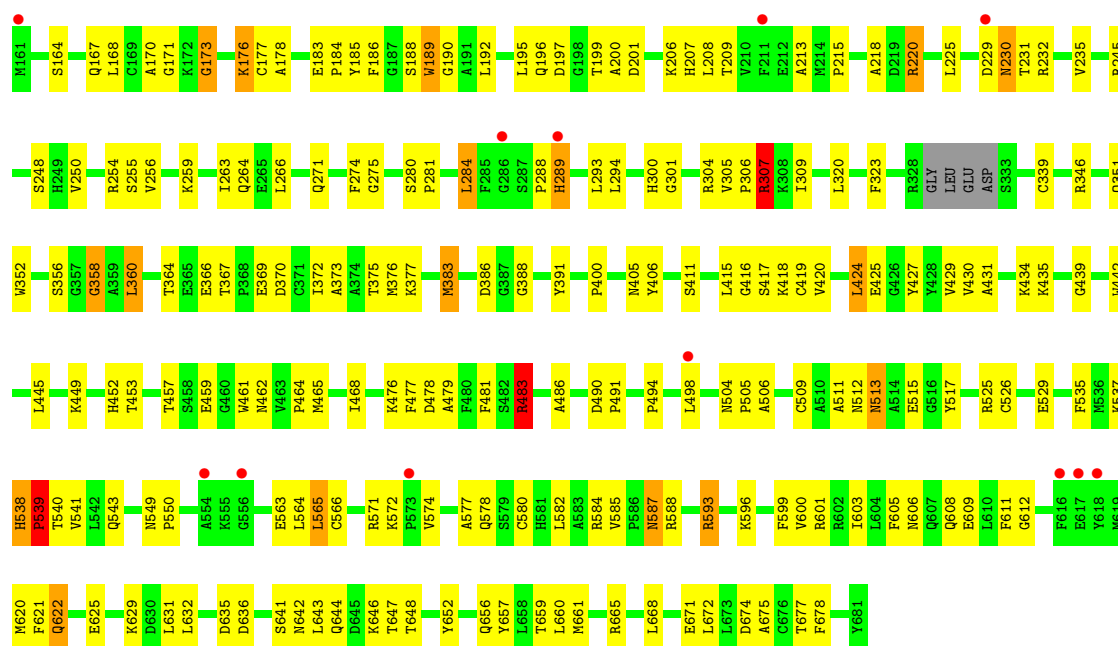
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Inhibitor of Carbonic Anhydrase

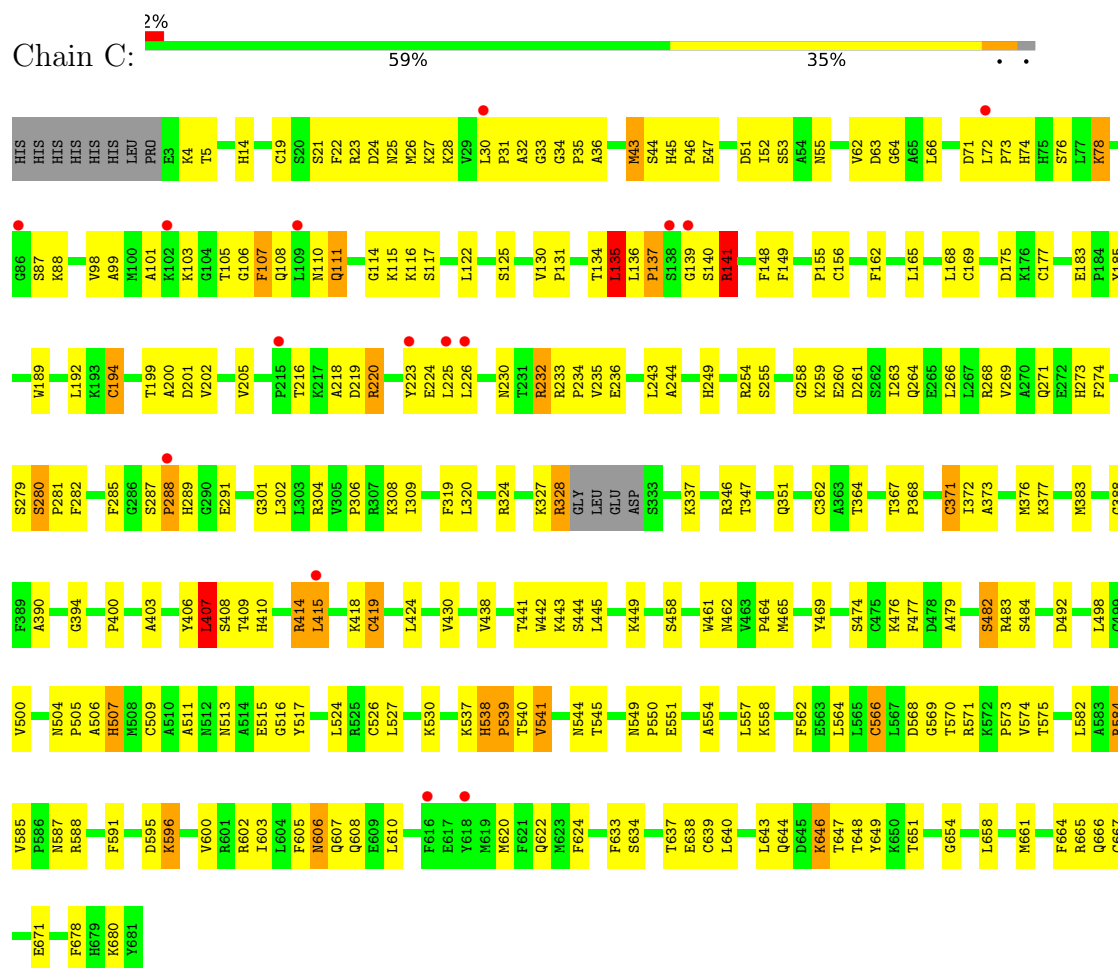


#### • Molecule 1: Inhibitor of Carbonic Anhydrase

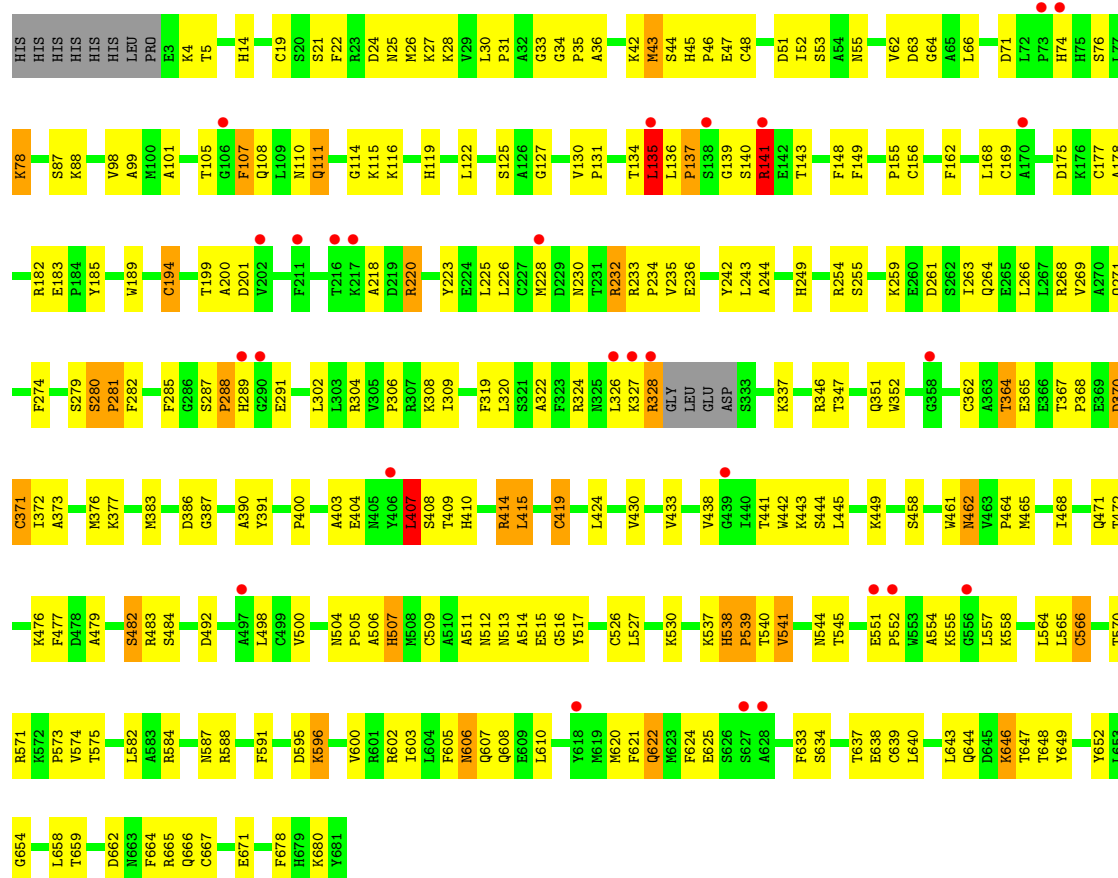




### • Molecule 1: Inhibitor of Carbonic Anhydrase



### • Molecule 1: Inhibitor of Carbonic Anhydrase



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 68.56Å 136.93Å 155.57Å<br>90.00° 90.11° 90.00°              | Depositor        |
| Resolution (Å)  | 19.00 – 2.40<br>18.95 – 2.40                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.2 (19.00-2.40)<br>93.9 (18.95-2.40)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.07  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.12 (at 2.41Å)   | Xtriage          |
| Refinement program  | CNS, REFMAC   | Depositor        |
| R, $R_{free}$   | 0.239 , 0.301<br>0.241 , 0.304                              | Depositor<br>DCC |
| $R_{free}$ test set   | 10093 reflections (9.56%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 52.1  | Xtriage          |
| Anisotropy  | 0.797   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 36.8   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$ | Xtriage          |
| Estimated twinning fraction   | 0.478 for h,-k,-l   | Xtriage          |
| Reported twinning fraction  | 0.500 for h,-k,-l   | Depositor        |
| Outliers  | 1 of 105600 reflections (0.001%)                            | Xtriage          |
| $F_o, F_c$ correlation  | 0.94  | EDS              |
| Total number of atoms   | 20772   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 75.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7286e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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     | 0.61         | 4/5312 (0.1%)   | 1.04        | 10/7179 (0.1%)  |
| 1   | B     | 0.58         | 4/5312 (0.1%)   | 0.99        | 8/7179 (0.1%)   |
| 1   | C     | 0.51         | 3/5312 (0.1%)   | 0.75        | 8/7179 (0.1%)   |
| 1   | D     | 0.47         | 3/5312 (0.1%)   | 0.73        | 7/7179 (0.1%)   |
| All | All   | 0.55         | 14/21248 (0.1%) | 0.89        | 33/28716 (0.1%) |

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

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

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | B     | 307 | ARG  | CZ-NH1 | -14.12 | 1.14        | 1.33     |
| 1   | A     | 307 | ARG  | CZ-NH1 | -13.47 | 1.15        | 1.33     |
| 1   | A     | 254 | ARG  | CZ-NH2 | -13.44 | 1.15        | 1.33     |
| 1   | B     | 307 | ARG  | CZ-NH2 | -12.93 | 1.16        | 1.33     |
| 1   | A     | 307 | ARG  | CZ-NH2 | -11.93 | 1.17        | 1.33     |
| 1   | A     | 254 | ARG  | CZ-NH1 | -11.89 | 1.17        | 1.33     |
| 1   | B     | 254 | ARG  | CZ-NH2 | -11.65 | 1.18        | 1.33     |
| 1   | B     | 254 | ARG  | CZ-NH1 | -11.44 | 1.18        | 1.33     |
| 1   | C     | 141 | ARG  | CZ-NH1 | -8.94  | 1.21        | 1.33     |
| 1   | C     | 141 | ARG  | CZ-NH2 | -8.81  | 1.21        | 1.33     |
| 1   | D     | 141 | ARG  | CZ-NH2 | -8.73  | 1.21        | 1.33     |
| 1   | C     | 232 | ARG  | CD-NE  | -6.82  | 1.34        | 1.46     |
| 1   | D     | 141 | ARG  | CZ-NH1 | -6.81  | 1.24        | 1.33     |
| 1   | D     | 232 | ARG  | CD-NE  | -6.76  | 1.34        | 1.46     |

All (33) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 307 | ARG  | NE-CZ-NH2  | 34.14  | 137.37      | 120.30   |
| 1   | B     | 254 | ARG  | NE-CZ-NH1  | 31.73  | 136.16      | 120.30   |
| 1   | B     | 307 | ARG  | NE-CZ-NH1  | 29.80  | 135.20      | 120.30   |
| 1   | A     | 254 | ARG  | NE-CZ-NH2  | 29.11  | 134.85      | 120.30   |
| 1   | B     | 307 | ARG  | NH1-CZ-NH2 | -23.68 | 93.36       | 119.40   |
| 1   | A     | 254 | ARG  | NH1-CZ-NH2 | -23.34 | 93.73       | 119.40   |
| 1   | B     | 254 | ARG  | NH1-CZ-NH2 | -22.94 | 94.17       | 119.40   |
| 1   | A     | 307 | ARG  | NH1-CZ-NH2 | -22.63 | 94.51       | 119.40   |
| 1   | B     | 307 | ARG  | NE-CZ-NH2  | 22.27  | 131.44      | 120.30   |
| 1   | A     | 254 | ARG  | NE-CZ-NH1  | 20.22  | 130.41      | 120.30   |
| 1   | D     | 141 | ARG  | NE-CZ-NH1  | 18.41  | 129.51      | 120.30   |
| 1   | B     | 254 | ARG  | NE-CZ-NH2  | 18.33  | 129.46      | 120.30   |
| 1   | A     | 601 | ARG  | NE-CZ-NH2  | -18.13 | 111.23      | 120.30   |
| 1   | A     | 601 | ARG  | NE-CZ-NH1  | 16.09  | 128.34      | 120.30   |
| 1   | C     | 141 | ARG  | NE-CZ-NH1  | 15.79  | 128.19      | 120.30   |
| 1   | C     | 141 | ARG  | NE-CZ-NH2  | 15.62  | 128.11      | 120.30   |
| 1   | A     | 307 | ARG  | NE-CZ-NH1  | 15.38  | 127.99      | 120.30   |
| 1   | D     | 141 | ARG  | NH1-CZ-NH2 | -14.87 | 103.05      | 119.40   |
| 1   | C     | 141 | ARG  | NH1-CZ-NH2 | -14.36 | 103.61      | 119.40   |
| 1   | D     | 141 | ARG  | NE-CZ-NH2  | 14.03  | 127.31      | 120.30   |
| 1   | A     | 304 | ARG  | NE-CZ-NH1  | 13.79  | 127.19      | 120.30   |
| 1   | C     | 602 | ARG  | NE-CZ-NH1  | 12.28  | 126.44      | 120.30   |
| 1   | D     | 602 | ARG  | NE-CZ-NH2  | 10.15  | 125.38      | 120.30   |
| 1   | C     | 602 | ARG  | NE-CZ-NH2  | -9.95  | 115.33      | 120.30   |
| 1   | A     | 304 | ARG  | NE-CZ-NH2  | -9.89  | 115.36      | 120.30   |
| 1   | C     | 232 | ARG  | NE-CZ-NH1  | 9.21   | 124.91      | 120.30   |
| 1   | B     | 304 | ARG  | NE-CZ-NH2  | 9.18   | 124.89      | 120.30   |
| 1   | D     | 602 | ARG  | NE-CZ-NH1  | -8.31  | 116.15      | 120.30   |
| 1   | D     | 232 | ARG  | NE-CZ-NH2  | 8.16   | 124.38      | 120.30   |
| 1   | C     | 602 | ARG  | CD-NE-CZ   | 5.91   | 131.87      | 123.60   |
| 1   | B     | 601 | ARG  | NE-CZ-NH1  | -5.63  | 117.49      | 120.30   |
| 1   | D     | 602 | ARG  | CD-NE-CZ   | 5.43   | 131.20      | 123.60   |
| 1   | C     | 232 | ARG  | NE-CZ-NH2  | -5.18  | 117.71      | 120.30   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 652 | TYR  | Sidechain |
| 1   | B     | 652 | TYR  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5193  | 0        | 5024     | 224     | 0            |
| 1   | B     | 5193  | 0        | 5024     | 210     | 0            |
| 1   | C     | 5193  | 0        | 5024     | 233     | 0            |
| 1   | D     | 5193  | 0        | 5024     | 222     | 0            |
| All | All   | 20772 | 0        | 20096    | 884     | 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 22.

All (884) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:414:ARG:HG2  | 1:C:415:LEU:H    | 1.21                     | 1.05              |
| 1:D:414:ARG:HG2  | 1:D:415:LEU:H    | 1.21                     | 1.03              |
| 1:C:558:LYS:HB3  | 1:C:558:LYS:HZ2  | 1.22                     | 1.02              |
| 1:D:558:LYS:HZ2  | 1:D:558:LYS:HB3  | 1.22                     | 1.00              |
| 1:A:572:LYS:HE2  | 1:A:580:CYS:HB2  | 1.43                     | 0.99              |
| 1:B:587:ASN:N    | 1:B:587:ASN:HD22 | 1.57                     | 0.98              |
| 1:C:218:ALA:HA   | 1:C:220:ARG:HE   | 1.27                     | 0.96              |
| 1:D:218:ALA:HA   | 1:D:220:ARG:HE   | 1.30                     | 0.96              |
| 1:A:587:ASN:HD22 | 1:A:587:ASN:N    | 1.59                     | 0.96              |
| 1:B:572:LYS:HE2  | 1:B:580:CYS:HB2  | 1.46                     | 0.95              |
| 1:B:112:LEU:HA   | 1:B:115:LYS:HE2  | 1.50                     | 0.94              |
| 1:B:587:ASN:H    | 1:B:587:ASN:ND2  | 1.59                     | 0.93              |
| 1:A:587:ASN:ND2  | 1:A:587:ASN:H    | 1.61                     | 0.92              |
| 1:C:371:CYS:HB3  | 1:C:383:MET:SD   | 2.12                     | 0.90              |
| 1:C:108:GLN:NE2  | 1:C:232:ARG:HG3  | 1.90                     | 0.86              |
| 1:D:220:ARG:HD3  | 1:D:220:ARG:H    | 1.40                     | 0.85              |
| 1:A:416:GLY:C    | 1:A:418:LYS:H    | 1.79                     | 0.85              |
| 1:C:220:ARG:H    | 1:C:220:ARG:HD3  | 1.39                     | 0.85              |
| 1:D:371:CYS:HB3  | 1:D:383:MET:SD   | 2.17                     | 0.85              |
| 1:B:416:GLY:C    | 1:B:418:LYS:H    | 1.80                     | 0.85              |
| 1:C:441:THR:HG22 | 1:C:444:SER:OG   | 1.77                     | 0.84              |
| 1:A:587:ASN:H    | 1:A:587:ASN:HD22 | 0.88                     | 0.84              |
| 1:C:337:LYS:HB2  | 1:C:337:LYS:NZ   | 1.92                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:400:PRO:HD2  | 1:D:647:THR:O    | 1.79                     | 0.83              |
| 1:A:564:LEU:HG   | 1:A:574:VAL:HA   | 1.61                     | 0.82              |
| 1:B:587:ASN:H    | 1:B:587:ASN:HD22 | 0.84                     | 0.81              |
| 1:D:558:LYS:HB3  | 1:D:558:LYS:NZ   | 1.96                     | 0.81              |
| 1:D:337:LYS:HB2  | 1:D:337:LYS:NZ   | 1.95                     | 0.80              |
| 1:C:558:LYS:HB3  | 1:C:558:LYS:NZ   | 1.97                     | 0.80              |
| 1:C:400:PRO:HD2  | 1:C:647:THR:O    | 1.82                     | 0.79              |
| 1:A:442:TRP:HA   | 1:A:445:LEU:HD11 | 1.65                     | 0.78              |
| 1:B:564:LEU:HG   | 1:B:574:VAL:HA   | 1.65                     | 0.78              |
| 1:C:108:GLN:HE22 | 1:C:232:ARG:HG3  | 1.48                     | 0.78              |
| 1:D:441:THR:H    | 1:D:444:SER:HB2  | 1.49                     | 0.78              |
| 1:C:103:LYS:HA   | 1:C:224:GLU:HG2  | 1.64                     | 0.77              |
| 1:B:442:TRP:HA   | 1:B:445:LEU:HD11 | 1.67                     | 0.77              |
| 1:D:541:VAL:CG1  | 1:D:574:VAL:HG21 | 2.14                     | 0.77              |
| 1:A:644:GLN:HE21 | 1:A:644:GLN:HA   | 1.50                     | 0.77              |
| 1:B:406:TYR:OH   | 1:B:588:ARG:HG3  | 1.85                     | 0.76              |
| 1:B:656:GLN:O    | 1:B:659:THR:HG22 | 1.84                     | 0.76              |
| 1:C:14:HIS:ND1   | 1:C:289:HIS:HB3  | 2.00                     | 0.76              |
| 1:B:70:ALA:HB1   | 1:B:75:HIS:O     | 1.87                     | 0.75              |
| 1:C:5:THR:HG23   | 1:C:36:ALA:HB3   | 1.68                     | 0.75              |
| 1:A:171:GLY:HA3  | 1:A:176:LYS:HA   | 1.69                     | 0.75              |
| 1:C:216:THR:OG1  | 1:C:219:ASP:HB2  | 1.87                     | 0.74              |
| 1:D:14:HIS:ND1   | 1:D:289:HIS:HB3  | 2.01                     | 0.74              |
| 1:A:665:ARG:HA   | 1:A:668:LEU:HD12 | 1.69                     | 0.74              |
| 1:A:70:ALA:HB1   | 1:A:75:HIS:O     | 1.88                     | 0.74              |
| 1:B:644:GLN:HA   | 1:B:644:GLN:HE21 | 1.51                     | 0.74              |
| 1:C:441:THR:H    | 1:C:444:SER:HB2  | 1.53                     | 0.74              |
| 1:D:441:THR:HG22 | 1:D:444:SER:OG   | 1.86                     | 0.74              |
| 1:D:108:GLN:HB2  | 1:D:111:GLN:HE22 | 1.53                     | 0.74              |
| 1:C:541:VAL:CG1  | 1:C:574:VAL:HG21 | 2.18                     | 0.73              |
| 1:C:108:GLN:HB2  | 1:C:111:GLN:HE22 | 1.53                     | 0.73              |
| 1:A:280:SER:OG   | 1:A:281:PRO:HD3  | 1.88                     | 0.73              |
| 1:B:171:GLY:HA3  | 1:B:176:LYS:HA   | 1.71                     | 0.73              |
| 1:C:328:ARG:HE   | 1:C:328:ARG:C    | 1.91                     | 0.73              |
| 1:A:110:ASN:CG   | 1:A:230:ASN:HD21 | 1.92                     | 0.73              |
| 1:C:259:LYS:O    | 1:C:263:ILE:HG13 | 1.89                     | 0.72              |
| 1:A:27:LYS:NZ    | 1:D:659:THR:HG23 | 2.03                     | 0.72              |
| 1:B:110:ASN:CG   | 1:B:230:ASN:HD21 | 1.93                     | 0.72              |
| 1:D:328:ARG:HE   | 1:D:328:ARG:C    | 1.91                     | 0.72              |
| 1:A:656:GLN:O    | 1:A:659:THR:HG22 | 1.88                     | 0.72              |
| 1:B:30:LEU:HD11  | 1:B:33:GLY:O     | 1.88                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:30:LEU:HD11  | 1:A:33:GLY:O     | 1.88                     | 0.72              |
| 1:B:372:ILE:O    | 1:B:376:MET:HG3  | 1.90                     | 0.72              |
| 1:D:88:LYS:HA    | 1:D:88:LYS:HE3   | 1.72                     | 0.72              |
| 1:C:279:SER:OG   | 1:C:281:PRO:HD2  | 1.88                     | 0.72              |
| 1:D:367:THR:HG22 | 1:D:511:ALA:HB3  | 1.72                     | 0.72              |
| 1:D:368:PRO:O    | 1:D:372:ILE:HG13 | 1.89                     | 0.72              |
| 1:D:43:MET:HB2   | 1:D:47:GLU:OE1   | 1.88                     | 0.72              |
| 1:C:414:ARG:HG2  | 1:C:415:LEU:N    | 2.03                     | 0.71              |
| 1:B:72:LEU:HB3   | 1:B:73:PRO:HD2   | 1.73                     | 0.71              |
| 1:A:168:LEU:HD23 | 1:A:200:ALA:HB2  | 1.73                     | 0.71              |
| 1:D:654:GLY:O    | 1:D:658:LEU:HB2  | 1.90                     | 0.71              |
| 1:A:406:TYR:OH   | 1:A:588:ARG:HG3  | 1.91                     | 0.70              |
| 1:D:337:LYS:HB2  | 1:D:337:LYS:HZ2  | 1.56                     | 0.70              |
| 1:A:307:ARG:HG3  | 1:A:671:GLU:OE2  | 1.90                     | 0.70              |
| 1:C:88:LYS:HE3   | 1:C:88:LYS:HA    | 1.74                     | 0.70              |
| 1:D:414:ARG:HG2  | 1:D:415:LEU:N    | 2.03                     | 0.70              |
| 1:C:654:GLY:O    | 1:C:658:LEU:HB2  | 1.91                     | 0.70              |
| 1:D:110:ASN:HB2  | 1:D:230:ASN:HD21 | 1.56                     | 0.70              |
| 1:B:427:TYR:HB2  | 1:B:538:HIS:HB2  | 1.72                     | 0.70              |
| 1:A:72:LEU:HB3   | 1:A:73:PRO:HD2   | 1.74                     | 0.70              |
| 1:B:307:ARG:HG3  | 1:B:671:GLU:OE2  | 1.91                     | 0.70              |
| 1:D:279:SER:OG   | 1:D:281:PRO:HD2  | 1.91                     | 0.70              |
| 1:B:74:HIS:O     | 1:B:74:HIS:ND1   | 2.25                     | 0.69              |
| 1:C:110:ASN:HB2  | 1:C:230:ASN:HD21 | 1.57                     | 0.69              |
| 1:B:665:ARG:HA   | 1:B:668:LEU:HD12 | 1.74                     | 0.69              |
| 1:B:405:ASN:OD1  | 1:B:424:LEU:HB2  | 1.92                     | 0.69              |
| 1:A:605:PHE:HZ   | 1:A:642:ASN:OD1  | 1.75                     | 0.69              |
| 1:B:168:LEU:HD23 | 1:B:200:ALA:HB2  | 1.75                     | 0.69              |
| 1:B:352:TRP:CE2  | 1:B:360:LEU:HD22 | 2.28                     | 0.69              |
| 1:C:407:LEU:HD21 | 1:C:410:HIS:HB2  | 1.75                     | 0.69              |
| 1:B:105:THR:HB   | 1:B:107:PHE:CE2  | 2.27                     | 0.69              |
| 1:A:105:THR:HB   | 1:A:107:PHE:CE2  | 2.28                     | 0.69              |
| 1:D:5:THR:HG23   | 1:D:36:ALA:HB3   | 1.74                     | 0.69              |
| 1:A:440:ILE:HA   | 1:A:448:LYS:HE2  | 1.75                     | 0.68              |
| 1:A:427:TYR:HB2  | 1:A:538:HIS:HB2  | 1.73                     | 0.68              |
| 1:B:644:GLN:HA   | 1:B:644:GLN:NE2  | 2.08                     | 0.68              |
| 1:C:19:CYS:O     | 1:C:22:PHE:HB3   | 1.93                     | 0.68              |
| 1:A:405:ASN:OD1  | 1:A:424:LEU:HB2  | 1.93                     | 0.68              |
| 1:B:425:GLU:O    | 1:B:584:ARG:HD3  | 1.93                     | 0.68              |
| 1:A:277:ASP:HA   | 1:A:283:GLN:HE22 | 1.59                     | 0.68              |
| 1:A:459:GLU:HG3  | 1:A:537:LYS:HB3  | 1.74                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:611:PHE:CD2  | 1:B:621:PHE:HB3  | 2.28                     | 0.68              |
| 1:C:98:VAL:HB    | 1:C:225:LEU:HD11 | 1.76                     | 0.68              |
| 1:A:178:ALA:H    | 1:A:183:GLU:HB2  | 1.59                     | 0.67              |
| 1:B:605:PHE:HZ   | 1:B:642:ASN:OD1  | 1.76                     | 0.67              |
| 1:C:368:PRO:O    | 1:C:372:ILE:HG13 | 1.94                     | 0.67              |
| 1:D:98:VAL:HB    | 1:D:225:LEU:HD11 | 1.77                     | 0.67              |
| 1:A:644:GLN:NE2  | 1:A:644:GLN:HA   | 2.09                     | 0.67              |
| 1:C:224:GLU:HG3  | 1:C:232:ARG:HH21 | 1.58                     | 0.67              |
| 1:D:4:LYS:O      | 1:D:35:PRO:HA    | 1.94                     | 0.67              |
| 1:A:372:ILE:O    | 1:A:376:MET:HG3  | 1.95                     | 0.67              |
| 1:C:271:GLN:NE2  | 1:C:302:LEU:H    | 1.93                     | 0.67              |
| 1:C:458:SER:HA   | 1:C:462:ASN:HB2  | 1.76                     | 0.66              |
| 1:B:351:GLN:HE21 | 1:B:621:PHE:HE1  | 1.43                     | 0.66              |
| 1:C:500:VAL:CG1  | 1:C:516:GLY:HA3  | 2.25                     | 0.66              |
| 1:B:73:PRO:O     | 1:B:74:HIS:HB3   | 1.96                     | 0.66              |
| 1:D:259:LYS:O    | 1:D:263:ILE:HG13 | 1.95                     | 0.66              |
| 1:A:70:ALA:HA    | 1:A:75:HIS:HB3   | 1.76                     | 0.66              |
| 1:A:351:GLN:HE21 | 1:A:621:PHE:HE1  | 1.43                     | 0.66              |
| 1:B:459:GLU:HG3  | 1:B:537:LYS:HB3  | 1.77                     | 0.66              |
| 1:C:4:LYS:O      | 1:C:35:PRO:HA    | 1.95                     | 0.66              |
| 1:D:407:LEU:HD21 | 1:D:410:HIS:HB2  | 1.77                     | 0.66              |
| 1:B:70:ALA:HA    | 1:B:75:HIS:HB3   | 1.76                     | 0.66              |
| 1:D:134:THR:HG22 | 1:D:134:THR:O    | 1.96                     | 0.66              |
| 1:C:271:GLN:HE22 | 1:C:302:LEU:H    | 1.41                     | 0.65              |
| 1:B:178:ALA:H    | 1:B:183:GLU:HB2  | 1.61                     | 0.65              |
| 1:B:306:PRO:HD3  | 1:B:678:PHE:CD1  | 2.31                     | 0.65              |
| 1:C:108:GLN:CD   | 1:C:232:ARG:HG3  | 2.16                     | 0.65              |
| 1:A:425:GLU:O    | 1:A:584:ARG:HD3  | 1.96                     | 0.65              |
| 1:C:43:MET:HB2   | 1:C:47:GLU:OE1   | 1.96                     | 0.65              |
| 1:B:41:ARG:HG3   | 1:B:42:LYS:N     | 2.11                     | 0.65              |
| 1:C:122:LEU:HB3  | 1:C:156:CYS:HB2  | 1.78                     | 0.65              |
| 1:A:352:TRP:CE2  | 1:A:360:LEU:HD22 | 2.32                     | 0.65              |
| 1:B:70:ALA:CB    | 1:B:75:HIS:O     | 2.45                     | 0.65              |
| 1:C:306:PRO:HG2  | 1:C:309:ILE:CG2  | 2.26                     | 0.65              |
| 1:C:367:THR:HG22 | 1:C:511:ALA:HB3  | 1.79                     | 0.65              |
| 1:C:418:LYS:NZ   | 1:C:418:LYS:HB3  | 2.11                     | 0.65              |
| 1:A:416:GLY:C    | 1:A:418:LYS:N    | 2.48                     | 0.64              |
| 1:A:622:GLN:HB3  | 1:A:625:GLU:HB3  | 1.78                     | 0.64              |
| 1:B:416:GLY:C    | 1:B:418:LYS:N    | 2.48                     | 0.64              |
| 1:B:45:HIS:ND1   | 1:B:62:VAL:HG12  | 2.12                     | 0.64              |
| 1:A:611:PHE:CD2  | 1:A:621:PHE:HB3  | 2.31                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:306:PRO:O    | 1:D:309:ILE:HG22 | 1.97                     | 0.64              |
| 1:D:458:SER:HA   | 1:D:462:ASN:HB2  | 1.79                     | 0.64              |
| 1:A:306:PRO:HD3  | 1:A:678:PHE:CD1  | 2.32                     | 0.64              |
| 1:B:622:GLN:HB3  | 1:B:625:GLU:HB3  | 1.78                     | 0.64              |
| 1:A:400:PRO:HB2  | 1:A:643:LEU:CD1  | 2.28                     | 0.64              |
| 1:A:74:HIS:O     | 1:A:74:HIS:ND1   | 2.30                     | 0.64              |
| 1:D:271:GLN:NE2  | 1:D:302:LEU:H    | 1.96                     | 0.64              |
| 1:D:111:GLN:NE2  | 1:D:111:GLN:H    | 1.96                     | 0.63              |
| 1:A:70:ALA:CB    | 1:A:75:HIS:O     | 2.46                     | 0.63              |
| 1:C:415:LEU:HD11 | 1:C:419:CYS:HB2  | 1.79                     | 0.63              |
| 1:C:337:LYS:HZ2  | 1:C:337:LYS:HB2  | 1.63                     | 0.63              |
| 1:B:442:TRP:HB2  | 1:B:565:LEU:HD22 | 1.80                     | 0.63              |
| 1:D:19:CYS:O     | 1:D:22:PHE:HB3   | 1.98                     | 0.63              |
| 1:D:271:GLN:HE22 | 1:D:302:LEU:H    | 1.45                     | 0.63              |
| 1:B:400:PRO:HB2  | 1:B:643:LEU:CD1  | 2.29                     | 0.63              |
| 1:A:73:PRO:O     | 1:A:74:HIS:HB3   | 1.99                     | 0.63              |
| 1:B:611:PHE:HB3  | 1:B:621:PHE:O    | 1.98                     | 0.63              |
| 1:C:407:LEU:HD11 | 1:C:410:HIS:HA   | 1.79                     | 0.63              |
| 1:A:65:ALA:HB2   | 1:A:125:SER:HB3  | 1.79                     | 0.62              |
| 1:D:122:LEU:HB3  | 1:D:156:CYS:HB2  | 1.81                     | 0.62              |
| 1:C:134:THR:HG22 | 1:C:134:THR:O    | 1.99                     | 0.62              |
| 1:C:108:GLN:H    | 1:C:111:GLN:NE2  | 1.97                     | 0.62              |
| 1:A:665:ARG:HH21 | 1:A:677:THR:HG21 | 1.65                     | 0.62              |
| 1:C:106:GLY:HA2  | 1:C:232:ARG:NH1  | 2.15                     | 0.62              |
| 1:C:409:THR:O    | 1:C:410:HIS:HB3  | 2.00                     | 0.62              |
| 1:A:416:GLY:O    | 1:A:418:LYS:N    | 2.33                     | 0.61              |
| 1:A:442:TRP:HB2  | 1:A:565:LEU:HD22 | 1.81                     | 0.61              |
| 1:B:599:PHE:O    | 1:B:603:ILE:HG12 | 2.01                     | 0.61              |
| 1:D:500:VAL:CG1  | 1:D:516:GLY:HA3  | 2.29                     | 0.61              |
| 1:A:596:LYS:O    | 1:A:600:VAL:HG23 | 2.00                     | 0.61              |
| 1:B:186:PHE:H    | 1:B:190:GLY:HA3  | 1.63                     | 0.61              |
| 1:A:629:LYS:HD3  | 1:A:635:ASP:OD1  | 2.01                     | 0.61              |
| 1:A:30:LEU:HG    | 1:A:34:GLY:HA3   | 1.82                     | 0.61              |
| 1:D:407:LEU:HD11 | 1:D:410:HIS:HA   | 1.82                     | 0.61              |
| 1:B:517:TYR:CG   | 1:B:526:CYS:HB2  | 2.35                     | 0.61              |
| 1:B:30:LEU:HG    | 1:B:34:GLY:HA3   | 1.82                     | 0.60              |
| 1:C:45:HIS:ND1   | 1:C:62:VAL:HG12  | 2.16                     | 0.60              |
| 1:A:207:HIS:CE1  | 1:A:208:LEU:HG   | 2.36                     | 0.60              |
| 1:C:218:ALA:HA   | 1:C:220:ARG:NE   | 2.09                     | 0.60              |
| 1:C:573:PRO:HB2  | 1:C:575:THR:HG22 | 1.83                     | 0.60              |
| 1:D:306:PRO:HG2  | 1:D:309:ILE:CG2  | 2.31                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:188:SER:OG   | 1:A:206:LYS:HG2  | 2.01                     | 0.60              |
| 1:B:173:GLY:O    | 1:B:176:LYS:HG2  | 2.01                     | 0.60              |
| 1:A:27:LYS:HZ3   | 1:D:659:THR:HG23 | 1.66                     | 0.60              |
| 1:B:367:THR:HG22 | 1:B:511:ALA:HB3  | 1.83                     | 0.60              |
| 1:A:51:ASP:HB3   | 1:A:56:LYS:HB2   | 1.84                     | 0.60              |
| 1:A:170:ALA:O    | 1:A:184:PRO:HG2  | 2.02                     | 0.60              |
| 1:A:504:ASN:HB2  | 1:A:505:PRO:HD2  | 1.84                     | 0.60              |
| 1:B:505:PRO:O    | 1:B:506:ALA:HB3  | 2.02                     | 0.60              |
| 1:B:168:LEU:HG   | 1:B:199:THR:HG22 | 1.83                     | 0.60              |
| 1:B:416:GLY:O    | 1:B:418:LYS:N    | 2.35                     | 0.60              |
| 1:D:605:PHE:O    | 1:D:608:GLN:HG2  | 2.02                     | 0.60              |
| 1:A:611:PHE:HB3  | 1:A:621:PHE:O    | 2.02                     | 0.60              |
| 1:A:186:PHE:H    | 1:A:190:GLY:HA3  | 1.66                     | 0.59              |
| 1:A:663:ASN:HB3  | 1:C:23:ARG:NH1   | 2.17                     | 0.59              |
| 1:D:573:PRO:HB2  | 1:D:575:THR:HG22 | 1.83                     | 0.59              |
| 1:A:45:HIS:ND1   | 1:A:62:VAL:HG12  | 2.16                     | 0.59              |
| 1:B:188:SER:OG   | 1:B:206:LYS:HG2  | 2.01                     | 0.59              |
| 1:D:45:HIS:ND1   | 1:D:62:VAL:HG12  | 2.17                     | 0.59              |
| 1:C:21:SER:O     | 1:C:25:ASN:ND2   | 2.35                     | 0.59              |
| 1:A:41:ARG:HG3   | 1:A:42:LYS:N     | 2.17                     | 0.59              |
| 1:D:409:THR:O    | 1:D:410:HIS:HB3  | 2.02                     | 0.59              |
| 1:D:449:LYS:HE3  | 1:D:483:ARG:HH21 | 1.66                     | 0.59              |
| 1:B:65:ALA:HB2   | 1:B:125:SER:HB3  | 1.84                     | 0.59              |
| 1:B:207:HIS:CE1  | 1:B:208:LEU:HG   | 2.38                     | 0.59              |
| 1:B:587:ASN:N    | 1:B:587:ASN:ND2  | 2.32                     | 0.59              |
| 1:C:44:SER:HB2   | 1:C:46:PRO:HD2   | 1.83                     | 0.59              |
| 1:C:605:PHE:O    | 1:C:608:GLN:HG2  | 2.03                     | 0.59              |
| 1:A:517:TYR:CG   | 1:A:526:CYS:HB2  | 2.37                     | 0.59              |
| 1:D:108:GLN:H    | 1:D:111:GLN:NE2  | 2.00                     | 0.59              |
| 1:A:674:ASP:HA   | 1:A:677:THR:OG1  | 2.03                     | 0.59              |
| 1:B:596:LYS:O    | 1:B:600:VAL:HG23 | 2.02                     | 0.59              |
| 1:C:111:GLN:NE2  | 1:C:111:GLN:H    | 2.00                     | 0.59              |
| 1:D:449:LYS:HE3  | 1:D:483:ARG:NH2  | 2.18                     | 0.59              |
| 1:A:116:LYS:HB3  | 1:A:200:ALA:HA   | 1.84                     | 0.58              |
| 1:B:665:ARG:HH21 | 1:B:677:THR:HG21 | 1.68                     | 0.58              |
| 1:B:79:PRO:O     | 1:B:305:VAL:HG21 | 2.02                     | 0.58              |
| 1:C:443:LYS:NZ   | 1:C:443:LYS:HB3  | 2.18                     | 0.58              |
| 1:C:527:LEU:HD23 | 1:C:527:LEU:O    | 2.03                     | 0.58              |
| 1:C:634:SER:HB2  | 1:C:637:THR:OG1  | 2.03                     | 0.58              |
| 1:A:427:TYR:CE1  | 1:A:587:ASN:HA   | 2.39                     | 0.58              |
| 1:B:170:ALA:O    | 1:B:184:PRO:HG2  | 2.04                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:634:SER:HB2  | 1:D:637:THR:OG1  | 2.02                     | 0.58              |
| 1:B:48:CYS:O     | 1:B:52:ILE:HG13  | 2.04                     | 0.58              |
| 1:C:484:SER:HA   | 1:C:498:LEU:HD12 | 1.86                     | 0.58              |
| 1:A:352:TRP:HB2  | 1:A:621:PHE:CZ   | 2.39                     | 0.58              |
| 1:D:606:ASN:N    | 1:D:606:ASN:HD22 | 2.02                     | 0.58              |
| 1:C:504:ASN:HB3  | 1:C:507:HIS:CG   | 2.38                     | 0.58              |
| 1:D:44:SER:HB2   | 1:D:46:PRO:HD2   | 1.85                     | 0.58              |
| 1:D:606:ASN:N    | 1:D:606:ASN:ND2  | 2.51                     | 0.58              |
| 1:A:136:LEU:H    | 1:A:136:LEU:HD23 | 1.69                     | 0.57              |
| 1:B:504:ASN:HB2  | 1:B:505:PRO:HD2  | 1.86                     | 0.57              |
| 1:C:268:ARG:HE   | 1:C:269:VAL:CG1  | 2.16                     | 0.57              |
| 1:D:21:SER:O     | 1:D:25:ASN:ND2   | 2.37                     | 0.57              |
| 1:D:415:LEU:HD11 | 1:D:419:CYS:HB2  | 1.86                     | 0.57              |
| 1:C:337:LYS:HB2  | 1:C:337:LYS:HZ3  | 1.70                     | 0.57              |
| 1:A:427:TYR:HE1  | 1:A:587:ASN:HA   | 1.69                     | 0.57              |
| 1:A:48:CYS:O     | 1:A:52:ILE:HG13  | 2.04                     | 0.57              |
| 1:D:596:LYS:O    | 1:D:600:VAL:HG23 | 2.05                     | 0.57              |
| 1:A:461:TRP:O    | 1:A:465:MET:HB2  | 2.04                     | 0.57              |
| 1:C:596:LYS:NZ   | 1:C:596:LYS:HB2  | 2.18                     | 0.57              |
| 1:C:596:LYS:O    | 1:C:600:VAL:HG23 | 2.04                     | 0.57              |
| 1:A:599:PHE:O    | 1:A:603:ILE:HG12 | 2.05                     | 0.57              |
| 1:B:116:LYS:HB3  | 1:B:200:ALA:HA   | 1.86                     | 0.57              |
| 1:C:346:ARG:HH21 | 1:C:364:THR:HG22 | 1.69                     | 0.57              |
| 1:D:105:THR:HB   | 1:D:107:PHE:CE1  | 2.40                     | 0.57              |
| 1:D:430:VAL:HA   | 1:D:582:LEU:HD13 | 1.87                     | 0.57              |
| 1:A:108:GLN:H    | 1:A:111:GLN:HB2  | 1.70                     | 0.57              |
| 1:B:465:MET:HE2  | 1:B:465:MET:HA   | 1.86                     | 0.57              |
| 1:B:405:ASN:HB2  | 1:B:641:SER:OG   | 2.05                     | 0.57              |
| 1:A:665:ARG:NH2  | 1:A:677:THR:HG21 | 2.20                     | 0.57              |
| 1:B:57:VAL:HG12  | 1:B:58:ASP:H     | 1.70                     | 0.57              |
| 1:D:346:ARG:HH21 | 1:D:364:THR:HG22 | 1.69                     | 0.57              |
| 1:A:320:LEU:HA   | 1:A:323:PHE:HB3  | 1.86                     | 0.56              |
| 1:B:352:TRP:HB2  | 1:B:621:PHE:CZ   | 2.40                     | 0.56              |
| 1:B:665:ARG:NH2  | 1:B:677:THR:HG21 | 2.20                     | 0.56              |
| 1:C:140:SER:O    | 1:C:141:ARG:HB2  | 2.05                     | 0.56              |
| 1:C:233:ARG:HG2  | 1:C:234:PRO:HD2  | 1.87                     | 0.56              |
| 1:C:306:PRO:O    | 1:C:309:ILE:HG22 | 2.06                     | 0.56              |
| 1:C:566:CYS:SG   | 1:C:570:THR:HB   | 2.44                     | 0.56              |
| 1:D:140:SER:O    | 1:D:141:ARG:CB   | 2.53                     | 0.56              |
| 1:A:538:HIS:HD2  | 1:A:539:PRO:HD2  | 1.70                     | 0.56              |
| 1:A:57:VAL:HG12  | 1:A:58:ASP:H     | 1.68                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:170:ALA:HB3  | 1:B:185:TYR:HE2  | 1.69                     | 0.56              |
| 1:D:558:LYS:HZ2  | 1:D:558:LYS:CB   | 2.08                     | 0.56              |
| 1:D:433:VAL:HG11 | 1:D:565:LEU:HD11 | 1.87                     | 0.56              |
| 1:B:538:HIS:HD2  | 1:B:539:PRO:HD2  | 1.70                     | 0.56              |
| 1:C:140:SER:O    | 1:C:141:ARG:CB   | 2.53                     | 0.56              |
| 1:C:415:LEU:HB3  | 1:C:638:GLU:CB   | 2.35                     | 0.56              |
| 1:A:168:LEU:HG   | 1:A:199:THR:HG22 | 1.87                     | 0.56              |
| 1:A:415:LEU:HD23 | 1:A:415:LEU:H    | 1.71                     | 0.56              |
| 1:C:268:ARG:HE   | 1:C:269:VAL:HG13 | 1.68                     | 0.56              |
| 1:C:678:PHE:O    | 1:C:680:LYS:HD2  | 2.05                     | 0.56              |
| 1:B:427:TYR:CE1  | 1:B:587:ASN:HA   | 2.40                     | 0.56              |
| 1:B:674:ASP:HA   | 1:B:677:THR:OG1  | 2.05                     | 0.56              |
| 1:C:666:GLN:H    | 1:C:666:GLN:NE2  | 2.04                     | 0.56              |
| 1:D:414:ARG:CG   | 1:D:415:LEU:H    | 2.05                     | 0.56              |
| 1:A:445:LEU:HB3  | 1:A:481:PHE:HE2  | 1.70                     | 0.56              |
| 1:D:189:TRP:CE2  | 1:D:291:GLU:HB3  | 2.40                     | 0.56              |
| 1:C:517:TYR:CG   | 1:C:526:CYS:HB2  | 2.41                     | 0.56              |
| 1:C:280:SER:O    | 1:C:281:PRO:C    | 2.44                     | 0.55              |
| 1:D:666:GLN:NE2  | 1:D:666:GLN:H    | 2.04                     | 0.55              |
| 1:A:27:LYS:HZ2   | 1:D:659:THR:HG23 | 1.70                     | 0.55              |
| 1:A:554:ALA:HA   | 1:A:557:LEU:HD13 | 1.87                     | 0.55              |
| 1:D:527:LEU:HD23 | 1:D:527:LEU:O    | 2.06                     | 0.55              |
| 1:A:543:GLN:HE22 | 1:A:636:ASP:HB3  | 1.71                     | 0.55              |
| 1:B:108:GLN:H    | 1:B:111:GLN:HB2  | 1.72                     | 0.55              |
| 1:B:543:GLN:HE22 | 1:B:636:ASP:HB3  | 1.72                     | 0.55              |
| 1:B:442:TRP:H    | 1:B:565:LEU:HD21 | 1.72                     | 0.55              |
| 1:C:415:LEU:HB3  | 1:C:638:GLU:HG3  | 1.87                     | 0.55              |
| 1:D:268:ARG:HE   | 1:D:269:VAL:CG1  | 2.19                     | 0.55              |
| 1:A:674:ASP:HA   | 1:A:677:THR:HG1  | 1.71                     | 0.55              |
| 1:D:403:ALA:HB1  | 1:D:424:LEU:HD23 | 1.88                     | 0.55              |
| 1:D:541:VAL:HG13 | 1:D:574:VAL:HG21 | 1.88                     | 0.55              |
| 1:D:554:ALA:O    | 1:D:557:LEU:HD13 | 2.06                     | 0.55              |
| 1:C:189:TRP:CE2  | 1:C:291:GLU:HB3  | 2.42                     | 0.55              |
| 1:A:505:PRO:O    | 1:A:506:ALA:HB3  | 2.07                     | 0.55              |
| 1:B:46:PRO:HG3   | 1:B:66:LEU:HD22  | 1.87                     | 0.55              |
| 1:B:427:TYR:HE1  | 1:B:587:ASN:HA   | 1.72                     | 0.55              |
| 1:B:51:ASP:HB3   | 1:B:56:LYS:HB2   | 1.88                     | 0.55              |
| 1:C:449:LYS:HE3  | 1:C:483:ARG:NH2  | 2.22                     | 0.55              |
| 1:C:541:VAL:HG13 | 1:C:574:VAL:HG21 | 1.89                     | 0.55              |
| 1:B:400:PRO:C    | 1:B:643:LEU:HD11 | 2.27                     | 0.55              |
| 1:C:409:THR:O    | 1:C:410:HIS:CB   | 2.56                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:415:LEU:HB3  | 1:D:638:GLU:HG3  | 1.88                     | 0.54              |
| 1:D:218:ALA:HA   | 1:D:220:ARG:NE   | 2.12                     | 0.54              |
| 1:D:407:LEU:HG   | 1:D:408:SER:N    | 2.22                     | 0.54              |
| 1:A:79:PRO:O     | 1:A:305:VAL:HG21 | 2.07                     | 0.54              |
| 1:B:121:GLY:HA2  | 1:B:155:PRO:HD2  | 1.89                     | 0.54              |
| 1:B:400:PRO:HB2  | 1:B:643:LEU:HD11 | 1.89                     | 0.54              |
| 1:C:441:THR:HG23 | 1:C:444:SER:H    | 1.71                     | 0.54              |
| 1:D:415:LEU:HB3  | 1:D:638:GLU:CB   | 2.38                     | 0.54              |
| 1:D:424:LEU:HG   | 1:D:587:ASN:HD22 | 1.73                     | 0.54              |
| 1:C:103:LYS:HA   | 1:C:224:GLU:CG   | 2.34                     | 0.54              |
| 1:D:280:SER:O    | 1:D:281:PRO:C    | 2.45                     | 0.54              |
| 1:D:504:ASN:HB3  | 1:D:507:HIS:CG   | 2.43                     | 0.54              |
| 1:A:429:VAL:HG12 | 1:A:582:LEU:HD12 | 1.88                     | 0.54              |
| 1:A:465:MET:HE2  | 1:A:465:MET:HA   | 1.90                     | 0.54              |
| 1:C:407:LEU:HG   | 1:C:408:SER:N    | 2.23                     | 0.54              |
| 1:D:564:LEU:O    | 1:D:571:ARG:HA   | 2.07                     | 0.54              |
| 1:C:105:THR:HB   | 1:C:107:PHE:CE1  | 2.42                     | 0.54              |
| 1:C:554:ALA:O    | 1:C:557:LEU:HD13 | 2.07                     | 0.54              |
| 1:D:233:ARG:HG2  | 1:D:234:PRO:HD2  | 1.89                     | 0.54              |
| 1:D:538:HIS:O    | 1:D:540:THR:N    | 2.41                     | 0.54              |
| 1:C:346:ARG:NE   | 1:C:362:CYS:HB2  | 2.23                     | 0.54              |
| 1:B:445:LEU:HB3  | 1:B:481:PHE:HE2  | 1.72                     | 0.54              |
| 1:C:424:LEU:HG   | 1:C:587:ASN:HD22 | 1.73                     | 0.54              |
| 1:D:610:LEU:O    | 1:D:620:MET:HE1  | 2.08                     | 0.53              |
| 1:A:442:TRP:H    | 1:A:565:LEU:HD21 | 1.74                     | 0.53              |
| 1:B:164:SER:HA   | 1:B:167:GLN:HE21 | 1.73                     | 0.53              |
| 1:B:192:LEU:HD23 | 1:B:192:LEU:O    | 2.08                     | 0.53              |
| 1:B:435:LYS:HG3  | 1:B:563:GLU:OE2  | 2.08                     | 0.53              |
| 1:C:347:THR:O    | 1:C:351:GLN:HG3  | 2.08                     | 0.53              |
| 1:B:196:GLN:HE22 | 1:B:215:PRO:HD3  | 1.73                     | 0.53              |
| 1:C:108:GLN:OE1  | 1:C:232:ARG:HG3  | 2.08                     | 0.53              |
| 1:A:405:ASN:HB2  | 1:A:641:SER:OG   | 2.08                     | 0.53              |
| 1:A:277:ASP:HA   | 1:A:283:GLN:NE2  | 2.22                     | 0.53              |
| 1:A:367:THR:HG22 | 1:A:511:ALA:HB3  | 1.91                     | 0.53              |
| 1:B:306:PRO:O    | 1:B:309:ILE:HG22 | 2.07                     | 0.53              |
| 1:C:414:ARG:O    | 1:C:415:LEU:HB2  | 2.09                     | 0.53              |
| 1:C:414:ARG:CG   | 1:C:415:LEU:H    | 2.05                     | 0.53              |
| 1:C:136:LEU:H    | 1:C:136:LEU:HD23 | 1.73                     | 0.53              |
| 1:C:407:LEU:HD21 | 1:C:410:HIS:CB   | 2.38                     | 0.53              |
| 1:D:443:LYS:NZ   | 1:D:443:LYS:HB3  | 2.24                     | 0.53              |
| 1:C:103:LYS:CA   | 1:C:224:GLU:HG2  | 2.38                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:264:GLN:NE2  | 1:C:304:ARG:HD2  | 2.23                     | 0.53              |
| 1:D:99:ALA:HB3   | 1:D:226:LEU:HB2  | 1.91                     | 0.53              |
| 1:D:35:PRO:HB2   | 1:D:266:LEU:HD12 | 1.91                     | 0.53              |
| 1:D:372:ILE:O    | 1:D:376:MET:HG3  | 2.09                     | 0.53              |
| 1:A:170:ALA:HB3  | 1:A:185:TYR:HE2  | 1.73                     | 0.53              |
| 1:D:678:PHE:O    | 1:D:680:LYS:HD2  | 2.09                     | 0.53              |
| 1:B:429:VAL:HG12 | 1:B:582:LEU:HD12 | 1.90                     | 0.52              |
| 1:C:538:HIS:HB3  | 1:C:539:PRO:CD   | 2.39                     | 0.52              |
| 1:C:538:HIS:O    | 1:C:540:THR:N    | 2.41                     | 0.52              |
| 1:C:558:LYS:HZ2  | 1:C:558:LYS:CB   | 2.08                     | 0.52              |
| 1:D:140:SER:O    | 1:D:141:ARG:HB2  | 2.08                     | 0.52              |
| 1:A:515:GLU:HG3  | 1:A:517:TYR:H    | 1.74                     | 0.52              |
| 1:A:538:HIS:O    | 1:A:539:PRO:C    | 2.48                     | 0.52              |
| 1:A:435:LYS:HG3  | 1:A:563:GLU:OE2  | 2.10                     | 0.52              |
| 1:C:403:ALA:HB1  | 1:C:424:LEU:HD23 | 1.90                     | 0.52              |
| 1:C:540:THR:O    | 1:C:544:ASN:ND2  | 2.43                     | 0.52              |
| 1:C:588:ARG:NH1  | 1:C:633:PHE:HA   | 2.24                     | 0.52              |
| 1:D:441:THR:H    | 1:D:444:SER:CB   | 2.21                     | 0.52              |
| 1:B:320:LEU:HA   | 1:B:323:PHE:HB3  | 1.91                     | 0.52              |
| 1:B:538:HIS:O    | 1:B:539:PRO:C    | 2.48                     | 0.52              |
| 1:D:414:ARG:O    | 1:D:415:LEU:HB2  | 2.09                     | 0.52              |
| 1:A:400:PRO:HB2  | 1:A:643:LEU:HD13 | 1.90                     | 0.52              |
| 1:D:424:LEU:HD11 | 1:D:587:ASN:ND2  | 2.25                     | 0.52              |
| 1:D:517:TYR:CG   | 1:D:526:CYS:HB2  | 2.45                     | 0.52              |
| 1:A:188:SER:O    | 1:A:209:THR:HG21 | 2.10                     | 0.52              |
| 1:C:185:TYR:CD1  | 1:C:194:CYS:HB2  | 2.44                     | 0.52              |
| 1:C:449:LYS:HE3  | 1:C:483:ARG:HH21 | 1.75                     | 0.52              |
| 1:C:606:ASN:N    | 1:C:606:ASN:HD22 | 2.08                     | 0.52              |
| 1:D:136:LEU:HB2  | 1:D:139:GLY:O    | 2.10                     | 0.52              |
| 1:B:415:LEU:H    | 1:B:415:LEU:HD23 | 1.75                     | 0.52              |
| 1:B:629:LYS:HD3  | 1:B:635:ASP:OD1  | 2.10                     | 0.52              |
| 1:C:390:ALA:HB1  | 1:C:591:PHE:CZ   | 2.44                     | 0.52              |
| 1:C:441:THR:H    | 1:C:444:SER:CB   | 2.22                     | 0.52              |
| 1:D:268:ARG:HE   | 1:D:269:VAL:HG13 | 1.73                     | 0.52              |
| 1:C:509:CYS:N    | 1:C:515:GLU:OE1  | 2.39                     | 0.52              |
| 1:D:484:SER:HA   | 1:D:498:LEU:HD12 | 1.91                     | 0.51              |
| 1:B:459:GLU:CD   | 1:B:459:GLU:H    | 2.13                     | 0.51              |
| 1:C:346:ARG:NE   | 1:C:362:CYS:CB   | 2.73                     | 0.51              |
| 1:D:347:THR:O    | 1:D:351:GLN:HG3  | 2.10                     | 0.51              |
| 1:C:63:ASP:HB3   | 1:C:66:LEU:HD13  | 1.92                     | 0.51              |
| 1:C:78:LYS:HB2   | 1:C:78:LYS:NZ    | 2.25                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:606:ASN:ND2  | 1:C:606:ASN:N    | 2.58                     | 0.51              |
| 1:A:196:GLN:HE22 | 1:A:215:PRO:HD3  | 1.75                     | 0.51              |
| 1:A:400:PRO:C    | 1:A:643:LEU:HD11 | 2.31                     | 0.51              |
| 1:A:400:PRO:HB2  | 1:A:643:LEU:HD11 | 1.91                     | 0.51              |
| 1:B:188:SER:O    | 1:B:209:THR:HG21 | 2.11                     | 0.51              |
| 1:C:430:VAL:HA   | 1:C:582:LEU:HD13 | 1.91                     | 0.51              |
| 1:D:409:THR:O    | 1:D:410:HIS:CB   | 2.58                     | 0.51              |
| 1:C:135:LEU:O    | 1:C:135:LEU:HD12 | 2.11                     | 0.51              |
| 1:D:130:VAL:HB   | 1:D:131:PRO:HD3  | 1.93                     | 0.51              |
| 1:D:373:ALA:O    | 1:D:377:LYS:HG3  | 2.11                     | 0.51              |
| 1:B:461:TRP:O    | 1:B:465:MET:HB2  | 2.10                     | 0.51              |
| 1:B:525:ARG:O    | 1:B:529:GLU:HG2  | 2.10                     | 0.51              |
| 1:D:407:LEU:HD21 | 1:D:410:HIS:CB   | 2.40                     | 0.51              |
| 1:A:86:GLY:H     | 1:A:300:HIS:CD2  | 2.29                     | 0.51              |
| 1:B:453:THR:HG23 | 1:B:535:PHE:O    | 2.10                     | 0.51              |
| 1:C:320:LEU:O    | 1:C:324:ARG:HG2  | 2.11                     | 0.51              |
| 1:C:88:LYS:CE    | 1:C:88:LYS:HA    | 2.39                     | 0.51              |
| 1:B:73:PRO:O     | 1:B:74:HIS:CB    | 2.59                     | 0.51              |
| 1:C:588:ARG:HH11 | 1:C:633:PHE:HA   | 1.76                     | 0.51              |
| 1:A:164:SER:HA   | 1:A:167:GLN:HE21 | 1.75                     | 0.50              |
| 1:A:225:LEU:HG   | 1:A:235:VAL:HA   | 1.93                     | 0.50              |
| 1:B:106:GLY:HA2  | 1:B:232:ARG:CZ   | 2.40                     | 0.50              |
| 1:D:538:HIS:HB3  | 1:D:539:PRO:CD   | 2.42                     | 0.50              |
| 1:A:427:TYR:CD2  | 1:A:537:LYS:HB2  | 2.46                     | 0.50              |
| 1:C:52:ILE:O     | 1:C:254:ARG:HD3  | 2.12                     | 0.50              |
| 1:C:564:LEU:O    | 1:C:571:ARG:HA   | 2.10                     | 0.50              |
| 1:A:229:ASP:O    | 1:A:231:THR:N    | 2.44                     | 0.50              |
| 1:D:140:SER:O    | 1:D:141:ARG:HG3  | 2.11                     | 0.50              |
| 1:A:17:THR:HG22  | 1:D:471:GLN:HA   | 1.93                     | 0.50              |
| 1:A:459:GLU:CD   | 1:A:459:GLU:H    | 2.15                     | 0.50              |
| 1:B:218:ALA:HA   | 1:B:220:ARG:NE   | 2.27                     | 0.50              |
| 1:B:476:LYS:HB2  | 1:B:476:LYS:NZ   | 2.26                     | 0.50              |
| 1:B:674:ASP:HA   | 1:B:677:THR:HG1  | 1.76                     | 0.50              |
| 1:D:88:LYS:HA    | 1:D:88:LYS:CE    | 2.40                     | 0.50              |
| 1:A:121:GLY:HA2  | 1:A:155:PRO:HD2  | 1.93                     | 0.50              |
| 1:B:86:GLY:H     | 1:B:300:HIS:CD2  | 2.30                     | 0.50              |
| 1:C:101:ALA:O    | 1:C:223:TYR:HB3  | 2.11                     | 0.50              |
| 1:C:136:LEU:HB2  | 1:C:139:GLY:O    | 2.11                     | 0.50              |
| 1:D:105:THR:HB   | 1:D:107:PHE:CZ   | 2.47                     | 0.50              |
| 1:A:25:ASN:HB3   | 1:A:274:PHE:CZ   | 2.46                     | 0.50              |
| 1:C:306:PRO:HG2  | 1:C:309:ILE:HG21 | 1.92                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:424:LEU:HD11 | 1:C:587:ASN:ND2  | 2.27                     | 0.50              |
| 1:C:664:PHE:CD2  | 1:C:667:CYS:HB2  | 2.47                     | 0.50              |
| 1:D:461:TRP:O    | 1:D:464:PRO:HD2  | 2.12                     | 0.50              |
| 1:C:35:PRO:HB2   | 1:C:266:LEU:HD12 | 1.94                     | 0.50              |
| 1:A:155:PRO:O    | 1:A:156:CYS:HB2  | 2.12                     | 0.49              |
| 1:D:135:LEU:HD12 | 1:D:135:LEU:O    | 2.12                     | 0.49              |
| 1:A:373:ALA:O    | 1:A:377:LYS:HG3  | 2.11                     | 0.49              |
| 1:A:525:ARG:O    | 1:A:529:GLU:HG2  | 2.12                     | 0.49              |
| 1:B:388:GLY:HA3  | 1:B:462:ASN:HD21 | 1.78                     | 0.49              |
| 1:C:545:THR:HG22 | 1:C:557:LEU:HB3  | 1.95                     | 0.49              |
| 1:D:168:LEU:HD21 | 1:D:200:ALA:HB2  | 1.94                     | 0.49              |
| 1:D:477:PHE:C    | 1:D:479:ALA:H    | 2.16                     | 0.49              |
| 1:B:15:GLU:HG2   | 1:B:294:LEU:HD23 | 1.94                     | 0.49              |
| 1:B:427:TYR:CD2  | 1:B:537:LYS:HB2  | 2.47                     | 0.49              |
| 1:D:346:ARG:NE   | 1:D:362:CYS:CB   | 2.76                     | 0.49              |
| 1:A:306:PRO:O    | 1:A:309:ILE:HG22 | 2.11                     | 0.49              |
| 1:A:631:LEU:O    | 1:A:632:LEU:HB2  | 2.12                     | 0.49              |
| 1:A:543:GLN:NE2  | 1:A:636:ASP:HB3  | 2.28                     | 0.49              |
| 1:B:229:ASP:O    | 1:B:231:THR:N    | 2.46                     | 0.49              |
| 1:B:606:ASN:O    | 1:B:609:GLU:HB3  | 2.12                     | 0.49              |
| 1:C:136:LEU:N    | 1:C:136:LEU:HD23 | 2.28                     | 0.49              |
| 1:C:116:LYS:HB2  | 1:C:201:ASP:OD1  | 2.12                     | 0.49              |
| 1:A:106:GLY:HA2  | 1:A:232:ARG:CZ   | 2.42                     | 0.49              |
| 1:B:13:ASP:O     | 1:B:17:THR:HG23  | 2.11                     | 0.49              |
| 1:C:469:TYR:HD2  | 1:C:474:SER:O    | 1.95                     | 0.49              |
| 1:D:588:ARG:NH1  | 1:D:633:PHE:HA   | 2.27                     | 0.49              |
| 1:C:103:LYS:HG3  | 1:C:224:GLU:OE2  | 2.11                     | 0.49              |
| 1:C:388:GLY:HA2  | 1:C:661:MET:HE1  | 1.95                     | 0.49              |
| 1:C:130:VAL:HB   | 1:C:131:PRO:HD3  | 1.95                     | 0.49              |
| 1:D:62:VAL:O     | 1:D:249:HIS:HB3  | 2.13                     | 0.49              |
| 1:A:383:MET:HE2  | 1:A:384:SER:O    | 2.13                     | 0.49              |
| 1:B:65:ALA:O     | 1:B:68:ALA:HB3   | 2.13                     | 0.49              |
| 1:D:136:LEU:HD23 | 1:D:136:LEU:H    | 1.76                     | 0.49              |
| 1:D:45:HIS:N     | 1:D:46:PRO:CD    | 2.76                     | 0.49              |
| 1:D:648:THR:HG22 | 1:D:649:TYR:N    | 2.28                     | 0.49              |
| 1:A:13:ASP:O     | 1:A:17:THR:HG23  | 2.12                     | 0.49              |
| 1:A:70:ALA:CA    | 1:A:75:HIS:O     | 2.61                     | 0.48              |
| 1:B:155:PRO:O    | 1:B:156:CYS:HB2  | 2.13                     | 0.48              |
| 1:B:25:ASN:HB3   | 1:B:274:PHE:CZ   | 2.48                     | 0.48              |
| 1:B:274:PHE:O    | 1:B:284:LEU:HB2  | 2.13                     | 0.48              |
| 1:B:373:ALA:O    | 1:B:377:LYS:HG3  | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:543:GLN:NE2  | 1:B:636:ASP:HB3  | 2.27                     | 0.48              |
| 1:D:264:GLN:NE2  | 1:D:304:ARG:HD2  | 2.28                     | 0.48              |
| 1:D:390:ALA:HB1  | 1:D:591:PHE:CZ   | 2.47                     | 0.48              |
| 1:A:15:GLU:HG2   | 1:A:294:LEU:HD23 | 1.95                     | 0.48              |
| 1:A:452:HIS:HB2  | 1:A:486:ALA:HA   | 1.94                     | 0.48              |
| 1:A:644:GLN:HE21 | 1:A:644:GLN:CA   | 2.20                     | 0.48              |
| 1:D:136:LEU:HD23 | 1:D:136:LEU:N    | 2.28                     | 0.48              |
| 1:D:185:TYR:CD1  | 1:D:194:CYS:HB2  | 2.48                     | 0.48              |
| 1:D:346:ARG:NE   | 1:D:362:CYS:HB2  | 2.28                     | 0.48              |
| 1:C:346:ARG:HB2  | 1:C:364:THR:HB   | 1.95                     | 0.48              |
| 1:C:610:LEU:O    | 1:C:620:MET:HE1  | 2.13                     | 0.48              |
| 1:A:431:ALA:HB2  | 1:A:582:LEU:HD11 | 1.96                     | 0.48              |
| 1:A:67:VAL:HG12  | 1:A:67:VAL:O     | 2.13                     | 0.48              |
| 1:B:218:ALA:C    | 1:B:220:ARG:H    | 2.16                     | 0.48              |
| 1:B:400:PRO:HB2  | 1:B:643:LEU:HD13 | 1.94                     | 0.48              |
| 1:C:603:ILE:O    | 1:C:607:GLN:HG2  | 2.14                     | 0.48              |
| 1:C:624:PHE:CZ   | 1:C:640:LEU:HG   | 2.48                     | 0.48              |
| 1:A:608:GLN:O    | 1:A:612:GLY:HA3  | 2.14                     | 0.48              |
| 1:D:438:VAL:HA   | 1:D:571:ARG:HH12 | 1.79                     | 0.48              |
| 1:C:477:PHE:C    | 1:C:479:ALA:H    | 2.17                     | 0.48              |
| 1:C:99:ALA:HB3   | 1:C:226:LEU:HB2  | 1.96                     | 0.48              |
| 1:D:48:CYS:O     | 1:D:52:ILE:HG13  | 2.13                     | 0.48              |
| 1:A:218:ALA:C    | 1:A:220:ARG:H    | 2.17                     | 0.48              |
| 1:A:65:ALA:O     | 1:A:68:ALA:HB3   | 2.14                     | 0.48              |
| 1:A:73:PRO:O     | 1:A:74:HIS:CB    | 2.62                     | 0.48              |
| 1:B:68:ALA:C     | 1:B:69:GLU:OE2   | 2.51                     | 0.48              |
| 1:C:538:HIS:HB3  | 1:C:539:PRO:HD2  | 1.95                     | 0.48              |
| 1:C:498:LEU:O    | 1:C:530:LYS:HD2  | 2.14                     | 0.47              |
| 1:D:287:SER:HA   | 1:D:288:PRO:HD3  | 1.75                     | 0.47              |
| 1:D:304:ARG:HB3  | 1:D:304:ARG:NH1  | 2.29                     | 0.47              |
| 1:A:69:GLU:OE2   | 1:A:69:GLU:N     | 2.47                     | 0.47              |
| 1:B:229:ASP:O    | 1:B:231:THR:HG23 | 2.14                     | 0.47              |
| 1:B:225:LEU:HG   | 1:B:235:VAL:HA   | 1.95                     | 0.47              |
| 1:D:545:THR:HG22 | 1:D:557:LEU:HB3  | 1.96                     | 0.47              |
| 1:A:81:MET:O     | 1:A:250:VAL:HG12 | 2.14                     | 0.47              |
| 1:A:49:ILE:HD11  | 1:A:62:VAL:HG21  | 1.96                     | 0.47              |
| 1:A:587:ASN:ND2  | 1:A:587:ASN:N    | 2.33                     | 0.47              |
| 1:A:274:PHE:O    | 1:A:284:LEU:HB2  | 2.15                     | 0.47              |
| 1:A:445:LEU:HB3  | 1:A:481:PHE:CE2  | 2.48                     | 0.47              |
| 1:A:608:GLN:O    | 1:A:612:GLY:N    | 2.47                     | 0.47              |
| 1:B:367:THR:O    | 1:B:370:ASP:HB2  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:21:SER:O     | 1:B:25:ASN:ND2   | 2.25                     | 0.47              |
| 1:B:538:HIS:CD2  | 1:B:539:PRO:HD2  | 2.49                     | 0.47              |
| 1:B:605:PHE:CZ   | 1:B:642:ASN:OD1  | 2.62                     | 0.47              |
| 1:C:648:THR:HG22 | 1:C:649:TYR:N    | 2.30                     | 0.47              |
| 1:D:116:LYS:HB2  | 1:D:201:ASP:OD1  | 2.15                     | 0.47              |
| 1:D:136:LEU:O    | 1:D:136:LEU:HG   | 2.14                     | 0.47              |
| 1:D:235:VAL:HG23 | 1:D:236:GLU:N    | 2.30                     | 0.47              |
| 1:B:259:LYS:O    | 1:B:263:ILE:HG13 | 2.14                     | 0.47              |
| 1:B:293:LEU:O    | 1:B:294:LEU:HB2  | 2.14                     | 0.47              |
| 1:D:28:LYS:NZ    | 1:D:28:LYS:HB2   | 2.30                     | 0.47              |
| 1:D:261:ASP:N    | 1:D:261:ASP:OD2  | 2.47                     | 0.47              |
| 1:D:63:ASP:HB2   | 1:D:249:HIS:CE1  | 2.50                     | 0.47              |
| 1:A:218:ALA:HA   | 1:A:220:ARG:NE   | 2.30                     | 0.47              |
| 1:D:324:ARG:O    | 1:D:328:ARG:HB3  | 2.15                     | 0.47              |
| 1:A:557:LEU:HD12 | 1:A:557:LEU:N    | 2.30                     | 0.47              |
| 1:C:45:HIS:HB2   | 1:C:46:PRO:HD3   | 1.96                     | 0.47              |
| 1:D:407:LEU:HD21 | 1:D:410:HIS:CA   | 2.45                     | 0.47              |
| 1:B:70:ALA:CA    | 1:B:75:HIS:O     | 2.63                     | 0.47              |
| 1:C:309:ILE:HG23 | 1:C:309:ILE:O    | 2.15                     | 0.47              |
| 1:C:458:SER:HB3  | 1:C:585:VAL:HG11 | 1.97                     | 0.47              |
| 1:A:59:ALA:HB2   | 1:A:263:ILE:HD13 | 1.97                     | 0.47              |
| 1:A:476:LYS:HB2  | 1:A:476:LYS:NZ   | 2.30                     | 0.47              |
| 1:C:461:TRP:O    | 1:C:464:PRO:HD2  | 2.15                     | 0.47              |
| 1:D:175:ASP:OD1  | 1:D:182:ARG:HB3  | 2.15                     | 0.47              |
| 1:A:391:TYR:CE1  | 1:A:661:MET:HB2  | 2.50                     | 0.46              |
| 1:A:442:TRP:HA   | 1:A:445:LEU:CD1  | 2.42                     | 0.46              |
| 1:B:81:MET:SD    | 1:B:264:GLN:NE2  | 2.88                     | 0.46              |
| 1:B:391:TYR:CE1  | 1:B:661:MET:HB2  | 2.50                     | 0.46              |
| 1:C:643:LEU:O    | 1:C:644:GLN:HB2  | 2.14                     | 0.46              |
| 1:D:140:SER:O    | 1:D:141:ARG:CG   | 2.63                     | 0.46              |
| 1:D:175:ASP:O    | 1:D:183:GLU:HG2  | 2.15                     | 0.46              |
| 1:D:320:LEU:O    | 1:D:324:ARG:HG2  | 2.15                     | 0.46              |
| 1:A:155:PRO:HB3  | 1:A:178:ALA:O    | 2.15                     | 0.46              |
| 1:B:424:LEU:HD13 | 1:B:425:GLU:N    | 2.29                     | 0.46              |
| 1:D:309:ILE:HG23 | 1:D:309:ILE:O    | 2.14                     | 0.46              |
| 1:D:63:ASP:HB3   | 1:D:66:LEU:HD13  | 1.98                     | 0.46              |
| 1:A:229:ASP:O    | 1:A:231:THR:HG23 | 2.15                     | 0.46              |
| 1:A:388:GLY:HA3  | 1:A:462:ASN:HD21 | 1.80                     | 0.46              |
| 1:B:155:PRO:HB3  | 1:B:178:ALA:O    | 2.16                     | 0.46              |
| 1:D:624:PHE:CZ   | 1:D:640:LEU:HG   | 2.49                     | 0.46              |
| 1:B:209:THR:HG22 | 1:B:209:THR:O    | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:261:ASP:OD2  | 1:C:261:ASP:N    | 2.47                     | 0.46              |
| 1:D:115:LYS:O    | 1:D:149:PHE:HB3  | 2.15                     | 0.46              |
| 1:D:551:GLU:HA   | 1:D:552:PRO:HD3  | 1.74                     | 0.46              |
| 1:B:517:TYR:CZ   | 1:B:526:CYS:HA   | 2.50                     | 0.46              |
| 1:B:631:LEU:O    | 1:B:632:LEU:HB2  | 2.16                     | 0.46              |
| 1:C:235:VAL:HG23 | 1:C:236:GLU:N    | 2.31                     | 0.46              |
| 1:C:274:PHE:HB3  | 1:C:282:PHE:O    | 2.14                     | 0.46              |
| 1:D:274:PHE:HB3  | 1:D:282:PHE:O    | 2.14                     | 0.46              |
| 1:C:136:LEU:HG   | 1:C:136:LEU:O    | 2.15                     | 0.46              |
| 1:C:24:ASP:O     | 1:C:28:LYS:HG3   | 2.16                     | 0.46              |
| 1:C:438:VAL:HA   | 1:C:571:ARG:HH12 | 1.80                     | 0.46              |
| 1:D:101:ALA:O    | 1:D:223:TYR:HB3  | 2.14                     | 0.46              |
| 1:A:367:THR:O    | 1:A:370:ASP:HB2  | 2.16                     | 0.46              |
| 1:A:46:PRO:HG3   | 1:A:66:LEU:HD22  | 1.96                     | 0.46              |
| 1:B:464:PRO:O    | 1:B:468:ILE:HD13 | 2.15                     | 0.46              |
| 1:C:30:LEU:N     | 1:C:31:PRO:HD3   | 2.30                     | 0.46              |
| 1:C:45:HIS:N     | 1:C:46:PRO:CD    | 2.79                     | 0.46              |
| 1:D:408:SER:OG   | 1:D:415:LEU:HD13 | 2.16                     | 0.46              |
| 1:A:116:LYS:O    | 1:A:201:ASP:N    | 2.48                     | 0.46              |
| 1:C:125:SER:HB3  | 1:C:319:PHE:HZ   | 1.80                     | 0.46              |
| 1:C:505:PRO:O    | 1:C:506:ALA:HB3  | 2.15                     | 0.46              |
| 1:B:445:LEU:HB3  | 1:B:481:PHE:CE2  | 2.50                     | 0.46              |
| 1:C:666:GLN:H    | 1:C:666:GLN:CD   | 2.19                     | 0.46              |
| 1:D:122:LEU:HD22 | 1:D:156:CYS:O    | 2.16                     | 0.46              |
| 1:A:45:HIS:O     | 1:A:49:ILE:HG12  | 2.16                     | 0.46              |
| 1:A:585:VAL:HG12 | 1:A:657:TYR:CE1  | 2.51                     | 0.46              |
| 1:B:46:PRO:O     | 1:B:50:ARG:HG3   | 2.16                     | 0.46              |
| 1:C:105:THR:HB   | 1:C:107:PHE:CZ   | 2.51                     | 0.46              |
| 1:C:407:LEU:HD23 | 1:C:408:SER:O    | 2.16                     | 0.46              |
| 1:C:72:LEU:H     | 1:C:72:LEU:HD22  | 1.81                     | 0.46              |
| 1:A:124:TRP:O    | 1:A:128:TRP:HB3  | 2.16                     | 0.45              |
| 1:A:192:LEU:HD23 | 1:A:192:LEU:O    | 2.15                     | 0.45              |
| 1:B:442:TRP:N    | 1:B:565:LEU:HD21 | 2.30                     | 0.45              |
| 1:C:287:SER:HA   | 1:C:288:PRO:HD3  | 1.74                     | 0.45              |
| 1:C:324:ARG:O    | 1:C:328:ARG:HB3  | 2.17                     | 0.45              |
| 1:D:280:SER:H    | 1:D:281:PRO:HD2  | 1.80                     | 0.45              |
| 1:D:566:CYS:SG   | 1:D:570:THR:HB   | 2.56                     | 0.45              |
| 1:A:6:ILE:HD13   | 1:A:266:LEU:HD22 | 1.97                     | 0.45              |
| 1:B:346:ARG:NH2  | 1:B:364:THR:HG22 | 2.30                     | 0.45              |
| 1:A:346:ARG:NH2  | 1:A:364:THR:HG22 | 2.31                     | 0.45              |
| 1:A:442:TRP:N    | 1:A:565:LEU:HD21 | 2.31                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:605:PHE:CZ   | 1:A:642:ASN:OD1  | 2.62                     | 0.45              |
| 1:B:176:LYS:NZ   | 1:B:176:LYS:HB2  | 2.31                     | 0.45              |
| 1:C:280:SER:H    | 1:C:281:PRO:CD   | 2.30                     | 0.45              |
| 1:C:304:ARG:HB3  | 1:C:304:ARG:NH1  | 2.31                     | 0.45              |
| 1:D:53:SER:C     | 1:D:55:ASN:H     | 2.19                     | 0.45              |
| 1:A:256:VAL:O    | 1:A:256:VAL:HG13 | 2.16                     | 0.45              |
| 1:A:339:CYS:HB3  | 1:A:383:MET:HG2  | 1.96                     | 0.45              |
| 1:C:407:LEU:HD21 | 1:C:410:HIS:CA   | 2.45                     | 0.45              |
| 1:D:280:SER:H    | 1:D:281:PRO:CD   | 2.30                     | 0.45              |
| 1:D:306:PRO:HG2  | 1:D:309:ILE:HG21 | 1.98                     | 0.45              |
| 1:D:52:ILE:O     | 1:D:254:ARG:HD3  | 2.17                     | 0.45              |
| 1:A:22:PHE:O     | 1:A:26:MET:HG2   | 2.17                     | 0.45              |
| 1:B:452:HIS:HB2  | 1:B:486:ALA:HA   | 1.97                     | 0.45              |
| 1:B:69:GLU:N     | 1:B:69:GLU:OE2   | 2.49                     | 0.45              |
| 1:C:243:LEU:O    | 1:C:244:ALA:HB2  | 2.17                     | 0.45              |
| 1:C:5:THR:HG23   | 1:C:36:ALA:CB    | 2.44                     | 0.45              |
| 1:D:243:LEU:O    | 1:D:244:ALA:HB2  | 2.17                     | 0.45              |
| 1:B:49:ILE:HD11  | 1:B:62:VAL:HG21  | 1.99                     | 0.45              |
| 1:C:584:ARG:O    | 1:C:584:ARG:NH1  | 2.50                     | 0.45              |
| 1:C:646:LYS:HD2  | 1:C:651:THR:O    | 2.17                     | 0.45              |
| 1:A:150:SER:O    | 1:A:164:SER:HB3  | 2.17                     | 0.45              |
| 1:A:415:LEU:HD23 | 1:A:415:LEU:N    | 2.31                     | 0.45              |
| 1:A:538:HIS:CD2  | 1:A:539:PRO:HD2  | 2.50                     | 0.45              |
| 1:B:116:LYS:O    | 1:B:200:ALA:HB1  | 2.17                     | 0.45              |
| 1:B:420:VAL:HG13 | 1:B:605:PHE:CE1  | 2.51                     | 0.45              |
| 1:C:279:SER:OG   | 1:C:280:SER:N    | 2.45                     | 0.45              |
| 1:D:606:ASN:ND2  | 1:D:606:ASN:H    | 2.15                     | 0.45              |
| 1:A:375:THR:O    | 1:A:593:ARG:NH1  | 2.50                     | 0.45              |
| 1:C:372:ILE:O    | 1:C:376:MET:HG3  | 2.17                     | 0.45              |
| 1:D:509:CYS:N    | 1:D:515:GLU:OE1  | 2.45                     | 0.45              |
| 1:D:588:ARG:HH11 | 1:D:633:PHE:HA   | 1.81                     | 0.45              |
| 1:A:116:LYS:O    | 1:A:200:ALA:HB1  | 2.16                     | 0.45              |
| 1:B:430:VAL:HB   | 1:B:564:LEU:HD22 | 1.98                     | 0.45              |
| 1:C:373:ALA:O    | 1:C:377:LYS:HG3  | 2.17                     | 0.45              |
| 1:D:538:HIS:HB3  | 1:D:539:PRO:HD2  | 1.99                     | 0.45              |
| 1:D:424:LEU:CG   | 1:D:587:ASN:HD22 | 2.30                     | 0.45              |
| 1:D:441:THR:HG23 | 1:D:444:SER:H    | 1.81                     | 0.45              |
| 1:D:505:PRO:O    | 1:D:506:ALA:HB3  | 2.16                     | 0.45              |
| 1:D:78:LYS:HB2   | 1:D:78:LYS:NZ    | 2.31                     | 0.45              |
| 1:A:453:THR:HG23 | 1:A:535:PHE:O    | 2.17                     | 0.44              |
| 1:A:420:VAL:HG13 | 1:A:605:PHE:CE1  | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:124:TRP:O    | 1:B:128:TRP:HB3  | 2.17                     | 0.44              |
| 1:B:339:CYS:HB3  | 1:B:383:MET:HG2  | 1.98                     | 0.44              |
| 1:B:515:GLU:HG3  | 1:B:517:TYR:H    | 1.81                     | 0.44              |
| 1:B:375:THR:O    | 1:B:593:ARG:NH1  | 2.50                     | 0.44              |
| 1:C:406:TYR:HD2  | 1:C:637:THR:HA   | 1.82                     | 0.44              |
| 1:A:68:ALA:C     | 1:A:69:GLU:OE2   | 2.55                     | 0.44              |
| 1:B:256:VAL:O    | 1:B:256:VAL:HG13 | 2.17                     | 0.44              |
| 1:B:6:ILE:HD13   | 1:B:266:LEU:HD22 | 1.99                     | 0.44              |
| 1:C:280:SER:H    | 1:C:281:PRO:HD2  | 1.82                     | 0.44              |
| 1:C:415:LEU:HB3  | 1:C:638:GLU:CG   | 2.47                     | 0.44              |
| 1:C:568:ASP:OD1  | 1:C:569:GLY:N    | 2.50                     | 0.44              |
| 1:D:643:LEU:O    | 1:D:644:GLN:HB2  | 2.18                     | 0.44              |
| 1:A:125:SER:HA   | 1:A:129:TYR:HB2  | 1.99                     | 0.44              |
| 1:A:440:ILE:HG23 | 1:A:448:LYS:CD   | 2.47                     | 0.44              |
| 1:B:449:LYS:HB3  | 1:B:498:LEU:HD11 | 1.99                     | 0.44              |
| 1:D:22:PHE:CZ    | 1:D:266:LEU:HD21 | 2.52                     | 0.44              |
| 1:A:209:THR:O    | 1:A:209:THR:HG22 | 2.17                     | 0.44              |
| 1:A:415:LEU:HD12 | 1:A:419:CYS:HB2  | 1.98                     | 0.44              |
| 1:A:7:ARG:O      | 1:A:57:VAL:HG12  | 2.17                     | 0.44              |
| 1:B:100:MET:HB3  | 1:B:195:LEU:CD2  | 2.47                     | 0.44              |
| 1:C:34:GLY:HA3   | 1:C:35:PRO:HD2   | 1.85                     | 0.44              |
| 1:A:465:MET:HE1  | 1:A:481:PHE:HE1  | 1.82                     | 0.44              |
| 1:A:92:LYS:HG3   | 1:A:94:HIS:CE1   | 2.52                     | 0.44              |
| 1:C:25:ASN:HA    | 1:C:28:LYS:HE3   | 1.99                     | 0.44              |
| 1:C:28:LYS:NZ    | 1:C:28:LYS:HB2   | 2.33                     | 0.44              |
| 1:C:464:PRO:HB2  | 1:C:465:MET:HE3  | 1.99                     | 0.44              |
| 1:C:596:LYS:HZ1  | 1:C:596:LYS:HB2  | 1.82                     | 0.44              |
| 1:D:346:ARG:HB2  | 1:D:364:THR:HB   | 1.99                     | 0.44              |
| 1:D:541:VAL:HG11 | 1:D:574:VAL:HG21 | 1.97                     | 0.44              |
| 1:A:478:ASP:HB2  | 1:A:494:PRO:HD2  | 2.00                     | 0.44              |
| 1:B:431:ALA:HB2  | 1:B:582:LEU:HD11 | 1.99                     | 0.44              |
| 1:A:70:ALA:O     | 1:A:76:SER:HA    | 2.18                     | 0.44              |
| 1:D:155:PRO:O    | 1:D:156:CYS:HB2  | 2.18                     | 0.44              |
| 1:D:28:LYS:HZ2   | 1:D:28:LYS:HB2   | 1.82                     | 0.44              |
| 1:D:461:TRP:CD2  | 1:D:465:MET:HG3  | 2.53                     | 0.44              |
| 1:B:141:ARG:HB2  | 1:B:144:ALA:HB2  | 2.00                     | 0.44              |
| 1:B:45:HIS:CG    | 1:B:62:VAL:HG12  | 2.53                     | 0.44              |
| 1:B:540:THR:HG22 | 1:B:543:GLN:OE1  | 2.18                     | 0.44              |
| 1:C:367:THR:HB   | 1:C:368:PRO:CD   | 2.48                     | 0.44              |
| 1:D:498:LEU:O    | 1:D:530:LYS:HD2  | 2.18                     | 0.44              |
| 1:A:113:ARG:HA   | 1:A:148:PHE:CZ   | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:367:THR:OG1  | 1:D:370:ASP:OD1  | 2.34                     | 0.43              |
| 1:B:105:THR:HB   | 1:B:107:PHE:CD2  | 2.53                     | 0.43              |
| 1:B:400:PRO:HD2  | 1:B:647:THR:O    | 2.18                     | 0.43              |
| 1:C:461:TRP:CD2  | 1:C:465:MET:HG3  | 2.53                     | 0.43              |
| 1:D:44:SER:CB    | 1:D:46:PRO:HD2   | 2.48                     | 0.43              |
| 1:A:100:MET:HB3  | 1:A:195:LEU:CD2  | 2.48                     | 0.43              |
| 1:A:46:PRO:O     | 1:A:50:ARG:HG3   | 2.19                     | 0.43              |
| 1:A:81:MET:SD    | 1:A:264:GLN:NE2  | 2.91                     | 0.43              |
| 1:C:63:ASP:HB2   | 1:C:249:HIS:CE1  | 2.54                     | 0.43              |
| 1:D:42:LYS:HB3   | 1:D:47:GLU:OE2   | 2.18                     | 0.43              |
| 1:B:477:PHE:C    | 1:B:479:ALA:H    | 2.21                     | 0.43              |
| 1:C:328:ARG:C    | 1:C:328:ARG:NE   | 2.68                     | 0.43              |
| 1:C:549:ASN:HA   | 1:C:550:PRO:HD3  | 1.85                     | 0.43              |
| 1:D:666:GLN:CD   | 1:D:666:GLN:H    | 2.21                     | 0.43              |
| 1:A:45:HIS:O     | 1:A:48:CYS:HB2   | 2.18                     | 0.43              |
| 1:B:356:SER:C    | 1:B:358:GLY:H    | 2.22                     | 0.43              |
| 1:B:442:TRP:HA   | 1:B:445:LEU:CD1  | 2.44                     | 0.43              |
| 1:D:169:CYS:HA   | 1:D:185:TYR:HD2  | 1.84                     | 0.43              |
| 1:D:664:PHE:CD2  | 1:D:667:CYS:HB2  | 2.53                     | 0.43              |
| 1:A:114:GLY:HA2  | 1:A:149:PHE:HA   | 1.99                     | 0.43              |
| 1:A:188:SER:C    | 1:A:209:THR:HG21 | 2.39                     | 0.43              |
| 1:A:98:VAL:HB    | 1:A:225:LEU:HD22 | 2.01                     | 0.43              |
| 1:A:30:LEU:CG    | 1:A:34:GLY:HA3   | 2.48                     | 0.43              |
| 1:A:424:LEU:HD13 | 1:A:425:GLU:N    | 2.33                     | 0.43              |
| 1:A:45:HIS:CG    | 1:A:62:VAL:HG12  | 2.52                     | 0.43              |
| 1:B:130:VAL:HB   | 1:B:131:PRO:HD3  | 2.01                     | 0.43              |
| 1:B:164:SER:HA   | 1:B:167:GLN:NE2  | 2.33                     | 0.43              |
| 1:B:643:LEU:O    | 1:B:644:GLN:HB2  | 2.18                     | 0.43              |
| 1:B:70:ALA:O     | 1:B:76:SER:HA    | 2.19                     | 0.43              |
| 1:C:31:PRO:C     | 1:C:33:GLY:N     | 2.71                     | 0.43              |
| 1:D:24:ASP:O     | 1:D:28:LYS:HG3   | 2.18                     | 0.43              |
| 1:D:322:ALA:O    | 1:D:326:LEU:HD13 | 2.19                     | 0.43              |
| 1:D:415:LEU:HB3  | 1:D:638:GLU:CG   | 2.49                     | 0.43              |
| 1:B:430:VAL:HG11 | 1:B:577:ALA:HB1  | 1.99                     | 0.43              |
| 1:C:169:CYS:HA   | 1:C:185:TYR:HD2  | 1.83                     | 0.43              |
| 1:C:175:ASP:O    | 1:C:183:GLU:HG2  | 2.19                     | 0.43              |
| 1:C:117:SER:OG   | 1:C:202:VAL:HB   | 2.18                     | 0.43              |
| 1:C:285:PHE:HZ   | 1:C:302:LEU:CD1  | 2.32                     | 0.43              |
| 1:C:564:LEU:HD21 | 1:C:574:VAL:HG23 | 2.01                     | 0.43              |
| 1:A:549:ASN:HA   | 1:A:550:PRO:HD3  | 1.89                     | 0.43              |
| 1:B:465:MET:HE1  | 1:B:481:PHE:HE1  | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:29:VAL:HG23  | 1:A:30:LEU:N     | 2.33                     | 0.43              |
| 1:B:585:VAL:HG12 | 1:B:657:TYR:CE1  | 2.53                     | 0.43              |
| 1:A:195:LEU:HB3  | 1:A:223:TYR:CE2  | 2.54                     | 0.43              |
| 1:B:366:GLU:O    | 1:B:512:ASN:HB3  | 2.18                     | 0.43              |
| 1:B:45:HIS:O     | 1:B:48:CYS:HB2   | 2.19                     | 0.43              |
| 1:B:45:HIS:O     | 1:B:49:ILE:HG12  | 2.19                     | 0.43              |
| 1:C:122:LEU:CB   | 1:C:156:CYS:HB2  | 2.47                     | 0.43              |
| 1:C:328:ARG:O    | 1:C:328:ARG:NE   | 2.50                     | 0.43              |
| 1:C:441:THR:HG23 | 1:C:443:LYS:N    | 2.34                     | 0.43              |
| 1:D:441:THR:N    | 1:D:444:SER:HB2  | 2.25                     | 0.43              |
| 1:D:540:THR:O    | 1:D:544:ASN:ND2  | 2.52                     | 0.43              |
| 1:A:119:HIS:CG   | 1:A:154:VAL:HG22 | 2.54                     | 0.42              |
| 1:A:276:LYS:HE2  | 1:A:300:HIS:CE1  | 2.54                     | 0.42              |
| 1:A:348:LYS:O    | 1:A:348:LYS:HG2  | 2.19                     | 0.42              |
| 1:D:27:LYS:O     | 1:D:31:PRO:HB3   | 2.19                     | 0.42              |
| 1:A:352:TRP:CD1  | 1:A:352:TRP:O    | 2.72                     | 0.42              |
| 1:A:540:THR:HG22 | 1:A:543:GLN:OE1  | 2.19                     | 0.42              |
| 1:A:654:GLY:O    | 1:A:658:LEU:HB2  | 2.19                     | 0.42              |
| 1:B:505:PRO:O    | 1:B:506:ALA:CB   | 2.66                     | 0.42              |
| 1:D:125:SER:HB3  | 1:D:319:PHE:HZ   | 1.84                     | 0.42              |
| 1:A:356:SER:C    | 1:A:358:GLY:H    | 2.22                     | 0.42              |
| 1:B:114:GLY:HA2  | 1:B:149:PHE:HA   | 2.00                     | 0.42              |
| 1:B:346:ARG:NH2  | 1:B:364:THR:CG2  | 2.82                     | 0.42              |
| 1:B:352:TRP:O    | 1:B:352:TRP:CD1  | 2.73                     | 0.42              |
| 1:B:415:LEU:HD12 | 1:B:419:CYS:HB2  | 2.01                     | 0.42              |
| 1:C:168:LEU:HD21 | 1:C:200:ALA:HB2  | 2.01                     | 0.42              |
| 1:C:424:LEU:CG   | 1:C:587:ASN:HD22 | 2.32                     | 0.42              |
| 1:D:134:THR:CG2  | 1:D:134:THR:O    | 2.66                     | 0.42              |
| 1:A:320:LEU:O    | 1:A:324:ARG:HG3  | 2.19                     | 0.42              |
| 1:B:102:LYS:HD3  | 1:B:102:LYS:H    | 1.84                     | 0.42              |
| 1:B:22:PHE:O     | 1:B:26:MET:HG2   | 2.19                     | 0.42              |
| 1:B:483:ARG:HB3  | 1:B:483:ARG:HE   | 1.37                     | 0.42              |
| 1:C:442:TRP:CE3  | 1:C:445:LEU:HD11 | 2.55                     | 0.42              |
| 1:C:273:HIS:HB3  | 1:C:274:PHE:CE1  | 2.55                     | 0.42              |
| 1:C:27:LYS:O     | 1:C:31:PRO:HB3   | 2.19                     | 0.42              |
| 1:C:541:VAL:HG21 | 1:C:562:PHE:CD2  | 2.54                     | 0.42              |
| 1:C:564:LEU:HG   | 1:C:574:VAL:HA   | 2.00                     | 0.42              |
| 1:D:28:LYS:NZ    | 1:D:28:LYS:CB    | 2.82                     | 0.42              |
| 1:A:130:VAL:HB   | 1:A:131:PRO:HD3  | 2.02                     | 0.42              |
| 1:A:84:TYR:CE1   | 1:A:301:GLY:HA3  | 2.55                     | 0.42              |
| 1:C:108:GLN:H    | 1:C:111:GLN:HE21 | 1.65                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:430:VAL:CA   | 1:C:582:LEU:HD13 | 2.50                     | 0.42              |
| 1:D:643:LEU:HB3  | 1:D:646:LYS:O    | 2.19                     | 0.42              |
| 1:A:291:GLU:OE1  | 1:A:291:GLU:HA   | 2.19                     | 0.42              |
| 1:C:192:LEU:HG   | 1:C:205:VAL:HG11 | 2.01                     | 0.42              |
| 1:D:407:LEU:HD23 | 1:D:408:SER:O    | 2.19                     | 0.42              |
| 1:D:464:PRO:HB2  | 1:D:465:MET:HE3  | 2.01                     | 0.42              |
| 1:A:434:LYS:O    | 1:A:571:ARG:NH2  | 2.52                     | 0.42              |
| 1:A:449:LYS:HB3  | 1:A:498:LEU:HD11 | 2.02                     | 0.42              |
| 1:B:435:LYS:HG3  | 1:B:563:GLU:CD   | 2.39                     | 0.42              |
| 1:B:67:VAL:HG12  | 1:B:67:VAL:O     | 2.19                     | 0.42              |
| 1:C:418:LYS:HZ2  | 1:C:418:LYS:HB3  | 1.81                     | 0.42              |
| 1:D:285:PHE:HZ   | 1:D:302:LEU:HD12 | 1.85                     | 0.42              |
| 1:D:45:HIS:HB2   | 1:D:46:PRO:HD3   | 2.00                     | 0.42              |
| 1:A:483:ARG:HB3  | 1:A:483:ARG:HE   | 1.41                     | 0.42              |
| 1:B:549:ASN:HA   | 1:B:550:PRO:HD3  | 1.86                     | 0.42              |
| 1:B:608:GLN:O    | 1:B:612:GLY:HA3  | 2.18                     | 0.42              |
| 1:D:143:THR:HG23 | 1:D:162:PHE:HE2  | 1.85                     | 0.42              |
| 1:D:228:MET:HA   | 1:D:228:MET:HE3  | 2.02                     | 0.42              |
| 1:D:442:TRP:CE3  | 1:D:445:LEU:HD11 | 2.55                     | 0.42              |
| 1:A:13:ASP:OD1   | 1:A:41:ARG:NH1   | 2.49                     | 0.42              |
| 1:C:285:PHE:HZ   | 1:C:302:LEU:HD12 | 1.85                     | 0.42              |
| 1:D:119:HIS:HD2  | 1:D:127:GLY:O    | 2.03                     | 0.42              |
| 1:A:459:GLU:CG   | 1:A:537:LYS:HB3  | 2.46                     | 0.41              |
| 1:B:188:SER:C    | 1:B:209:THR:HG21 | 2.41                     | 0.41              |
| 1:B:309:ILE:HB   | 1:B:675:ALA:HB1  | 2.01                     | 0.41              |
| 1:C:137:PRO:HD3  | 1:C:148:PHE:HD1  | 1.85                     | 0.41              |
| 1:C:115:LYS:O    | 1:C:149:PHE:HB3  | 2.19                     | 0.41              |
| 1:C:549:ASN:C    | 1:C:551:GLU:H    | 2.23                     | 0.41              |
| 1:C:53:SER:C     | 1:C:55:ASN:H     | 2.23                     | 0.41              |
| 1:D:76:SER:O     | 1:D:255:SER:N    | 2.29                     | 0.41              |
| 1:A:541:VAL:HG11 | 1:A:574:VAL:HB   | 2.02                     | 0.41              |
| 1:B:478:ASP:HB2  | 1:B:494:PRO:HD2  | 2.02                     | 0.41              |
| 1:B:541:VAL:HG11 | 1:B:574:VAL:HB   | 2.00                     | 0.41              |
| 1:B:644:GLN:HE21 | 1:B:644:GLN:CA   | 2.20                     | 0.41              |
| 1:D:25:ASN:H     | 1:D:25:ASN:HD22  | 1.68                     | 0.41              |
| 1:B:189:TRP:CE2  | 1:B:213:ALA:HB2  | 2.55                     | 0.41              |
| 1:B:476:LYS:O    | 1:B:479:ALA:HB3  | 2.21                     | 0.41              |
| 1:B:84:TYR:CE1   | 1:B:301:GLY:HA3  | 2.56                     | 0.41              |
| 1:C:301:GLY:C    | 1:C:302:LEU:HD12 | 2.41                     | 0.41              |
| 1:D:108:GLN:HE22 | 1:D:232:ARG:N    | 2.18                     | 0.41              |
| 1:D:468:ILE:O    | 1:D:472:THR:HG23 | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:367:THR:HB   | 1:B:369:GLU:OE1  | 2.21                     | 0.41              |
| 1:C:406:TYR:C    | 1:C:638:GLU:HG2  | 2.40                     | 0.41              |
| 1:D:130:VAL:HG12 | 1:D:243:LEU:HD23 | 2.01                     | 0.41              |
| 1:D:31:PRO:C     | 1:D:33:GLY:N     | 2.72                     | 0.41              |
| 1:D:352:TRP:HB2  | 1:D:621:PHE:CE2  | 2.56                     | 0.41              |
| 1:D:30:LEU:N     | 1:D:31:PRO:HD3   | 2.35                     | 0.41              |
| 1:D:587:ASN:O    | 1:D:652:TYR:OH   | 2.36                     | 0.41              |
| 1:A:105:THR:HB   | 1:A:107:PHE:CD2  | 2.55                     | 0.41              |
| 1:A:310:ASP:OD2  | 1:A:377:LYS:NZ   | 2.40                     | 0.41              |
| 1:B:70:ALA:HA    | 1:B:75:HIS:CB    | 2.49                     | 0.41              |
| 1:C:308:LYS:HD3  | 1:C:671:GLU:HB2  | 2.03                     | 0.41              |
| 1:C:394:GLY:HA3  | 1:C:649:TYR:CG   | 2.55                     | 0.41              |
| 1:C:76:SER:O     | 1:C:255:SER:N    | 2.27                     | 0.41              |
| 1:D:178:ALA:HB3  | 1:D:183:GLU:HB2  | 2.01                     | 0.41              |
| 1:D:404:GLU:HB3  | 1:D:588:ARG:O    | 2.20                     | 0.41              |
| 1:A:155:PRO:O    | 1:A:156:CYS:CB   | 2.69                     | 0.41              |
| 1:A:438:VAL:HG23 | 1:A:438:VAL:O    | 2.21                     | 0.41              |
| 1:A:45:HIS:N     | 1:A:46:PRO:CD    | 2.83                     | 0.41              |
| 1:A:477:PHE:C    | 1:A:479:ALA:H    | 2.24                     | 0.41              |
| 1:B:94:HIS:CD2   | 1:B:245:ARG:NH2  | 2.89                     | 0.41              |
| 1:C:122:LEU:HD22 | 1:C:156:CYS:O    | 2.21                     | 0.41              |
| 1:C:254:ARG:HB2  | 1:C:258:GLY:HA3  | 2.02                     | 0.41              |
| 1:D:122:LEU:CB   | 1:D:156:CYS:HB2  | 2.49                     | 0.41              |
| 1:D:337:LYS:HB2  | 1:D:337:LYS:HZ3  | 1.81                     | 0.41              |
| 1:D:441:THR:HG23 | 1:D:443:LYS:H    | 1.86                     | 0.41              |
| 1:D:308:LYS:HD3  | 1:D:671:GLU:HB2  | 2.03                     | 0.41              |
| 1:A:430:VAL:HB   | 1:A:564:LEU:HD22 | 2.02                     | 0.41              |
| 1:A:533:VAL:HG12 | 1:A:534:ALA:N    | 2.35                     | 0.41              |
| 1:A:622:GLN:HE21 | 1:A:622:GLN:HB2  | 1.63                     | 0.41              |
| 1:B:111:GLN:N    | 1:B:111:GLN:OE1  | 2.54                     | 0.41              |
| 1:B:434:LYS:O    | 1:B:571:ARG:NH2  | 2.53                     | 0.41              |
| 1:B:657:TYR:O    | 1:B:660:LEU:HB3  | 2.21                     | 0.41              |
| 1:C:111:GLN:CD   | 1:C:111:GLN:H    | 2.24                     | 0.41              |
| 1:C:155:PRO:O    | 1:C:156:CYS:HB2  | 2.21                     | 0.41              |
| 1:C:28:LYS:HZ2   | 1:C:28:LYS:HB2   | 1.84                     | 0.41              |
| 1:C:524:LEU:CD2  | 1:C:544:ASN:HD22 | 2.33                     | 0.41              |
| 1:D:226:LEU:N    | 1:D:226:LEU:HD12 | 2.36                     | 0.41              |
| 1:D:242:TYR:HD1  | 1:D:244:ALA:N    | 2.18                     | 0.41              |
| 1:D:328:ARG:O    | 1:D:328:ARG:NE   | 2.53                     | 0.41              |
| 1:B:386:ASP:OD1  | 1:B:457:THR:HA   | 2.21                     | 0.41              |
| 1:D:603:ILE:O    | 1:D:607:GLN:HG2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:109:LEU:O    | 1:A:112:LEU:HD12 | 2.21                     | 0.41              |
| 1:A:288:PRO:HG2  | 1:A:289:HIS:H    | 1.86                     | 0.41              |
| 1:A:368:PRO:O    | 1:A:371:CYS:HB2  | 2.21                     | 0.41              |
| 1:A:476:LYS:O    | 1:A:479:ALA:HB3  | 2.21                     | 0.41              |
| 1:A:466:GLY:HA2  | 1:A:664:PHE:CD2  | 2.56                     | 0.41              |
| 1:D:391:TYR:OH   | 1:D:662:ASP:OD1  | 2.33                     | 0.41              |
| 1:A:72:LEU:HB3   | 1:A:73:PRO:CD    | 2.49                     | 0.41              |
| 1:C:31:PRO:O     | 1:C:32:ALA:C     | 2.59                     | 0.41              |
| 1:D:512:ASN:OD1  | 1:D:514:ALA:HB3  | 2.21                     | 0.41              |
| 1:A:490:ASP:HA   | 1:A:491:PRO:HD3  | 1.98                     | 0.40              |
| 1:B:116:LYS:O    | 1:B:201:ASP:N    | 2.51                     | 0.40              |
| 1:B:98:VAL:HB    | 1:B:225:LEU:HD22 | 2.03                     | 0.40              |
| 1:B:490:ASP:HA   | 1:B:491:PRO:HD3  | 1.95                     | 0.40              |
| 1:B:72:LEU:HB3   | 1:B:73:PRO:CD    | 2.47                     | 0.40              |
| 1:C:418:LYS:HZ3  | 1:C:418:LYS:HB3  | 1.84                     | 0.40              |
| 1:D:386:ASP:CG   | 1:D:387:GLY:N    | 2.74                     | 0.40              |
| 1:B:30:LEU:CG    | 1:B:34:GLY:HA3   | 2.50                     | 0.40              |
| 1:C:168:LEU:HD11 | 1:C:199:THR:O    | 2.22                     | 0.40              |
| 1:C:260:GLU:CD   | 1:C:260:GLU:H    | 2.24                     | 0.40              |
| 1:C:624:PHE:CE1  | 1:C:640:LEU:HG   | 2.57                     | 0.40              |
| 1:D:34:GLY:HA3   | 1:D:35:PRO:HD2   | 1.86                     | 0.40              |
| 1:A:113:ARG:HA   | 1:A:148:PHE:HZ   | 1.85                     | 0.40              |
| 1:B:271:GLN:NE2  | 1:B:301:GLY:HA3  | 2.36                     | 0.40              |
| 1:C:108:GLN:HE22 | 1:C:232:ARG:CG   | 2.27                     | 0.40              |
| 1:C:162:PHE:HB2  | 1:C:165:LEU:HD12 | 2.03                     | 0.40              |
| 1:D:365:GLU:HB2  | 1:D:371:CYS:SG   | 2.62                     | 0.40              |
| 1:D:564:LEU:HG   | 1:D:574:VAL:HA   | 2.03                     | 0.40              |
| 1:A:517:TYR:CZ   | 1:A:526:CYS:HA   | 2.56                     | 0.40              |
| 1:B:352:TRP:CE3  | 1:B:632:LEU:HD13 | 2.57                     | 0.40              |
| 1:B:420:VAL:O    | 1:B:641:SER:HA   | 2.22                     | 0.40              |
| 1:C:441:THR:CG2  | 1:C:444:SER:H    | 2.34                     | 0.40              |
| 1:D:168:LEU:HD11 | 1:D:199:THR:O    | 2.21                     | 0.40              |
| 1:D:441:THR:HG23 | 1:D:443:LYS:N    | 2.36                     | 0.40              |
| 1:D:622:GLN:HB2  | 1:D:625:GLU:HB3  | 2.04                     | 0.40              |
| 1:A:578:GLN:HB3  | 1:A:578:GLN:HE21 | 1.64                     | 0.40              |
| 1:B:119:HIS:CD2  | 1:B:154:VAL:HG22 | 2.57                     | 0.40              |
| 1:B:150:SER:O    | 1:B:164:SER:HB3  | 2.22                     | 0.40              |
| 1:C:337:LYS:CB   | 1:C:337:LYS:NZ   | 2.74                     | 0.40              |
| 1:C:644:GLN:OE1  | 1:C:644:GLN:HA   | 2.21                     | 0.40              |
| 1:D:137:PRO:HD3  | 1:D:148:PHE:HD1  | 1.86                     | 0.40              |
| 1:D:644:GLN:HA   | 1:D:644:GLN:OE1  | 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     | 671/687 (98%)   | 578 (86%)  | 74 (11%)  | 19 (3%)  | 5           | 5 |
| 1   | B     | 671/687 (98%)   | 574 (86%)  | 78 (12%)  | 19 (3%)  | 5           | 5 |
| 1   | C     | 671/687 (98%)   | 568 (85%)  | 83 (12%)  | 20 (3%)  | 5           | 4 |
| 1   | D     | 671/687 (98%)   | 563 (84%)  | 87 (13%)  | 21 (3%)  | 4           | 4 |
| All | All   | 2684/2748 (98%) | 2283 (85%) | 322 (12%) | 79 (3%)  | 5           | 4 |

All (79) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 230 | ASN  |
| 1   | A     | 280 | SER  |
| 1   | A     | 289 | HIS  |
| 1   | A     | 539 | PRO  |
| 1   | A     | 620 | MET  |
| 1   | B     | 230 | ASN  |
| 1   | B     | 280 | SER  |
| 1   | B     | 289 | HIS  |
| 1   | B     | 539 | PRO  |
| 1   | B     | 620 | MET  |
| 1   | C     | 141 | ARG  |
| 1   | C     | 280 | SER  |
| 1   | C     | 665 | ARG  |
| 1   | D     | 141 | ARG  |
| 1   | D     | 280 | SER  |
| 1   | D     | 665 | ARG  |
| 1   | A     | 140 | SER  |
| 1   | A     | 275 | GLY  |
| 1   | A     | 288 | PRO  |
| 1   | A     | 307 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 417 | SER  |
| 1   | B     | 140 | SER  |
| 1   | B     | 288 | PRO  |
| 1   | B     | 307 | ARG  |
| 1   | B     | 417 | SER  |
| 1   | C     | 646 | LYS  |
| 1   | D     | 646 | LYS  |
| 1   | A     | 114 | GLY  |
| 1   | A     | 281 | PRO  |
| 1   | A     | 513 | ASN  |
| 1   | B     | 114 | GLY  |
| 1   | B     | 275 | GLY  |
| 1   | B     | 281 | PRO  |
| 1   | C     | 537 | LYS  |
| 1   | C     | 538 | HIS  |
| 1   | D     | 407 | LEU  |
| 1   | A     | 439 | GLY  |
| 1   | A     | 646 | LYS  |
| 1   | B     | 411 | SER  |
| 1   | B     | 439 | GLY  |
| 1   | B     | 513 | ASN  |
| 1   | B     | 646 | LYS  |
| 1   | C     | 87  | SER  |
| 1   | C     | 107 | PHE  |
| 1   | C     | 407 | LEU  |
| 1   | C     | 414 | ARG  |
| 1   | C     | 482 | SER  |
| 1   | D     | 87  | SER  |
| 1   | D     | 414 | ARG  |
| 1   | D     | 537 | LYS  |
| 1   | D     | 538 | HIS  |
| 1   | A     | 358 | GLY  |
| 1   | A     | 411 | SER  |
| 1   | A     | 678 | PHE  |
| 1   | B     | 358 | GLY  |
| 1   | C     | 135 | LEU  |
| 1   | C     | 513 | ASN  |
| 1   | D     | 135 | LEU  |
| 1   | D     | 415 | LEU  |
| 1   | D     | 462 | ASN  |
| 1   | D     | 482 | SER  |
| 1   | B     | 483 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 114 | GLY  |
| 1   | C     | 288 | PRO  |
| 1   | C     | 415 | LEU  |
| 1   | D     | 107 | PHE  |
| 1   | D     | 114 | GLY  |
| 1   | D     | 513 | ASN  |
| 1   | D     | 539 | PRO  |
| 1   | C     | 73  | PRO  |
| 1   | C     | 539 | PRO  |
| 1   | D     | 288 | PRO  |
| 1   | B     | 173 | GLY  |
| 1   | C     | 64  | GLY  |
| 1   | D     | 64  | GLY  |
| 1   | D     | 137 | PRO  |
| 1   | C     | 137 | PRO  |
| 1   | D     | 281 | PRO  |
| 1   | A     | 173 | GLY  |

### 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     | 563/574 (98%)   | 532 (94%)  | 31 (6%)  | 24          | 37 |
| 1   | B     | 563/574 (98%)   | 530 (94%)  | 33 (6%)  | 21          | 34 |
| 1   | C     | 563/574 (98%)   | 535 (95%)  | 28 (5%)  | 27          | 43 |
| 1   | D     | 563/574 (98%)   | 532 (94%)  | 31 (6%)  | 24          | 37 |
| All | All   | 2252/2296 (98%) | 2129 (94%) | 123 (6%) | 24          | 37 |

All (123) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | ILE  |
| 1   | A     | 14  | HIS  |
| 1   | A     | 69  | GLU  |
| 1   | A     | 74  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 78  | LYS  |
| 1   | A     | 135 | LEU  |
| 1   | A     | 176 | LYS  |
| 1   | A     | 177 | CYS  |
| 1   | A     | 189 | TRP  |
| 1   | A     | 197 | ASP  |
| 1   | A     | 220 | ARG  |
| 1   | A     | 248 | SER  |
| 1   | A     | 250 | VAL  |
| 1   | A     | 255 | SER  |
| 1   | A     | 284 | LEU  |
| 1   | A     | 289 | HIS  |
| 1   | A     | 360 | LEU  |
| 1   | A     | 362 | CYS  |
| 1   | A     | 383 | MET  |
| 1   | A     | 424 | LEU  |
| 1   | A     | 483 | ARG  |
| 1   | A     | 538 | HIS  |
| 1   | A     | 539 | PRO  |
| 1   | A     | 565 | LEU  |
| 1   | A     | 566 | CYS  |
| 1   | A     | 578 | GLN  |
| 1   | A     | 587 | ASN  |
| 1   | A     | 593 | ARG  |
| 1   | A     | 622 | GLN  |
| 1   | A     | 648 | THR  |
| 1   | A     | 672 | LEU  |
| 1   | B     | 6   | ILE  |
| 1   | B     | 13  | ASP  |
| 1   | B     | 14  | HIS  |
| 1   | B     | 69  | GLU  |
| 1   | B     | 74  | HIS  |
| 1   | B     | 78  | LYS  |
| 1   | B     | 135 | LEU  |
| 1   | B     | 176 | LYS  |
| 1   | B     | 177 | CYS  |
| 1   | B     | 189 | TRP  |
| 1   | B     | 197 | ASP  |
| 1   | B     | 220 | ARG  |
| 1   | B     | 248 | SER  |
| 1   | B     | 250 | VAL  |
| 1   | B     | 255 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 284 | LEU  |
| 1   | B     | 289 | HIS  |
| 1   | B     | 360 | LEU  |
| 1   | B     | 383 | MET  |
| 1   | B     | 424 | LEU  |
| 1   | B     | 483 | ARG  |
| 1   | B     | 509 | CYS  |
| 1   | B     | 513 | ASN  |
| 1   | B     | 538 | HIS  |
| 1   | B     | 539 | PRO  |
| 1   | B     | 565 | LEU  |
| 1   | B     | 566 | CYS  |
| 1   | B     | 578 | GLN  |
| 1   | B     | 587 | ASN  |
| 1   | B     | 593 | ARG  |
| 1   | B     | 622 | GLN  |
| 1   | B     | 648 | THR  |
| 1   | B     | 672 | LEU  |
| 1   | C     | 26  | MET  |
| 1   | C     | 43  | MET  |
| 1   | C     | 51  | ASP  |
| 1   | C     | 71  | ASP  |
| 1   | C     | 74  | HIS  |
| 1   | C     | 78  | LYS  |
| 1   | C     | 111 | GLN  |
| 1   | C     | 135 | LEU  |
| 1   | C     | 177 | CYS  |
| 1   | C     | 194 | CYS  |
| 1   | C     | 220 | ARG  |
| 1   | C     | 327 | LYS  |
| 1   | C     | 328 | ARG  |
| 1   | C     | 371 | CYS  |
| 1   | C     | 407 | LEU  |
| 1   | C     | 419 | CYS  |
| 1   | C     | 476 | LYS  |
| 1   | C     | 482 | SER  |
| 1   | C     | 492 | ASP  |
| 1   | C     | 507 | HIS  |
| 1   | C     | 541 | VAL  |
| 1   | C     | 566 | CYS  |
| 1   | C     | 584 | ARG  |
| 1   | C     | 595 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 596 | LYS  |
| 1   | C     | 606 | ASN  |
| 1   | C     | 622 | GLN  |
| 1   | C     | 639 | CYS  |
| 1   | D     | 26  | MET  |
| 1   | D     | 43  | MET  |
| 1   | D     | 51  | ASP  |
| 1   | D     | 71  | ASP  |
| 1   | D     | 74  | HIS  |
| 1   | D     | 78  | LYS  |
| 1   | D     | 111 | GLN  |
| 1   | D     | 135 | LEU  |
| 1   | D     | 177 | CYS  |
| 1   | D     | 194 | CYS  |
| 1   | D     | 220 | ARG  |
| 1   | D     | 327 | LYS  |
| 1   | D     | 328 | ARG  |
| 1   | D     | 364 | THR  |
| 1   | D     | 370 | ASP  |
| 1   | D     | 371 | CYS  |
| 1   | D     | 407 | LEU  |
| 1   | D     | 419 | CYS  |
| 1   | D     | 476 | LYS  |
| 1   | D     | 482 | SER  |
| 1   | D     | 492 | ASP  |
| 1   | D     | 507 | HIS  |
| 1   | D     | 541 | VAL  |
| 1   | D     | 555 | LYS  |
| 1   | D     | 566 | CYS  |
| 1   | D     | 584 | ARG  |
| 1   | D     | 595 | ASP  |
| 1   | D     | 596 | LYS  |
| 1   | D     | 606 | ASN  |
| 1   | D     | 622 | GLN  |
| 1   | D     | 639 | CYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 55  | ASN  |
| 1   | A     | 110 | ASN  |
| 1   | A     | 167 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 207 | HIS  |
| 1   | A     | 230 | ASN  |
| 1   | A     | 300 | HIS  |
| 1   | A     | 334 | GLN  |
| 1   | A     | 351 | GLN  |
| 1   | A     | 421 | ASN  |
| 1   | A     | 462 | ASN  |
| 1   | A     | 578 | GLN  |
| 1   | A     | 587 | ASN  |
| 1   | A     | 622 | GLN  |
| 1   | A     | 642 | ASN  |
| 1   | A     | 644 | GLN  |
| 1   | A     | 656 | GLN  |
| 1   | A     | 663 | ASN  |
| 1   | A     | 666 | GLN  |
| 1   | B     | 55  | ASN  |
| 1   | B     | 110 | ASN  |
| 1   | B     | 167 | GLN  |
| 1   | B     | 207 | HIS  |
| 1   | B     | 230 | ASN  |
| 1   | B     | 300 | HIS  |
| 1   | B     | 334 | GLN  |
| 1   | B     | 351 | GLN  |
| 1   | B     | 421 | ASN  |
| 1   | B     | 462 | ASN  |
| 1   | B     | 587 | ASN  |
| 1   | B     | 606 | ASN  |
| 1   | B     | 622 | GLN  |
| 1   | B     | 644 | GLN  |
| 1   | B     | 656 | GLN  |
| 1   | B     | 663 | ASN  |
| 1   | B     | 666 | GLN  |
| 1   | C     | 111 | GLN  |
| 1   | C     | 167 | GLN  |
| 1   | C     | 230 | ASN  |
| 1   | C     | 249 | HIS  |
| 1   | C     | 264 | GLN  |
| 1   | C     | 271 | GLN  |
| 1   | C     | 283 | GLN  |
| 1   | C     | 405 | ASN  |
| 1   | C     | 518 | HIS  |
| 1   | C     | 544 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 578 | GLN  |
| 1   | C     | 587 | ASN  |
| 1   | C     | 606 | ASN  |
| 1   | C     | 614 | ASN  |
| 1   | C     | 622 | GLN  |
| 1   | C     | 663 | ASN  |
| 1   | C     | 679 | HIS  |
| 1   | D     | 111 | GLN  |
| 1   | D     | 119 | HIS  |
| 1   | D     | 167 | GLN  |
| 1   | D     | 230 | ASN  |
| 1   | D     | 249 | HIS  |
| 1   | D     | 264 | GLN  |
| 1   | D     | 271 | GLN  |
| 1   | D     | 283 | GLN  |
| 1   | D     | 405 | ASN  |
| 1   | D     | 518 | HIS  |
| 1   | D     | 544 | ASN  |
| 1   | D     | 578 | GLN  |
| 1   | D     | 587 | ASN  |
| 1   | D     | 606 | ASN  |
| 1   | D     | 608 | GLN  |
| 1   | D     | 614 | ASN  |
| 1   | D     | 622 | GLN  |
| 1   | D     | 663 | ASN  |
| 1   | D     | 679 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

There are no ligands in this entry.

## 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     | 675/687 (98%)   | -0.14  | 19 (2%)   | 53 | 50 | 15, 64, 105, 116      | 18 (2%) |
| 1   | B     | 675/687 (98%)   | 0.03   | 16 (2%)   | 59 | 56 | 19, 79, 112, 128      | 25 (3%) |
| 1   | C     | 675/687 (98%)   | -0.10  | 15 (2%)   | 62 | 59 | 36, 68, 109, 125      | 16 (2%) |
| 1   | D     | 675/687 (98%)   | 0.15   | 27 (4%)   | 38 | 37 | 48, 83, 114, 134      | 19 (2%) |
| All | All   | 2700/2748 (98%) | -0.01  | 77 (2%)   | 51 | 49 | 15, 74, 110, 134      | 78 (2%) |

All (77) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 215 | PRO  | 6.8  |
| 1   | D     | 290 | GLY  | 6.1  |
| 1   | D     | 326 | LEU  | 5.9  |
| 1   | D     | 618 | TYR  | 5.1  |
| 1   | D     | 170 | ALA  | 5.1  |
| 1   | D     | 138 | SER  | 4.8  |
| 1   | D     | 289 | HIS  | 4.8  |
| 1   | A     | 138 | SER  | 4.8  |
| 1   | C     | 72  | LEU  | 4.3  |
| 1   | C     | 139 | GLY  | 4.1  |
| 1   | C     | 138 | SER  | 4.0  |
| 1   | D     | 556 | GLY  | 3.8  |
| 1   | B     | 618 | TYR  | 3.7  |
| 1   | A     | 73  | PRO  | 3.7  |
| 1   | B     | 556 | GLY  | 3.5  |
| 1   | A     | 327 | LYS  | 3.4  |
| 1   | D     | 628 | ALA  | 3.4  |
| 1   | B     | 286 | GLY  | 3.3  |
| 1   | C     | 109 | LEU  | 3.3  |
| 1   | D     | 327 | LYS  | 3.2  |
| 1   | D     | 141 | ARG  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 415 | LEU  | 3.1  |
| 1   | B     | 554 | ALA  | 3.1  |
| 1   | A     | 618 | TYR  | 3.0  |
| 1   | D     | 135 | LEU  | 3.0  |
| 1   | A     | 74  | HIS  | 2.8  |
| 1   | D     | 439 | GLY  | 2.8  |
| 1   | D     | 211 | PHE  | 2.8  |
| 1   | B     | 161 | MET  | 2.8  |
| 1   | D     | 627 | SER  | 2.8  |
| 1   | A     | 575 | THR  | 2.8  |
| 1   | C     | 226 | LEU  | 2.7  |
| 1   | D     | 358 | GLY  | 2.7  |
| 1   | A     | 172 | LYS  | 2.6  |
| 1   | C     | 102 | LYS  | 2.6  |
| 1   | D     | 217 | LYS  | 2.6  |
| 1   | D     | 202 | VAL  | 2.5  |
| 1   | A     | 113 | ARG  | 2.5  |
| 1   | B     | 136 | LEU  | 2.5  |
| 1   | C     | 86  | GLY  | 2.4  |
| 1   | B     | 211 | PHE  | 2.4  |
| 1   | B     | 138 | SER  | 2.4  |
| 1   | A     | 198 | GLY  | 2.3  |
| 1   | A     | 210 | VAL  | 2.3  |
| 1   | B     | 616 | PHE  | 2.3  |
| 1   | A     | 104 | GLY  | 2.3  |
| 1   | C     | 30  | LEU  | 2.3  |
| 1   | C     | 415 | LEU  | 2.3  |
| 1   | D     | 106 | GLY  | 2.3  |
| 1   | A     | 215 | PRO  | 2.3  |
| 1   | C     | 288 | PRO  | 2.3  |
| 1   | D     | 216 | THR  | 2.3  |
| 1   | D     | 74  | HIS  | 2.2  |
| 1   | A     | 414 | ARG  | 2.2  |
| 1   | C     | 223 | TYR  | 2.2  |
| 1   | D     | 497 | ALA  | 2.2  |
| 1   | D     | 228 | MET  | 2.2  |
| 1   | A     | 616 | PHE  | 2.2  |
| 1   | D     | 73  | PRO  | 2.2  |
| 1   | B     | 229 | ASP  | 2.2  |
| 1   | D     | 551 | GLU  | 2.2  |
| 1   | B     | 289 | HIS  | 2.1  |
| 1   | B     | 617 | GLU  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 618 | TYR  | 2.1  |
| 1   | D     | 552 | PRO  | 2.1  |
| 1   | B     | 150 | SER  | 2.1  |
| 1   | C     | 225 | LEU  | 2.1  |
| 1   | A     | 75  | HIS  | 2.1  |
| 1   | B     | 498 | LEU  | 2.0  |
| 1   | A     | 139 | GLY  | 2.0  |
| 1   | D     | 328 | ARG  | 2.0  |
| 1   | A     | 222 | GLN  | 2.0  |
| 1   | B     | 151 | SER  | 2.0  |
| 1   | D     | 406 | TYR  | 2.0  |
| 1   | B     | 573 | PRO  | 2.0  |
| 1   | C     | 616 | PHE  | 2.0  |
| 1   | A     | 619 | MET  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.