



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:32 PM GMT

PDB ID : 3TYH  
Title : Crystal structure of oxo-copper clusters binding to ferric binding protein from *Neisseria gonorrhoeae*  
Authors : Chen, W.J.; Wang, H.F.; Zhou, C.J.; Ye, D.R.; Huang, J.; Tan, X.S.; Zhong, W.Q.  
Deposited on : 2011-09-26  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

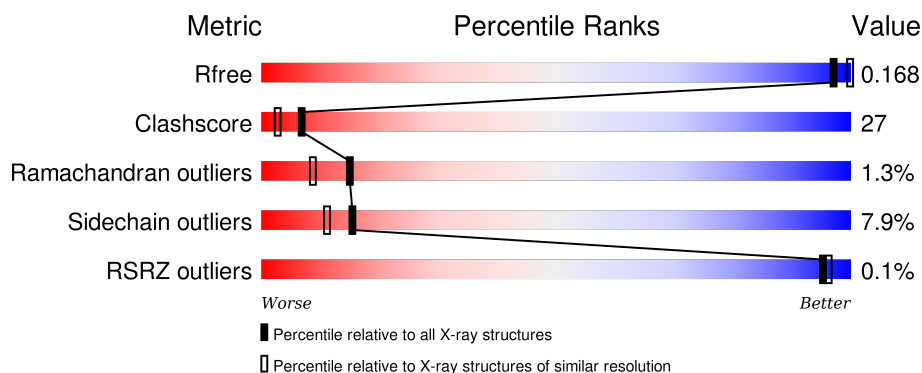
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 3939 (2.10-2.10)                                      |
| Clashscore            | 102246                      | 4460 (2.10-2.10)                                      |
| Ramachandran outliers | 100387                      | 4413 (2.10-2.10)                                      |
| Sidechain outliers    | 100360                      | 4414 (2.10-2.10)                                      |
| RSRZ outliers         | 91569                       | 3948 (2.10-2.10)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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     | 309    | <div> <div>61%</div> <div>36%</div> <div>.</div> </div>               |
| 1   | B     | 309    | <div> <div>57%</div> <div>38%</div> <div>5%</div> </div>              |
| 1   | C     | 309    | <div> <div>62%</div> <div>33%</div> <div>.</div> </div>               |
| 1   | D     | 309    | <div> <div>55%</div> <div>37%</div> <div>6%</div> <div>.</div> </div> |
| 1   | E     | 309    | <div> <div>65%</div> <div>29%</div> <div>5%</div> </div>              |

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| Mol | Chain | Length | Quality of chain                                      |
|-----|-------|--------|---|
| 1   | F     | 309    | <div><div></div><div>61%34%5% •</div></div>           |
| 1   | G     | 309    | <div><div></div><div>60%35%5%</div></div>             |
| 1   | H     | 309    | <div><div>%<div></div></div><div>48%47%5%</div></div> |
| 1   | I     | 309    | <div><div></div><div>47%47%6%</div></div>             |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22889 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 FbpA protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | B     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | C     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | D     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | E     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | F     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | G     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | H     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | I     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | G     | 2        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | D     | 2        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | E     | 2        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | H     | 2        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | B     | 2        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | I     | 2        | Total<br>2 | Cu<br>2 | 0       | 0       |
| 2   | C     | 2        | Total<br>2 | Cu<br>2 | 0       | 0       |
| 2   | A     | 2        | Total<br>2 | Cu<br>2 | 0       | 0       |
| 2   | F     | 2        | Total<br>2 | Cu<br>2 | 0       | 0       |

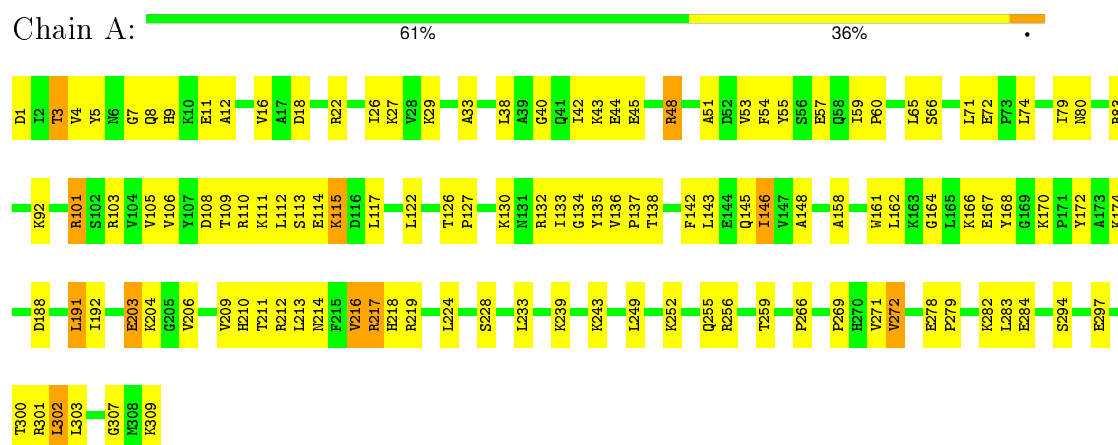
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 3   | A     | 217      | Total<br>217 | O<br>217 | 0       | 0       |
| 3   | B     | 166      | Total<br>166 | O<br>166 | 0       | 0       |
| 3   | C     | 188      | Total<br>188 | O<br>188 | 0       | 0       |
| 3   | D     | 177      | Total<br>177 | O<br>177 | 0       | 0       |
| 3   | E     | 178      | Total<br>178 | O<br>178 | 0       | 0       |
| 3   | F     | 181      | Total<br>181 | O<br>181 | 0       | 0       |
| 3   | G     | 123      | Total<br>123 | O<br>123 | 0       | 0       |
| 3   | H     | 120      | Total<br>120 | O<br>120 | 0       | 0       |
| 3   | I     | 119      | Total<br>119 | O<br>119 | 0       | 0       |

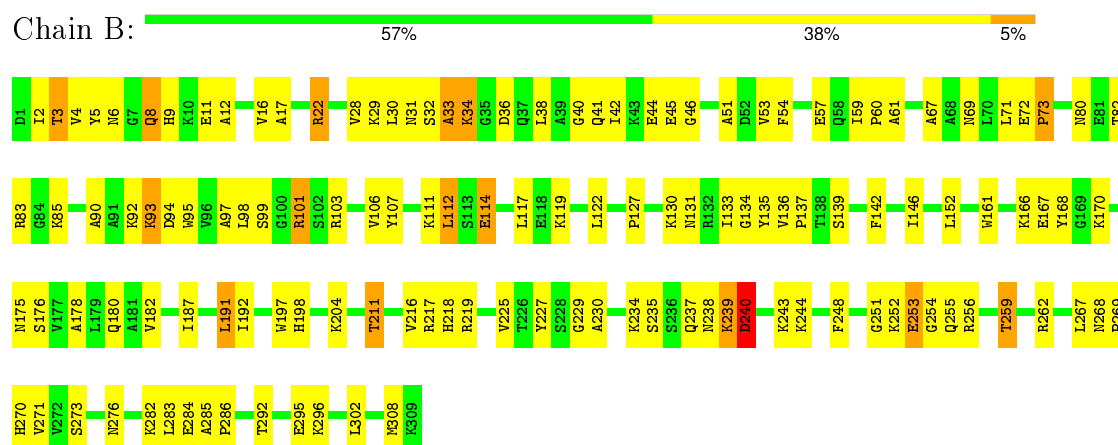
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

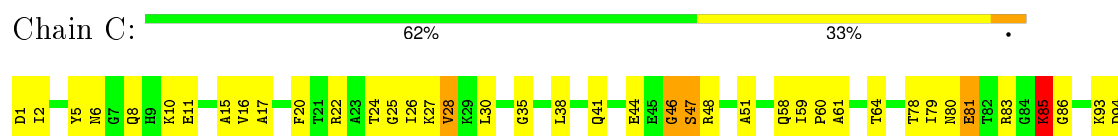
#### • Molecule 1: FbpA protein

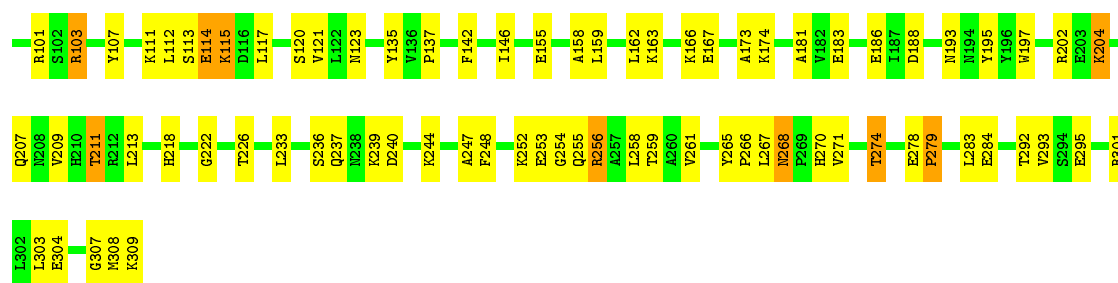


#### • Molecule 1: FbpA protein



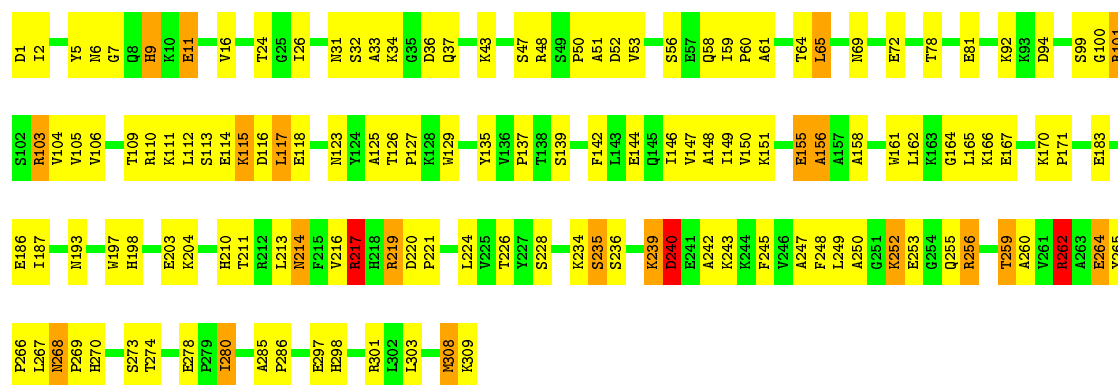
#### • Molecule 1: FbpA protein





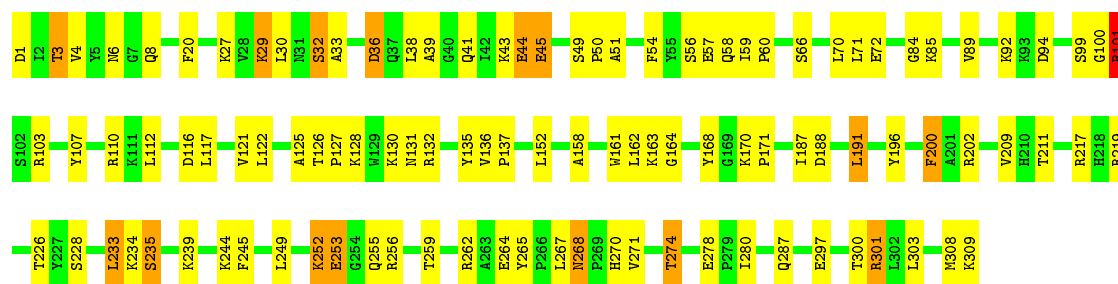
- Molecule 1: FbpA protein

Chain D: 55% 37% 6% .



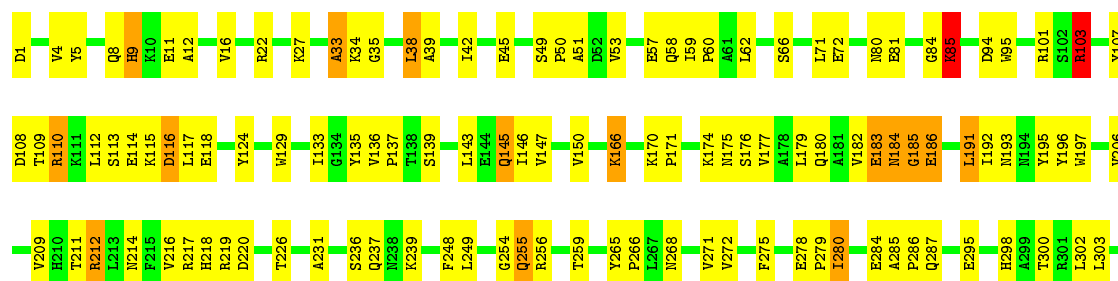
- Molecule 1: FbpA protein

Chain E: 65% 29% 5%



- Molecule 1: FbpA protein

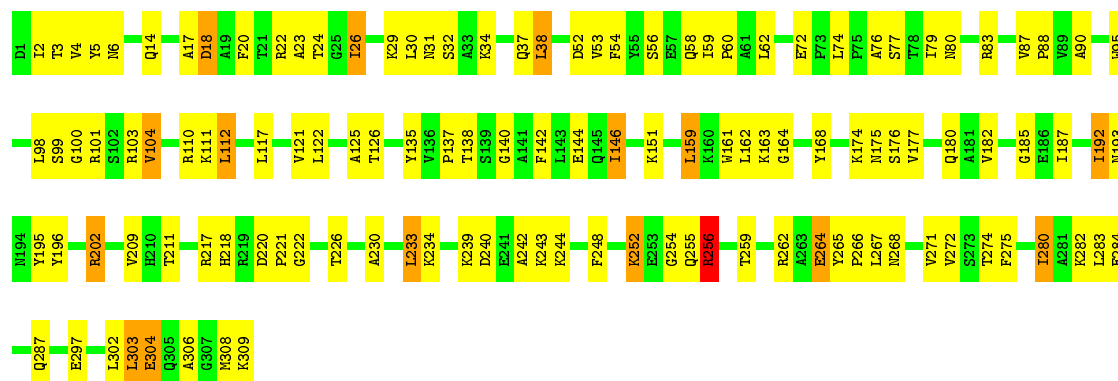
Chain F: 61% 34% 5% .



G307  
K308  
K309

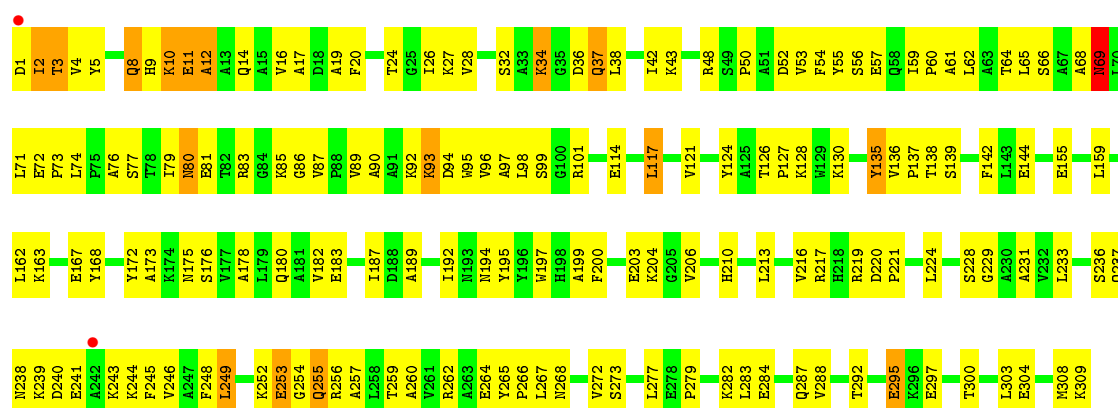
• Molecule 1: FbpA protein

Chain G: 



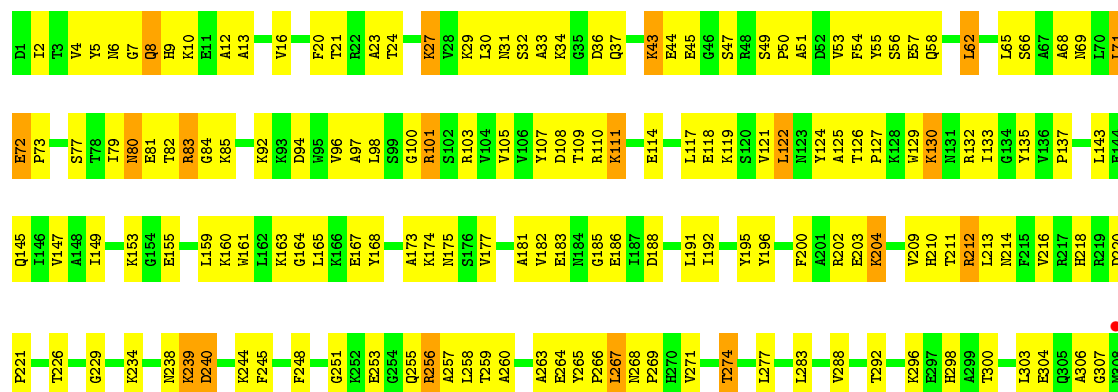
• Molecule 1: FbpA protein

Chain H: 



• Molecule 1: FbpA protein

Chain I: 





K309

## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 32   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 146.51Å 146.51Å 114.59Å<br>90.00° 90.00° 120.00°   | Depositor        |
| Resolution (Å)  | 47.96 – 2.10<br>47.96 – 2.10   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (47.96-2.10)<br>100.0 (47.96-2.10)  | Depositor<br>EDS |
| $R_{merge}$   | 0.14   | Depositor        |
| $R_{sym}$   | 0.16   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.30 (at 2.10Å)  | Xtriage          |
| Refinement program  | REFMAC 5.5.0102  | Depositor        |
| R, $R_{free}$   | 0.143 , 0.169<br>0.147 , 0.168   | Depositor<br>DCC |
| $R_{free}$ test set   | 8174 reflections (5.37%)   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 26.5   | Xtriage          |
| Anisotropy  | 0.001  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 41.7  | EDS              |
| Estimated twinning fraction   | 0.541 for H, K, L<br>0.459 for H+K, -K, -L<br>0.004 for -h,-k,l<br>0.018 for h,-h-k,-l<br>0.045 for -k,-h,-l | Xtriage          |
| Reported twinning fraction  | 0.541 for H, K, L<br>0.459 for H+K, -K, -L   | Depositor        |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$  | Xtriage          |
| Outliers  | 0 of 160455 reflections  | Xtriage          |
| $F_o, F_c$ correlation  | 0.97   | EDS              |
| Total number of atoms   | 22889  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 28.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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     | 0.69         | 0/2423         | 0.93        | 3/3280 (0.1%)   |
| 1   | B     | 0.64         | 0/2423         | 0.97        | 3/3280 (0.1%)   |
| 1   | C     | 0.65         | 0/2423         | 0.95        | 2/3280 (0.1%)   |
| 1   | D     | 0.60         | 0/2423         | 0.92        | 3/3280 (0.1%)   |
| 1   | E     | 0.63         | 0/2423         | 0.94        | 5/3280 (0.2%)   |
| 1   | F     | 0.73         | 1/2423 (0.0%)  | 1.01        | 9/3280 (0.3%)   |
| 1   | G     | 0.55         | 0/2423         | 0.90        | 2/3280 (0.1%)   |
| 1   | H     | 0.48         | 0/2423         | 0.87        | 1/3280 (0.0%)   |
| 1   | I     | 0.48         | 0/2423         | 0.88        | 2/3280 (0.1%)   |
| All | All   | 0.61         | 1/21807 (0.0%) | 0.93        | 30/29520 (0.1%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 85  | LYS  | C-N   | -6.11 | 1.22        | 1.33     |

All (30) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | C     | 103 | ARG  | NE-CZ-NH2 | -12.65 | 113.97      | 120.30   |
| 1   | F     | 85  | LYS  | C-N-CA    | -9.06  | 103.27      | 122.30   |
| 1   | E     | 101 | ARG  | NE-CZ-NH1 | -8.52  | 116.04      | 120.30   |
| 1   | A     | 101 | ARG  | NE-CZ-NH2 | -7.37  | 116.61      | 120.30   |
| 1   | E     | 103 | ARG  | NE-CZ-NH1 | 7.10   | 123.85      | 120.30   |
| 1   | F     | 84  | GLY  | O-C-N     | -6.94  | 111.59      | 122.70   |
| 1   | F     | 103 | ARG  | NE-CZ-NH1 | 6.92   | 123.76      | 120.30   |
| 1   | D     | 262 | ARG  | NE-CZ-NH1 | 6.72   | 123.66      | 120.30   |
| 1   | I     | 256 | ARG  | NE-CZ-NH2 | -6.65  | 116.97      | 120.30   |
| 1   | F     | 103 | ARG  | NE-CZ-NH2 | -6.58  | 117.01      | 120.30   |
| 1   | H     | 262 | ARG  | NE-CZ-NH1 | -6.47  | 117.06      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | I     | 101 | ARG  | NE-CZ-NH1 | 6.34  | 123.47      | 120.30   |
| 1   | A     | 301 | ARG  | NE-CZ-NH1 | 6.19  | 123.40      | 120.30   |
| 1   | B     | 22  | ARG  | NE-CZ-NH1 | 6.17  | 123.38      | 120.30   |
| 1   | F     | 85  | LYS  | O-C-N     | 6.16  | 133.67      | 123.20   |
| 1   | F     | 84  | GLY  | C-N-CA    | 6.02  | 136.75      | 121.70   |
| 1   | D     | 217 | ARG  | NE-CZ-NH1 | -5.91 | 117.35      | 120.30   |
| 1   | F     | 22  | ARG  | NE-CZ-NH1 | 5.89  | 123.25      | 120.30   |
| 1   | G     | 256 | ARG  | NE-CZ-NH1 | 5.73  | 123.17      | 120.30   |
| 1   | F     | 212 | ARG  | NE-CZ-NH2 | 5.71  | 123.16      | 120.30   |
| 1   | A     | 217 | ARG  | NE-CZ-NH1 | -5.66 | 117.47      | 120.30   |
| 1   | D     | 219 | ARG  | NE-CZ-NH1 | -5.61 | 117.50      | 120.30   |
| 1   | E     | 103 | ARG  | NE-CZ-NH2 | -5.35 | 117.62      | 120.30   |
| 1   | C     | 256 | ARG  | NE-CZ-NH2 | -5.27 | 117.67      | 120.30   |
| 1   | E     | 110 | ARG  | NE-CZ-NH1 | 5.21  | 122.90      | 120.30   |
| 1   | F     | 110 | ARG  | NE-CZ-NH2 | 5.15  | 122.87      | 120.30   |
| 1   | G     | 202 | ARG  | NE-CZ-NH1 | -5.07 | 117.76      | 120.30   |
| 1   | E     | 191 | LEU  | CA-CB-CG  | 5.07  | 126.96      | 115.30   |
| 1   | B     | 262 | ARG  | NE-CZ-NH1 | -5.04 | 117.78      | 120.30   |
| 1   | B     | 101 | ARG  | NE-CZ-NH2 | -5.01 | 117.80      | 120.30   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2378  | 0        | 2424     | 124     | 0            |
| 1   | B     | 2378  | 0        | 2424     | 118     | 0            |
| 1   | C     | 2378  | 0        | 2424     | 111     | 0            |
| 1   | D     | 2378  | 0        | 2424     | 154     | 0            |
| 1   | E     | 2378  | 0        | 2424     | 88      | 0            |
| 1   | F     | 2378  | 0        | 2423     | 133     | 0            |
| 1   | G     | 2378  | 0        | 2425     | 112     | 0            |
| 1   | H     | 2378  | 0        | 2424     | 172     | 0            |
| 1   | I     | 2378  | 0        | 2424     | 155     | 0            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| 2   | C     | 2     | 0        | 0        | 0       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 2   | E     | 2     | 0        | 0        | 0       | 0            |
| 2   | F     | 2     | 0        | 0        | 0       | 0            |
| 2   | G     | 2     | 0        | 0        | 0       | 0            |
| 2   | H     | 2     | 0        | 0        | 0       | 0            |
| 2   | I     | 2     | 0        | 0        | 0       | 0            |
| 3   | A     | 217   | 0        | 0        | 17      | 0            |
| 3   | B     | 166   | 0        | 0        | 14      | 0            |
| 3   | C     | 188   | 0        | 0        | 11      | 0            |
| 3   | D     | 177   | 0        | 0        | 19      | 0            |
| 3   | E     | 178   | 0        | 0        | 3       | 0            |
| 3   | F     | 181   | 0        | 0        | 14      | 0            |
| 3   | G     | 123   | 0        | 0        | 8       | 0            |
| 3   | H     | 120   | 0        | 0        | 30      | 0            |
| 3   | I     | 119   | 0        | 0        | 18      | 0            |
| All | All   | 22889 | 0        | 21816    | 1160    | 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 27.

All (1160) 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:B:252:LYS:HE2  | 1:B:256:ARG:NH2  | 1.45                     | 1.30              |
| 1:C:202:ARG:HH22 | 1:C:274:THR:HG23 | 1.07                     | 1.12              |
| 1:A:284:GLU:HB3  | 3:A:1406:HOH:O   | 1.49                     | 1.11              |
| 1:I:202:ARG:HH22 | 1:I:274:THR:HG23 | 1.14                     | 1.11              |
| 1:F:192:ILE:HG22 | 1:F:193:ASN:H    | 1.13                     | 1.08              |
| 1:E:202:ARG:HH22 | 1:E:274:THR:HG23 | 0.93                     | 1.06              |
| 1:A:279:PRO:HD2  | 1:A:282:LYS:HE2  | 1.34                     | 1.05              |
| 1:H:80:ASN:HA    | 1:H:83:ARG:HD3   | 1.39                     | 1.04              |
| 1:C:121:VAL:HG21 | 1:C:222:GLY:HA3  | 1.32                     | 1.04              |
| 1:A:101:ARG:HH22 | 1:A:228:SER:HB3  | 1.22                     | 1.01              |
| 1:D:125:ALA:HB1  | 1:D:164:GLY:HA3  | 1.42                     | 1.00              |
| 1:F:308:MET:O    | 1:F:308:MET:HG2  | 1.60                     | 1.00              |
| 1:B:4:VAL:HG22   | 1:B:53:VAL:HB    | 1.43                     | 0.98              |
| 1:H:54:PHE:HB3   | 1:H:231:ALA:HB3  | 1.45                     | 0.98              |
| 1:E:202:ARG:NH2  | 1:E:274:THR:HG23 | 1.79                     | 0.98              |
| 1:G:202:ARG:NH2  | 1:G:274:THR:HG22 | 1.79                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:1:ASP:OD1    | 1:H:27:LYS:HB2   | 1.64                     | 0.97              |
| 1:F:265:TYR:HB3  | 1:F:280:ILE:HG12 | 1.45                     | 0.97              |
| 1:E:170:LYS:HD2  | 1:E:187:ILE:HD12 | 1.43                     | 0.97              |
| 1:B:197:TRP:NE1  | 1:B:211:THR:HG22 | 1.82                     | 0.95              |
| 1:F:85:LYS:CE    | 1:F:219:ARG:HH22 | 1.80                     | 0.94              |
| 1:B:197:TRP:HE1  | 1:B:211:THR:HG22 | 1.27                     | 0.93              |
| 1:I:304:GLU:HG2  | 1:I:309:LYS:OXT  | 1.67                     | 0.93              |
| 1:A:146:ILE:HD13 | 1:A:162:LEU:HD11 | 1.49                     | 0.93              |
| 1:H:303:LEU:HB3  | 1:H:309:LYS:HG3  | 1.48                     | 0.93              |
| 1:H:32:SER:HA    | 3:H:1604:HOH:O   | 1.68                     | 0.92              |
| 1:B:252:LYS:HE2  | 1:B:256:ARG:HH21 | 1.11                     | 0.92              |
| 1:H:80:ASN:CA    | 1:H:83:ARG:HD3   | 2.00                     | 0.92              |
| 1:F:133:ILE:HB   | 3:F:1325:HOH:O   | 1.68                     | 0.92              |
| 1:H:99:SER:HA    | 1:H:267:LEU:HG   | 1.52                     | 0.92              |
| 1:F:192:ILE:HG22 | 1:F:193:ASN:N    | 1.81                     | 0.91              |
| 1:C:121:VAL:CG2  | 1:C:222:GLY:HA3  | 2.00                     | 0.91              |
| 1:H:17:ALA:HB1   | 1:H:28:VAL:HG21  | 1.52                     | 0.89              |
| 1:A:279:PRO:HD2  | 1:A:282:LYS:CE   | 2.03                     | 0.89              |
| 1:A:101:ARG:NH2  | 1:A:228:SER:HB3  | 1.88                     | 0.88              |
| 1:E:72:GLU:HG2   | 1:E:234:LYS:HA   | 1.56                     | 0.88              |
| 1:C:202:ARG:HH22 | 1:C:274:THR:CG2  | 1.87                     | 0.88              |
| 1:I:200:PHE:CE1  | 1:I:204:LYS:HG3  | 2.09                     | 0.88              |
| 1:D:267:LEU:HA   | 1:D:280:ILE:HD11 | 1.56                     | 0.87              |
| 1:F:85:LYS:NZ    | 1:F:219:ARG:HH22 | 1.70                     | 0.87              |
| 1:I:56:SER:HB3   | 3:I:1137:HOH:O   | 1.74                     | 0.87              |
| 1:A:111:LYS:O    | 1:A:112:LEU:HD23 | 1.75                     | 0.86              |
| 1:H:4:VAL:HG22   | 1:H:53:VAL:HB    | 1.54                     | 0.86              |
| 1:I:159:LEU:HD11 | 1:I:163:LYS:HE3  | 1.57                     | 0.86              |
| 1:B:252:LYS:CE   | 1:B:256:ARG:NH2  | 2.36                     | 0.86              |
| 1:C:162:LEU:HB3  | 1:C:308:MET:HE1  | 1.56                     | 0.85              |
| 1:C:202:ARG:NH2  | 1:C:274:THR:HG23 | 1.90                     | 0.85              |
| 1:F:147:VAL:HG22 | 1:F:295:GLU:HG3  | 1.58                     | 0.85              |
| 1:I:125:ALA:HB1  | 1:I:164:GLY:HA3  | 1.56                     | 0.85              |
| 1:A:278:GLU:HB3  | 1:A:282:LYS:HE2  | 1.58                     | 0.85              |
| 1:F:85:LYS:HZ1   | 1:F:219:ARG:NH2  | 1.73                     | 0.85              |
| 1:A:9:HIS:HD2    | 1:A:11:GLU:H     | 1.25                     | 0.85              |
| 1:H:303:LEU:HD13 | 1:H:309:LYS:HD2  | 1.59                     | 0.85              |
| 1:F:85:LYS:NZ    | 1:F:219:ARG:NH2  | 2.25                     | 0.84              |
| 1:B:80:ASN:OD1   | 1:B:83:ARG:HD3   | 1.77                     | 0.84              |
| 1:D:101:ARG:HH12 | 1:D:264:GLU:CG   | 1.91                     | 0.84              |
| 1:I:127:PRO:HA   | 1:I:130:LYS:HG3  | 1.58                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:275:PHE:HD1  | 3:F:1091:HOH:O   | 1.60                     | 0.83              |
| 1:F:85:LYS:HE2   | 1:F:219:ARG:HH22 | 1.41                     | 0.83              |
| 1:G:256:ARG:NH2  | 1:G:272:VAL:H    | 1.76                     | 0.83              |
| 1:E:202:ARG:HH22 | 1:E:274:THR:CG2  | 1.87                     | 0.83              |
| 1:H:38:LEU:O     | 1:H:42:ILE:HD12  | 1.79                     | 0.83              |
| 1:G:202:ARG:HH22 | 1:G:274:THR:HG22 | 1.42                     | 0.83              |
| 1:I:259:THR:CG2  | 1:I:266:PRO:HG3  | 2.09                     | 0.83              |
| 1:C:61:ALA:O     | 1:C:64:THR:HG22  | 1.78                     | 0.83              |
| 1:F:192:ILE:CG2  | 1:F:193:ASN:H    | 1.90                     | 0.82              |
| 1:F:129:TRP:HB3  | 3:F:1325:HOH:O   | 1.80                     | 0.82              |
| 1:H:80:ASN:C     | 1:H:83:ARG:HD3   | 2.00                     | 0.82              |
| 1:E:262:ARG:HG3  | 1:E:264:GLU:HG3  | 1.60                     | 0.81              |
| 1:A:252:LYS:HE2  | 1:A:256:ARG:HH12 | 1.45                     | 0.81              |
| 1:D:101:ARG:NH1  | 1:D:264:GLU:HG2  | 1.96                     | 0.81              |
| 1:I:82:THR:HB    | 1:I:267:LEU:HB3  | 1.61                     | 0.81              |
| 1:D:101:ARG:HH12 | 1:D:264:GLU:HG2  | 1.46                     | 0.81              |
| 1:B:41:GLN:HA    | 1:B:44:GLU:OE2   | 1.80                     | 0.81              |
| 1:H:62:LEU:HD13  | 1:H:95:TRP:HB2   | 1.63                     | 0.81              |
| 1:A:278:GLU:HB3  | 1:A:282:LYS:CE   | 2.11                     | 0.80              |
| 1:H:259:THR:HG21 | 1:H:266:PRO:HG3  | 1.62                     | 0.80              |
| 1:D:101:ARG:NH1  | 1:D:264:GLU:CB   | 2.45                     | 0.80              |
| 1:G:104:VAL:HG12 | 1:G:192:ILE:HG13 | 1.63                     | 0.80              |
| 1:F:110:ARG:HH22 | 1:F:183:GLU:C    | 1.83                     | 0.80              |
| 1:G:304:GLU:HA   | 1:G:309:LYS:HB2  | 1.64                     | 0.80              |
| 1:H:182:VAL:HG22 | 3:H:1274:HOH:O   | 1.82                     | 0.80              |
| 1:H:220:ASP:OD1  | 1:H:221:PRO:HD2  | 1.80                     | 0.80              |
| 1:F:147:VAL:HG13 | 1:F:295:GLU:HG2  | 1.62                     | 0.79              |
| 1:A:115:LYS:HB2  | 1:A:115:LYS:NZ   | 1.96                     | 0.79              |
| 1:F:265:TYR:HB3  | 1:F:280:ILE:CG1  | 2.12                     | 0.79              |
| 1:E:196:TYR:O    | 1:E:200:PHE:CD1  | 2.35                     | 0.79              |
| 1:F:129:TRP:HE3  | 3:F:1325:HOH:O   | 1.65                     | 0.79              |
| 1:G:5:TYR:HE1    | 1:G:31:ASN:HD22  | 1.29                     | 0.79              |
| 1:B:5:TYR:CE1    | 1:B:51:ALA:HB2   | 2.17                     | 0.79              |
| 1:I:182:VAL:HG13 | 1:I:211:THR:HG21 | 1.64                     | 0.79              |
| 1:H:20:PHE:CE1   | 1:H:24:THR:HG21  | 2.18                     | 0.79              |
| 1:B:252:LYS:CE   | 1:B:256:ARG:HH21 | 1.95                     | 0.78              |
| 1:C:51:ALA:HA    | 3:C:351:HOH:O    | 1.83                     | 0.78              |
| 1:I:202:ARG:NH2  | 1:I:274:THR:HG23 | 1.97                     | 0.78              |
| 1:G:259:THR:HG21 | 1:G:266:PRO:HG3  | 1.66                     | 0.77              |
| 1:A:7:GLY:HA2    | 1:A:33:ALA:O     | 1.84                     | 0.77              |
| 1:C:135:TYR:CE2  | 1:C:137:PRO:HG3  | 2.18                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:9:HIS:HB3    | 1:I:12:ALA:HB3   | 1.67                     | 0.76              |
| 1:D:101:ARG:N    | 1:D:101:ARG:HD2  | 1.98                     | 0.76              |
| 1:A:146:ILE:HD11 | 1:A:302:LEU:HD12 | 1.67                     | 0.76              |
| 1:I:72:GLU:HG3   | 1:I:239:LYS:HD2  | 1.67                     | 0.76              |
| 1:D:259:THR:HG23 | 1:D:273:SER:HA   | 1.69                     | 0.75              |
| 1:H:93:LYS:HA    | 3:H:1233:HOH:O   | 1.86                     | 0.75              |
| 1:G:303:LEU:HD12 | 1:G:309:LYS:HE2  | 1.68                     | 0.75              |
| 1:C:22:ARG:NH2   | 1:D:186:GLU:HG2  | 2.02                     | 0.75              |
| 1:E:72:GLU:CG    | 1:E:234:LYS:HA   | 2.17                     | 0.74              |
| 1:G:135:TYR:CE2  | 1:G:137:PRO:HG3  | 2.22                     | 0.74              |
| 1:D:114:GLU:HA   | 1:D:117:LEU:HD12 | 1.69                     | 0.74              |
| 1:H:137:PRO:HB3  | 1:H:308:MET:HE3  | 1.68                     | 0.74              |
| 1:D:16:VAL:HG11  | 1:D:249:LEU:CD2  | 2.17                     | 0.74              |
| 1:D:262:ARG:HB3  | 1:D:264:GLU:OE2  | 1.88                     | 0.74              |
| 1:A:112:LEU:HD11 | 1:A:188:ASP:HB3  | 1.68                     | 0.73              |
| 1:D:11:GLU:CD    | 1:D:11:GLU:H     | 1.91                     | 0.73              |
| 1:H:163:LYS:HD2  | 3:H:806:HOH:O    | 1.88                     | 0.73              |
| 1:E:158:ALA:O    | 1:E:162:LEU:HD13 | 1.88                     | 0.73              |
| 1:H:187:ILE:HG23 | 3:H:1274:HOH:O   | 1.89                     | 0.73              |
| 1:F:278:GLU:HB2  | 1:F:279:PRO:HD2  | 1.69                     | 0.73              |
| 1:C:35:GLY:HA3   | 3:C:424:HOH:O    | 1.88                     | 0.73              |
| 1:D:101:ARG:HH12 | 1:D:264:GLU:CB   | 2.01                     | 0.73              |
| 1:D:267:LEU:HD23 | 1:D:280:ILE:HD13 | 1.69                     | 0.73              |
| 1:D:264:GLU:HG2  | 3:D:1451:HOH:O   | 1.88                     | 0.72              |
| 1:I:29:LYS:HE3   | 1:I:31:ASN:HD21  | 1.54                     | 0.72              |
| 1:H:253:GLU:H    | 1:H:253:GLU:CD   | 1.93                     | 0.72              |
| 1:H:80:ASN:HA    | 1:H:83:ARG:CD    | 2.18                     | 0.72              |
| 1:G:159:LEU:HD23 | 1:G:302:LEU:HD22 | 1.72                     | 0.72              |
| 1:E:164:GLY:O    | 1:E:168:TYR:HD1  | 1.72                     | 0.72              |
| 1:I:309:LYS:HE3  | 3:I:841:HOH:O    | 1.89                     | 0.71              |
| 1:A:110:ARG:HE   | 1:A:210:HIS:CG   | 2.08                     | 0.71              |
| 1:E:43:LYS:HG2   | 1:E:70:LEU:CD1   | 2.20                     | 0.71              |
| 1:E:36:ASP:O     | 1:E:39:ALA:HB3   | 1.90                     | 0.71              |
| 1:H:71:LEU:HB2   | 1:H:94:ASP:HB3   | 1.72                     | 0.71              |
| 1:E:72:GLU:HG2   | 1:E:234:LYS:CA   | 2.20                     | 0.71              |
| 1:I:80:ASN:HB3   | 1:I:83:ARG:NH2   | 2.06                     | 0.71              |
| 1:C:80:ASN:HA    | 1:C:83:ARG:HG3   | 1.73                     | 0.71              |
| 1:I:114:GLU:HA   | 1:I:117:LEU:HD12 | 1.72                     | 0.70              |
| 1:G:252:LYS:HD2  | 1:G:252:LYS:H    | 1.56                     | 0.70              |
| 1:G:3:THR:OG1    | 1:G:29:LYS:HE3   | 1.91                     | 0.70              |
| 1:I:57:GLU:HG2   | 1:I:58:GLN:HG3   | 1.73                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:265:TYR:HB3  | 1:G:280:ILE:CG1  | 2.21                     | 0.70              |
| 1:F:16:VAL:HG11  | 1:F:249:LEU:HD23 | 1.72                     | 0.70              |
| 1:I:303:LEU:HD13 | 1:I:309:LYS:HG3  | 1.74                     | 0.70              |
| 1:D:155:GLU:OE2  | 1:D:298:HIS:HE1  | 1.75                     | 0.69              |
| 1:G:252:LYS:N    | 1:G:252:LYS:HD2  | 2.07                     | 0.69              |
| 1:F:265:TYR:CB   | 1:F:280:ILE:HG12 | 2.19                     | 0.69              |
| 1:E:252:LYS:HE2  | 1:E:252:LYS:H    | 1.57                     | 0.69              |
| 1:A:224:LEU:HB2  | 3:A:351:HOH:O    | 1.93                     | 0.69              |
| 1:D:61:ALA:O     | 1:D:65:LEU:HD22  | 1.93                     | 0.69              |
| 1:B:255:GLN:HB2  | 1:B:271:VAL:HG21 | 1.73                     | 0.69              |
| 1:A:279:PRO:CD   | 1:A:282:LYS:HE2  | 2.17                     | 0.69              |
| 1:C:303:LEU:HD12 | 1:C:308:MET:HE3  | 1.75                     | 0.69              |
| 1:C:240:ASP:O    | 1:C:244:LYS:HG3  | 1.92                     | 0.68              |
| 1:C:268:ASN:HD22 | 1:C:270:HIS:H    | 1.41                     | 0.68              |
| 1:D:197:TRP:HE1  | 1:D:211:THR:HG23 | 1.57                     | 0.68              |
| 1:H:66:SER:HB2   | 1:H:94:ASP:HB2   | 1.75                     | 0.68              |
| 1:I:135:TYR:CE2  | 1:I:137:PRO:HG3  | 2.28                     | 0.68              |
| 1:D:58:GLN:HB2   | 1:D:60:PRO:HD2   | 1.76                     | 0.68              |
| 1:B:5:TYR:CD1    | 1:B:51:ALA:HB2   | 2.28                     | 0.68              |
| 1:F:256:ARG:HH22 | 1:F:272:VAL:H    | 1.41                     | 0.68              |
| 1:D:47:SER:HA    | 1:D:235:SER:HB2  | 1.76                     | 0.68              |
| 1:H:20:PHE:O     | 1:H:24:THR:HG23  | 1.94                     | 0.68              |
| 1:I:122:LEU:HA   | 1:I:161:TRP:CD1  | 2.29                     | 0.67              |
| 1:B:41:GLN:HG2   | 3:B:550:HOH:O    | 1.93                     | 0.67              |
| 1:F:183:GLU:C    | 1:F:184:ASN:OD1  | 2.33                     | 0.67              |
| 1:H:128:LYS:HB3  | 3:H:1184:HOH:O   | 1.94                     | 0.67              |
| 1:H:4:VAL:HG22   | 1:H:53:VAL:CB    | 2.25                     | 0.67              |
| 1:A:259:THR:HG21 | 1:A:266:PRO:HG3  | 1.77                     | 0.66              |
| 1:A:101:ARG:HH22 | 1:A:228:SER:CB   | 2.04                     | 0.66              |
| 1:D:9:HIS:CG     | 1:D:11:GLU:OE1   | 2.49                     | 0.66              |
| 1:D:101:ARG:HG3  | 1:D:101:ARG:HH11 | 1.60                     | 0.66              |
| 1:F:184:ASN:O    | 1:F:186:GLU:N    | 2.28                     | 0.66              |
| 1:B:176:SER:O    | 1:B:180:GLN:HG3  | 1.94                     | 0.66              |
| 1:I:255:GLN:HB2  | 1:I:271:VAL:HG21 | 1.76                     | 0.66              |
| 1:C:204:LYS:HE3  | 3:C:1506:HOH:O   | 1.93                     | 0.66              |
| 1:C:265:TYR:CE2  | 1:C:283:LEU:HD11 | 2.30                     | 0.66              |
| 1:A:48:ARG:HA    | 1:A:48:ARG:NE    | 2.10                     | 0.66              |
| 1:F:248:PHE:O    | 1:F:254:GLY:HA3  | 1.95                     | 0.66              |
| 1:F:191:LEU:N    | 1:F:191:LEU:HD22 | 2.11                     | 0.66              |
| 1:D:5:TYR:CE1    | 1:D:51:ALA:HB2   | 2.31                     | 0.65              |
| 1:B:5:TYR:HA     | 1:B:31:ASN:HB3   | 1.79                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:255:GLN:O    | 1:D:259:THR:HB   | 1.97                     | 0.65              |
| 1:B:135:TYR:CE2  | 1:B:137:PRO:HG3  | 2.31                     | 0.65              |
| 1:C:85:LYS:HG3   | 1:C:86:GLY:H     | 1.60                     | 0.65              |
| 1:H:219:ARG:HG3  | 3:H:1532:HOH:O   | 1.96                     | 0.65              |
| 1:C:301:ARG:HG2  | 3:C:1111:HOH:O   | 1.95                     | 0.65              |
| 1:D:16:VAL:HG11  | 1:D:249:LEU:HD23 | 1.79                     | 0.65              |
| 1:D:72:GLU:HG3   | 1:D:239:LYS:HE2  | 1.77                     | 0.65              |
| 1:D:259:THR:CG2  | 1:D:273:SER:HA   | 2.27                     | 0.65              |
| 1:H:12:ALA:O     | 1:H:16:VAL:HG23  | 1.97                     | 0.65              |
| 1:B:127:PRO:HG3  | 1:B:168:TYR:CZ   | 2.31                     | 0.65              |
| 1:B:197:TRP:CD1  | 1:B:211:THR:HG22 | 2.31                     | 0.64              |
| 1:F:9:HIS:CD2    | 1:F:11:GLU:HG2   | 2.32                     | 0.64              |
| 1:E:41:GLN:O     | 1:E:44:GLU:HB2   | 1.97                     | 0.64              |
| 1:B:9:HIS:HD2    | 1:B:12:ALA:H     | 1.43                     | 0.64              |
| 1:C:121:VAL:HG21 | 1:C:222:GLY:CA   | 2.20                     | 0.64              |
| 1:A:9:HIS:CD2    | 1:A:11:GLU:H     | 2.12                     | 0.64              |
| 1:D:101:ARG:NH1  | 1:D:264:GLU:HB2  | 2.12                     | 0.64              |
| 1:E:268:ASN:HD22 | 1:E:268:ASN:C    | 2.01                     | 0.64              |
| 1:D:268:ASN:HD22 | 1:D:270:HIS:H    | 1.46                     | 0.64              |
| 1:I:72:GLU:OE1   | 1:I:73:PRO:HD2   | 1.98                     | 0.64              |
| 1:A:4:VAL:HG13   | 1:A:53:VAL:HB    | 1.79                     | 0.64              |
| 1:D:219:ARG:NH1  | 1:D:285:ALA:O    | 2.29                     | 0.64              |
| 1:I:259:THR:HG21 | 1:I:266:PRO:HG3  | 1.79                     | 0.64              |
| 1:A:57:GLU:HG2   | 1:A:101:ARG:NH1  | 2.12                     | 0.64              |
| 3:A:1431:HOH:O   | 1:H:50:PRO:HB3   | 1.97                     | 0.64              |
| 1:D:104:VAL:HG22 | 1:D:105:VAL:N    | 2.13                     | 0.64              |
| 1:D:111:LYS:O    | 1:D:112:LEU:HD23 | 1.97                     | 0.64              |
| 1:D:183:GLU:OE1  | 1:D:211:THR:HG22 | 1.97                     | 0.64              |
| 1:H:236:SER:HB2  | 1:H:239:LYS:HE2  | 1.79                     | 0.64              |
| 1:A:106:VAL:HG22 | 1:A:213:LEU:CD2  | 2.28                     | 0.64              |
| 1:G:304:GLU:OE2  | 1:G:309:LYS:HD3  | 1.98                     | 0.64              |
| 1:D:101:ARG:NH1  | 1:D:264:GLU:CG   | 2.55                     | 0.63              |
| 1:F:135:TYR:CE2  | 1:F:137:PRO:HG3  | 2.33                     | 0.63              |
| 1:D:5:TYR:CD1    | 1:D:51:ALA:HB2   | 2.33                     | 0.63              |
| 1:B:296:LYS:HG2  | 3:B:1149:HOH:O   | 1.97                     | 0.63              |
| 1:E:4:VAL:HB     | 1:E:30:LEU:HD23  | 1.79                     | 0.63              |
| 1:H:144:GLU:HG3  | 1:H:224:LEU:HD21 | 1.81                     | 0.63              |
| 1:B:197:TRP:CD1  | 1:B:211:THR:CG2  | 2.82                     | 0.63              |
| 1:I:200:PHE:HE1  | 1:I:204:LYS:HG3  | 1.59                     | 0.63              |
| 1:E:101:ARG:HH11 | 1:E:101:ARG:HG3  | 1.63                     | 0.63              |
| 1:F:256:ARG:NH2  | 1:F:272:VAL:H    | 1.96                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:34:LYS:NZ    | 1:F:58:GLN:OE1   | 2.31                     | 0.63              |
| 1:B:57:GLU:HG2   | 3:B:320:HOH:O    | 1.97                     | 0.63              |
| 1:I:119:LYS:O    | 1:I:216:VAL:HG23 | 2.00                     | 0.62              |
| 1:I:145:GLN:O    | 1:I:149:ILE:HG13 | 2.00                     | 0.62              |
| 1:B:166:LYS:HD3  | 1:B:308:MET:HG2  | 1.81                     | 0.62              |
| 1:C:5:TYR:CE1    | 1:C:51:ALA:HB2   | 2.33                     | 0.62              |
| 1:C:80:ASN:OD1   | 1:C:83:ARG:HD3   | 1.99                     | 0.62              |
| 1:I:121:VAL:HG13 | 1:I:122:LEU:HD23 | 1.81                     | 0.62              |
| 1:D:297:GLU:O    | 1:D:301:ARG:HG2  | 1.98                     | 0.62              |
| 1:E:112:LEU:HD12 | 1:E:116:ASP:HB2  | 1.80                     | 0.62              |
| 1:H:303:LEU:CD1  | 1:H:309:LYS:HD2  | 2.29                     | 0.62              |
| 1:C:79:ILE:HD12  | 1:C:93:LYS:HG3   | 1.82                     | 0.62              |
| 1:A:133:ILE:HD11 | 1:A:191:LEU:HD13 | 1.81                     | 0.62              |
| 1:C:22:ARG:HH22  | 1:D:186:GLU:HG2  | 1.65                     | 0.62              |
| 1:H:11:GLU:O     | 1:H:12:ALA:C     | 2.38                     | 0.62              |
| 1:I:143:LEU:O    | 1:I:147:VAL:HG23 | 2.00                     | 0.62              |
| 1:F:101:ARG:NH2  | 1:F:226:THR:HG22 | 2.15                     | 0.62              |
| 1:G:4:VAL:HB     | 1:G:30:LEU:HD23  | 1.81                     | 0.62              |
| 1:H:183:GLU:OE2  | 1:H:210:HIS:CD2  | 2.53                     | 0.62              |
| 1:F:129:TRP:CE3  | 3:F:1325:HOH:O   | 2.42                     | 0.62              |
| 1:D:224:LEU:HD11 | 3:D:1605:HOH:O   | 1.98                     | 0.62              |
| 1:F:112:LEU:HD22 | 3:F:520:HOH:O    | 1.99                     | 0.62              |
| 1:D:118:GLU:HB3  | 1:D:123:ASN:HB2  | 1.80                     | 0.62              |
| 1:A:219:ARG:N    | 3:A:1406:HOH:O   | 2.32                     | 0.62              |
| 1:I:108:ASP:HB3  | 3:I:1227:HOH:O   | 1.98                     | 0.62              |
| 1:G:53:VAL:HG23  | 1:G:242:ALA:HB1  | 1.82                     | 0.62              |
| 1:D:217:ARG:NH1  | 1:D:278:GLU:OE2  | 2.31                     | 0.62              |
| 1:I:9:HIS:HB3    | 1:I:12:ALA:CB    | 2.30                     | 0.61              |
| 1:I:177:VAL:HG23 | 3:I:365:HOH:O    | 1.98                     | 0.61              |
| 1:B:36:ASP:OD1   | 1:B:61:ALA:HB2   | 2.00                     | 0.61              |
| 1:I:81:GLU:OE1   | 1:I:268:ASN:ND2  | 2.32                     | 0.61              |
| 1:H:17:ALA:HB1   | 1:H:28:VAL:CG2   | 2.28                     | 0.61              |
| 1:H:66:SER:O     | 1:H:92:LYS:HE3   | 2.00                     | 0.61              |
| 1:H:245:PHE:O    | 1:H:249:LEU:HB2  | 1.99                     | 0.61              |
| 1:I:127:PRO:HA   | 1:I:130:LYS:CG   | 2.30                     | 0.61              |
| 1:H:80:ASN:O     | 1:H:83:ARG:HD3   | 2.00                     | 0.61              |
| 1:I:71:LEU:HB3   | 1:I:94:ASP:HB2   | 1.81                     | 0.61              |
| 1:H:61:ALA:O     | 1:H:64:THR:HG22  | 2.01                     | 0.61              |
| 1:F:66:SER:HB2   | 1:F:71:LEU:HD12  | 1.82                     | 0.61              |
| 1:B:218:HIS:HA   | 1:B:284:GLU:OE2  | 2.00                     | 0.61              |
| 1:D:252:LYS:HE3  | 1:D:252:LYS:H    | 1.66                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:234:LYS:O    | 1:E:239:LYS:NZ   | 2.33                     | 0.61              |
| 1:H:8:GLN:HG3    | 1:H:9:HIS:N      | 2.14                     | 0.61              |
| 1:C:303:LEU:HD12 | 1:C:308:MET:CE   | 2.31                     | 0.61              |
| 1:G:303:LEU:HB3  | 1:G:309:LYS:HE2  | 1.82                     | 0.61              |
| 1:G:287:GLN:HB2  | 3:G:1054:HOH:O   | 2.01                     | 0.61              |
| 1:H:53:VAL:HG23  | 3:H:1069:HOH:O   | 2.01                     | 0.61              |
| 1:I:114:GLU:CD   | 1:I:214:ASN:HD22 | 2.04                     | 0.61              |
| 1:A:164:GLY:O    | 1:A:168:TYR:HD1  | 1.84                     | 0.61              |
| 1:D:267:LEU:CD2  | 1:D:280:ILE:HD13 | 2.30                     | 0.60              |
| 1:G:99:SER:HB2   | 1:G:264:GLU:HG2  | 1.83                     | 0.60              |
| 1:G:303:LEU:HB3  | 1:G:309:LYS:CE   | 2.30                     | 0.60              |
| 1:A:115:LYS:HB2  | 1:A:115:LYS:HZ2  | 1.66                     | 0.60              |
| 1:B:34:LYS:HE3   | 3:B:1298:HOH:O   | 2.00                     | 0.60              |
| 1:B:237:GLN:CD   | 1:B:237:GLN:H    | 2.03                     | 0.60              |
| 1:D:267:LEU:HD23 | 1:D:280:ILE:CD1  | 2.32                     | 0.60              |
| 1:G:255:GLN:HE22 | 1:G:267:LEU:H    | 1.49                     | 0.60              |
| 1:C:236:SER:HB3  | 1:C:239:LYS:HE2  | 1.84                     | 0.60              |
| 1:H:279:PRO:HD2  | 1:H:282:LYS:HG3  | 1.82                     | 0.60              |
| 1:I:130:LYS:HA   | 1:I:168:TYR:O    | 2.01                     | 0.60              |
| 1:E:66:SER:HB2   | 1:E:71:LEU:HD12  | 1.84                     | 0.60              |
| 1:I:105:VAL:HG22 | 1:I:191:LEU:HD23 | 1.82                     | 0.60              |
| 1:I:5:TYR:CE1    | 1:I:51:ALA:HB2   | 2.35                     | 0.60              |
| 1:C:309:LYS:HB2  | 3:C:629:HOH:O    | 2.01                     | 0.60              |
| 1:I:143:LEU:HD21 | 1:I:296:LYS:HG3  | 1.84                     | 0.60              |
| 1:G:142:PHE:O    | 1:G:146:ILE:HD13 | 2.02                     | 0.60              |
| 1:H:76:ALA:HA    | 1:H:79:ILE:HD12  | 1.83                     | 0.60              |
| 1:I:259:THR:HG22 | 1:I:266:PRO:HG3  | 1.84                     | 0.60              |
| 1:E:3:THR:HG22   | 1:E:29:LYS:NZ    | 2.17                     | 0.60              |
| 1:G:99:SER:CB    | 1:G:264:GLU:HG2  | 2.32                     | 0.60              |
| 1:C:59:ILE:HB    | 1:C:60:PRO:HD3   | 1.84                     | 0.60              |
| 1:C:114:GLU:HA   | 1:C:117:LEU:HD12 | 1.84                     | 0.59              |
| 1:H:62:LEU:HB3   | 1:H:95:TRP:CD1   | 2.36                     | 0.59              |
| 1:E:43:LYS:HG2   | 1:E:70:LEU:HD11  | 1.83                     | 0.59              |
| 1:B:239:LYS:NZ   | 1:B:239:LYS:HB3  | 2.17                     | 0.59              |
| 1:A:117:LEU:HD22 | 1:A:214:ASN:CB   | 2.32                     | 0.59              |
| 1:I:62:LEU:CD1   | 1:I:62:LEU:N     | 2.64                     | 0.59              |
| 1:F:114:GLU:HG2  | 1:F:214:ASN:ND2  | 2.18                     | 0.59              |
| 1:G:20:PHE:HE1   | 1:G:244:LYS:HG2  | 1.67                     | 0.59              |
| 1:H:34:LYS:HD3   | 1:H:37:GLN:HE21  | 1.67                     | 0.59              |
| 1:D:110:ARG:HA   | 3:D:1007:HOH:O   | 2.03                     | 0.59              |
| 1:I:234:LYS:O    | 1:I:239:LYS:NZ   | 2.35                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:167:GLU:HG3  | 1:H:168:TYR:CD2  | 2.38                     | 0.59              |
| 1:C:166:LYS:HE3  | 1:C:307:GLY:O    | 2.03                     | 0.59              |
| 1:D:239:LYS:O    | 1:D:243:LYS:HG3  | 2.03                     | 0.58              |
| 1:A:252:LYS:HE2  | 1:A:256:ARG:NH1  | 2.14                     | 0.58              |
| 1:B:133:ILE:HD11 | 1:B:191:LEU:HD13 | 1.85                     | 0.58              |
| 1:H:62:LEU:HD13  | 1:H:95:TRP:CB    | 2.33                     | 0.58              |
| 1:I:135:TYR:CD2  | 1:I:137:PRO:HG3  | 2.39                     | 0.58              |
| 1:B:122:LEU:HA   | 1:B:161:TRP:CD1  | 2.38                     | 0.58              |
| 1:I:72:GLU:HG3   | 1:I:239:LYS:CD   | 2.33                     | 0.58              |
| 1:A:145:GLN:NE2  | 3:A:351:HOH:O    | 2.37                     | 0.58              |
| 1:E:51:ALA:HB3   | 1:E:233:LEU:HD11 | 1.85                     | 0.58              |
| 1:F:308:MET:O    | 1:F:308:MET:CG   | 2.40                     | 0.58              |
| 1:B:36:ASP:HB2   | 3:B:1298:HOH:O   | 2.03                     | 0.58              |
| 1:D:99:SER:OG    | 1:D:101:ARG:NH2  | 2.36                     | 0.58              |
| 1:F:34:LYS:HD3   | 1:F:35:GLY:N     | 2.18                     | 0.58              |
| 1:F:166:LYS:HD3  | 1:F:307:GLY:O    | 2.04                     | 0.58              |
| 1:E:125:ALA:HB1  | 1:E:164:GLY:HA3  | 1.85                     | 0.58              |
| 1:A:48:ARG:C     | 1:A:48:ARG:HE    | 2.06                     | 0.58              |
| 1:D:7:GLY:HA2    | 1:D:33:ALA:O     | 2.02                     | 0.58              |
| 1:A:136:VAL:HG13 | 1:A:172:TYR:O    | 2.04                     | 0.58              |
| 1:G:34:LYS:O     | 1:G:37:GLN:HB3   | 2.03                     | 0.58              |
| 1:H:38:LEU:HD21  | 3:H:1604:HOH:O   | 2.03                     | 0.58              |
| 1:I:129:TRP:O    | 1:I:130:LYS:C    | 2.42                     | 0.58              |
| 1:F:136:VAL:O    | 1:F:139:SER:HB3  | 2.03                     | 0.58              |
| 1:A:126:THR:HB   | 1:A:127:PRO:HD2  | 1.86                     | 0.58              |
| 1:D:197:TRP:NE1  | 1:D:211:THR:HG23 | 2.19                     | 0.58              |
| 1:A:106:VAL:HG21 | 1:A:192:ILE:HD11 | 1.86                     | 0.58              |
| 1:C:120:SER:HB3  | 1:C:123:ASN:OD1  | 2.03                     | 0.58              |
| 1:A:203:GLU:HG3  | 1:A:204:LYS:N    | 2.17                     | 0.58              |
| 1:F:182:VAL:C    | 1:F:184:ASN:H    | 2.07                     | 0.58              |
| 1:D:236:SER:HB3  | 1:D:239:LYS:HD2  | 1.85                     | 0.58              |
| 1:C:81:GLU:HA    | 1:C:81:GLU:OE1   | 2.04                     | 0.58              |
| 1:G:110:ARG:C    | 1:G:111:LYS:HD2  | 2.24                     | 0.58              |
| 1:H:77:SER:HA    | 3:H:1079:HOH:O   | 2.03                     | 0.57              |
| 1:I:118:GLU:HB2  | 1:I:124:TYR:CE2  | 2.39                     | 0.57              |
| 1:D:72:GLU:HG2   | 1:D:234:LYS:HA   | 1.86                     | 0.57              |
| 1:A:233:LEU:H    | 1:A:233:LEU:HD12 | 1.69                     | 0.57              |
| 1:E:85:LYS:N     | 1:E:85:LYS:HD2   | 2.18                     | 0.57              |
| 1:H:17:ALA:CB    | 1:H:28:VAL:HG21  | 2.28                     | 0.57              |
| 1:G:6:ASN:O      | 1:G:32:SER:HA    | 2.04                     | 0.57              |
| 1:F:1:ASP:CG     | 1:F:27:LYS:HB2   | 2.25                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:54:PHE:CE2   | 1:I:62:LEU:HD12  | 2.39                     | 0.57              |
| 1:C:58:GLN:HB2   | 3:C:424:HOH:O    | 2.04                     | 0.57              |
| 1:F:166:LYS:O    | 1:F:166:LYS:HE2  | 2.03                     | 0.57              |
| 1:D:101:ARG:CZ   | 3:D:1451:HOH:O   | 2.53                     | 0.57              |
| 1:A:48:ARG:NE    | 1:A:48:ARG:CA    | 2.67                     | 0.57              |
| 1:F:81:GLU:HG2   | 3:F:729:HOH:O    | 2.04                     | 0.57              |
| 1:D:101:ARG:HG3  | 1:D:101:ARG:NH1  | 2.20                     | 0.57              |
| 1:F:16:VAL:HG11  | 1:F:249:LEU:CD2  | 2.34                     | 0.57              |
| 1:H:54:PHE:HB3   | 1:H:231:ALA:CB   | 2.29                     | 0.57              |
| 1:I:9:HIS:HA     | 3:I:1201:HOH:O   | 2.03                     | 0.57              |
| 1:F:278:GLU:HB2  | 1:F:279:PRO:CD   | 2.35                     | 0.57              |
| 1:B:106:VAL:CG2  | 1:B:211:THR:HG23 | 2.34                     | 0.57              |
| 1:D:256:ARG:HG3  | 3:D:350:HOH:O    | 2.04                     | 0.57              |
| 1:D:37:GLN:HG3   | 3:D:757:HOH:O    | 2.05                     | 0.57              |
| 1:B:106:VAL:HG23 | 1:B:211:THR:HG23 | 1.86                     | 0.57              |
| 1:I:163:LYS:HE2  | 1:I:306:ALA:HA   | 1.87                     | 0.57              |
| 1:H:273:SER:HA   | 3:H:1390:HOH:O   | 2.04                     | 0.56              |
| 1:H:216:VAL:HG21 | 1:H:220:ASP:OD2  | 2.04                     | 0.56              |
| 1:B:5:TYR:HB3    | 1:B:38:LEU:HD13  | 1.88                     | 0.56              |
| 1:D:9:HIS:ND1    | 1:D:11:GLU:OE1   | 2.38                     | 0.56              |
| 1:A:110:ARG:NH1  | 3:A:1141:HOH:O   | 2.38                     | 0.56              |
| 1:H:86:GLY:HA2   | 1:H:287:GLN:NE2  | 2.21                     | 0.56              |
| 1:A:146:ILE:HD12 | 1:A:158:ALA:HB1  | 1.87                     | 0.56              |
| 1:F:259:THR:HG21 | 1:F:266:PRO:HG3  | 1.87                     | 0.56              |
| 1:A:135:TYR:CD2  | 1:A:137:PRO:HD3  | 2.40                     | 0.56              |
| 1:B:5:TYR:HA     | 1:B:31:ASN:O     | 2.05                     | 0.56              |
| 1:F:147:VAL:HG13 | 1:F:295:GLU:CG   | 2.34                     | 0.56              |
| 1:A:130:LYS:O    | 1:A:132:ARG:HG3  | 2.06                     | 0.56              |
| 1:F:184:ASN:C    | 1:F:186:GLU:H    | 2.08                     | 0.56              |
| 1:A:300:THR:HG23 | 1:A:309:LYS:HE3  | 1.87                     | 0.56              |
| 1:D:142:PHE:HE2  | 1:D:308:MET:HE1  | 1.70                     | 0.56              |
| 1:G:233:LEU:HD12 | 1:G:233:LEU:N    | 2.20                     | 0.56              |
| 1:D:118:GLU:OE2  | 1:D:129:TRP:NE1  | 2.28                     | 0.56              |
| 1:D:308:MET:O    | 1:D:309:LYS:HD2  | 2.06                     | 0.56              |
| 1:H:268:ASN:ND2  | 3:H:1198:HOH:O   | 2.39                     | 0.56              |
| 1:D:220:ASP:O    | 1:D:286:PRO:HG3  | 2.05                     | 0.56              |
| 1:G:282:LYS:HE3  | 3:G:1294:HOH:O   | 2.06                     | 0.56              |
| 1:C:24:THR:OG1   | 1:C:26:ILE:HG12  | 2.05                     | 0.56              |
| 1:F:80:ASN:HD21  | 1:I:47:SER:CB    | 2.18                     | 0.56              |
| 1:C:255:GLN:HE22 | 1:C:267:LEU:H    | 1.54                     | 0.56              |
| 1:E:6:ASN:O      | 1:E:32:SER:HA    | 2.04                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:200:PHE:CD1  | 1:E:200:PHE:N    | 2.74                     | 0.56              |
| 1:B:178:ALA:O    | 1:B:182:VAL:HG23 | 2.06                     | 0.56              |
| 1:H:80:ASN:HB2   | 3:H:1079:HOH:O   | 2.06                     | 0.55              |
| 1:F:300:THR:HA   | 1:F:303:LEU:HD12 | 1.87                     | 0.55              |
| 1:C:94:ASP:N     | 1:C:94:ASP:OD1   | 2.39                     | 0.55              |
| 1:I:83:ARG:NH2   | 3:I:774:HOH:O    | 2.38                     | 0.55              |
| 1:E:126:THR:HB   | 1:E:127:PRO:HD2  | 1.88                     | 0.55              |
| 1:E:128:LYS:HZ2  | 1:E:132:ARG:HH12 | 1.54                     | 0.55              |
| 1:H:38:LEU:HB2   | 1:H:54:PHE:HE1   | 1.70                     | 0.55              |
| 1:E:4:VAL:HB     | 1:E:30:LEU:CD2   | 2.36                     | 0.55              |
| 1:F:34:LYS:HE2   | 1:F:57:GLU:OE1   | 2.06                     | 0.55              |
| 1:A:117:LEU:HD22 | 1:A:214:ASN:HB2  | 1.88                     | 0.55              |
| 1:F:108:ASP:OD2  | 1:F:110:ARG:HB2  | 2.07                     | 0.55              |
| 1:H:252:LYS:N    | 3:H:1198:HOH:O   | 2.25                     | 0.55              |
| 1:B:142:PHE:O    | 1:B:146:ILE:HG13 | 2.07                     | 0.55              |
| 1:E:122:LEU:HA   | 1:E:161:TRP:CD1  | 2.42                     | 0.55              |
| 1:I:34:LYS:HG3   | 1:I:37:GLN:HB2   | 1.87                     | 0.55              |
| 1:H:256:ARG:HH11 | 1:H:256:ARG:HB2  | 1.70                     | 0.55              |
| 1:C:304:GLU:OE2  | 1:C:309:LYS:HD2  | 2.05                     | 0.55              |
| 1:E:200:PHE:HD1  | 1:E:200:PHE:N    | 2.05                     | 0.55              |
| 1:I:7:GLY:HA2    | 1:I:33:ALA:O     | 2.07                     | 0.55              |
| 1:H:2:ILE:HG22   | 1:H:238:ASN:CB   | 2.37                     | 0.55              |
| 1:H:139:SER:HB3  | 1:H:142:PHE:HB2  | 1.89                     | 0.55              |
| 1:D:101:ARG:HD2  | 1:D:226:THR:O    | 2.07                     | 0.55              |
| 1:D:101:ARG:HH12 | 1:D:264:GLU:HB2  | 1.67                     | 0.55              |
| 1:D:59:ILE:N     | 1:D:60:PRO:CD    | 2.70                     | 0.55              |
| 1:B:225:VAL:HG23 | 1:B:285:ALA:HB2  | 1.88                     | 0.55              |
| 1:I:65:LEU:HB3   | 1:I:71:LEU:CD1   | 2.37                     | 0.55              |
| 1:I:100:GLY:O    | 1:I:264:GLU:HG2  | 2.05                     | 0.55              |
| 1:F:184:ASN:N    | 1:F:184:ASN:OD1  | 2.41                     | 0.55              |
| 1:F:108:ASP:OD1  | 1:F:185:GLY:HA3  | 2.07                     | 0.55              |
| 1:D:69:ASN:OD1   | 1:D:92:LYS:NZ    | 2.37                     | 0.55              |
| 1:G:38:LEU:HD23  | 1:G:54:PHE:HE1   | 1.72                     | 0.55              |
| 1:A:256:ARG:HG2  | 1:A:271:VAL:HG13 | 1.89                     | 0.54              |
| 1:C:80:ASN:HA    | 1:C:83:ARG:CG    | 2.36                     | 0.54              |
| 1:I:34:LYS:HG3   | 1:I:37:GLN:CB    | 2.36                     | 0.54              |
| 1:H:96:VAL:O     | 1:H:229:GLY:HA2  | 2.06                     | 0.54              |
| 1:A:211:THR:O    | 1:A:212:ARG:HD3  | 2.08                     | 0.54              |
| 1:A:1:ASP:HB3    | 1:A:26:ILE:HG23  | 1.88                     | 0.54              |
| 1:H:180:GLN:HG3  | 3:H:1269:HOH:O   | 2.06                     | 0.54              |
| 1:I:54:PHE:HE2   | 1:I:62:LEU:HD12  | 1.71                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:34:LYS:HB3   | 3:D:757:HOH:O    | 2.06                     | 0.54              |
| 1:D:162:LEU:HD22 | 1:D:308:MET:SD   | 2.47                     | 0.54              |
| 1:E:101:ARG:HG3  | 1:E:101:ARG:NH1  | 2.22                     | 0.54              |
| 1:B:90:ALA:HB2   | 1:B:95:TRP:CD2   | 2.43                     | 0.54              |
| 1:B:72:GLU:OE1   | 1:B:234:LYS:HA   | 2.07                     | 0.54              |
| 1:A:111:LYS:C    | 1:A:112:LEU:HD23 | 2.28                     | 0.54              |
| 1:A:239:LYS:O    | 1:A:243:LYS:HG3  | 2.07                     | 0.54              |
| 1:D:50:PRO:HD3   | 3:D:338:HOH:O    | 2.06                     | 0.54              |
| 1:F:39:ALA:HA    | 1:F:42:ILE:HD12  | 1.89                     | 0.54              |
| 1:I:240:ASP:O    | 1:I:244:LYS:HG2  | 2.07                     | 0.54              |
| 1:A:3:THR:HG22   | 1:A:29:LYS:HB3   | 1.88                     | 0.54              |
| 1:C:1:ASP:OD2    | 1:C:27:LYS:HB2   | 2.08                     | 0.54              |
| 1:G:18:ASP:O     | 1:G:22:ARG:HG3   | 2.08                     | 0.54              |
| 1:B:73:PRO:HG3   | 3:B:726:HOH:O    | 2.07                     | 0.54              |
| 1:H:42:ILE:H     | 1:H:42:ILE:HD12  | 1.72                     | 0.54              |
| 1:H:24:THR:HG22  | 1:H:244:LYS:HE2  | 1.90                     | 0.54              |
| 1:G:193:ASN:HB2  | 1:G:196:TYR:CE1  | 2.43                     | 0.54              |
| 1:G:146:ILE:HG13 | 1:G:162:LEU:HD21 | 1.90                     | 0.53              |
| 1:G:112:LEU:HD13 | 1:G:117:LEU:HD21 | 1.90                     | 0.53              |
| 1:C:255:GLN:HG3  | 1:C:268:ASN:HB2  | 1.91                     | 0.53              |
| 1:A:109:THR:HG21 | 1:A:212:ARG:HG2  | 1.90                     | 0.53              |
| 1:H:240:ASP:HB2  | 1:H:243:LYS:HZ1  | 1.73                     | 0.53              |
| 1:B:2:ILE:HG13   | 1:B:28:VAL:HG13  | 1.90                     | 0.53              |
| 1:B:6:ASN:N      | 1:B:31:ASN:O     | 2.39                     | 0.53              |
| 1:H:5:TYR:HB3    | 1:H:38:LEU:HD22  | 1.91                     | 0.53              |
| 1:H:2:ILE:HB     | 3:H:1069:HOH:O   | 2.08                     | 0.53              |
| 1:A:115:LYS:HZ3  | 1:A:115:LYS:HB2  | 1.72                     | 0.53              |
| 1:H:253:GLU:CD   | 1:H:253:GLU:N    | 2.61                     | 0.53              |
| 1:G:209:VAL:HG12 | 1:G:211:THR:H    | 1.73                     | 0.53              |
| 1:D:114:GLU:O    | 1:D:115:LYS:C    | 2.45                     | 0.53              |
| 1:G:54:PHE:CZ    | 1:G:56:SER:HB2   | 2.44                     | 0.53              |
| 1:A:294:SER:O    | 1:A:297:GLU:HB3  | 2.08                     | 0.53              |
| 1:A:174:LYS:NZ   | 1:I:23:ALA:O     | 2.41                     | 0.53              |
| 1:D:31:ASN:ND2   | 3:D:649:HOH:O    | 2.42                     | 0.53              |
| 1:H:52:ASP:HB2   | 3:H:1069:HOH:O   | 2.08                     | 0.53              |
| 1:E:164:GLY:O    | 1:E:168:TYR:CD1  | 2.58                     | 0.53              |
| 1:C:255:GLN:HB3  | 1:C:271:VAL:HG21 | 1.91                     | 0.53              |
| 1:D:36:ASP:CB    | 3:D:757:HOH:O    | 2.56                     | 0.53              |
| 1:G:38:LEU:HD23  | 1:G:54:PHE:CE1   | 2.44                     | 0.53              |
| 1:B:204:LYS:NZ   | 3:B:1603:HOH:O   | 2.41                     | 0.53              |
| 1:I:4:VAL:HG22   | 1:I:53:VAL:HB    | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:26:ILE:HG12  | 3:H:1222:HOH:O   | 2.08                     | 0.53              |
| 1:B:8:GLN:HA     | 1:B:57:GLU:HG3   | 1.90                     | 0.53              |
| 1:G:151:LYS:HG3  | 3:G:314:HOH:O    | 2.08                     | 0.53              |
| 1:C:6:ASN:O      | 1:C:38:LEU:HD11  | 2.08                     | 0.53              |
| 1:B:42:ILE:O     | 1:B:45:GLU:HG2   | 2.09                     | 0.53              |
| 1:H:136:VAL:HB   | 1:H:139:SER:HB2  | 1.91                     | 0.53              |
| 1:A:9:HIS:HD2    | 1:A:11:GLU:N     | 2.01                     | 0.53              |
| 1:F:9:HIS:CG     | 1:F:11:GLU:HG2   | 2.43                     | 0.53              |
| 1:F:174:LYS:HD3  | 1:F:176:SER:OG   | 2.09                     | 0.53              |
| 1:C:15:ALA:HB2   | 1:C:261:VAL:HG11 | 1.91                     | 0.53              |
| 1:A:269:PRO:HG2  | 1:H:48:ARG:HG2   | 1.91                     | 0.53              |
| 1:H:55:TYR:CE1   | 1:H:249:LEU:HD21 | 2.43                     | 0.52              |
| 1:G:252:LYS:O    | 1:G:256:ARG:HG3  | 2.09                     | 0.52              |
| 1:I:65:LEU:HB3   | 1:I:71:LEU:HD11  | 1.91                     | 0.52              |
| 1:F:133:ILE:N    | 3:F:1325:HOH:O   | 2.41                     | 0.52              |
| 1:H:71:LEU:HB2   | 1:H:94:ASP:CB    | 2.38                     | 0.52              |
| 1:D:252:LYS:O    | 1:D:256:ARG:HB2  | 2.10                     | 0.52              |
| 1:D:9:HIS:CD2    | 1:D:11:GLU:OE2   | 2.62                     | 0.52              |
| 1:D:252:LYS:HD2  | 1:D:253:GLU:N    | 2.24                     | 0.52              |
| 1:D:135:TYR:CE2  | 1:D:137:PRO:HG3  | 2.45                     | 0.52              |
| 1:D:16:VAL:CG1   | 1:D:248:PHE:HE2  | 2.23                     | 0.52              |
| 1:I:114:GLU:HB2  | 3:I:862:HOH:O    | 2.08                     | 0.52              |
| 1:A:218:HIS:O    | 1:A:218:HIS:CD2  | 2.62                     | 0.52              |
| 1:B:38:LEU:O     | 1:B:42:ILE:HG13  | 2.09                     | 0.52              |
| 1:G:100:GLY:O    | 1:G:264:GLU:HG3  | 2.09                     | 0.52              |
| 1:D:104:VAL:HG23 | 1:D:214:ASN:O    | 2.09                     | 0.52              |
| 1:I:185:GLY:HA2  | 3:I:1232:HOH:O   | 2.08                     | 0.52              |
| 1:E:6:ASN:ND2    | 1:E:8:GLN:H      | 2.06                     | 0.52              |
| 1:G:121:VAL:CG1  | 1:G:222:GLY:HA3  | 2.40                     | 0.52              |
| 1:C:101:ARG:HH21 | 1:C:226:THR:CG2  | 2.22                     | 0.52              |
| 1:C:197:TRP:HE1  | 1:C:211:THR:HG23 | 1.74                     | 0.52              |
| 1:A:16:VAL:HG11  | 1:A:249:LEU:CD2  | 2.40                     | 0.52              |
| 1:H:93:LYS:HD2   | 1:H:93:LYS:N     | 2.25                     | 0.52              |
| 1:A:113:SER:O    | 1:A:117:LEU:HD12 | 2.09                     | 0.52              |
| 1:A:3:THR:HG22   | 1:A:29:LYS:HG2   | 1.91                     | 0.52              |
| 1:F:179:LEU:HD22 | 1:F:196:TYR:O    | 2.09                     | 0.52              |
| 1:C:41:GLN:HA    | 1:C:44:GLU:HB2   | 1.91                     | 0.52              |
| 1:D:101:ARG:NH1  | 3:D:1451:HOH:O   | 2.42                     | 0.52              |
| 1:E:262:ARG:CG   | 1:E:264:GLU:HG3  | 2.35                     | 0.52              |
| 1:I:182:VAL:HG13 | 1:I:211:THR:CG2  | 2.35                     | 0.52              |
| 1:F:255:GLN:HB2  | 1:F:271:VAL:HG21 | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:9:HIS:CD2    | 1:B:12:ALA:H     | 2.27                     | 0.52              |
| 1:I:111:LYS:HB2  | 3:I:1227:HOH:O   | 2.10                     | 0.52              |
| 1:G:99:SER:OG    | 1:G:264:GLU:HG2  | 2.10                     | 0.52              |
| 1:A:233:LEU:N    | 1:A:233:LEU:HD12 | 2.24                     | 0.52              |
| 1:A:43:LYS:HG3   | 3:A:1402:HOH:O   | 2.08                     | 0.52              |
| 1:E:99:SER:HA    | 1:E:267:LEU:HG   | 1.90                     | 0.52              |
| 1:G:140:GLY:O    | 1:G:144:GLU:HG2  | 2.10                     | 0.52              |
| 1:H:126:THR:HB   | 1:H:127:PRO:CD   | 2.39                     | 0.52              |
| 1:C:197:TRP:HB3  | 1:C:213:LEU:HD11 | 1.91                     | 0.52              |
| 1:F:195:TYR:C    | 1:F:197:TRP:H    | 2.13                     | 0.52              |
| 1:B:99:SER:HA    | 1:B:267:LEU:HG   | 1.92                     | 0.52              |
| 1:C:197:TRP:NE1  | 1:C:211:THR:HG23 | 2.25                     | 0.51              |
| 1:I:6:ASN:HD21   | 1:I:8:GLN:HB3    | 1.74                     | 0.51              |
| 1:G:234:LYS:HB2  | 3:G:706:HOH:O    | 2.09                     | 0.51              |
| 1:B:46:GLY:O     | 1:B:235:SER:HB3  | 2.09                     | 0.51              |
| 1:B:114:GLU:HA   | 1:B:117:LEU:HD12 | 1.92                     | 0.51              |
| 1:C:79:ILE:O     | 1:C:83:ARG:HG3   | 2.10                     | 0.51              |
| 1:I:143:LEU:HB3  | 3:I:1112:HOH:O   | 2.10                     | 0.51              |
| 1:I:62:LEU:H     | 1:I:62:LEU:HD13  | 1.75                     | 0.51              |
| 1:C:142:PHE:O    | 1:C:146:ILE:HG13 | 2.11                     | 0.51              |
| 1:E:217:ARG:HH21 | 1:E:278:GLU:CD   | 2.14                     | 0.51              |
| 1:I:181:ALA:O    | 1:I:186:GLU:HB2  | 2.10                     | 0.51              |
| 1:G:90:ALA:HB2   | 1:G:95:TRP:CE2   | 2.46                     | 0.51              |
| 1:G:218:HIS:N    | 1:G:284:GLU:OE2  | 2.43                     | 0.51              |
| 1:F:192:ILE:CG2  | 1:F:193:ASN:N    | 2.54                     | 0.51              |
| 1:A:43:LYS:HE3   | 3:A:1402:HOH:O   | 2.10                     | 0.51              |
| 1:H:130:LYS:HE3  | 3:H:500:HOH:O    | 2.10                     | 0.51              |
| 1:A:272:VAL:O    | 1:A:272:VAL:HG22 | 2.09                     | 0.51              |
| 1:D:198:HIS:CD2  | 3:D:1446:HOH:O   | 2.64                     | 0.51              |
| 1:H:2:ILE:HG23   | 1:H:241:GLU:HB3  | 1.93                     | 0.51              |
| 1:D:2:ILE:HG13   | 1:D:2:ILE:O      | 2.11                     | 0.51              |
| 1:F:113:SER:OG   | 1:F:115:LYS:HG2  | 2.10                     | 0.51              |
| 1:H:55:TYR:CD1   | 1:H:249:LEU:HD21 | 2.45                     | 0.51              |
| 1:F:108:ASP:C    | 1:F:108:ASP:OD2  | 2.49                     | 0.51              |
| 1:A:110:ARG:HE   | 1:A:210:HIS:CD2  | 2.29                     | 0.51              |
| 1:I:114:GLU:CD   | 1:I:214:ASN:ND2  | 2.63                     | 0.51              |
| 1:A:106:VAL:HG22 | 1:A:213:LEU:HD23 | 1.92                     | 0.51              |
| 1:H:256:ARG:HB2  | 1:H:256:ARG:NH1  | 2.25                     | 0.51              |
| 1:I:132:ARG:HB3  | 1:I:188:ASP:HB2  | 1.92                     | 0.51              |
| 1:C:255:GLN:HE22 | 1:C:267:LEU:N    | 2.09                     | 0.51              |
| 1:H:43:LYS:NZ    | 1:H:65:LEU:HD23  | 2.25                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:135:TYR:O    | 1:D:137:PRO:HD3  | 2.11                     | 0.51              |
| 1:C:278:GLU:O    | 1:C:279:PRO:C    | 2.48                     | 0.51              |
| 1:D:9:HIS:CE1    | 1:D:11:GLU:OE2   | 2.63                     | 0.50              |
| 1:G:3:THR:HG23   | 1:G:29:LYS:HD2   | 1.93                     | 0.50              |
| 1:E:300:THR:O    | 1:E:303:LEU:HB2  | 2.11                     | 0.50              |
| 1:H:42:ILE:HG21  | 1:H:233:LEU:HD12 | 1.94                     | 0.50              |
| 1:H:304:GLU:HG3  | 1:H:309:LYS:HB2  | 1.92                     | 0.50              |
| 1:F:107:TYR:CE2  | 1:F:109:THR:HG22 | 2.46                     | 0.50              |
| 1:D:256:ARG:CZ   | 1:D:256:ARG:HB3  | 2.42                     | 0.50              |
| 1:E:6:ASN:HD21   | 1:E:8:GLN:HB2    | 1.76                     | 0.50              |
| 1:A:3:THR:HG21   | 1:A:29:LYS:NZ    | 2.25                     | 0.50              |
| 1:D:204:LYS:HD3  | 1:D:204:LYS:N    | 2.26                     | 0.50              |
| 1:H:74:LEU:HB2   | 1:H:93:LYS:O     | 2.11                     | 0.50              |
| 1:I:43:LYS:NZ    | 1:I:68:ALA:HB1   | 2.26                     | 0.50              |
| 1:F:298:HIS:O    | 1:F:302:LEU:HG   | 2.12                     | 0.50              |
| 1:H:80:ASN:CB    | 3:H:1079:HOH:O   | 2.60                     | 0.50              |
| 1:H:272:VAL:C    | 3:H:1390:HOH:O   | 2.49                     | 0.50              |
| 1:H:176:SER:O    | 1:H:180:GLN:NE2  | 2.44                     | 0.50              |
| 1:G:185:GLY:HA2  | 3:G:1285:HOH:O   | 2.12                     | 0.50              |
| 1:C:46:GLY:O     | 1:C:47:SER:C     | 2.50                     | 0.50              |
| 1:G:163:LYS:HD2  | 1:G:306:ALA:HA   | 1.94                     | 0.50              |
| 1:C:255:GLN:O    | 1:C:259:THR:HG22 | 2.12                     | 0.50              |
| 1:B:133:ILE:N    | 1:B:187:ILE:HD11 | 2.27                     | 0.50              |
| 1:H:42:ILE:HG12  | 1:H:233:LEU:HD11 | 1.92                     | 0.50              |
| 1:C:256:ARG:HA   | 1:C:259:THR:HG22 | 1.94                     | 0.50              |
| 1:B:175:ASN:HD22 | 1:B:192:ILE:HG22 | 1.76                     | 0.50              |
| 1:F:217:ARG:NH1  | 1:F:278:GLU:OE2  | 2.45                     | 0.50              |
| 1:I:79:ILE:O     | 1:I:83:ARG:HB3   | 2.11                     | 0.50              |
| 1:C:93:LYS:HG2   | 1:C:93:LYS:O     | 2.11                     | 0.50              |
| 1:A:142:PHE:O    | 1:A:146:ILE:HG22 | 2.12                     | 0.50              |
| 1:I:255:GLN:CB   | 1:I:271:VAL:HG21 | 2.42                     | 0.50              |
| 1:B:283:LEU:O    | 1:B:284:GLU:HB2  | 2.12                     | 0.50              |
| 1:E:209:VAL:HG12 | 1:E:211:THR:H    | 1.77                     | 0.50              |
| 1:C:292:THR:OG1  | 1:C:295:GLU:HG3  | 2.12                     | 0.50              |
| 1:H:121:VAL:HA   | 1:H:124:TYR:HD2  | 1.76                     | 0.50              |
| 1:H:83:ARG:HD2   | 1:H:83:ARG:N     | 2.26                     | 0.50              |
| 1:I:80:ASN:HA    | 1:I:83:ARG:HB3   | 1.93                     | 0.50              |
| 1:B:170:LYS:HE2  | 1:B:187:ILE:HD12 | 1.94                     | 0.50              |
| 1:G:174:LYS:HB2  | 1:G:177:VAL:HG23 | 1.94                     | 0.50              |
| 1:H:300:THR:O    | 1:H:303:LEU:HB2  | 2.12                     | 0.49              |
| 1:H:28:VAL:HG22  | 3:H:1139:HOH:O   | 2.11                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:2:ILE:HD13   | 1:H:26:ILE:CG2   | 2.41                     | 0.49              |
| 1:I:117:LEU:HD13 | 1:I:214:ASN:HB2  | 1.93                     | 0.49              |
| 1:H:64:THR:HG23  | 1:H:65:LEU:HG    | 1.94                     | 0.49              |
| 1:A:164:GLY:O    | 1:A:168:TYR:CD1  | 2.65                     | 0.49              |
| 1:I:44:GLU:HG3   | 1:I:45:GLU:N     | 2.27                     | 0.49              |
| 1:A:74:LEU:HB2   | 1:A:79:ILE:HD11  | 1.93                     | 0.49              |
| 1:B:80:ASN:HB3   | 3:G:1158:HOH:O   | 2.12                     | 0.49              |
| 1:G:256:ARG:HG2  | 1:G:271:VAL:HG13 | 1.94                     | 0.49              |
| 1:D:268:ASN:HD22 | 1:D:268:ASN:C    | 2.15                     | 0.49              |
| 1:H:162:LEU:HD22 | 1:H:308:MET:HE1  | 1.93                     | 0.49              |
| 1:F:135:TYR:CD2  | 1:F:137:PRO:HG3  | 2.47                     | 0.49              |
| 1:D:118:GLU:CB   | 1:D:123:ASN:HB2  | 2.41                     | 0.49              |
| 1:F:214:ASN:HB3  | 3:F:347:HOH:O    | 2.12                     | 0.49              |
| 1:A:216:VAL:HG22 | 3:A:316:HOH:O    | 2.13                     | 0.49              |
| 1:H:5:TYR:OH     | 1:H:50:PRO:HD2   | 2.13                     | 0.49              |
| 1:D:56:SER:O     | 1:D:228:SER:HB3  | 2.13                     | 0.49              |
| 1:C:197:TRP:CD1  | 1:C:211:THR:HG23 | 2.48                     | 0.49              |
| 1:B:107:TYR:HB2  | 1:B:112:LEU:HD11 | 1.94                     | 0.49              |
| 1:C:308:MET:C    | 3:C:629:HOH:O    | 2.50                     | 0.49              |
| 1:G:255:GLN:NE2  | 1:G:268:ASN:H    | 2.10                     | 0.49              |
| 1:C:135:TYR:HE2  | 1:C:137:PRO:HG3  | 1.74                     | 0.49              |
| 1:I:80:ASN:HB3   | 1:I:83:ARG:CZ    | 2.42                     | 0.49              |
| 1:A:148:ALA:HB3  | 3:A:351:HOH:O    | 2.11                     | 0.49              |
| 1:A:12:ALA:O     | 1:A:16:VAL:HG23  | 2.12                     | 0.49              |
| 1:G:137:PRO:O    | 1:G:138:THR:HG23 | 2.12                     | 0.49              |
| 1:C:252:LYS:HE2  | 1:C:270:HIS:CB   | 2.41                     | 0.49              |
| 1:G:265:TYR:HB3  | 1:G:280:ILE:HG12 | 1.95                     | 0.49              |
| 1:I:77:SER:O     | 1:I:80:ASN:ND2   | 2.46                     | 0.49              |
| 1:D:34:LYS:HB3   | 1:D:37:GLN:HG3   | 1.94                     | 0.49              |
| 1:B:17:ALA:HB1   | 3:B:1209:HOH:O   | 2.11                     | 0.49              |
| 1:C:159:LEU:HG   | 1:C:163:LYS:HE3  | 1.95                     | 0.49              |
| 1:A:59:ILE:N     | 1:A:60:PRO:CD    | 2.76                     | 0.49              |
| 1:H:57:GLU:N     | 1:H:57:GLU:OE2   | 2.35                     | 0.49              |
| 1:H:28:VAL:HB    | 3:H:425:HOH:O    | 2.12                     | 0.49              |
| 1:D:109:THR:HA   | 1:D:112:LEU:O    | 2.13                     | 0.49              |
| 1:D:303:LEU:HB3  | 1:D:309:LYS:HB2  | 1.95                     | 0.49              |
| 1:B:32:SER:O     | 1:B:33:ALA:HB2   | 2.13                     | 0.49              |
| 1:H:199:ALA:O    | 1:H:203:GLU:HG3  | 2.13                     | 0.49              |
| 1:A:9:HIS:O      | 1:A:12:ALA:HB3   | 2.12                     | 0.49              |
| 1:D:155:GLU:OE2  | 1:D:298:HIS:CE1  | 2.59                     | 0.49              |
| 1:I:81:GLU:OE1   | 1:I:251:GLY:HA2  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:18:ASP:O     | 1:A:22:ARG:HG3   | 2.13                     | 0.49              |
| 1:C:233:LEU:N    | 1:C:233:LEU:HD12 | 2.28                     | 0.49              |
| 1:I:130:LYS:HG2  | 1:I:168:TYR:HB3  | 1.93                     | 0.49              |
| 1:F:256:ARG:HH22 | 1:F:272:VAL:N    | 2.08                     | 0.49              |
| 1:I:43:LYS:HZ2   | 1:I:68:ALA:HB1   | 1.78                     | 0.49              |
| 1:C:48:ARG:HE    | 1:C:237:GLN:CD   | 2.16                     | 0.49              |
| 1:H:68:ALA:O     | 1:H:69:ASN:C     | 2.51                     | 0.49              |
| 1:F:275:PHE:CD1  | 3:F:1091:HOH:O   | 2.47                     | 0.48              |
| 1:C:5:TYR:CD1    | 1:C:51:ALA:HB2   | 2.47                     | 0.48              |
| 1:D:114:GLU:HA   | 1:D:117:LEU:CD1  | 2.41                     | 0.48              |
| 1:D:155:GLU:O    | 1:D:158:ALA:N    | 2.46                     | 0.48              |
| 1:I:257:ALA:O    | 1:I:260:ALA:HB3  | 2.13                     | 0.48              |
| 1:D:81:GLU:HB2   | 1:D:250:ALA:HB1  | 1.95                     | 0.48              |
| 1:G:265:TYR:HB3  | 1:G:280:ILE:HG13 | 1.95                     | 0.48              |
| 1:I:265:TYR:N    | 1:I:265:TYR:CD1  | 2.81                     | 0.48              |
| 1:D:245:PHE:O    | 1:D:248:PHE:HB3  | 2.12                     | 0.48              |
| 1:F:136:VAL:HG11 | 1:F:174:LYS:HA   | 1.95                     | 0.48              |
| 1:F:237:GLN:N    | 1:F:237:GLN:CD   | 2.66                     | 0.48              |
| 1:G:303:LEU:HD13 | 1:G:308:MET:HB2  | 1.94                     | 0.48              |
| 1:E:135:TYR:O    | 1:E:171:PRO:HA   | 2.12                     | 0.48              |
| 1:B:41:GLN:O     | 1:B:44:GLU:HG2   | 2.14                     | 0.48              |
| 1:H:2:ILE:HG22   | 1:H:238:ASN:HB2  | 1.94                     | 0.48              |
| 1:I:209:VAL:O    | 1:I:212:ARG:NH2  | 2.46                     | 0.48              |
| 1:H:257:ALA:O    | 1:H:260:ALA:HB3  | 2.13                     | 0.48              |
| 1:A:8:GLN:NE2    | 1:A:55:TYR:CE1   | 2.81                     | 0.48              |
| 1:H:38:LEU:HD11  | 3:H:1604:HOH:O   | 2.14                     | 0.48              |
| 1:A:110:ARG:NE   | 1:A:210:HIS:CG   | 2.80                     | 0.48              |
| 1:D:106:VAL:HG22 | 1:D:211:THR:OG1  | 2.13                     | 0.48              |
| 1:D:256:ARG:HB3  | 1:D:256:ARG:NH1  | 2.28                     | 0.48              |
| 1:B:238:ASN:O    | 1:B:239:LYS:C    | 2.51                     | 0.48              |
| 1:G:24:THR:CG2   | 1:G:244:LYS:HE2  | 2.44                     | 0.48              |
| 1:E:8:GLN:NE2    | 1:E:228:SER:HB3  | 2.29                     | 0.48              |
| 1:F:118:GLU:HB2  | 1:F:124:TYR:CZ   | 2.49                     | 0.48              |
| 1:B:252:LYS:HE3  | 1:B:270:HIS:O    | 2.14                     | 0.48              |
| 1:B:34:LYS:HB2   | 3:B:1298:HOH:O   | 2.13                     | 0.48              |
| 1:H:303:LEU:HB3  | 1:H:309:LYS:CG   | 2.33                     | 0.48              |
| 1:D:265:TYR:CD1  | 1:D:265:TYR:N    | 2.81                     | 0.48              |
| 1:C:17:ALA:O     | 1:C:20:PHE:HB3   | 2.14                     | 0.48              |
| 1:G:182:VAL:HG22 | 1:G:187:ILE:HG23 | 1.95                     | 0.48              |
| 1:A:122:LEU:HA   | 1:A:161:TRP:CD1  | 2.48                     | 0.48              |
| 1:F:108:ASP:OD2  | 1:F:110:ARG:N    | 2.47                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:80:ASN:HA    | 1:C:83:ARG:CD    | 2.44                     | 0.48              |
| 1:G:18:ASP:N     | 1:G:18:ASP:OD1   | 2.45                     | 0.48              |
| 1:H:121:VAL:HA   | 1:H:124:TYR:CD2  | 2.48                     | 0.48              |
| 1:H:173:ALA:N    | 3:H:578:HOH:O    | 2.42                     | 0.48              |
| 1:E:84:GLY:HA2   | 3:E:551:HOH:O    | 2.14                     | 0.48              |
| 1:B:69:ASN:OD1   | 1:B:92:LYS:HE2   | 2.13                     | 0.48              |
| 1:A:33:ALA:HB3   | 1:A:38:LEU:HG    | 1.96                     | 0.48              |
| 1:A:108:ASP:OD2  | 1:A:110:ARG:HG3  | 2.13                     | 0.48              |
| 1:H:11:GLU:O     | 1:H:14:GLN:N     | 2.46                     | 0.48              |
| 1:E:233:LEU:HD12 | 1:E:235:SER:OG   | 2.14                     | 0.48              |
| 1:A:218:HIS:O    | 1:A:218:HIS:HD2  | 1.97                     | 0.48              |
| 1:B:3:THR:HG23   | 1:B:29:LYS:HE3   | 1.95                     | 0.48              |
| 1:I:62:LEU:HD12  | 1:I:62:LEU:N     | 2.29                     | 0.47              |
| 1:F:184:ASN:HB2  | 1:F:186:GLU:HG2  | 1.95                     | 0.47              |
| 1:B:72:GLU:CA    | 1:B:234:LYS:HG3  | 2.44                     | 0.47              |
| 1:C:183:GLU:HG3  | 3:C:1146:HOH:O   | 2.14                     | 0.47              |
| 1:H:72:GLU:HA    | 1:H:73:PRO:HD3   | 1.75                     | 0.47              |
| 1:H:178:ALA:O    | 1:H:182:VAL:HG23 | 2.13                     | 0.47              |
| 1:B:239:LYS:HE2  | 1:B:243:LYS:HZ2  | 1.79                     | 0.47              |
| 1:E:128:LYS:NZ   | 1:E:132:ARG:HH12 | 2.12                     | 0.47              |
| 1:C:197:TRP:HE1  | 1:C:211:THR:CG2  | 2.28                     | 0.47              |
| 1:B:136:VAL:CG1  | 1:B:139:SER:HB3  | 2.44                     | 0.47              |
| 1:H:200:PHE:CE1  | 1:H:204:LYS:HG3  | 2.49                     | 0.47              |
| 1:H:135:TYR:HD2  | 1:H:142:PHE:CZ   | 2.32                     | 0.47              |
| 1:G:100:GLY:HA2  | 1:G:226:THR:O    | 2.14                     | 0.47              |
| 1:C:255:GLN:NE2  | 1:C:268:ASN:H    | 2.11                     | 0.47              |
| 1:F:255:GLN:NE2  | 1:F:268:ASN:H    | 2.13                     | 0.47              |
| 1:E:268:ASN:HD22 | 1:E:270:HIS:H    | 1.62                     | 0.47              |
| 1:E:130:LYS:O    | 1:E:132:ARG:HG3  | 2.15                     | 0.47              |
| 1:H:76:ALA:O     | 1:H:80:ASN:HB2   | 2.14                     | 0.47              |
| 1:F:107:TYR:O    | 1:F:211:THR:HA   | 2.14                     | 0.47              |
| 1:C:239:LYS:HE3  | 1:C:239:LYS:HB2  | 1.62                     | 0.47              |
| 1:A:126:THR:HB   | 1:A:127:PRO:CD   | 2.44                     | 0.47              |
| 1:G:14:GLN:O     | 1:G:18:ASP:OD1   | 2.31                     | 0.47              |
| 1:I:92:LYS:HE3   | 3:I:354:HOH:O    | 2.13                     | 0.47              |
| 1:F:146:ILE:O    | 1:F:150:VAL:HG23 | 2.15                     | 0.47              |
| 1:I:82:THR:HB    | 1:I:267:LEU:CB   | 2.38                     | 0.47              |
| 1:B:73:PRO:HA    | 1:B:94:ASP:HA    | 1.95                     | 0.47              |
| 1:I:20:PHE:O     | 1:I:23:ALA:HB3   | 2.15                     | 0.47              |
| 1:F:103:ARG:HD3  | 3:F:316:HOH:O    | 2.15                     | 0.47              |
| 1:B:252:LYS:HG2  | 1:B:256:ARG:CZ   | 2.45                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:265:TYR:CE2  | 1:G:283:LEU:HD11 | 2.49                     | 0.47              |
| 1:E:200:PHE:HD1  | 1:E:200:PHE:H    | 1.63                     | 0.47              |
| 1:I:9:HIS:O      | 1:I:13:ALA:N     | 2.44                     | 0.47              |
| 1:E:44:GLU:O     | 1:E:45:GLU:C     | 2.52                     | 0.47              |
| 1:F:237:GLN:H    | 1:F:237:GLN:NE2  | 2.12                     | 0.47              |
| 1:F:236:SER:HB3  | 1:F:239:LYS:HG3  | 1.97                     | 0.47              |
| 1:E:268:ASN:ND2  | 1:E:270:HIS:H    | 2.13                     | 0.47              |
| 1:E:101:ARG:HH11 | 1:E:101:ARG:CG   | 2.23                     | 0.47              |
| 1:B:57:GLU:O     | 1:B:101:ARG:NH2  | 2.46                     | 0.47              |
| 1:F:174:LYS:HG3  | 1:F:177:VAL:HG23 | 1.97                     | 0.47              |
| 1:A:130:LYS:HG3  | 3:A:1610:HOH:O   | 2.15                     | 0.47              |
| 1:A:1:ASP:CB     | 1:A:26:ILE:HG23  | 2.45                     | 0.47              |
| 1:D:2:ILE:HA     | 1:D:52:ASP:OD1   | 2.15                     | 0.47              |
| 1:F:45:GLU:OE1   | 1:F:50:PRO:HD2   | 2.14                     | 0.47              |
| 1:I:10:LYS:HE3   | 1:I:32:SER:HB2   | 1.97                     | 0.47              |
| 1:D:101:ARG:NE   | 1:D:228:SER:OG   | 2.39                     | 0.47              |
| 1:F:217:ARG:HB3  | 1:F:284:GLU:OE2  | 2.15                     | 0.47              |
| 1:I:258:LEU:C    | 1:I:260:ALA:H    | 2.18                     | 0.47              |
| 1:I:216:VAL:O    | 1:I:218:HIS:HD2  | 1.96                     | 0.47              |
| 1:I:110:ARG:HH11 | 1:I:210:HIS:CG   | 2.33                     | 0.47              |
| 1:I:34:LYS:HE2   | 1:I:37:GLN:OE1   | 2.15                     | 0.47              |
| 1:H:19:ALA:HB1   | 1:H:248:PHE:HZ   | 1.80                     | 0.47              |
| 1:F:118:GLU:HB2  | 1:F:124:TYR:CE2  | 2.50                     | 0.47              |
| 1:G:101:ARG:HD2  | 1:G:195:TYR:CE1  | 2.50                     | 0.47              |
| 1:I:155:GLU:OE1  | 1:I:298:HIS:HE1  | 1.98                     | 0.47              |
| 1:B:237:GLN:N    | 1:B:237:GLN:OE1  | 2.46                     | 0.47              |
| 1:A:1:ASP:OD2    | 1:A:27:LYS:HB2   | 2.14                     | 0.47              |
| 1:D:43:LYS:HE3   | 1:D:64:THR:HG22  | 1.97                     | 0.47              |
| 1:H:4:VAL:HG23   | 3:H:425:HOH:O    | 2.15                     | 0.47              |
| 1:H:167:GLU:HG3  | 1:H:168:TYR:CE2  | 2.50                     | 0.47              |
| 1:H:252:LYS:HA   | 1:H:255:GLN:HB2  | 1.97                     | 0.47              |
| 1:B:136:VAL:HG12 | 1:B:139:SER:HB3  | 1.97                     | 0.47              |
| 1:F:4:VAL:HG22   | 1:F:53:VAL:HB    | 1.97                     | 0.47              |
| 1:H:265:TYR:CZ   | 1:H:277:LEU:HD22 | 2.49                     | 0.47              |
| 1:A:9:HIS:CD2    | 1:A:11:GLU:HB2   | 2.50                     | 0.46              |
| 1:E:92:LYS:HB2   | 1:E:94:ASP:CG    | 2.35                     | 0.46              |
| 1:D:303:LEU:HD13 | 1:D:309:LYS:HE3  | 1.96                     | 0.46              |
| 1:E:130:LYS:HD2  | 1:E:131:ASN:N    | 2.29                     | 0.46              |
| 1:B:67:ALA:C     | 1:B:69:ASN:H     | 2.18                     | 0.46              |
| 1:G:101:ARG:HD3  | 1:G:262:ARG:NH2  | 2.29                     | 0.46              |
| 1:D:147:VAL:HG13 | 1:D:151:LYS:HE3  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:54:PHE:O     | 1:B:230:ALA:HA   | 2.15                     | 0.46              |
| 1:G:99:SER:HB2   | 1:G:265:TYR:O    | 2.15                     | 0.46              |
| 1:H:71:LEU:CB    | 1:H:94:ASP:HB3   | 2.43                     | 0.46              |
| 1:D:103:ARG:HH21 | 1:D:193:ASN:ND2  | 2.12                     | 0.46              |
| 1:B:259:THR:HG23 | 1:B:273:SER:HA   | 1.97                     | 0.46              |
| 1:I:110:ARG:HH22 | 1:I:185:GLY:CA   | 2.29                     | 0.46              |
| 1:D:36:ASP:HB3   | 3:D:757:HOH:O    | 2.14                     | 0.46              |
| 1:B:72:GLU:HB2   | 1:B:234:LYS:HA   | 1.96                     | 0.46              |
| 1:G:58:GLN:HG2   | 1:G:60:PRO:HD2   | 1.96                     | 0.46              |
| 1:A:278:GLU:HB3  | 1:A:282:LYS:HE3  | 1.93                     | 0.46              |
| 1:G:202:ARG:HH22 | 1:G:274:THR:CG2  | 2.21                     | 0.46              |
| 1:F:11:GLU:HG3   | 1:F:12:ALA:N     | 2.30                     | 0.46              |
| 1:D:155:GLU:O    | 1:D:156:ALA:C    | 2.53                     | 0.46              |
| 1:G:220:ASP:OD1  | 1:G:221:PRO:HD2  | 2.15                     | 0.46              |
| 1:I:265:TYR:HA   | 1:I:266:PRO:HD3  | 1.66                     | 0.46              |
| 1:I:103:ARG:NH2  | 1:I:192:ILE:HA   | 2.31                     | 0.46              |
| 1:I:183:GLU:OE1  | 1:I:209:VAL:HA   | 2.16                     | 0.46              |
| 1:C:22:ARG:HH22  | 1:D:186:GLU:CG   | 2.28                     | 0.46              |
| 1:G:121:VAL:HG11 | 1:G:222:GLY:HA3  | 1.97                     | 0.46              |
| 1:H:126:THR:HB   | 1:H:127:PRO:HD2  | 1.97                     | 0.46              |
| 1:F:45:GLU:HB3   | 1:F:49:SER:HA    | 1.96                     | 0.46              |
| 1:H:20:PHE:CD2   | 1:H:245:PHE:HD1  | 2.34                     | 0.46              |
| 1:D:267:LEU:HA   | 1:D:280:ILE:CD1  | 2.37                     | 0.46              |
| 1:E:85:LYS:H     | 1:E:85:LYS:HD2   | 1.80                     | 0.46              |
| 1:C:101:ARG:NH2  | 1:C:226:THR:CG2  | 2.78                     | 0.46              |
| 1:C:278:GLU:HG2  | 1:C:278:GLU:O    | 2.15                     | 0.46              |
| 1:G:135:TYR:CD2  | 1:G:137:PRO:HG3  | 2.51                     | 0.46              |
| 1:I:161:TRP:CZ2  | 1:I:165:LEU:HD11 | 2.51                     | 0.46              |
| 1:C:114:GLU:C    | 1:C:115:LYS:HD2  | 2.37                     | 0.46              |
| 1:G:126:THR:HA   | 1:G:168:TYR:CE1  | 2.51                     | 0.46              |
| 1:I:175:ASN:OD1  | 1:I:196:TYR:CE1  | 2.69                     | 0.46              |
| 1:I:27:LYS:NZ    | 3:I:1010:HOH:O   | 2.48                     | 0.46              |
| 1:E:244:LYS:HD2  | 3:E:1109:HOH:O   | 2.14                     | 0.46              |
| 1:H:2:ILE:HD13   | 1:H:26:ILE:HG22  | 1.98                     | 0.46              |
| 1:I:255:GLN:O    | 1:I:258:LEU:HB3  | 2.16                     | 0.46              |
| 1:I:8:GLN:HE21   | 1:I:8:GLN:HB2    | 1.58                     | 0.46              |
| 1:D:170:LYS:HD2  | 1:D:187:ILE:HD12 | 1.98                     | 0.46              |
| 1:I:72:GLU:HG2   | 1:I:234:LYS:HA   | 1.97                     | 0.46              |
| 1:F:34:LYS:HD3   | 1:F:34:LYS:C     | 2.36                     | 0.46              |
| 1:F:57:GLU:O     | 1:F:101:ARG:NH2  | 2.49                     | 0.46              |
| 1:A:167:GLU:HG2  | 1:A:168:TYR:CZ   | 2.52                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:239:LYS:O    | 1:G:243:LYS:HG3  | 2.16                     | 0.46              |
| 1:B:255:GLN:O    | 1:B:259:THR:HB   | 2.16                     | 0.45              |
| 1:H:240:ASP:HA   | 1:H:243:LYS:HB2  | 1.98                     | 0.45              |
| 1:C:173:ALA:O    | 1:C:174:LYS:HG2  | 2.17                     | 0.45              |
| 1:C:25:GLY:HA3   | 3:C:439:HOH:O    | 2.15                     | 0.45              |
| 1:G:255:GLN:HB2  | 1:G:271:VAL:HG21 | 1.98                     | 0.45              |
| 1:C:265:TYR:HA   | 1:C:266:PRO:HD3  | 1.82                     | 0.45              |
| 1:A:174:LYS:HA   | 1:A:174:LYS:HD3  | 1.69                     | 0.45              |
| 1:F:115:LYS:C    | 1:F:117:LEU:H    | 2.20                     | 0.45              |
| 1:G:248:PHE:O    | 1:G:254:GLY:HA3  | 2.16                     | 0.45              |
| 1:D:58:GLN:HA    | 3:D:319:HOH:O    | 2.16                     | 0.45              |
| 1:B:59:ILE:HB    | 1:B:60:PRO:HD3   | 1.97                     | 0.45              |
| 1:A:40:GLY:O     | 1:A:44:GLU:HG2   | 2.16                     | 0.45              |
| 1:A:219:ARG:HG2  | 3:A:1406:HOH:O   | 2.17                     | 0.45              |
| 1:H:135:TYR:HE2  | 1:H:308:MET:CE   | 2.30                     | 0.45              |
| 1:D:100:GLY:O    | 1:D:264:GLU:CB   | 2.64                     | 0.45              |
| 1:D:144:GLU:CG   | 1:D:224:LEU:HD21 | 2.46                     | 0.45              |
| 1:I:8:GLN:NE2    | 1:I:55:TYR:CE1   | 2.83                     | 0.45              |
| 1:H:117:LEU:HD12 | 1:H:124:TYR:OH   | 2.15                     | 0.45              |
| 1:E:301:ARG:HD3  | 1:E:301:ARG:HA   | 1.50                     | 0.45              |
| 1:D:203:GLU:HG3  | 1:D:204:LYS:HD3  | 1.99                     | 0.45              |
| 1:G:122:LEU:HA   | 1:G:161:TRP:CD1  | 2.52                     | 0.45              |
| 1:B:198:HIS:HE1  | 3:B:1444:HOH:O   | 1.98                     | 0.45              |
| 1:I:2:ILE:HG22   | 1:I:238:ASN:HB2  | 1.99                     | 0.45              |
| 1:E:255:GLN:O    | 1:E:259:THR:HG22 | 2.16                     | 0.45              |
| 1:E:170:LYS:CD   | 1:E:187:ILE:HD12 | 2.31                     | 0.45              |
| 1:A:106:VAL:HG21 | 1:A:192:ILE:CD1  | 2.46                     | 0.45              |
| 1:G:72:GLU:OE1   | 1:G:234:LYS:HA   | 2.16                     | 0.45              |
| 1:C:218:HIS:HA   | 1:C:284:GLU:OE2  | 2.16                     | 0.45              |
| 1:E:49:SER:HA    | 1:E:50:PRO:HD3   | 1.85                     | 0.45              |
| 1:B:34:LYS:O     | 1:B:38:LEU:HG    | 2.17                     | 0.45              |
| 1:H:95:TRP:O     | 1:H:95:TRP:CE3   | 2.70                     | 0.45              |
| 1:C:268:ASN:ND2  | 1:C:270:HIS:H    | 2.12                     | 0.45              |
| 1:B:9:HIS:CD2    | 1:B:11:GLU:HB2   | 2.52                     | 0.45              |
| 1:H:240:ASP:CB   | 1:H:243:LYS:HZ1  | 2.30                     | 0.45              |
| 1:H:194:ASN:CG   | 1:H:195:TYR:N    | 2.70                     | 0.45              |
| 1:F:109:THR:HG21 | 1:F:212:ARG:HG2  | 1.99                     | 0.45              |
| 1:H:71:LEU:HB2   | 1:H:94:ASP:CG    | 2.37                     | 0.45              |
| 1:C:85:LYS:HG3   | 1:C:86:GLY:N     | 2.30                     | 0.45              |
| 1:C:113:SER:O    | 1:C:115:LYS:N    | 2.41                     | 0.45              |
| 1:F:237:GLN:H    | 1:F:237:GLN:CD   | 2.18                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:33:ALA:HB3   | 1:F:38:LEU:HD13  | 1.97                     | 0.45              |
| 1:F:206:VAL:HG22 | 1:F:212:ARG:NH2  | 2.32                     | 0.45              |
| 1:C:255:GLN:CB   | 1:C:271:VAL:HG21 | 2.47                     | 0.45              |
| 1:F:115:LYS:O    | 1:F:116:ASP:CG   | 2.55                     | 0.45              |
| 1:A:112:LEU:CD1  | 1:A:188:ASP:HB3  | 2.43                     | 0.45              |
| 1:A:51:ALA:HB3   | 1:A:233:LEU:HD22 | 1.97                     | 0.45              |
| 1:G:79:ILE:HG22  | 1:G:83:ARG:NH1   | 2.32                     | 0.45              |
| 1:I:49:SER:HA    | 1:I:50:PRO:HD3   | 1.83                     | 0.45              |
| 1:B:38:LEU:HB2   | 1:B:54:PHE:CE1   | 2.52                     | 0.44              |
| 1:H:172:TYR:CB   | 1:H:178:ALA:HB2  | 2.47                     | 0.44              |
| 1:D:114:GLU:O    | 1:D:116:ASP:N    | 2.51                     | 0.44              |
| 1:A:110:ARG:CZ   | 3:A:1141:HOH:O   | 2.65                     | 0.44              |
| 1:I:57:GLU:OE1   | 1:I:58:GLN:NE2   | 2.50                     | 0.44              |
| 1:C:244:LYS:O    | 1:C:247:ALA:HB3  | 2.17                     | 0.44              |
| 1:I:119:LYS:O    | 1:I:216:VAL:CG2  | 2.64                     | 0.44              |
| 1:D:217:ARG:HH11 | 1:D:217:ARG:HG2  | 1.82                     | 0.44              |
| 1:G:110:ARG:O    | 1:G:111:LYS:HD2  | 2.17                     | 0.44              |
| 1:D:139:SER:HB3  | 1:D:142:PHE:HB2  | 1.99                     | 0.44              |
| 1:B:59:ILE:HD11  | 1:B:227:TYR:HB2  | 1.98                     | 0.44              |
| 1:D:24:THR:HB    | 1:D:26:ILE:HD12  | 1.98                     | 0.44              |
| 1:E:54:PHE:CZ    | 1:E:56:SER:HB3   | 2.51                     | 0.44              |
| 1:B:248:PHE:O    | 1:B:254:GLY:HA3  | 2.17                     | 0.44              |
| 1:A:83:ARG:HG3   | 3:A:1125:HOH:O   | 2.17                     | 0.44              |
| 1:F:133:ILE:CB   | 3:F:1325:HOH:O   | 2.43                     | 0.44              |
| 1:I:259:THR:HG21 | 1:I:266:PRO:CG   | 2.46                     | 0.44              |
| 1:I:108:ASP:C    | 1:I:110:ARG:H    | 2.20                     | 0.44              |
| 1:H:197:TRP:CB   | 1:H:213:LEU:HD21 | 2.48                     | 0.44              |
| 1:B:302:LEU:HA   | 1:B:302:LEU:HD23 | 1.80                     | 0.44              |
| 1:E:255:GLN:HB2  | 1:E:271:VAL:HG21 | 1.99                     | 0.44              |
| 1:E:112:LEU:HD12 | 1:E:116:ASP:CB   | 2.47                     | 0.44              |
| 1:C:101:ARG:HH21 | 1:C:226:THR:HG22 | 1.81                     | 0.44              |
| 1:H:121:VAL:HG12 | 1:H:124:TYR:CE2  | 2.52                     | 0.44              |
| 1:H:248:PHE:O    | 1:H:254:GLY:HA3  | 2.18                     | 0.44              |
| 1:G:176:SER:O    | 1:G:180:GLN:HG2  | 2.18                     | 0.44              |
| 1:H:175:ASN:HD22 | 1:H:192:ILE:HG22 | 1.83                     | 0.44              |
| 1:H:159:LEU:HD12 | 1:H:159:LEU:O    | 2.17                     | 0.44              |
| 1:D:280:ILE:H    | 1:D:280:ILE:HG13 | 1.50                     | 0.44              |
| 1:D:101:ARG:H    | 1:D:101:ARG:HD2  | 1.82                     | 0.44              |
| 1:A:42:ILE:HD13  | 1:A:233:LEU:HD21 | 1.98                     | 0.44              |
| 1:F:145:GLN:HA   | 1:F:145:GLN:NE2  | 2.33                     | 0.44              |
| 1:E:297:GLU:HA   | 1:E:297:GLU:OE1  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:2:ILE:HG22   | 1:H:238:ASN:HB3  | 1.98                     | 0.44              |
| 1:I:54:PHE:CE2   | 1:I:62:LEU:CD1   | 3.00                     | 0.44              |
| 1:F:256:ARG:NH1  | 1:F:272:VAL:O    | 2.45                     | 0.44              |
| 1:F:179:LEU:CD2  | 1:F:196:TYR:O    | 2.66                     | 0.44              |
| 1:E:20:PHE:CD2   | 1:E:245:PHE:HD1  | 2.35                     | 0.44              |
| 1:B:111:LYS:HA   | 1:B:111:LYS:HD2  | 1.64                     | 0.44              |
| 1:G:202:ARG:CZ   | 1:G:274:THR:HG22 | 2.46                     | 0.44              |
| 1:I:126:THR:HB   | 1:I:127:PRO:HD2  | 2.00                     | 0.44              |
| 1:E:162:LEU:O    | 1:E:308:MET:HE3  | 2.18                     | 0.44              |
| 1:H:219:ARG:HD3  | 1:H:284:GLU:O    | 2.17                     | 0.44              |
| 1:D:239:LYS:HB3  | 1:D:243:LYS:HE3  | 1.99                     | 0.44              |
| 1:A:105:VAL:HB   | 1:A:214:ASN:HB3  | 1.99                     | 0.44              |
| 1:B:72:GLU:N     | 1:B:234:LYS:HG3  | 2.33                     | 0.44              |
| 1:F:143:LEU:O    | 1:F:146:ILE:HB   | 2.17                     | 0.44              |
| 1:H:139:SER:HB3  | 1:H:142:PHE:CB   | 2.48                     | 0.44              |
| 1:I:256:ARG:HA   | 1:I:259:THR:OG1  | 2.17                     | 0.44              |
| 1:B:259:THR:CG2  | 1:B:273:SER:HA   | 2.48                     | 0.44              |
| 1:C:78:THR:O     | 1:C:81:GLU:HB2   | 2.16                     | 0.44              |
| 1:B:71:LEU:CB    | 1:B:94:ASP:HB2   | 2.48                     | 0.44              |
| 1:F:72:GLU:OE1   | 1:F:239:LYS:NZ   | 2.46                     | 0.44              |
| 1:G:125:ALA:HB1  | 1:G:164:GLY:HA3  | 1.99                     | 0.44              |
| 1:E:59:ILE:N     | 1:E:60:PRO:CD    | 2.81                     | 0.44              |
| 1:C:248:PHE:CE2  | 1:C:254:GLY:HA2  | 2.53                     | 0.44              |
| 1:G:98:LEU:O     | 1:G:267:LEU:HG   | 2.18                     | 0.44              |
| 1:F:182:VAL:HG12 | 1:F:211:THR:HG22 | 1.99                     | 0.44              |
| 1:F:209:VAL:O    | 1:F:212:ARG:NH1  | 2.48                     | 0.44              |
| 1:I:83:ARG:HG3   | 1:I:83:ARG:O     | 2.16                     | 0.44              |
| 1:A:133:ILE:HD11 | 1:A:191:LEU:CD1  | 2.46                     | 0.44              |
| 1:B:217:ARG:HA   | 1:B:283:LEU:O    | 2.18                     | 0.44              |
| 1:C:2:ILE:O      | 1:C:28:VAL:HA    | 2.17                     | 0.44              |
| 1:F:110:ARG:NH2  | 1:F:183:GLU:C    | 2.63                     | 0.44              |
| 1:H:189:ALA:N    | 3:H:1274:HOH:O   | 2.50                     | 0.44              |
| 1:D:53:VAL:HG11  | 1:D:245:PHE:HD2  | 1.83                     | 0.44              |
| 1:D:234:LYS:O    | 1:D:239:LYS:HE3  | 2.18                     | 0.44              |
| 1:B:219:ARG:HD3  | 1:B:284:GLU:O    | 2.18                     | 0.44              |
| 1:B:239:LYS:HE2  | 1:B:243:LYS:NZ   | 2.33                     | 0.44              |
| 1:C:16:VAL:HG23  | 1:C:17:ALA:N     | 2.33                     | 0.44              |
| 1:I:101:ARG:CG   | 1:I:195:TYR:HE1  | 2.31                     | 0.44              |
| 1:I:245:PHE:O    | 1:I:248:PHE:HB3  | 2.18                     | 0.44              |
| 1:I:133:ILE:O    | 1:I:133:ILE:HG23 | 2.18                     | 0.44              |
| 1:H:54:PHE:HE2   | 1:H:62:LEU:HD23  | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:20:PHE:HE1   | 1:H:244:LYS:HG2  | 1.83                     | 0.43              |
| 1:I:80:ASN:HB3   | 1:I:83:ARG:HH21  | 1.80                     | 0.43              |
| 1:F:103:ARG:NH2  | 3:F:313:HOH:O    | 2.34                     | 0.43              |
| 1:I:10:LYS:HE3   | 1:I:32:SER:CB    | 2.48                     | 0.43              |
| 1:D:147:VAL:CG1  | 1:D:151:LYS:HE3  | 2.48                     | 0.43              |
| 1:I:103:ARG:HH21 | 1:I:192:ILE:HA   | 1.82                     | 0.43              |
| 1:I:195:TYR:CE2  | 1:I:196:TYR:CE1  | 3.06                     | 0.43              |
| 1:A:134:GLY:HA2  | 1:A:170:LYS:O    | 2.18                     | 0.43              |
| 1:E:58:GLN:HA    | 1:E:58:GLN:OE1   | 2.17                     | 0.43              |
| 1:B:5:TYR:CZ     | 1:B:31:ASN:ND2   | 2.87                     | 0.43              |
| 1:H:137:PRO:HA   | 1:H:142:PHE:CD2  | 2.53                     | 0.43              |
| 1:H:273:SER:N    | 3:H:1390:HOH:O   | 2.50                     | 0.43              |
| 1:G:87:VAL:HA    | 1:G:88:PRO:HD3   | 1.82                     | 0.43              |
| 1:A:110:ARG:HH21 | 1:A:210:HIS:CD2  | 2.36                     | 0.43              |
| 1:I:110:ARG:HH11 | 1:I:210:HIS:CD2  | 2.36                     | 0.43              |
| 1:C:114:GLU:O    | 1:C:115:LYS:HG3  | 2.18                     | 0.43              |
| 1:D:308:MET:HE2  | 1:D:308:MET:HB2  | 1.50                     | 0.43              |
| 1:I:220:ASP:CG   | 1:I:221:PRO:HD2  | 2.38                     | 0.43              |
| 1:H:54:PHE:CE2   | 1:H:62:LEU:HD23  | 2.52                     | 0.43              |
| 1:G:59:ILE:N     | 1:G:60:PRO:CD    | 2.82                     | 0.43              |
| 1:I:84:GLY:N     | 3:I:1374:HOH:O   | 2.51                     | 0.43              |
| 1:F:219:ARG:NH1  | 1:F:285:ALA:O    | 2.43                     | 0.43              |
| 1:A:252:LYS:HE2  | 1:A:256:ARG:HH22 | 1.82                     | 0.43              |
| 1:B:82:THR:HG21  | 1:B:97:ALA:O     | 2.18                     | 0.43              |
| 1:G:26:ILE:H     | 1:G:26:ILE:HG13  | 1.54                     | 0.43              |
| 1:G:202:ARG:NH2  | 1:G:275:PHE:CD1  | 2.87                     | 0.43              |
| 1:H:136:VAL:C    | 1:H:138:THR:H    | 2.21                     | 0.43              |
| 1:F:191:LEU:H    | 1:F:191:LEU:HD22 | 1.80                     | 0.43              |
| 1:G:17:ALA:O     | 1:G:20:PHE:HB3   | 2.18                     | 0.43              |
| 1:D:36:ASP:N     | 3:D:757:HOH:O    | 2.52                     | 0.43              |
| 1:E:33:ALA:HB3   | 1:E:38:LEU:HD21  | 2.00                     | 0.43              |
| 1:F:216:VAL:O    | 1:F:218:HIS:HD2  | 2.02                     | 0.43              |
| 1:A:143:LEU:HA   | 1:A:146:ILE:CG2  | 2.49                     | 0.43              |
| 1:H:246:VAL:HA   | 1:H:249:LEU:HB3  | 1.99                     | 0.43              |
| 1:H:20:PHE:CE2   | 1:H:26:ILE:HB    | 2.54                     | 0.43              |
| 1:C:85:LYS:NZ    | 1:C:85:LYS:HB3   | 2.34                     | 0.43              |
| 1:I:34:LYS:HD2   | 1:I:36:ASP:OD1   | 2.19                     | 0.43              |
| 1:F:175:ASN:OD1  | 1:F:196:TYR:CE1  | 2.72                     | 0.43              |
| 1:F:33:ALA:HB3   | 1:F:38:LEU:CD1   | 2.48                     | 0.43              |
| 1:F:265:TYR:CB   | 1:F:280:ILE:CG1  | 2.87                     | 0.43              |
| 1:F:85:LYS:HE2   | 1:F:219:ARG:NH2  | 2.22                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:98:LEU:O     | 1:H:267:LEU:HB2  | 2.16                     | 0.43              |
| 1:D:269:PRO:HD2  | 1:D:270:HIS:CD2  | 2.54                     | 0.43              |
| 1:E:92:LYS:HB2   | 1:E:94:ASP:OD1   | 2.19                     | 0.43              |
| 1:D:220:ASP:CG   | 1:D:221:PRO:HD2  | 2.38                     | 0.43              |
| 1:B:71:LEU:HB2   | 1:B:94:ASP:HB2   | 2.00                     | 0.43              |
| 1:I:160:LYS:HD3  | 3:I:1383:HOH:O   | 2.19                     | 0.43              |
| 1:I:174:LYS:HB2  | 3:I:365:HOH:O    | 2.18                     | 0.43              |
| 1:B:239:LYS:HZ3  | 1:B:239:LYS:HB3  | 1.81                     | 0.43              |
| 1:C:48:ARG:HE    | 1:C:237:GLN:NE2  | 2.15                     | 0.43              |
| 1:B:282:LYS:HA   | 1:B:282:LYS:HD3  | 1.78                     | 0.43              |
| 1:B:119:LYS:HG2  | 3:B:669:HOH:O    | 2.18                     | 0.43              |
| 1:C:162:LEU:HD22 | 1:C:308:MET:HE3  | 2.01                     | 0.43              |
| 1:H:10:LYS:O     | 1:H:14:GLN:HG3   | 2.19                     | 0.43              |
| 1:D:126:THR:HB   | 1:D:127:PRO:HD2  | 2.00                     | 0.43              |
| 1:C:181:ALA:O    | 1:C:186:GLU:HB2  | 2.18                     | 0.43              |
| 1:E:268:ASN:ND2  | 1:E:268:ASN:C    | 2.70                     | 0.42              |
| 1:A:114:GLU:HA   | 1:A:117:LEU:HD13 | 2.01                     | 0.42              |
| 1:D:146:ILE:O    | 1:D:150:VAL:HG23 | 2.19                     | 0.42              |
| 1:G:163:LYS:CD   | 1:G:306:ALA:HA   | 2.49                     | 0.42              |
| 1:E:100:GLY:HA2  | 1:E:226:THR:O    | 2.19                     | 0.42              |
| 1:H:80:ASN:HD22  | 1:H:80:ASN:HA    | 1.62                     | 0.42              |
| 1:H:56:SER:HB2   | 1:H:62:LEU:HD21  | 2.01                     | 0.42              |
| 1:A:255:GLN:HB2  | 1:A:271:VAL:HG21 | 2.01                     | 0.42              |
| 1:F:184:ASN:C    | 1:F:186:GLU:N    | 2.72                     | 0.42              |
| 1:C:265:TYR:CZ   | 1:C:283:LEU:HD11 | 2.54                     | 0.42              |
| 1:G:53:VAL:CG2   | 1:G:242:ALA:HB1  | 2.49                     | 0.42              |
| 1:G:54:PHE:CE1   | 1:G:56:SER:HB2   | 2.54                     | 0.42              |
| 1:H:254:GLY:O    | 1:H:257:ALA:HB3  | 2.18                     | 0.42              |
| 1:D:216:VAL:HG13 | 3:D:314:HOH:O    | 2.18                     | 0.42              |
| 1:A:217:ARG:HA   | 1:A:283:LEU:O    | 2.19                     | 0.42              |
| 1:B:38:LEU:HB2   | 1:B:54:PHE:HE1   | 1.84                     | 0.42              |
| 1:H:90:ALA:HA    | 1:H:95:TRP:CH2   | 2.53                     | 0.42              |
| 1:G:99:SER:HA    | 1:G:267:LEU:HG   | 2.01                     | 0.42              |
| 1:A:110:ARG:NH2  | 3:A:1141:HOH:O   | 2.52                     | 0.42              |
| 1:A:106:VAL:HG23 | 1:A:192:ILE:HG12 | 2.02                     | 0.42              |
| 1:G:20:PHE:CE1   | 1:G:244:LYS:HG2  | 2.50                     | 0.42              |
| 1:G:54:PHE:O     | 1:G:230:ALA:HA   | 2.19                     | 0.42              |
| 1:D:239:LYS:O    | 1:D:240:ASP:C    | 2.57                     | 0.42              |
| 1:C:20:PHE:CE2   | 1:C:26:ILE:HB    | 2.54                     | 0.42              |
| 1:C:112:LEU:HD11 | 1:C:188:ASP:HB3  | 2.02                     | 0.42              |
| 1:A:166:LYS:HD3  | 1:A:307:GLY:O    | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:94:ASP:OD1   | 1:F:94:ASP:N     | 2.52                     | 0.42              |
| 1:B:252:LYS:NZ   | 1:B:270:HIS:HB3  | 2.34                     | 0.42              |
| 1:H:162:LEU:HD13 | 1:H:303:LEU:HA   | 2.02                     | 0.42              |
| 1:G:252:LYS:CD   | 1:G:252:LYS:H    | 2.30                     | 0.42              |
| 1:F:182:VAL:C    | 1:F:184:ASN:N    | 2.70                     | 0.42              |
| 1:H:273:SER:CA   | 3:H:1390:HOH:O   | 2.65                     | 0.42              |
| 1:G:72:GLU:OE1   | 1:G:239:LYS:NZ   | 2.43                     | 0.42              |
| 1:I:186:GLU:HB3  | 3:I:1382:HOH:O   | 2.19                     | 0.42              |
| 1:E:245:PHE:O    | 1:E:249:LEU:HG   | 2.19                     | 0.42              |
| 1:A:54:PHE:CD2   | 1:A:65:LEU:HD12  | 2.55                     | 0.42              |
| 1:F:95:TRP:HB3   | 1:F:231:ALA:HB2  | 2.01                     | 0.42              |
| 1:A:7:GLY:O      | 1:A:57:GLU:HB2   | 2.19                     | 0.42              |
| 1:C:303:LEU:HA   | 1:C:303:LEU:HD12 | 1.93                     | 0.42              |
| 1:E:112:LEU:CD1  | 1:E:116:ASP:HB2  | 2.49                     | 0.42              |
| 1:G:182:VAL:HA   | 1:G:187:ILE:O    | 2.20                     | 0.42              |
| 1:F:62:LEU:HD13  | 1:F:95:TRP:HB2   | 2.01                     | 0.42              |
| 1:I:132:ARG:NE   | 1:I:188:ASP:OD2  | 2.47                     | 0.42              |
| 1:E:107:TYR:CD1  | 1:E:117:LEU:HD11 | 2.55                     | 0.42              |
| 1:F:59:ILE:N     | 1:F:60:PRO:CD    | 2.82                     | 0.42              |
| 1:I:153:LYS:HD3  | 1:I:153:LYS:HA   | 1.80                     | 0.42              |
| 1:F:147:VAL:CG2  | 1:F:295:GLU:HG3  | 2.41                     | 0.42              |
| 1:G:265:TYR:HA   | 1:G:266:PRO:HD3  | 1.91                     | 0.42              |
| 1:C:256:ARG:HA   | 1:C:259:THR:CG2  | 2.50                     | 0.42              |
| 1:E:233:LEU:HD23 | 1:E:233:LEU:N    | 2.34                     | 0.42              |
| 1:D:142:PHE:CE2  | 1:D:308:MET:HE1  | 2.54                     | 0.42              |
| 1:G:233:LEU:CD1  | 1:G:233:LEU:N    | 2.82                     | 0.42              |
| 1:H:265:TYR:CE2  | 1:H:283:LEU:HD11 | 2.54                     | 0.42              |
| 1:C:248:PHE:CE2  | 1:C:254:GLY:CA   | 3.03                     | 0.42              |
| 1:G:175:ASN:HD22 | 1:G:192:ILE:HG22 | 1.85                     | 0.42              |
| 1:D:144:GLU:HG2  | 1:D:224:LEU:HD21 | 2.02                     | 0.42              |
| 1:I:268:ASN:HA   | 1:I:269:PRO:HD3  | 1.87                     | 0.42              |
| 1:I:5:TYR:CZ     | 1:I:51:ALA:HB2   | 2.55                     | 0.42              |
| 1:G:146:ILE:CG1  | 1:G:162:LEU:HD21 | 2.49                     | 0.42              |
| 1:F:175:ASN:CB   | 1:F:196:TYR:CE1  | 3.02                     | 0.42              |
| 1:I:43:LYS:O     | 1:I:43:LYS:HD2   | 2.19                     | 0.42              |
| 1:F:300:THR:O    | 1:F:303:LEU:HB2  | 2.19                     | 0.42              |
| 1:H:240:ASP:HA   | 1:H:243:LYS:HZ3  | 1.85                     | 0.42              |
| 1:F:195:TYR:C    | 1:F:197:TRP:N    | 2.73                     | 0.42              |
| 1:I:195:TYR:HE2  | 1:I:196:TYR:CZ   | 2.38                     | 0.42              |
| 1:G:79:ILE:C     | 3:G:1518:HOH:O   | 2.59                     | 0.41              |
| 1:C:30:LEU:HA    | 1:C:30:LEU:HD23  | 1.77                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:1:ASP:OD1    | 1:E:27:LYS:HB2   | 2.20                     | 0.41              |
| 1:A:142:PHE:HE2  | 1:A:303:LEU:HD21 | 1.86                     | 0.41              |
| 1:D:265:TYR:HB3  | 1:D:280:ILE:HG12 | 2.01                     | 0.41              |
| 1:C:283:LEU:HD23 | 1:C:283:LEU:HA   | 1.83                     | 0.41              |
| 1:E:112:LEU:CD1  | 1:E:116:ASP:CB   | 2.98                     | 0.41              |
| 1:D:217:ARG:HH11 | 1:D:217:ARG:CG   | 2.33                     | 0.41              |
| 1:D:146:ILE:HD11 | 1:D:303:LEU:HD21 | 2.01                     | 0.41              |
| 1:A:59:ILE:N     | 1:A:60:PRO:HD2   | 2.35                     | 0.41              |
| 1:B:119:LYS:O    | 1:B:216:VAL:HG13 | 2.20                     | 0.41              |
| 1:G:76:ALA:O     | 1:G:77:SER:C     | 2.58                     | 0.41              |
| 3:A:1457:HOH:O   | 1:H:237:GLN:NE2  | 2.54                     | 0.41              |
| 1:D:113:SER:HB3  | 1:D:115:LYS:HD3  | 2.01                     | 0.41              |
| 1:I:174:LYS:HE2  | 1:I:174:LYS:HB3  | 1.83                     | 0.41              |
| 1:D:220:ASP:OD1  | 1:D:221:PRO:HD2  | 2.20                     | 0.41              |
| 1:H:59:ILE:N     | 1:H:60:PRO:CD    | 2.83                     | 0.41              |
| 1:D:266:PRO:O    | 1:D:280:ILE:HD11 | 2.21                     | 0.41              |
| 1:I:118:GLU:HG2  | 1:I:129:TRP:CZ2  | 2.55                     | 0.41              |
| 1:G:265:TYR:HB2  | 1:G:280:ILE:HD11 | 2.01                     | 0.41              |
| 1:G:267:LEU:HD23 | 1:G:280:ILE:HD12 | 2.02                     | 0.41              |
| 1:D:9:HIS:NE2    | 1:D:11:GLU:OE2   | 2.54                     | 0.41              |
| 1:F:12:ALA:O     | 1:F:16:VAL:HG23  | 2.19                     | 0.41              |
| 1:D:301:ARG:HD2  | 1:D:301:ARG:HA   | 1.83                     | 0.41              |
| 1:A:5:TYR:CE1    | 1:A:51:ALA:HB2   | 2.55                     | 0.41              |
| 1:I:55:TYR:HE1   | 1:I:98:LEU:HD12  | 1.86                     | 0.41              |
| 1:C:159:LEU:CG   | 1:C:163:LYS:HE3  | 2.50                     | 0.41              |
| 1:I:96:VAL:HG22  | 1:I:97:ALA:O     | 2.21                     | 0.41              |
| 1:B:268:ASN:OD1  | 1:B:269:PRO:HD2  | 2.21                     | 0.41              |
| 1:B:152:LEU:HD11 | 1:B:286:PRO:HB2  | 2.02                     | 0.41              |
| 1:E:287:GLN:HG2  | 1:E:287:GLN:H    | 1.73                     | 0.41              |
| 1:H:66:SER:OG    | 1:H:92:LYS:HB2   | 2.20                     | 0.41              |
| 1:F:256:ARG:HG2  | 1:F:271:VAL:HG13 | 2.01                     | 0.41              |
| 1:A:300:THR:CG2  | 1:A:309:LYS:HE3  | 2.50                     | 0.41              |
| 1:G:101:ARG:HG2  | 1:G:195:TYR:CD1  | 2.56                     | 0.41              |
| 1:H:265:TYR:CZ   | 1:H:283:LEU:HD11 | 2.55                     | 0.41              |
| 1:G:80:ASN:OD1   | 1:G:83:ARG:NH2   | 2.42                     | 0.41              |
| 1:H:85:LYS:C     | 1:H:87:VAL:H     | 2.24                     | 0.41              |
| 1:I:292:THR:HG23 | 3:I:763:HOH:O    | 2.20                     | 0.41              |
| 1:B:4:VAL:O      | 1:B:31:ASN:N     | 2.53                     | 0.41              |
| 1:F:133:ILE:HD11 | 1:F:191:LEU:CD2  | 2.50                     | 0.41              |
| 1:B:243:LYS:HB3  | 3:B:1385:HOH:O   | 2.20                     | 0.41              |
| 1:A:72:GLU:OE1   | 1:A:239:LYS:HE2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:240:ASP:O    | 1:B:244:LYS:HG3  | 2.20                     | 0.41              |
| 1:F:5:TYR:CD1    | 1:F:51:ALA:HB2   | 2.56                     | 0.41              |
| 1:E:136:VAL:HA   | 1:E:137:PRO:HD2  | 1.89                     | 0.41              |
| 1:H:3:THR:N      | 3:H:1069:HOH:O   | 2.52                     | 0.41              |
| 1:H:216:VAL:O    | 1:H:217:ARG:HB2  | 2.21                     | 0.41              |
| 1:I:21:THR:C     | 1:I:23:ALA:H     | 2.23                     | 0.41              |
| 1:G:62:LEU:HD13  | 1:G:95:TRP:HB2   | 2.02                     | 0.41              |
| 1:D:170:LYS:HA   | 1:D:171:PRO:HD3  | 1.93                     | 0.41              |
| 1:I:96:VAL:O     | 1:I:229:GLY:HA2  | 2.21                     | 0.41              |
| 1:F:170:LYS:HE2  | 3:F:1488:HOH:O   | 2.21                     | 0.41              |
| 1:E:265:TYR:CD1  | 1:E:265:TYR:N    | 2.89                     | 0.41              |
| 1:I:258:LEU:C    | 1:I:260:ALA:N    | 2.73                     | 0.41              |
| 1:D:104:VAL:CG2  | 1:D:105:VAL:N    | 2.83                     | 0.41              |
| 1:I:195:TYR:HA   | 1:I:263:ALA:HB3  | 2.01                     | 0.41              |
| 1:F:220:ASP:O    | 1:F:286:PRO:HG3  | 2.21                     | 0.41              |
| 1:E:89:VAL:HG13  | 3:E:1259:HOH:O   | 2.20                     | 0.41              |
| 1:B:251:GLY:O    | 1:B:252:LYS:C    | 2.59                     | 0.41              |
| 1:E:256:ARG:HA   | 1:E:259:THR:HG22 | 2.02                     | 0.41              |
| 1:I:54:PHE:CE2   | 1:I:56:SER:HB2   | 2.55                     | 0.41              |
| 1:B:40:GLY:O     | 1:B:41:GLN:C     | 2.59                     | 0.41              |
| 1:D:16:VAL:HG13  | 1:D:248:PHE:HE2  | 1.85                     | 0.41              |
| 1:C:79:ILE:CD1   | 1:C:93:LYS:HG3   | 2.49                     | 0.41              |
| 1:E:66:SER:OG    | 1:E:92:LYS:HD3   | 2.21                     | 0.41              |
| 1:B:198:HIS:CE1  | 3:B:1444:HOH:O   | 2.73                     | 0.41              |
| 1:A:65:LEU:O     | 1:A:71:LEU:HG    | 2.21                     | 0.41              |
| 1:H:97:ALA:HA    | 1:H:228:SER:O    | 2.21                     | 0.41              |
| 1:C:193:ASN:HB3  | 1:C:195:TYR:CE1  | 2.56                     | 0.41              |
| 1:D:6:ASN:O      | 1:D:32:SER:HA    | 2.21                     | 0.41              |
| 1:F:85:LYS:HZ3   | 1:F:219:ARG:NH1  | 2.19                     | 0.41              |
| 1:C:309:LYS:N    | 3:C:629:HOH:O    | 2.53                     | 0.41              |
| 1:I:129:TRP:O    | 1:I:130:LYS:O    | 2.37                     | 0.41              |
| 1:I:265:TYR:CE2  | 1:I:283:LEU:HD11 | 2.56                     | 0.41              |
| 1:D:53:VAL:HG12  | 1:D:242:ALA:HB1  | 2.03                     | 0.41              |
| 1:D:148:ALA:HB2  | 3:D:324:HOH:O    | 2.20                     | 0.41              |
| 1:D:94:ASP:N     | 1:D:94:ASP:OD1   | 2.49                     | 0.41              |
| 1:H:54:PHE:O     | 1:H:231:ALA:N    | 2.53                     | 0.40              |
| 1:I:159:LEU:O    | 1:I:160:LYS:C    | 2.58                     | 0.40              |
| 1:G:265:TYR:CB   | 1:G:280:ILE:HD11 | 2.51                     | 0.40              |
| 1:B:134:GLY:HA2  | 1:B:170:LYS:O    | 2.21                     | 0.40              |
| 1:D:149:ILE:HG13 | 1:D:221:PRO:HB3  | 2.03                     | 0.40              |
| 1:D:198:HIS:NE2  | 3:D:1446:HOH:O   | 2.37                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:66:SER:HB2   | 1:A:71:LEU:HD12  | 2.03                     | 0.40              |
| 1:D:161:TRP:CZ2  | 1:D:165:LEU:HD11 | 2.56                     | 0.40              |
| 1:E:259:THR:O    | 1:E:274:THR:HG22 | 2.22                     | 0.40              |
| 1:G:265:TYR:N    | 1:G:265:TYR:CD1  | 2.89                     | 0.40              |
| 1:F:182:VAL:O    | 1:F:184:ASN:N    | 2.55                     | 0.40              |
| 1:E:57:GLU:O     | 1:E:101:ARG:NH2  | 2.54                     | 0.40              |
| 1:G:244:LYS:NZ   | 3:G:712:HOH:O    | 2.54                     | 0.40              |
| 1:B:130:LYS:HE3  | 1:B:131:ASN:ND2  | 2.36                     | 0.40              |
| 1:B:98:LEU:HG    | 1:B:229:GLY:HA2  | 2.04                     | 0.40              |
| 1:D:78:THR:HG23  | 1:D:247:ALA:HA   | 2.03                     | 0.40              |
| 1:B:292:THR:OG1  | 1:B:295:GLU:HB2  | 2.21                     | 0.40              |
| 1:B:253:GLU:H    | 1:B:253:GLU:HG3  | 1.51                     | 0.40              |
| 1:H:42:ILE:HG21  | 1:H:233:LEU:CD1  | 2.52                     | 0.40              |
| 1:A:252:LYS:HD2  | 1:H:237:GLN:CD   | 2.41                     | 0.40              |
| 1:I:183:GLU:OE2  | 1:I:211:THR:HG23 | 2.21                     | 0.40              |
| 1:D:104:VAL:HG21 | 1:D:213:LEU:HB3  | 2.04                     | 0.40              |
| 1:B:59:ILE:N     | 1:B:60:PRO:CD    | 2.84                     | 0.40              |
| 1:I:248:PHE:HA   | 3:I:873:HOH:O    | 2.20                     | 0.40              |
| 1:D:210:HIS:CE1  | 3:D:795:HOH:O    | 2.73                     | 0.40              |
| 1:C:155:GLU:O    | 1:C:158:ALA:HB3  | 2.21                     | 0.40              |
| 1:G:2:ILE:HA     | 1:G:52:ASP:OD1   | 2.21                     | 0.40              |
| 1:B:256:ARG:HD3  | 3:B:796:HOH:O    | 2.21                     | 0.40              |
| 1:C:303:LEU:CD1  | 1:C:308:MET:HE3  | 2.48                     | 0.40              |
| 1:I:173:ALA:O    | 1:I:174:LYS:HG2  | 2.22                     | 0.40              |
| 3:A:1179:HOH:O   | 1:H:48:ARG:HG2   | 2.20                     | 0.40              |
| 1:F:170:LYS:HA   | 1:F:171:PRO:HD3  | 1.93                     | 0.40              |
| 1:H:292:THR:H    | 1:H:295:GLU:HB2  | 1.86                     | 0.40              |
| 1:E:253:GLU:H    | 1:E:253:GLU:CD   | 2.25                     | 0.40              |
| 1:C:111:LYS:HE2  | 1:C:111:LYS:HB3  | 1.54                     | 0.40              |
| 1:D:260:ALA:HA   | 1:D:274:THR:CG2  | 2.52                     | 0.40              |
| 1:A:115:LYS:CB   | 1:A:115:LYS:NZ   | 2.77                     | 0.40              |
| 1:I:107:TYR:CD1  | 1:I:117:LEU:HD11 | 2.57                     | 0.40              |
| 1:C:204:LYS:CE   | 3:C:1506:HOH:O   | 2.61                     | 0.40              |
| 1:B:170:LYS:CE   | 1:B:187:ILE:HD12 | 2.51                     | 0.40              |
| 1:C:107:TYR:O    | 1:C:211:THR:HA   | 2.22                     | 0.40              |
| 1:A:80:ASN:CG    | 1:A:83:ARG:HH21  | 2.25                     | 0.40              |
| 1:A:170:LYS:HE3  | 1:A:170:LYS:HB2  | 1.93                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 307/309 (99%)   | 297 (97%)  | 10 (3%)  | 0        | 100         | 100 |
| 1   | B     | 307/309 (99%)   | 280 (91%)  | 21 (7%)  | 6 (2%)   | 9           | 4   |
| 1   | C     | 307/309 (99%)   | 284 (92%)  | 18 (6%)  | 5 (2%)   | 12          | 6   |
| 1   | D     | 307/309 (99%)   | 286 (93%)  | 16 (5%)  | 5 (2%)   | 12          | 6   |
| 1   | E     | 307/309 (99%)   | 296 (96%)  | 9 (3%)   | 2 (1%)   | 26          | 21  |
| 1   | F     | 307/309 (99%)   | 284 (92%)  | 18 (6%)  | 5 (2%)   | 12          | 6   |
| 1   | G     | 307/309 (99%)   | 284 (92%)  | 19 (6%)  | 4 (1%)   | 15          | 9   |
| 1   | H     | 307/309 (99%)   | 262 (85%)  | 39 (13%) | 6 (2%)   | 9           | 4   |
| 1   | I     | 307/309 (99%)   | 274 (89%)  | 30 (10%) | 3 (1%)   | 19          | 13  |
| All | All   | 2763/2781 (99%) | 2547 (92%) | 180 (6%) | 36 (1%)  | 15          | 9   |

All (36) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 85  | LYS  |
| 1   | H     | 8   | GLN  |
| 1   | H     | 81  | GLU  |
| 1   | B     | 33  | ALA  |
| 1   | B     | 85  | LYS  |
| 1   | C     | 85  | LYS  |
| 1   | C     | 114 | GLU  |
| 1   | D     | 240 | ASP  |
| 1   | E     | 44  | GLU  |
| 1   | F     | 183 | GLU  |
| 1   | F     | 185 | GLY  |
| 1   | G     | 26  | ILE  |
| 1   | H     | 12  | ALA  |
| 1   | C     | 46  | GLY  |
| 1   | C     | 47  | SER  |
| 1   | C     | 279 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 217 | ARG  |
| 1   | D     | 239 | LYS  |
| 1   | F     | 116 | ASP  |
| 1   | H     | 11  | GLU  |
| 1   | I     | 130 | LYS  |
| 1   | I     | 307 | GLY  |
| 1   | D     | 155 | GLU  |
| 1   | E     | 45  | GLU  |
| 1   | F     | 33  | ALA  |
| 1   | G     | 23  | ALA  |
| 1   | G     | 217 | ARG  |
| 1   | H     | 10  | LYS  |
| 1   | H     | 69  | ASN  |
| 1   | I     | 203 | GLU  |
| 1   | B     | 93  | LYS  |
| 1   | D     | 156 | ALA  |
| 1   | B     | 240 | ASP  |
| 1   | B     | 276 | ASN  |
| 1   | G     | 192 | ILE  |
| 1   | B     | 73  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 245/245 (100%) | 230 (94%) | 15 (6%)  | 23          | 19 |
| 1   | B     | 245/245 (100%) | 228 (93%) | 17 (7%)  | 19          | 15 |
| 1   | C     | 245/245 (100%) | 227 (93%) | 18 (7%)  | 17          | 13 |
| 1   | D     | 245/245 (100%) | 223 (91%) | 22 (9%)  | 12          | 8  |
| 1   | E     | 245/245 (100%) | 224 (91%) | 21 (9%)  | 13          | 9  |
| 1   | F     | 245/245 (100%) | 232 (95%) | 13 (5%)  | 28          | 25 |
| 1   | G     | 245/245 (100%) | 228 (93%) | 17 (7%)  | 19          | 15 |
| 1   | H     | 245/245 (100%) | 223 (91%) | 22 (9%)  | 12          | 8  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | I     | 245/245 (100%)   | 215 (88%)  | 30 (12%) | 6           | 3  |
| All | All   | 2205/2205 (100%) | 2030 (92%) | 175 (8%) | 15          | 11 |

All (175) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | THR  |
| 1   | A     | 45  | GLU  |
| 1   | A     | 48  | ARG  |
| 1   | A     | 92  | LYS  |
| 1   | A     | 103 | ARG  |
| 1   | A     | 115 | LYS  |
| 1   | A     | 138 | THR  |
| 1   | A     | 146 | ILE  |
| 1   | A     | 191 | LEU  |
| 1   | A     | 203 | GLU  |
| 1   | A     | 206 | VAL  |
| 1   | A     | 209 | VAL  |
| 1   | A     | 216 | VAL  |
| 1   | A     | 272 | VAL  |
| 1   | A     | 302 | LEU  |
| 1   | B     | 3   | THR  |
| 1   | B     | 8   | GLN  |
| 1   | B     | 16  | VAL  |
| 1   | B     | 22  | ARG  |
| 1   | B     | 30  | LEU  |
| 1   | B     | 34  | LYS  |
| 1   | B     | 93  | LYS  |
| 1   | B     | 103 | ARG  |
| 1   | B     | 112 | LEU  |
| 1   | B     | 114 | GLU  |
| 1   | B     | 167 | GLU  |
| 1   | B     | 191 | LEU  |
| 1   | B     | 211 | THR  |
| 1   | B     | 239 | LYS  |
| 1   | B     | 240 | ASP  |
| 1   | B     | 253 | GLU  |
| 1   | B     | 259 | THR  |
| 1   | C     | 8   | GLN  |
| 1   | C     | 10  | LYS  |
| 1   | C     | 11  | GLU  |
| 1   | C     | 28  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 81  | GLU  |
| 1   | C     | 85  | LYS  |
| 1   | C     | 103 | ARG  |
| 1   | C     | 115 | LYS  |
| 1   | C     | 167 | GLU  |
| 1   | C     | 204 | LYS  |
| 1   | C     | 207 | GLN  |
| 1   | C     | 209 | VAL  |
| 1   | C     | 211 | THR  |
| 1   | C     | 253 | GLU  |
| 1   | C     | 258 | LEU  |
| 1   | C     | 268 | ASN  |
| 1   | C     | 274 | THR  |
| 1   | C     | 293 | VAL  |
| 1   | D     | 1   | ASP  |
| 1   | D     | 9   | HIS  |
| 1   | D     | 11  | GLU  |
| 1   | D     | 48  | ARG  |
| 1   | D     | 65  | LEU  |
| 1   | D     | 101 | ARG  |
| 1   | D     | 103 | ARG  |
| 1   | D     | 115 | LYS  |
| 1   | D     | 117 | LEU  |
| 1   | D     | 166 | LYS  |
| 1   | D     | 167 | GLU  |
| 1   | D     | 214 | ASN  |
| 1   | D     | 235 | SER  |
| 1   | D     | 240 | ASP  |
| 1   | D     | 252 | LYS  |
| 1   | D     | 256 | ARG  |
| 1   | D     | 259 | THR  |
| 1   | D     | 262 | ARG  |
| 1   | D     | 264 | GLU  |
| 1   | D     | 268 | ASN  |
| 1   | D     | 280 | ILE  |
| 1   | D     | 308 | MET  |
| 1   | E     | 3   | THR  |
| 1   | E     | 29  | LYS  |
| 1   | E     | 32  | SER  |
| 1   | E     | 36  | ASP  |
| 1   | E     | 101 | ARG  |
| 1   | E     | 121 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 152 | LEU  |
| 1   | E     | 163 | LYS  |
| 1   | E     | 188 | ASP  |
| 1   | E     | 191 | LEU  |
| 1   | E     | 200 | PHE  |
| 1   | E     | 219 | ARG  |
| 1   | E     | 233 | LEU  |
| 1   | E     | 235 | SER  |
| 1   | E     | 252 | LYS  |
| 1   | E     | 253 | GLU  |
| 1   | E     | 268 | ASN  |
| 1   | E     | 274 | THR  |
| 1   | E     | 280 | ILE  |
| 1   | E     | 301 | ARG  |
| 1   | E     | 309 | LYS  |
| 1   | F     | 8   | GLN  |
| 1   | F     | 9   | HIS  |
| 1   | F     | 38  | LEU  |
| 1   | F     | 103 | ARG  |
| 1   | F     | 145 | GLN  |
| 1   | F     | 166 | LYS  |
| 1   | F     | 180 | GLN  |
| 1   | F     | 184 | ASN  |
| 1   | F     | 186 | GLU  |
| 1   | F     | 191 | LEU  |
| 1   | F     | 255 | GLN  |
| 1   | F     | 280 | ILE  |
| 1   | F     | 287 | GLN  |
| 1   | G     | 18  | ASP  |
| 1   | G     | 38  | LEU  |
| 1   | G     | 74  | LEU  |
| 1   | G     | 103 | ARG  |
| 1   | G     | 104 | VAL  |
| 1   | G     | 112 | LEU  |
| 1   | G     | 146 | ILE  |
| 1   | G     | 159 | LEU  |
| 1   | G     | 233 | LEU  |
| 1   | G     | 240 | ASP  |
| 1   | G     | 252 | LYS  |
| 1   | G     | 256 | ARG  |
| 1   | G     | 264 | GLU  |
| 1   | G     | 280 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 297 | GLU  |
| 1   | G     | 303 | LEU  |
| 1   | G     | 304 | GLU  |
| 1   | H     | 2   | ILE  |
| 1   | H     | 3   | THR  |
| 1   | H     | 34  | LYS  |
| 1   | H     | 36  | ASP  |
| 1   | H     | 37  | GLN  |
| 1   | H     | 69  | ASN  |
| 1   | H     | 80  | ASN  |
| 1   | H     | 89  | VAL  |
| 1   | H     | 93  | LYS  |
| 1   | H     | 101 | ARG  |
| 1   | H     | 114 | GLU  |
| 1   | H     | 117 | LEU  |
| 1   | H     | 135 | TYR  |
| 1   | H     | 155 | GLU  |
| 1   | H     | 206 | VAL  |
| 1   | H     | 249 | LEU  |
| 1   | H     | 253 | GLU  |
| 1   | H     | 255 | GLN  |
| 1   | H     | 264 | GLU  |
| 1   | H     | 288 | VAL  |
| 1   | H     | 295 | GLU  |
| 1   | H     | 297 | GLU  |
| 1   | I     | 8   | GLN  |
| 1   | I     | 16  | VAL  |
| 1   | I     | 24  | THR  |
| 1   | I     | 27  | LYS  |
| 1   | I     | 30  | LEU  |
| 1   | I     | 43  | LYS  |
| 1   | I     | 62  | LEU  |
| 1   | I     | 66  | SER  |
| 1   | I     | 69  | ASN  |
| 1   | I     | 71  | LEU  |
| 1   | I     | 72  | GLU  |
| 1   | I     | 80  | ASN  |
| 1   | I     | 83  | ARG  |
| 1   | I     | 85  | LYS  |
| 1   | I     | 109 | THR  |
| 1   | I     | 111 | LYS  |
| 1   | I     | 122 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 167 | GLU  |
| 1   | I     | 204 | LYS  |
| 1   | I     | 212 | ARG  |
| 1   | I     | 213 | LEU  |
| 1   | I     | 226 | THR  |
| 1   | I     | 239 | LYS  |
| 1   | I     | 240 | ASP  |
| 1   | I     | 253 | GLU  |
| 1   | I     | 267 | LEU  |
| 1   | I     | 274 | THR  |
| 1   | I     | 277 | LEU  |
| 1   | I     | 288 | VAL  |
| 1   | I     | 300 | THR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | HIS  |
| 1   | A     | 208 | ASN  |
| 1   | A     | 218 | HIS  |
| 1   | A     | 298 | HIS  |
| 1   | B     | 9   | HIS  |
| 1   | B     | 31  | ASN  |
| 1   | B     | 41  | GLN  |
| 1   | B     | 58  | GLN  |
| 1   | B     | 131 | ASN  |
| 1   | B     | 175 | ASN  |
| 1   | B     | 193 | ASN  |
| 1   | B     | 198 | HIS  |
| 1   | B     | 210 | HIS  |
| 1   | B     | 214 | ASN  |
| 1   | B     | 218 | HIS  |
| 1   | C     | 8   | GLN  |
| 1   | C     | 31  | ASN  |
| 1   | C     | 208 | ASN  |
| 1   | C     | 255 | GLN  |
| 1   | C     | 268 | ASN  |
| 1   | D     | 14  | GLN  |
| 1   | D     | 123 | ASN  |
| 1   | D     | 175 | ASN  |
| 1   | D     | 193 | ASN  |
| 1   | D     | 238 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 268 | ASN  |
| 1   | D     | 270 | HIS  |
| 1   | D     | 298 | HIS  |
| 1   | E     | 6   | ASN  |
| 1   | E     | 69  | ASN  |
| 1   | E     | 238 | ASN  |
| 1   | E     | 255 | GLN  |
| 1   | E     | 268 | ASN  |
| 1   | F     | 80  | ASN  |
| 1   | F     | 175 | ASN  |
| 1   | F     | 198 | HIS  |
| 1   | F     | 214 | ASN  |
| 1   | F     | 218 | HIS  |
| 1   | F     | 237 | GLN  |
| 1   | F     | 255 | GLN  |
| 1   | F     | 287 | GLN  |
| 1   | F     | 298 | HIS  |
| 1   | G     | 69  | ASN  |
| 1   | G     | 175 | ASN  |
| 1   | G     | 184 | ASN  |
| 1   | G     | 208 | ASN  |
| 1   | G     | 218 | HIS  |
| 1   | G     | 237 | GLN  |
| 1   | G     | 238 | ASN  |
| 1   | G     | 255 | GLN  |
| 1   | H     | 37  | GLN  |
| 1   | H     | 69  | ASN  |
| 1   | H     | 80  | ASN  |
| 1   | H     | 131 | ASN  |
| 1   | H     | 175 | ASN  |
| 1   | H     | 180 | GLN  |
| 1   | H     | 184 | ASN  |
| 1   | H     | 208 | ASN  |
| 1   | H     | 237 | GLN  |
| 1   | H     | 255 | GLN  |
| 1   | I     | 6   | ASN  |
| 1   | I     | 8   | GLN  |
| 1   | I     | 14  | GLN  |
| 1   | I     | 31  | ASN  |
| 1   | I     | 69  | ASN  |
| 1   | I     | 80  | ASN  |
| 1   | I     | 175 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 214 | ASN  |
| 1   | I     | 298 | HIS  |
| 1   | I     | 305 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|--------------|-----------------------|-------|
| 1   | A     | 309/309 (100%)   | -0.77  | 0 100 100    | 12, 20, 31, 41        | 0     |
| 1   | B     | 309/309 (100%)   | -0.66  | 0 100 100    | 11, 23, 45, 62        | 0     |
| 1   | C     | 309/309 (100%)   | -0.74  | 0 100 100    | 12, 23, 37, 55        | 0     |
| 1   | D     | 309/309 (100%)   | -0.72  | 0 100 100    | 15, 26, 38, 51        | 0     |
| 1   | E     | 309/309 (100%)   | -0.79  | 0 100 100    | 13, 23, 34, 46        | 0     |
| 1   | F     | 309/309 (100%)   | -0.78  | 0 100 100    | 13, 22, 36, 48        | 0     |
| 1   | G     | 309/309 (100%)   | -0.71  | 0 100 100    | 18, 29, 41, 50        | 0     |
| 1   | H     | 309/309 (100%)   | -0.37  | 2 (0%) 90 92 | 23, 38, 59, 65        | 0     |
| 1   | I     | 309/309 (100%)   | -0.55  | 1 (0%) 94 95 | 22, 36, 49, 67        | 0     |
| All | All   | 2781/2781 (100%) | -0.68  | 3 (0%) 95 96 | 11, 27, 48, 67        | 0     |

All (3) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 308 | MET  | 3.0  |
| 1   | H     | 242 | ALA  | 2.2  |
| 1   | H     | 1   | ASP  | 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 2   | CU   | B     | 310 | 1/1   | 0.98 | 0.09 | -0.10 | 41,41,41,41                | 0     |
| 2   | CU   | F     | 311 | 1/1   | 0.92 | 0.09 | -     | 61,61,61,61                | 0     |
| 2   | CU   | D     | 311 | 1/1   | 0.95 | 0.10 | -     | 50,50,50,50                | 0     |
| 2   | CU   | H     | 311 | 1/1   | 0.94 | 0.06 | -     | 71,71,71,71                | 0     |
| 2   | CU   | C     | 311 | 1/1   | 0.99 | 0.09 | -     | 37,37,37,37                | 0     |
| 2   | CU   | A     | 311 | 1/1   | 1.00 | 0.09 | -     | 37,37,37,37                | 0     |
| 2   | CU   | G     | 311 | 1/1   | 0.96 | 0.07 | -     | 55,55,55,55                | 0     |
| 2   | CU   | E     | 311 | 1/1   | 0.99 | 0.09 | -     | 45,45,45,45                | 0     |
| 2   | CU   | I     | 310 | 1/1   | 0.99 | 0.05 | -     | 46,46,46,46                | 0     |
| 2   | CU   | I     | 311 | 1/1   | 0.95 | 0.06 | -     | 64,64,64,64                | 0     |
| 2   | CU   | C     | 310 | 1/1   | 0.99 | 0.07 | -     | 49,49,49,49                | 0     |
| 2   | CU   | F     | 310 | 1/1   | 0.91 | 0.08 | -     | 53,53,53,53                | 0     |
| 2   | CU   | A     | 310 | 1/1   | 0.99 | 0.09 | -     | 38,38,38,38                | 0     |
| 2   | CU   | D     | 310 | 1/1   | 0.97 | 0.12 | -     | 45,45,45,45                | 0     |
| 2   | CU   | G     | 310 | 1/1   | 0.98 | 0.05 | -     | 53,53,53,53                | 0     |
| 2   | CU   | E     | 310 | 1/1   | 0.99 | 0.08 | -     | 46,46,46,46                | 0     |
| 2   | CU   | H     | 310 | 1/1   | 0.96 | 0.06 | -     | 56,56,56,56                | 0     |
| 2   | CU   | B     | 311 | 1/1   | 0.98 | 0.09 | -     | 46,46,46,46                | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.