



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:45 PM GMT

PDB ID : 1V02  
Title : CRYSTAL STRUCTURE OF THE SORGHUM BICOLOR DHURRINASE 1  
Authors : Moriniere, J.; Verdoucq, L.; Bevan, D.R.; Esen, A.; Henrissat, B.; Czjzek, M.  
Deposited on : 2004-03-22  
Resolution : 1.80 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

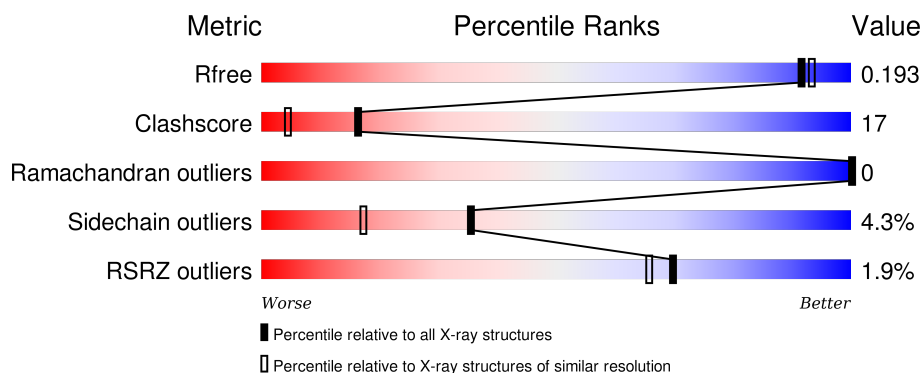
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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                       | 4533 (1.80-1.80)                                      |
| Clashscore            | 102246                      | 5383 (1.80-1.80)                                      |
| Ramachandran outliers | 100387                      | 5320 (1.80-1.80)                                      |
| Sidechain outliers    | 100360                      | 5319 (1.80-1.80)                                      |
| RSRZ outliers         | 91569                       | 4547 (1.80-1.80)                                      |

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     | 565    | <div> <div></div> <div>70% 14% • 14%</div> </div>   |
| 1   | B     | 565    | <div> <div>2%</div> <div>72% 12% • 14%</div> </div> |
| 1   | C     | 565    | <div> <div></div> <div>68% 16% • 14%</div> </div>   |
| 1   | D     | 565    | <div> <div>2%</div> <div>72% 12% • 14%</div> </div> |
| 1   | F     | 565    | <div> <div>2%</div> <div>67% 16% • 14%</div> </div> |

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| Mol | Chain | Length | Quality of chain      |
|-----|-------|--------|-----------------------|
| 2   | E     | 565    | <p>2% 68% 15% 14%</p> |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28327 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 DHURRINASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 484      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3875  | 2476 | 652 | 728 | 19 |         |         |       |
| 1   | B     | 484      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3875  | 2476 | 652 | 728 | 19 |         |         |       |
| 1   | C     | 484      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3875  | 2476 | 652 | 728 | 19 |         |         |       |
| 1   | D     | 484      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3875  | 2476 | 652 | 728 | 19 |         |         |       |
| 1   | F     | 484      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3875  | 2476 | 652 | 728 | 19 |         |         |       |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 119     | ARG      | GLY    | CONFLICT | UNP Q41290 |
| A     | 161     | ARG      | GLU    | CONFLICT | UNP Q41290 |
| A     | 162     | ILE      | ASP    | CONFLICT | UNP Q41290 |
| A     | 163     | ILE      | TYR    | CONFLICT | UNP Q41290 |
| B     | 119     | ARG      | GLY    | CONFLICT | UNP Q41290 |
| B     | 161     | ARG      | GLU    | CONFLICT | UNP Q41290 |
| B     | 162     | ILE      | ASP    | CONFLICT | UNP Q41290 |
| B     | 163     | ILE      | TYR    | CONFLICT | UNP Q41290 |
| C     | 119     | ARG      | GLY    | CONFLICT | UNP Q41290 |
| C     | 161     | ARG      | GLU    | CONFLICT | UNP Q41290 |
| C     | 162     | ILE      | ASP    | CONFLICT | UNP Q41290 |
| C     | 163     | ILE      | TYR    | CONFLICT | UNP Q41290 |
| D     | 119     | ARG      | GLY    | CONFLICT | UNP Q41290 |
| D     | 161     | ARG      | GLU    | CONFLICT | UNP Q41290 |
| D     | 162     | ILE      | ASP    | CONFLICT | UNP Q41290 |
| D     | 163     | ILE      | TYR    | CONFLICT | UNP Q41290 |
| F     | 119     | ARG      | GLY    | CONFLICT | UNP Q41290 |
| F     | 161     | ARG      | GLU    | CONFLICT | UNP Q41290 |
| F     | 162     | ILE      | ASP    | CONFLICT | UNP Q41290 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| F     | 163     | ILE      | TYR    | CONFLICT | UNP Q41290 |

- Molecule 2 is a protein called DHURRINASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | E     | 484      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3884  | 2482 | 656 | 727 | 19 |         |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| E     | 119     | ARG      | GLY    | CONFLICT | UNP Q41290 |
| E     | 161     | ARG      | GLU    | CONFLICT | UNP Q41290 |
| E     | 162     | ILE      | ASP    | CONFLICT | UNP Q41290 |
| E     | 163     | ILE      | TYR    | CONFLICT | UNP Q41290 |
| E     | 180     | LYS      | THR    | CONFLICT | UNP Q41290 |

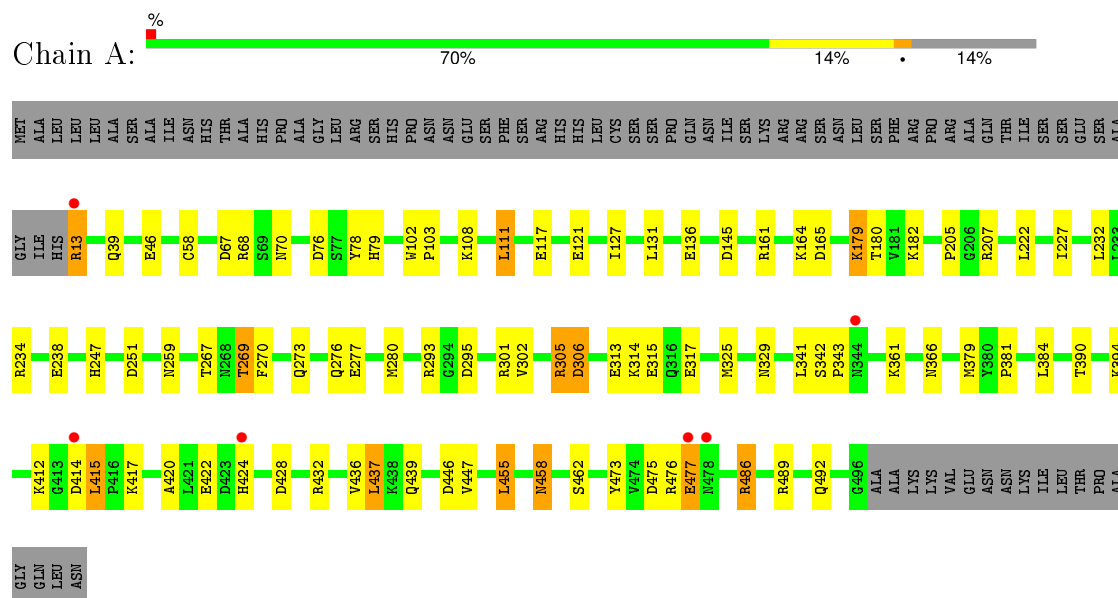
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 846      | Total | O   | 0       | 0       |
|     |       |          | 846   | 846 |         |         |
| 3   | B     | 860      | Total | O   | 0       | 0       |
|     |       |          | 860   | 860 |         |         |
| 3   | C     | 832      | Total | O   | 0       | 0       |
|     |       |          | 832   | 832 |         |         |
| 3   | D     | 827      | Total | O   | 0       | 0       |
|     |       |          | 827   | 827 |         |         |
| 3   | E     | 869      | Total | O   | 0       | 0       |
|     |       |          | 869   | 869 |         |         |
| 3   | F     | 834      | Total | O   | 0       | 0       |
|     |       |          | 834   | 834 |         |         |

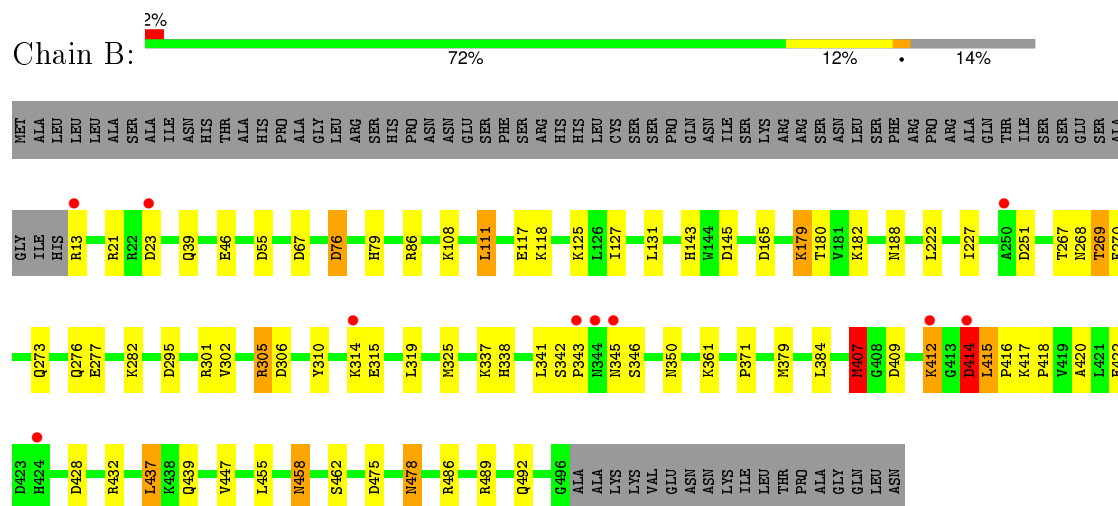
### 3 Residue-property plots

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: DHURRINASE

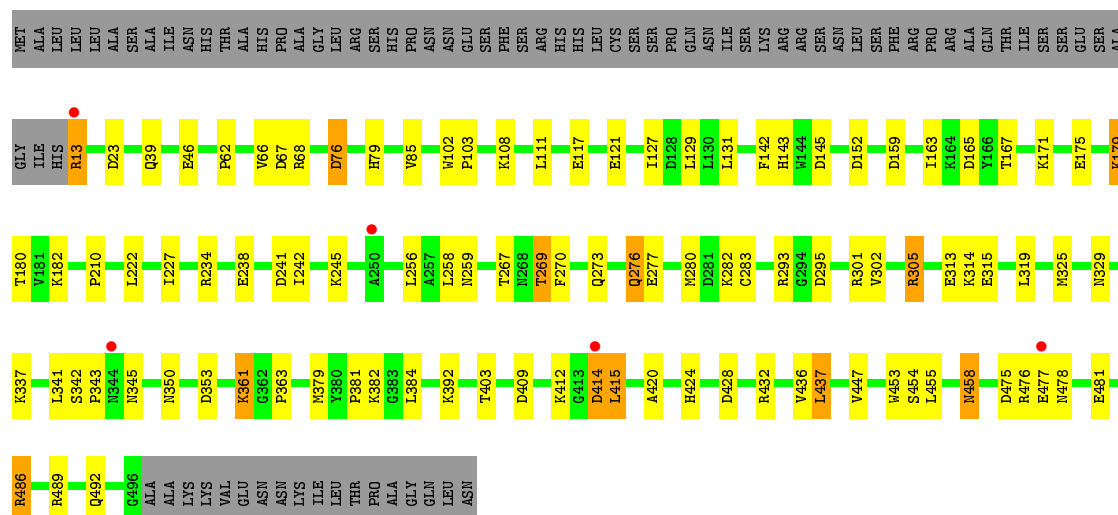


#### • Molecule 1: DHURRINASE

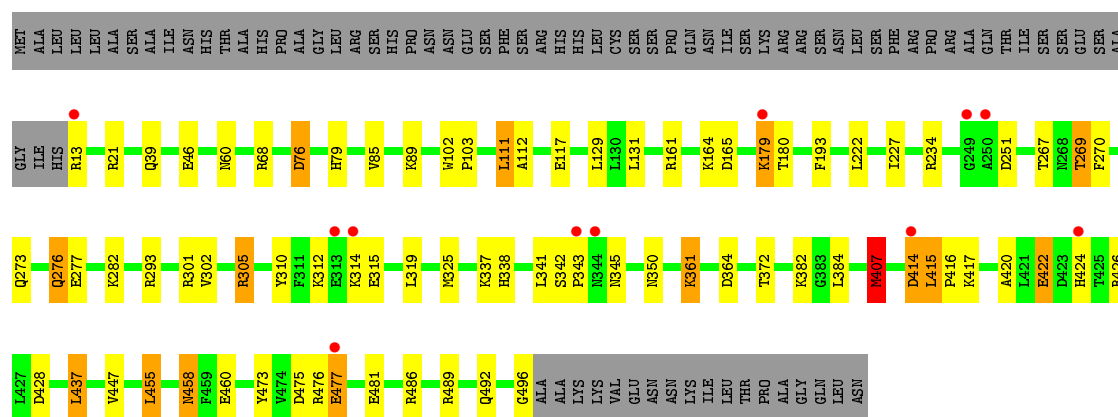


#### • Molecule 1: DHURRINASE

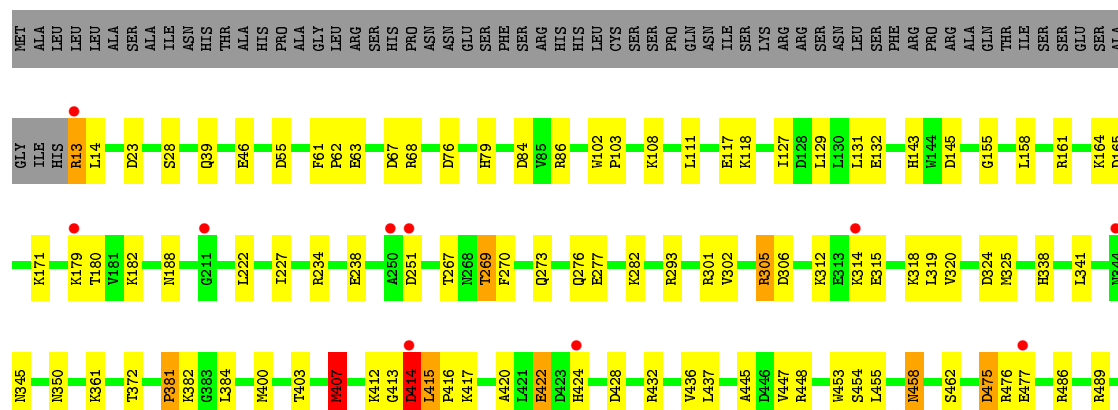




### • Molecule 1: DHURRINASE

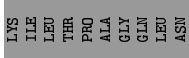
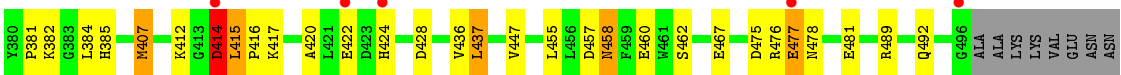
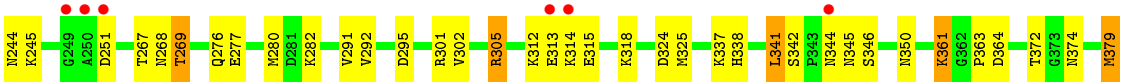
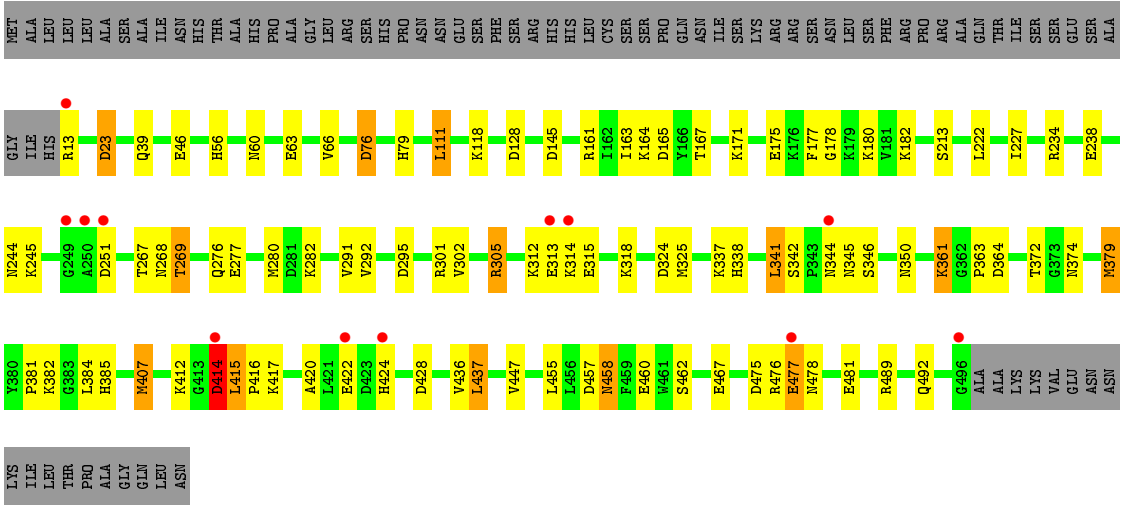


### • Molecule 1: DHURRINASE





● Molecule 2: DHURRINASE





## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 31   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 101.05Å 101.05Å 279.05Å<br>90.00° 90.00° 120.00°               | Depositor        |
| Resolution (Å)  | 30.00 – 1.80<br>19.92 – 1.80                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.6 (30.00-1.80)<br>98.6 (19.92-1.80)                         | Depositor<br>EDS |
| $R_{merge}$   | 0.07   | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.71 (at 1.80Å)  | Xtriage          |
| Refinement program  | REFMAC 5.1.24  | Depositor        |
| R, $R_{free}$   | 0.172 , 0.210<br>0.152 , 0.193                                 | Depositor<br>DCC |
| $R_{free}$ test set   | 14720 reflections (5.33%)                                      | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 17.3   | Xtriage          |
| Anisotropy  | 0.478  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.38 , 69.3  | EDS              |
| Estimated twinning fraction   | 0.000 for -h,-k,l<br>0.023 for h,-h-k,-l<br>0.013 for -k,-h,-l | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$    | Xtriage          |
| Outliers  | 0 of 291091 reflections  | Xtriage          |
| $F_o, F_c$ correlation  | 0.97   | EDS              |
| Total number of atoms   | 28327  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 31.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.43% 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

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     | 0.62         | 0/3990         | 0.80        | 10/5421 (0.2%)  |
| 1   | B     | 0.62         | 2/3990 (0.1%)  | 0.80        | 12/5421 (0.2%)  |
| 1   | C     | 0.61         | 0/3990         | 0.80        | 14/5421 (0.3%)  |
| 1   | D     | 0.63         | 1/3990 (0.0%)  | 0.79        | 8/5421 (0.1%)   |
| 1   | F     | 0.66         | 1/3990 (0.0%)  | 0.80        | 10/5421 (0.2%)  |
| 2   | E     | 0.62         | 1/3999 (0.0%)  | 0.81        | 12/5431 (0.2%)  |
| All | All   | 0.63         | 5/23949 (0.0%) | 0.80        | 66/32536 (0.2%) |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | F     | 407 | MET  | SD-CE | -13.31 | 1.03        | 1.77     |
| 1   | D     | 407 | MET  | SD-CE | -10.35 | 1.19        | 1.77     |
| 1   | B     | 407 | MET  | SD-CE | -6.03  | 1.44        | 1.77     |
| 2   | E     | 379 | MET  | CG-SD | -5.46  | 1.67        | 1.81     |
| 1   | B     | 407 | MET  | CG-SD | -5.13  | 1.67        | 1.81     |

All (66) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 305 | ARG  | NE-CZ-NH1 | 9.27  | 124.93      | 120.30   |
| 2   | E     | 305 | ARG  | NE-CZ-NH1 | 9.17  | 124.89      | 120.30   |
| 1   | D     | 305 | ARG  | NE-CZ-NH1 | 9.05  | 124.82      | 120.30   |
| 1   | B     | 305 | ARG  | NE-CZ-NH1 | 8.60  | 124.60      | 120.30   |
| 2   | E     | 305 | ARG  | NE-CZ-NH2 | -7.70 | 116.45      | 120.30   |
| 1   | A     | 305 | ARG  | NE-CZ-NH1 | 7.41  | 124.01      | 120.30   |
| 1   | F     | 305 | ARG  | NE-CZ-NH2 | -7.17 | 116.71      | 120.30   |
| 1   | B     | 305 | ARG  | NE-CZ-NH2 | -6.93 | 116.83      | 120.30   |
| 1   | A     | 165 | ASP  | CB-CG-OD2 | 6.84  | 124.46      | 118.30   |
| 2   | E     | 165 | ASP  | CB-CG-OD2 | 6.83  | 124.45      | 118.30   |
| 1   | C     | 305 | ARG  | NE-CZ-NH1 | 6.57  | 123.58      | 120.30   |
| 1   | F     | 67  | ASP  | CB-CG-OD2 | 6.55  | 124.19      | 118.30   |
| 1   | B     | 145 | ASP  | CB-CG-OD2 | 6.49  | 124.14      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 145 | ASP  | CB-CG-OD2 | 6.46  | 124.12      | 118.30   |
| 1   | C     | 145 | ASP  | CB-CG-OD2 | 6.45  | 124.10      | 118.30   |
| 1   | D     | 165 | ASP  | CB-CG-OD2 | 6.30  | 123.97      | 118.30   |
| 1   | B     | 414 | ASP  | CB-CG-OD2 | 6.29  | 123.96      | 118.30   |
| 1   | A     | 145 | ASP  | CB-CG-OD2 | 6.29  | 123.96      | 118.30   |
| 1   | B     | 475 | ASP  | CB-CG-OD2 | 6.11  | 123.80      | 118.30   |
| 1   | B     | 67  | ASP  | CB-CG-OD2 | 6.11  | 123.80      | 118.30   |
| 1   | D     | 305 | ARG  | NE-CZ-NH2 | -6.09 | 117.25      | 120.30   |
| 1   | C     | 475 | ASP  | CB-CG-OD2 | 5.92  | 123.62      | 118.30   |
| 1   | A     | 475 | ASP  | CB-CG-OD2 | 5.92  | 123.62      | 118.30   |
| 1   | A     | 305 | ARG  | NE-CZ-NH2 | -5.91 | 117.35      | 120.30   |
| 2   | E     | 145 | ASP  | CB-CG-OD2 | 5.88  | 123.59      | 118.30   |
| 1   | A     | 455 | LEU  | CB-CG-CD2 | 5.87  | 120.98      | 111.00   |
| 1   | C     | 409 | ASP  | CB-CG-OD2 | 5.83  | 123.55      | 118.30   |
| 1   | B     | 428 | ASP  | CB-CG-OD2 | 5.83  | 123.54      | 118.30   |
| 1   | F     | 324 | ASP  | CB-CG-OD2 | 5.80  | 123.52      | 118.30   |
| 1   | F     | 165 | ASP  | CB-CG-OD2 | 5.78  | 123.51      | 118.30   |
| 2   | E     | 23  | ASP  | CB-CG-OD2 | 5.73  | 123.46      | 118.30   |
| 1   | D     | 414 | ASP  | CB-CG-OD2 | 5.66  | 123.39      | 118.30   |
| 1   | C     | 165 | ASP  | CB-CG-OD2 | 5.65  | 123.39      | 118.30   |
| 1   | F     | 55  | ASP  | CB-CG-OD2 | 5.60  | 123.34      | 118.30   |
| 1   | C     | 428 | ASP  | CB-CG-OD2 | 5.59  | 123.33      | 118.30   |
| 2   | E     | 457 | ASP  | CB-CG-OD2 | 5.58  | 123.32      | 118.30   |
| 1   | A     | 295 | ASP  | CB-CG-OD2 | 5.57  | 123.31      | 118.30   |
| 1   | C     | 23  | ASP  | CB-CG-OD2 | 5.55  | 123.30      | 118.30   |
| 1   | A     | 446 | ASP  | CB-CG-OD2 | 5.51  | 123.26      | 118.30   |
| 2   | E     | 295 | ASP  | CB-CG-OD2 | 5.50  | 123.25      | 118.30   |
| 2   | E     | 324 | ASP  | CB-CG-OD2 | 5.42  | 123.18      | 118.30   |
| 1   | B     | 76  | ASP  | CB-CG-OD2 | 5.42  | 123.17      | 118.30   |
| 1   | C     | 295 | ASP  | CB-CG-OD2 | 5.38  | 123.15      | 118.30   |
| 1   | B     | 295 | ASP  | CB-CG-OD2 | 5.34  | 123.11      | 118.30   |
| 1   | C     | 305 | ARG  | NE-CZ-NH2 | -5.28 | 117.66      | 120.30   |
| 2   | E     | 414 | ASP  | CB-CG-OD2 | 5.26  | 123.04      | 118.30   |
| 1   | C     | 241 | ASP  | CB-CG-OD2 | 5.24  | 123.02      | 118.30   |
| 1   | F     | 475 | ASP  | CB-CG-OD2 | 5.23  | 123.01      | 118.30   |
| 1   | D     | 475 | ASP  | CB-CG-OD2 | 5.22  | 123.00      | 118.30   |
| 1   | B     | 165 | ASP  | CB-CG-OD2 | 5.20  | 122.98      | 118.30   |
| 2   | E     | 128 | ASP  | CB-CG-OD2 | 5.18  | 122.97      | 118.30   |
| 1   | D     | 455 | LEU  | CB-CG-CD2 | 5.14  | 119.74      | 111.00   |
| 1   | F     | 414 | ASP  | CB-CG-OD2 | 5.13  | 122.92      | 118.30   |
| 1   | C     | 159 | ASP  | CB-CG-OD2 | 5.13  | 122.91      | 118.30   |
| 1   | C     | 67  | ASP  | CB-CG-OD2 | 5.11  | 122.89      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2   | E     | 76  | ASP  | CB-CG-OD2 | 5.11 | 122.89      | 118.30   |
| 1   | C     | 76  | ASP  | CB-CG-OD2 | 5.10 | 122.89      | 118.30   |
| 1   | A     | 67  | ASP  | CB-CG-OD2 | 5.07 | 122.86      | 118.30   |
| 2   | E     | 341 | LEU  | CA-CB-CG  | 5.06 | 126.95      | 115.30   |
| 1   | B     | 409 | ASP  | CB-CG-OD2 | 5.06 | 122.85      | 118.30   |
| 1   | D     | 364 | ASP  | CB-CG-OD2 | 5.05 | 122.85      | 118.30   |
| 1   | B     | 55  | ASP  | CB-CG-OD2 | 5.03 | 122.83      | 118.30   |
| 1   | D     | 76  | ASP  | CB-CG-OD2 | 5.03 | 122.83      | 118.30   |
| 1   | C     | 353 | ASP  | CB-CG-OD2 | 5.00 | 122.80      | 118.30   |
| 1   | A     | 306 | ASP  | CB-CG-OD2 | 5.00 | 122.80      | 118.30   |
| 1   | F     | 84  | ASP  | CB-CG-OD2 | 5.00 | 122.80      | 118.30   |

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     | 3875  | 0        | 3686     | 124     | 0            |
| 1   | B     | 3875  | 0        | 3686     | 102     | 0            |
| 1   | C     | 3875  | 0        | 3686     | 129     | 0            |
| 1   | D     | 3875  | 0        | 3686     | 115     | 0            |
| 1   | F     | 3875  | 0        | 3686     | 155     | 0            |
| 2   | E     | 3884  | 0        | 3704     | 137     | 1            |
| 3   | A     | 846   | 0        | 0        | 75      | 2            |
| 3   | B     | 860   | 0        | 0        | 71      | 1            |
| 3   | C     | 832   | 0        | 0        | 86      | 3            |
| 3   | D     | 827   | 0        | 0        | 71      | 2            |
| 3   | E     | 869   | 0        | 0        | 99      | 2            |
| 3   | F     | 834   | 0        | 0        | 110     | 1            |
| All | All   | 28327 | 0        | 22134    | 757     | 6            |

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 17.

All (757) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:117:GLU:HB2  | 3:D:2299:HOH:O   | 1.22                     | 1.39              |
| 2:E:372:THR:HB   | 2:E:407:MET:CE   | 1.51                     | 1.39              |
| 1:F:277:GLU:HG3  | 3:F:2551:HOH:O   | 1.22                     | 1.33              |
| 1:B:417:LYS:HB3  | 3:B:2765:HOH:O   | 1.22                     | 1.31              |
| 1:D:407:MET:CE   | 1:D:407:MET:SD   | 1.19                     | 1.28              |
| 1:A:462:SER:HB2  | 3:A:2792:HOH:O   | 1.16                     | 1.28              |
| 1:B:462:SER:HB2  | 3:B:2815:HOH:O   | 1.17                     | 1.28              |
| 1:C:277:GLU:HG3  | 3:C:2542:HOH:O   | 1.25                     | 1.28              |
| 1:A:227:ILE:HG13 | 3:A:2255:HOH:O   | 1.14                     | 1.27              |
| 1:C:245:LYS:HD3  | 3:C:2497:HOH:O   | 1.27                     | 1.26              |
| 1:C:379:MET:HE2  | 3:C:2743:HOH:O   | 1.32                     | 1.26              |
| 1:A:251:ASP:HB3  | 3:A:2532:HOH:O   | 1.30                     | 1.26              |
| 1:B:407:MET:HE1  | 3:B:2709:HOH:O   | 1.27                     | 1.25              |
| 1:F:227:ILE:HG13 | 3:F:2493:HOH:O   | 1.32                     | 1.25              |
| 2:E:315:GLU:CD   | 3:E:2641:HOH:O   | 1.72                     | 1.23              |
| 1:C:227:ILE:HG13 | 3:C:2240:HOH:O   | 1.30                     | 1.23              |
| 1:C:171:LYS:HB2  | 3:C:2406:HOH:O   | 1.37                     | 1.23              |
| 1:F:132:GLU:HB3  | 3:F:2314:HOH:O   | 1.38                     | 1.22              |
| 2:E:372:THR:CB   | 2:E:407:MET:HE2  | 1.69                     | 1.21              |
| 1:C:179:LYS:HE3  | 3:C:2434:HOH:O   | 1.41                     | 1.20              |
| 2:E:422:GLU:HB2  | 3:E:2854:HOH:O   | 1.38                     | 1.19              |
| 1:D:424:HIS:HB2  | 3:D:2740:HOH:O   | 1.39                     | 1.19              |
| 1:F:422:GLU:HB2  | 3:F:2819:HOH:O   | 1.39                     | 1.19              |
| 1:A:424:HIS:ND1  | 3:A:2751:HOH:O   | 1.73                     | 1.19              |
| 2:E:23:ASP:HB3   | 3:E:2040:HOH:O   | 1.42                     | 1.18              |
| 1:D:68:ARG:CA    | 3:D:2181:HOH:O   | 1.88                     | 1.18              |
| 2:E:424:HIS:ND1  | 3:E:2779:HOH:O   | 1.78                     | 1.17              |
| 1:F:407:MET:CE   | 1:F:407:MET:CG   | 2.22                     | 1.17              |
| 1:A:13:ARG:CG    | 1:A:432:ARG:HH21 | 1.57                     | 1.17              |
| 2:E:251:ASP:HB3  | 3:E:2559:HOH:O   | 1.43                     | 1.16              |
| 1:B:345:ASN:OD1  | 3:B:2666:HOH:O   | 1.61                     | 1.16              |
| 1:F:182:LYS:HG2  | 3:F:2518:HOH:O   | 1.46                     | 1.15              |
| 2:E:462:SER:HB2  | 3:E:2822:HOH:O   | 0.98                     | 1.14              |
| 1:B:182:LYS:HG2  | 3:B:2455:HOH:O   | 1.47                     | 1.14              |
| 2:E:407:MET:SD   | 3:E:2759:HOH:O   | 2.04                     | 1.14              |
| 1:F:227:ILE:CG1  | 3:F:2493:HOH:O   | 1.88                     | 1.14              |
| 1:A:422:GLU:HB2  | 3:A:2828:HOH:O   | 1.46                     | 1.13              |
| 1:D:131:LEU:HD11 | 1:D:180:THR:HG22 | 1.29                     | 1.13              |
| 1:F:407:MET:SD   | 1:F:407:MET:CE   | 1.03                     | 1.12              |
| 1:D:407:MET:SD   | 1:D:407:MET:HE1  | 1.77                     | 1.12              |
| 1:C:179:LYS:HB2  | 1:C:179:LYS:HZ3  | 1.10                     | 1.12              |
| 1:F:477:GLU:HB3  | 3:F:2799:HOH:O   | 1.46                     | 1.12              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:234:ARG:NH2  | 3:D:2492:HOH:O   | 1.83                     | 1.12              |
| 1:C:179:LYS:HB2  | 1:C:179:LYS:NZ   | 1.65                     | 1.11              |
| 2:E:277:GLU:HG3  | 3:E:2303:HOH:O   | 1.48                     | 1.10              |
| 2:E:269:THR:CG2  | 3:E:2576:HOH:O   | 2.00                     | 1.10              |
| 1:A:227:ILE:CG1  | 3:A:2255:HOH:O   | 1.73                     | 1.10              |
| 2:E:318:LYS:HD2  | 3:E:2540:HOH:O   | 1.52                     | 1.10              |
| 1:A:131:LEU:HD11 | 1:A:180:THR:CG2  | 1.81                     | 1.10              |
| 2:E:269:THR:HG23 | 3:E:2576:HOH:O   | 1.50                     | 1.10              |
| 1:D:407:MET:SD   | 1:D:407:MET:HE2  | 1.77                     | 1.09              |
| 1:F:86:ARG:HG3   | 3:F:2117:HOH:O   | 1.52                     | 1.09              |
| 1:F:129:LEU:HA   | 3:F:2314:HOH:O   | 1.51                     | 1.08              |
| 1:C:345:ASN:OD1  | 3:C:2625:HOH:O   | 1.67                     | 1.08              |
| 1:D:407:MET:SD   | 1:D:407:MET:HE3  | 1.77                     | 1.08              |
| 1:F:161:ARG:HD3  | 3:F:2400:HOH:O   | 1.51                     | 1.08              |
| 1:B:407:MET:SD   | 3:B:2709:HOH:O   | 2.04                     | 1.08              |
| 1:A:13:ARG:HG2   | 1:A:432:ARG:HH21 | 0.96                     | 1.07              |
| 1:C:227:ILE:CG1  | 3:C:2240:HOH:O   | 1.90                     | 1.07              |
| 1:D:312:LYS:NZ   | 3:D:2588:HOH:O   | 1.72                     | 1.07              |
| 2:E:111:LEU:HG   | 3:E:2449:HOH:O   | 1.52                     | 1.07              |
| 1:A:13:ARG:HA    | 3:A:2005:HOH:O   | 1.52                     | 1.07              |
| 1:B:23:ASP:HB3   | 3:B:2039:HOH:O   | 1.54                     | 1.07              |
| 1:C:131:LEU:HD11 | 1:C:180:THR:HG23 | 1.35                     | 1.06              |
| 2:E:56:HIS:CE1   | 3:E:2160:HOH:O   | 2.08                     | 1.06              |
| 2:E:372:THR:CB   | 2:E:407:MET:CE   | 2.30                     | 1.06              |
| 1:F:361:LYS:HD2  | 3:F:2654:HOH:O   | 1.55                     | 1.06              |
| 1:A:108:LYS:HE3  | 3:A:2294:HOH:O   | 1.55                     | 1.05              |
| 1:C:131:LEU:CD1  | 1:C:180:THR:HG23 | 1.86                     | 1.05              |
| 1:D:407:MET:CE   | 1:D:407:MET:CG   | 2.34                     | 1.05              |
| 2:E:313:GLU:OE1  | 3:E:2633:HOH:O   | 1.72                     | 1.04              |
| 2:E:417:LYS:HB3  | 3:E:2483:HOH:O   | 1.57                     | 1.04              |
| 1:D:338:HIS:HD2  | 3:D:2616:HOH:O   | 1.40                     | 1.03              |
| 1:D:131:LEU:HD11 | 1:D:180:THR:CG2  | 1.87                     | 1.03              |
| 1:D:234:ARG:CZ   | 3:D:2492:HOH:O   | 2.07                     | 1.03              |
| 2:E:227:ILE:HG13 | 3:E:2275:HOH:O   | 0.85                     | 1.03              |
| 1:F:407:MET:HE3  | 1:F:407:MET:SD   | 1.63                     | 1.01              |
| 2:E:313:GLU:HB2  | 3:E:2634:HOH:O   | 1.59                     | 1.01              |
| 1:F:407:MET:HE1  | 1:F:407:MET:SD   | 1.63                     | 1.01              |
| 1:B:227:ILE:HG13 | 3:B:2515:HOH:O   | 0.85                     | 1.01              |
| 1:C:131:LEU:HD11 | 1:C:180:THR:CG2  | 1.90                     | 1.00              |
| 2:E:291:VAL:HG23 | 3:E:2601:HOH:O   | 1.58                     | 1.00              |
| 1:F:407:MET:HE2  | 1:F:407:MET:SD   | 1.63                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:227:ILE:HG13 | 3:D:2252:HOH:O   | 0.84                     | 1.00              |
| 1:B:118:LYS:HG2  | 3:B:2314:HOH:O   | 1.61                     | 1.00              |
| 1:D:282:LYS:HG2  | 3:D:2638:HOH:O   | 1.60                     | 0.99              |
| 1:D:179:LYS:HZ2  | 1:D:179:LYS:HB2  | 1.28                     | 0.98              |
| 1:D:111:LEU:HG   | 3:D:2412:HOH:O   | 1.62                     | 0.98              |
| 1:A:13:ARG:HG2   | 1:A:432:ARG:NH2  | 1.77                     | 0.98              |
| 1:B:346:SER:HB3  | 3:B:2667:HOH:O   | 1.62                     | 0.97              |
| 1:C:392:LYS:HD3  | 3:C:2694:HOH:O   | 1.65                     | 0.97              |
| 1:F:382:LYS:HE3  | 3:F:2684:HOH:O   | 1.63                     | 0.96              |
| 1:A:131:LEU:CD1  | 1:A:180:THR:HG23 | 1.94                     | 0.96              |
| 1:A:131:LEU:CD1  | 1:A:180:THR:CG2  | 2.44                     | 0.96              |
| 2:E:56:HIS:ND1   | 3:E:2160:HOH:O   | 1.95                     | 0.95              |
| 2:E:312:LYS:NZ   | 3:E:2629:HOH:O   | 1.98                     | 0.95              |
| 1:D:179:LYS:NZ   | 1:D:179:LYS:HB2  | 1.82                     | 0.95              |
| 1:A:277:GLU:CD   | 3:A:2559:HOH:O   | 2.04                     | 0.95              |
| 1:F:117:GLU:HB2  | 3:F:2287:HOH:O   | 1.67                     | 0.95              |
| 2:E:345:ASN:OD1  | 3:E:2673:HOH:O   | 1.84                     | 0.94              |
| 1:A:394:LYS:HB2  | 3:A:2709:HOH:O   | 1.67                     | 0.94              |
| 2:E:56:HIS:CG    | 3:E:2160:HOH:O   | 2.19                     | 0.94              |
| 1:B:118:LYS:HD3  | 3:B:2311:HOH:O   | 1.65                     | 0.94              |
| 1:D:422:GLU:HG2  | 3:D:2733:HOH:O   | 1.66                     | 0.94              |
| 1:F:63:GLU:OE1   | 3:F:2157:HOH:O   | 1.86                     | 0.94              |
| 1:D:131:LEU:CD1  | 1:D:180:THR:CG2  | 2.47                     | 0.93              |
| 1:F:131:LEU:HD11 | 1:F:180:THR:CG2  | 1.98                     | 0.93              |
| 1:F:447:VAL:HG23 | 3:F:2771:HOH:O   | 1.68                     | 0.93              |
| 2:E:56:HIS:HD2   | 2:E:60:ASN:HD22  | 1.14                     | 0.92              |
| 2:E:56:HIS:HD2   | 2:E:60:ASN:ND2   | 1.67                     | 0.92              |
| 1:F:462:SER:HB2  | 3:F:2782:HOH:O   | 0.75                     | 0.92              |
| 1:D:486:ARG:NH1  | 3:D:2811:HOH:O   | 1.78                     | 0.91              |
| 1:A:131:LEU:HD11 | 1:A:180:THR:HG23 | 1.48                     | 0.91              |
| 1:B:118:LYS:CG   | 3:B:2314:HOH:O   | 2.17                     | 0.91              |
| 1:C:182:LYS:HE3  | 3:C:2438:HOH:O   | 1.70                     | 0.91              |
| 1:D:164:LYS:HE2  | 3:D:2401:HOH:O   | 1.71                     | 0.90              |
| 1:A:379:MET:HG2  | 3:A:2008:HOH:O   | 1.70                     | 0.90              |
| 2:E:238:GLU:HG3  | 3:E:2541:HOH:O   | 1.70                     | 0.90              |
| 1:A:238:GLU:OE2  | 3:A:2511:HOH:O   | 1.88                     | 0.90              |
| 2:E:56:HIS:CD2   | 2:E:60:ASN:ND2   | 2.40                     | 0.90              |
| 1:C:258:LEU:HG   | 3:C:2512:HOH:O   | 1.70                     | 0.89              |
| 1:C:293:ARG:NE   | 3:C:2557:HOH:O   | 1.66                     | 0.89              |
| 1:F:238:GLU:HG3  | 3:F:2504:HOH:O   | 1.70                     | 0.89              |
| 1:F:417:LYS:HD3  | 3:F:2447:HOH:O   | 1.72                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:112:ALA:HB3  | 3:D:2288:HOH:O   | 1.73                     | 0.89              |
| 1:B:108:LYS:HG2  | 3:B:2138:HOH:O   | 1.72                     | 0.89              |
| 1:A:179:LYS:HZ2  | 1:A:179:LYS:HB2  | 1.37                     | 0.89              |
| 1:A:179:LYS:HB2  | 1:A:179:LYS:NZ   | 1.86                     | 0.88              |
| 1:F:407:MET:HE2  | 1:F:407:MET:CG   | 1.94                     | 0.88              |
| 1:F:413:GLY:HA2  | 3:F:2724:HOH:O   | 1.72                     | 0.88              |
| 1:C:280:MET:HG3  | 3:C:2543:HOH:O   | 1.74                     | 0.88              |
| 1:F:400:MET:HE3  | 3:F:2771:HOH:O   | 1.72                     | 0.88              |
| 1:C:179:LYS:CB   | 1:C:179:LYS:NZ   | 2.38                     | 0.87              |
| 1:F:117:GLU:HG3  | 3:F:2286:HOH:O   | 1.73                     | 0.87              |
| 1:F:158:LEU:HB2  | 3:F:2379:HOH:O   | 1.72                     | 0.87              |
| 1:F:118:LYS:HG3  | 3:F:2295:HOH:O   | 1.74                     | 0.86              |
| 1:C:293:ARG:NH2  | 3:C:2557:HOH:O   | 2.06                     | 0.86              |
| 1:F:118:LYS:CG   | 3:F:2295:HOH:O   | 2.23                     | 0.86              |
| 1:A:477:GLU:HB3  | 3:A:2810:HOH:O   | 1.76                     | 0.86              |
| 1:F:13:ARG:HD2   | 3:F:2018:HOH:O   | 1.76                     | 0.85              |
| 1:F:131:LEU:HD11 | 1:F:180:THR:HG23 | 1.55                     | 0.85              |
| 1:C:171:LYS:HD2  | 3:C:2187:HOH:O   | 1.74                     | 0.85              |
| 1:F:182:LYS:HE3  | 3:F:2203:HOH:O   | 1.76                     | 0.85              |
| 1:B:314:LYS:HB2  | 3:B:2620:HOH:O   | 1.76                     | 0.84              |
| 1:A:131:LEU:HD11 | 1:A:180:THR:HG22 | 1.59                     | 0.84              |
| 1:C:379:MET:CE   | 3:C:2743:HOH:O   | 2.01                     | 0.84              |
| 1:F:422:GLU:HG2  | 3:F:2740:HOH:O   | 1.76                     | 0.84              |
| 1:F:131:LEU:CD1  | 1:F:180:THR:HG23 | 2.06                     | 0.84              |
| 1:A:46:GLU:HG3   | 3:A:2126:HOH:O   | 1.78                     | 0.84              |
| 1:B:46:GLU:HB3   | 3:B:2129:HOH:O   | 1.78                     | 0.84              |
| 1:F:412:LYS:HB2  | 3:F:2720:HOH:O   | 1.77                     | 0.83              |
| 1:B:277:GLU:CD   | 3:B:2579:HOH:O   | 2.16                     | 0.83              |
| 1:B:131:LEU:CD1  | 1:B:180:THR:HG23 | 2.08                     | 0.83              |
| 1:F:415:LEU:HD13 | 1:F:420:ALA:HB2  | 1.59                     | 0.83              |
| 1:A:476:ARG:HD3  | 3:A:2807:HOH:O   | 1.78                     | 0.82              |
| 1:B:125:LYS:HD3  | 3:B:2324:HOH:O   | 1.78                     | 0.82              |
| 1:B:478:ASN:CG   | 3:B:2832:HOH:O   | 2.18                     | 0.82              |
| 1:B:131:LEU:CD1  | 1:B:180:THR:CG2  | 2.57                     | 0.82              |
| 2:E:417:LYS:HE2  | 2:E:477:GLU:OE1  | 1.79                     | 0.82              |
| 1:D:277:GLU:HG3  | 3:D:2553:HOH:O   | 1.79                     | 0.81              |
| 2:E:280:MET:HE2  | 3:E:2304:HOH:O   | 1.80                     | 0.81              |
| 1:A:314:LYS:HE3  | 3:A:2615:HOH:O   | 1.78                     | 0.81              |
| 1:D:312:LYS:HE3  | 3:D:2492:HOH:O   | 1.79                     | 0.81              |
| 1:D:76:ASP:OD1   | 1:D:79:HIS:HD2   | 1.63                     | 0.81              |
| 1:C:68:ARG:CA    | 3:C:2170:HOH:O   | 2.28                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:417:LYS:HD2  | 3:E:2483:HOH:O   | 1.81                     | 0.81              |
| 1:C:280:MET:HE2  | 3:C:2690:HOH:O   | 1.81                     | 0.81              |
| 1:C:117:GLU:HG3  | 3:C:2284:HOH:O   | 1.79                     | 0.81              |
| 1:C:379:MET:HG2  | 3:C:2743:HOH:O   | 1.78                     | 0.81              |
| 1:C:131:LEU:CD1  | 1:C:180:THR:CG2  | 2.55                     | 0.81              |
| 1:A:394:LYS:CB   | 3:A:2709:HOH:O   | 2.25                     | 0.81              |
| 1:A:489:ARG:HH11 | 1:A:492:GLN:HE22 | 1.28                     | 0.81              |
| 1:F:417:LYS:HE3  | 3:F:2803:HOH:O   | 1.79                     | 0.80              |
| 1:F:489:ARG:HH11 | 1:F:492:GLN:HE22 | 1.25                     | 0.80              |
| 1:B:417:LYS:HD2  | 3:B:2410:HOH:O   | 1.80                     | 0.80              |
| 1:A:280:MET:HE3  | 3:A:2568:HOH:O   | 1.81                     | 0.80              |
| 1:F:306:ASP:HB2  | 3:F:2582:HOH:O   | 1.82                     | 0.80              |
| 1:C:13:ARG:CG    | 3:C:2753:HOH:O   | 2.30                     | 0.80              |
| 1:D:46:GLU:HG3   | 3:D:2128:HOH:O   | 1.80                     | 0.80              |
| 1:F:417:LYS:HE2  | 1:F:475:ASP:OD1  | 1.82                     | 0.80              |
| 2:E:338:HIS:HB3  | 3:E:2577:HOH:O   | 1.81                     | 0.79              |
| 1:B:131:LEU:HD11 | 1:B:180:THR:CG2  | 2.13                     | 0.79              |
| 1:B:111:LEU:HG   | 3:B:2431:HOH:O   | 1.82                     | 0.79              |
| 1:A:13:ARG:CG    | 1:A:432:ARG:NH2  | 2.42                     | 0.78              |
| 1:D:486:ARG:HD2  | 3:D:2735:HOH:O   | 1.83                     | 0.78              |
| 1:B:117:GLU:OE1  | 3:B:2307:HOH:O   | 2.01                     | 0.78              |
| 1:B:23:ASP:CG    | 1:F:448:ARG:HH22 | 1.86                     | 0.78              |
| 1:A:13:ARG:CA    | 3:A:2005:HOH:O   | 2.20                     | 0.78              |
| 1:C:13:ARG:N     | 3:C:2001:HOH:O   | 2.17                     | 0.78              |
| 1:F:407:MET:CE   | 3:F:2669:HOH:O   | 2.32                     | 0.78              |
| 1:B:314:LYS:HE3  | 3:B:2621:HOH:O   | 1.82                     | 0.78              |
| 1:A:462:SER:CB   | 3:A:2792:HOH:O   | 1.90                     | 0.77              |
| 1:C:382:LYS:HE2  | 3:C:2682:HOH:O   | 1.83                     | 0.77              |
| 2:E:111:LEU:CG   | 3:E:2449:HOH:O   | 2.19                     | 0.77              |
| 1:F:61:PHE:HA    | 1:F:63:GLU:OE2   | 1.84                     | 0.77              |
| 2:E:467:GLU:OE1  | 3:E:2828:HOH:O   | 2.02                     | 0.77              |
| 1:C:337:LYS:NZ   | 3:C:2609:HOH:O   | 2.13                     | 0.77              |
| 2:E:280:MET:CE   | 3:E:2304:HOH:O   | 2.33                     | 0.77              |
| 1:D:361:LYS:HD3  | 3:D:2343:HOH:O   | 1.85                     | 0.77              |
| 1:C:13:ARG:NH1   | 3:C:2002:HOH:O   | 2.18                     | 0.77              |
| 1:B:412:LYS:HE3  | 3:B:2402:HOH:O   | 1.84                     | 0.77              |
| 1:F:413:GLY:CA   | 3:F:2724:HOH:O   | 2.32                     | 0.76              |
| 1:B:306:ASP:HB2  | 3:B:2609:HOH:O   | 1.84                     | 0.76              |
| 1:A:277:GLU:OE1  | 3:A:2559:HOH:O   | 2.01                     | 0.76              |
| 2:E:372:THR:HB   | 2:E:407:MET:HE2  | 0.79                     | 0.76              |
| 1:C:489:ARG:HH11 | 1:C:492:GLN:HE22 | 1.31                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:477:GLU:CB   | 3:A:2810:HOH:O   | 2.32                     | 0.76              |
| 1:F:345:ASN:OD1  | 3:F:2626:HOH:O   | 2.03                     | 0.75              |
| 2:E:76:ASP:OD1   | 2:E:79:HIS:HD2   | 1.70                     | 0.75              |
| 1:A:68:ARG:CA    | 3:A:2185:HOH:O   | 2.34                     | 0.75              |
| 1:D:21:ARG:NH2   | 3:D:2032:HOH:O   | 2.18                     | 0.75              |
| 1:A:13:ARG:NH2   | 3:A:2009:HOH:O   | 2.20                     | 0.74              |
| 1:C:476:ARG:HG2  | 3:C:2196:HOH:O   | 1.87                     | 0.74              |
| 1:B:46:GLU:OE2   | 3:B:2129:HOH:O   | 2.05                     | 0.74              |
| 1:D:89:LYS:HD2   | 3:D:2246:HOH:O   | 1.88                     | 0.74              |
| 1:B:462:SER:CB   | 3:B:2815:HOH:O   | 1.93                     | 0.74              |
| 2:E:292:VAL:HG23 | 3:E:2601:HOH:O   | 1.88                     | 0.74              |
| 1:F:164:LYS:HE3  | 3:F:2189:HOH:O   | 1.87                     | 0.74              |
| 1:B:46:GLU:CG    | 3:B:2129:HOH:O   | 2.36                     | 0.74              |
| 1:C:238:GLU:OE1  | 3:C:2487:HOH:O   | 2.05                     | 0.74              |
| 1:F:171:LYS:HE3  | 3:F:2421:HOH:O   | 1.89                     | 0.73              |
| 1:C:76:ASP:OD1   | 1:C:79:HIS:HD2   | 1.70                     | 0.73              |
| 1:F:314:LYS:CE   | 3:F:2604:HOH:O   | 2.35                     | 0.73              |
| 1:D:422:GLU:HB2  | 3:D:2811:HOH:O   | 1.87                     | 0.73              |
| 2:E:489:ARG:HH11 | 2:E:492:GLN:HE22 | 1.36                     | 0.73              |
| 1:B:422:GLU:OE1  | 1:B:486:ARG:NH1  | 2.22                     | 0.73              |
| 1:F:131:LEU:CD1  | 1:F:180:THR:CG2  | 2.64                     | 0.73              |
| 1:C:13:ARG:HG2   | 3:C:2753:HOH:O   | 1.87                     | 0.73              |
| 1:C:127:ILE:HG22 | 1:C:180:THR:HG21 | 1.70                     | 0.73              |
| 1:F:314:LYS:HD2  | 3:F:2604:HOH:O   | 1.88                     | 0.73              |
| 1:C:242:ILE:HD11 | 3:C:2405:HOH:O   | 1.88                     | 0.73              |
| 2:E:182:LYS:HG2  | 3:E:2469:HOH:O   | 1.88                     | 0.72              |
| 1:F:23:ASP:HB3   | 3:F:2036:HOH:O   | 1.88                     | 0.72              |
| 1:D:407:MET:CE   | 3:D:2672:HOH:O   | 2.36                     | 0.72              |
| 1:F:424:HIS:HB2  | 3:F:2743:HOH:O   | 1.90                     | 0.72              |
| 1:D:179:LYS:HD2  | 3:D:2209:HOH:O   | 1.89                     | 0.72              |
| 2:E:227:ILE:CG1  | 3:E:2275:HOH:O   | 1.66                     | 0.72              |
| 1:F:422:GLU:O    | 1:F:422:GLU:HG2  | 1.90                     | 0.72              |
| 1:C:108:LYS:NZ   | 3:C:2264:HOH:O   | 2.23                     | 0.71              |
| 1:F:227:ILE:HD11 | 3:F:2296:HOH:O   | 1.89                     | 0.71              |
| 1:B:346:SER:CB   | 3:B:2667:HOH:O   | 2.27                     | 0.71              |
| 1:F:302:VAL:O    | 1:F:305:ARG:HD3  | 1.91                     | 0.71              |
| 1:D:407:MET:CG   | 1:D:407:MET:HE2  | 2.10                     | 0.70              |
| 1:C:127:ILE:CG2  | 1:C:180:THR:HG21 | 2.21                     | 0.70              |
| 1:F:179:LYS:HG3  | 3:F:2437:HOH:O   | 1.91                     | 0.70              |
| 2:E:372:THR:CG2  | 2:E:407:MET:CE   | 2.70                     | 0.70              |
| 1:F:108:LYS:NZ   | 3:F:2263:HOH:O   | 2.22                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:314:LYS:CD   | 3:F:2604:HOH:O   | 2.40                     | 0.70              |
| 1:B:131:LEU:HD11 | 1:B:180:THR:HG22 | 1.74                     | 0.70              |
| 2:E:417:LYS:CB   | 3:E:2483:HOH:O   | 2.26                     | 0.70              |
| 1:A:476:ARG:NH2  | 3:A:2809:HOH:O   | 2.25                     | 0.69              |
| 1:D:417:LYS:HG2  | 1:D:473:TYR:OH   | 1.91                     | 0.69              |
| 1:C:171:LYS:HE3  | 3:C:2419:HOH:O   | 1.92                     | 0.69              |
| 1:D:112:ALA:CB   | 3:D:2288:HOH:O   | 2.35                     | 0.69              |
| 1:F:493:GLU:OE1  | 3:F:2828:HOH:O   | 2.09                     | 0.69              |
| 1:D:302:VAL:O    | 1:D:305:ARG:HD3  | 1.92                     | 0.69              |
| 2:E:313:GLU:HB3  | 3:E:2630:HOH:O   | 1.91                     | 0.69              |
| 2:E:182:LYS:HE3  | 3:E:2476:HOH:O   | 1.92                     | 0.69              |
| 1:B:337:LYS:NZ   | 3:B:2648:HOH:O   | 2.14                     | 0.69              |
| 1:B:108:LYS:NZ   | 3:B:2280:HOH:O   | 2.25                     | 0.69              |
| 1:B:131:LEU:HD12 | 1:B:180:THR:CG2  | 2.21                     | 0.69              |
| 1:B:227:ILE:HD11 | 3:B:2319:HOH:O   | 1.92                     | 0.69              |
| 1:C:280:MET:CE   | 3:C:2690:HOH:O   | 2.39                     | 0.69              |
| 1:F:424:HIS:ND1  | 3:F:2741:HOH:O   | 2.26                     | 0.68              |
| 2:E:462:SER:CB   | 3:E:2822:HOH:O   | 1.79                     | 0.68              |
| 1:D:293:ARG:NH1  | 3:D:2560:HOH:O   | 1.80                     | 0.68              |
| 2:E:477:GLU:CB   | 3:E:2838:HOH:O   | 2.41                     | 0.68              |
| 2:E:244:ASN:CG   | 3:E:2548:HOH:O   | 2.31                     | 0.68              |
| 1:F:28:SER:HB3   | 3:F:2060:HOH:O   | 1.94                     | 0.68              |
| 1:B:46:GLU:HG3   | 3:B:2130:HOH:O   | 1.94                     | 0.68              |
| 1:D:489:ARG:HH11 | 1:D:492:GLN:HE22 | 1.42                     | 0.68              |
| 1:B:13:ARG:NH2   | 3:B:2008:HOH:O   | 2.26                     | 0.68              |
| 1:C:238:GLU:HG3  | 3:C:2487:HOH:O   | 1.94                     | 0.68              |
| 1:B:46:GLU:CB    | 3:B:2129:HOH:O   | 2.37                     | 0.67              |
| 1:F:179:LYS:HD3  | 3:F:2199:HOH:O   | 1.94                     | 0.67              |
| 2:E:315:GLU:OE2  | 3:E:2641:HOH:O   | 1.91                     | 0.67              |
| 1:F:76:ASP:OD1   | 1:F:79:HIS:HD2   | 1.78                     | 0.67              |
| 2:E:111:LEU:HD13 | 3:E:2148:HOH:O   | 1.92                     | 0.67              |
| 1:D:13:ARG:HD2   | 3:D:2006:HOH:O   | 1.93                     | 0.67              |
| 1:F:314:LYS:HD3  | 3:F:2303:HOH:O   | 1.95                     | 0.67              |
| 1:A:280:MET:CE   | 3:A:2568:HOH:O   | 2.42                     | 0.66              |
| 1:A:13:ARG:CG    | 3:A:2005:HOH:O   | 2.43                     | 0.66              |
| 2:E:164:LYS:HE2  | 3:E:2228:HOH:O   | 1.94                     | 0.66              |
| 1:C:412:LYS:NZ   | 3:C:2722:HOH:O   | 2.10                     | 0.66              |
| 1:C:415:LEU:HD13 | 1:C:420:ALA:HB2  | 1.78                     | 0.66              |
| 1:A:117:GLU:OE1  | 3:A:2300:HOH:O   | 2.13                     | 0.66              |
| 1:A:366:ASN:ND2  | 3:A:2680:HOH:O   | 2.28                     | 0.66              |
| 1:B:371:PRO:O    | 3:B:2707:HOH:O   | 2.14                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:302:VAL:O    | 1:B:305:ARG:HD3  | 1.95                     | 0.66              |
| 1:F:417:LYS:HG3  | 3:F:2735:HOH:O   | 1.94                     | 0.66              |
| 1:D:312:LYS:HE2  | 3:D:2589:HOH:O   | 1.95                     | 0.66              |
| 1:B:361:LYS:HD2  | 3:B:2695:HOH:O   | 1.94                     | 0.66              |
| 2:E:477:GLU:HB3  | 3:E:2838:HOH:O   | 1.96                     | 0.66              |
| 2:E:56:HIS:CD2   | 3:E:2160:HOH:O   | 2.43                     | 0.66              |
| 1:A:179:LYS:NZ   | 1:A:179:LYS:CB   | 2.59                     | 0.66              |
| 1:F:227:ILE:HG12 | 3:F:2493:HOH:O   | 1.73                     | 0.65              |
| 1:F:117:GLU:OE2  | 3:F:2286:HOH:O   | 2.13                     | 0.65              |
| 1:D:417:LYS:HE3  | 3:D:2731:HOH:O   | 1.96                     | 0.65              |
| 1:F:117:GLU:CG   | 3:F:2286:HOH:O   | 2.38                     | 0.65              |
| 1:A:117:GLU:O    | 1:A:121:GLU:HG3  | 1.96                     | 0.65              |
| 2:E:302:VAL:O    | 2:E:305:ARG:HD3  | 1.95                     | 0.65              |
| 1:D:338:HIS:CD2  | 3:D:2616:HOH:O   | 2.27                     | 0.65              |
| 1:C:277:GLU:CD   | 3:C:2539:HOH:O   | 2.35                     | 0.65              |
| 1:C:182:LYS:HD3  | 3:C:2507:HOH:O   | 1.97                     | 0.65              |
| 1:D:417:LYS:HB3  | 3:D:2440:HOH:O   | 1.96                     | 0.65              |
| 1:F:486:ARG:NH1  | 3:F:2819:HOH:O   | 2.28                     | 0.65              |
| 2:E:363:PRO:HD2  | 3:E:2704:HOH:O   | 1.97                     | 0.65              |
| 1:B:21:ARG:NH2   | 3:B:2028:HOH:O   | 1.96                     | 0.64              |
| 2:E:227:ILE:HD12 | 3:E:2277:HOH:O   | 1.97                     | 0.64              |
| 1:F:476:ARG:NH2  | 3:F:2795:HOH:O   | 2.30                     | 0.64              |
| 1:C:477:GLU:HG3  | 3:C:2802:HOH:O   | 1.97                     | 0.64              |
| 1:F:417:LYS:HD2  | 3:F:2736:HOH:O   | 1.96                     | 0.64              |
| 1:F:46:GLU:HG3   | 3:F:2119:HOH:O   | 1.98                     | 0.64              |
| 2:E:412:LYS:HE2  | 3:E:2767:HOH:O   | 1.98                     | 0.64              |
| 2:E:227:ILE:HD12 | 3:E:2276:HOH:O   | 1.98                     | 0.64              |
| 1:B:489:ARG:HH11 | 1:B:492:GLN:HE22 | 1.45                     | 0.64              |
| 1:A:417:LYS:HB3  | 3:A:2453:HOH:O   | 1.96                     | 0.64              |
| 1:F:13:ARG:HB2   | 3:F:2001:HOH:O   | 1.97                     | 0.64              |
| 2:E:314:LYS:HD2  | 3:E:2635:HOH:O   | 1.97                     | 0.64              |
| 2:E:314:LYS:CD   | 3:E:2635:HOH:O   | 2.46                     | 0.64              |
| 1:F:117:GLU:CD   | 3:F:2286:HOH:O   | 2.36                     | 0.63              |
| 1:C:13:ARG:O     | 3:C:2004:HOH:O   | 2.15                     | 0.63              |
| 1:A:205:PRO:HB2  | 3:A:2473:HOH:O   | 1.97                     | 0.63              |
| 1:F:413:GLY:O    | 3:F:2724:HOH:O   | 2.15                     | 0.63              |
| 1:A:302:VAL:O    | 1:A:305:ARG:HD3  | 1.97                     | 0.63              |
| 1:B:76:ASP:OD1   | 1:B:79:HIS:HD2   | 1.81                     | 0.63              |
| 1:F:171:LYS:HD2  | 3:F:2187:HOH:O   | 1.98                     | 0.63              |
| 1:A:13:ARG:CB    | 3:A:2005:HOH:O   | 2.44                     | 0.63              |
| 1:F:63:GLU:H     | 1:F:63:GLU:CD    | 2.01                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:131:LEU:HD12 | 1:B:180:THR:HG23 | 1.80                     | 0.63              |
| 1:A:13:ARG:NH1   | 1:A:428:ASP:OD2  | 2.32                     | 0.63              |
| 1:C:13:ARG:HB3   | 3:C:2753:HOH:O   | 1.98                     | 0.63              |
| 1:D:314:LYS:HE3  | 3:D:2593:HOH:O   | 1.99                     | 0.63              |
| 1:B:407:MET:CE   | 3:B:2709:HOH:O   | 1.90                     | 0.62              |
| 1:D:179:LYS:HD2  | 3:D:2103:HOH:O   | 1.99                     | 0.62              |
| 1:D:424:HIS:CB   | 3:D:2740:HOH:O   | 2.16                     | 0.62              |
| 1:F:422:GLU:CG   | 1:F:422:GLU:O    | 2.48                     | 0.62              |
| 2:E:213:SER:HB2  | 3:E:2510:HOH:O   | 1.99                     | 0.62              |
| 1:C:302:VAL:O    | 1:C:305:ARG:HD3  | 1.99                     | 0.62              |
| 1:A:390:THR:HG23 | 3:A:2709:HOH:O   | 1.98                     | 0.62              |
| 1:C:242:ILE:CD1  | 3:C:2405:HOH:O   | 2.46                     | 0.62              |
| 1:F:407:MET:HE1  | 3:F:2669:HOH:O   | 1.99                     | 0.61              |
| 2:E:412:LYS:HA   | 3:E:2765:HOH:O   | 1.99                     | 0.61              |
| 1:F:417:LYS:HB3  | 3:F:2447:HOH:O   | 2.00                     | 0.61              |
| 1:C:167:THR:CB   | 3:C:2405:HOH:O   | 2.49                     | 0.61              |
| 1:C:108:LYS:HG2  | 3:C:2063:HOH:O   | 1.99                     | 0.61              |
| 2:E:111:LEU:CD1  | 3:E:2148:HOH:O   | 2.47                     | 0.61              |
| 1:F:413:GLY:C    | 3:F:2724:HOH:O   | 2.39                     | 0.61              |
| 1:D:345:ASN:OD1  | 3:D:2631:HOH:O   | 2.16                     | 0.61              |
| 1:B:379:MET:CE   | 1:B:432:ARG:HD2  | 2.31                     | 0.61              |
| 2:E:13:ARG:HA    | 3:E:2003:HOH:O   | 1.99                     | 0.60              |
| 1:B:416:PRO:HD3  | 3:B:2762:HOH:O   | 2.02                     | 0.60              |
| 2:E:478:ASN:HB3  | 3:E:2843:HOH:O   | 2.00                     | 0.60              |
| 1:F:13:ARG:NH1   | 3:F:2004:HOH:O   | 2.34                     | 0.60              |
| 1:D:417:LYS:HD3  | 1:D:473:TYR:CE2  | 2.36                     | 0.60              |
| 1:C:13:ARG:HH11  | 1:C:13:ARG:CG    | 2.13                     | 0.60              |
| 1:F:108:LYS:NZ   | 3:F:2262:HOH:O   | 2.20                     | 0.60              |
| 1:A:227:ILE:HD11 | 3:A:2311:HOH:O   | 2.01                     | 0.60              |
| 1:D:276:GLN:NE2  | 3:D:2547:HOH:O   | 0.75                     | 0.60              |
| 1:F:131:LEU:HD11 | 1:F:180:THR:HG22 | 1.81                     | 0.60              |
| 1:A:136:GLU:HG2  | 3:A:2348:HOH:O   | 2.02                     | 0.60              |
| 1:C:486:ARG:HD3  | 3:C:2817:HOH:O   | 2.02                     | 0.59              |
| 1:B:127:ILE:HG22 | 1:B:180:THR:HG21 | 1.84                     | 0.59              |
| 1:D:415:LEU:HD13 | 1:D:420:ALA:HB2  | 1.84                     | 0.59              |
| 1:B:315:GLU:HG3  | 3:B:2626:HOH:O   | 2.02                     | 0.59              |
| 1:C:179:LYS:HB2  | 1:C:179:LYS:HZ2  | 1.64                     | 0.59              |
| 1:F:164:LYS:CE   | 3:F:2189:HOH:O   | 2.48                     | 0.59              |
| 2:E:382:LYS:HG3  | 3:E:2731:HOH:O   | 2.01                     | 0.59              |
| 1:F:238:GLU:CG   | 3:F:2504:HOH:O   | 2.40                     | 0.59              |
| 1:F:171:LYS:CE   | 3:F:2420:HOH:O   | 2.51                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:111:LEU:HG   | 3:A:2422:HOH:O   | 2.03                     | 0.59              |
| 1:A:317:GLU:HB3  | 3:A:2616:HOH:O   | 2.01                     | 0.59              |
| 1:A:13:ARG:HG3   | 1:A:432:ARG:HH21 | 1.59                     | 0.58              |
| 1:A:207:ARG:HG3  | 3:A:2473:HOH:O   | 2.02                     | 0.58              |
| 1:A:486:ARG:NH1  | 3:A:2828:HOH:O   | 2.29                     | 0.58              |
| 1:F:476:ARG:NH1  | 3:F:2797:HOH:O   | 2.18                     | 0.58              |
| 1:B:417:LYS:CD   | 3:B:2410:HOH:O   | 2.47                     | 0.58              |
| 1:F:407:MET:HE2  | 1:F:407:MET:HG2  | 1.82                     | 0.58              |
| 1:C:171:LYS:O    | 1:C:175:GLU:HG3  | 2.03                     | 0.57              |
| 2:E:417:LYS:HG3  | 3:E:2773:HOH:O   | 2.03                     | 0.57              |
| 1:C:13:ARG:HG3   | 1:C:13:ARG:HH11  | 1.68                     | 0.57              |
| 1:B:417:LYS:HG3  | 3:B:2767:HOH:O   | 2.04                     | 0.57              |
| 1:F:475:ASP:OD2  | 1:F:477:GLU:HG2  | 2.04                     | 0.57              |
| 1:A:476:ARG:NH1  | 3:A:2803:HOH:O   | 2.26                     | 0.57              |
| 1:F:179:LYS:HE2  | 3:F:2095:HOH:O   | 2.05                     | 0.57              |
| 1:D:407:MET:HE1  | 3:D:2672:HOH:O   | 2.03                     | 0.57              |
| 1:D:227:ILE:HD11 | 3:D:2307:HOH:O   | 2.03                     | 0.57              |
| 1:C:283:CYS:HB2  | 3:C:2521:HOH:O   | 2.05                     | 0.57              |
| 1:D:422:GLU:O    | 1:D:422:GLU:CG   | 2.52                     | 0.57              |
| 1:A:131:LEU:HD12 | 1:A:180:THR:CG2  | 2.33                     | 0.57              |
| 1:A:476:ARG:HH21 | 1:A:476:ARG:HG2  | 1.69                     | 0.57              |
| 1:C:13:ARG:CB    | 3:C:2753:HOH:O   | 2.53                     | 0.57              |
| 1:D:337:LYS:NZ   | 3:D:2615:HOH:O   | 2.24                     | 0.57              |
| 1:D:117:GLU:HG3  | 3:D:2297:HOH:O   | 2.03                     | 0.56              |
| 1:D:417:LYS:HD3  | 1:D:473:TYR:HE2  | 1.68                     | 0.56              |
| 1:D:13:ARG:NH2   | 3:D:2005:HOH:O   | 2.24                     | 0.56              |
| 1:B:268:ASN:ND2  | 3:B:2564:HOH:O   | 2.38                     | 0.56              |
| 2:E:161:ARG:NH1  | 3:E:2428:HOH:O   | 2.38                     | 0.56              |
| 1:A:317:GLU:HG2  | 3:A:2616:HOH:O   | 2.05                     | 0.56              |
| 2:E:161:ARG:CZ   | 3:E:2428:HOH:O   | 2.53                     | 0.56              |
| 1:A:161:ARG:NH2  | 1:C:152:ASP:O    | 2.38                     | 0.56              |
| 1:C:314:LYS:HG2  | 3:C:2588:HOH:O   | 2.04                     | 0.56              |
| 2:E:234:ARG:NE   | 2:E:315:GLU:OE2  | 2.31                     | 0.56              |
| 1:D:301:ARG:O    | 1:D:305:ARG:HD2  | 2.05                     | 0.56              |
| 2:E:382:LYS:HE3  | 3:E:2387:HOH:O   | 2.05                     | 0.56              |
| 1:A:293:ARG:NH1  | 3:A:2572:HOH:O   | 2.25                     | 0.56              |
| 1:A:68:ARG:CA    | 3:A:2186:HOH:O   | 2.53                     | 0.56              |
| 1:D:417:LYS:HD2  | 3:D:2440:HOH:O   | 2.05                     | 0.56              |
| 1:C:424:HIS:HB2  | 3:C:2736:HOH:O   | 2.06                     | 0.56              |
| 2:E:244:ASN:ND2  | 3:E:2548:HOH:O   | 2.37                     | 0.56              |
| 2:E:422:GLU:O    | 2:E:422:GLU:HG2  | 2.06                     | 0.56              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:E:227:ILE:CD1  | 3:E:2276:HOH:O  | 2.54                     | 0.56              |
| 1:A:164:LYS:HE3  | 3:A:2411:HOH:O  | 2.06                     | 0.56              |
| 2:E:385:HIS:CE1  | 3:E:2730:HOH:O  | 2.58                     | 0.56              |
| 1:D:179:LYS:NZ   | 1:D:179:LYS:CB  | 2.60                     | 0.56              |
| 1:F:171:LYS:HE2  | 3:F:2420:HOH:O  | 2.05                     | 0.56              |
| 2:E:379:MET:HE2  | 3:E:2008:HOH:O  | 2.06                     | 0.56              |
| 1:C:13:ARG:HD2   | 3:C:2005:HOH:O  | 2.06                     | 0.56              |
| 1:A:13:ARG:HB3   | 1:A:428:ASP:OD1 | 2.06                     | 0.55              |
| 1:B:314:LYS:HD2  | 3:B:2625:HOH:O  | 2.05                     | 0.55              |
| 1:C:256:LEU:O    | 3:C:2512:HOH:O  | 2.17                     | 0.55              |
| 1:C:117:GLU:O    | 1:C:121:GLU:HG3 | 2.05                     | 0.55              |
| 1:C:167:THR:HB   | 3:C:2405:HOH:O  | 2.06                     | 0.55              |
| 1:F:320:VAL:HG21 | 3:F:2600:HOH:O  | 2.06                     | 0.55              |
| 1:A:182:LYS:HE3  | 3:A:2446:HOH:O  | 2.05                     | 0.55              |
| 1:B:269:THR:HA   | 3:B:2565:HOH:O  | 2.06                     | 0.55              |
| 1:C:315:GLU:HG3  | 3:C:2592:HOH:O  | 2.06                     | 0.55              |
| 1:D:476:ARG:NH2  | 3:D:2789:HOH:O  | 2.39                     | 0.55              |
| 1:C:127:ILE:CG2  | 1:C:180:THR:CG2 | 2.84                     | 0.55              |
| 1:D:477:GLU:HB3  | 3:D:2794:HOH:O  | 2.05                     | 0.55              |
| 1:D:76:ASP:OD1   | 1:D:79:HIS:CD2  | 2.53                     | 0.55              |
| 1:B:179:LYS:HA   | 1:B:179:LYS:HE3 | 1.88                     | 0.55              |
| 1:F:171:LYS:CD   | 3:F:2187:HOH:O  | 2.54                     | 0.55              |
| 1:D:13:ARG:NH1   | 1:D:428:ASP:OD2 | 2.40                     | 0.55              |
| 1:B:343:PRO:HB2  | 3:B:2659:HOH:O  | 2.06                     | 0.55              |
| 1:C:227:ILE:HD11 | 3:C:2297:HOH:O  | 2.07                     | 0.55              |
| 1:A:267:THR:OG1  | 1:A:269:THR:HB  | 2.07                     | 0.55              |
| 2:E:374:ASN:ND2  | 3:E:2828:HOH:O  | 2.39                     | 0.54              |
| 1:C:167:THR:HG21 | 3:C:2405:HOH:O  | 2.07                     | 0.54              |
| 3:B:2008:HOH:O   | 2:E:364:ASP:HA  | 2.06                     | 0.54              |
| 1:B:414:ASP:HB2  | 3:B:2754:HOH:O  | 2.07                     | 0.54              |
| 1:F:118:LYS:HE3  | 3:F:2295:HOH:O  | 2.06                     | 0.54              |
| 1:A:313:GLU:HB2  | 3:C:2155:HOH:O  | 2.07                     | 0.54              |
| 1:A:314:LYS:HE2  | 3:A:2609:HOH:O  | 2.07                     | 0.54              |
| 2:E:13:ARG:NH1   | 2:E:428:ASP:OD2 | 2.40                     | 0.54              |
| 2:E:337:LYS:NZ   | 3:E:2660:HOH:O  | 2.25                     | 0.54              |
| 1:A:13:ARG:HB2   | 3:A:2003:HOH:O  | 2.07                     | 0.54              |
| 1:B:39:GLN:O     | 1:B:458:ASN:HB2 | 2.08                     | 0.54              |
| 1:F:422:GLU:HG3  | 1:F:424:HIS:CE1 | 2.42                     | 0.54              |
| 1:A:179:LYS:HE3  | 1:A:179:LYS:HA  | 1.90                     | 0.54              |
| 1:A:227:ILE:HG12 | 3:A:2255:HOH:O  | 1.66                     | 0.54              |
| 2:E:267:THR:OG1  | 2:E:269:THR:HB  | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:417:LYS:HG2  | 1:D:473:TYR:CZ   | 2.43                     | 0.53              |
| 1:A:417:LYS:CD   | 3:A:2453:HOH:O   | 2.56                     | 0.53              |
| 1:F:414:ASP:CB   | 3:F:2725:HOH:O   | 2.56                     | 0.53              |
| 1:F:414:ASP:HB3  | 3:F:2725:HOH:O   | 2.07                     | 0.53              |
| 1:F:445:ALA:HB1  | 3:F:2771:HOH:O   | 2.06                     | 0.53              |
| 1:F:68:ARG:CA    | 3:F:2169:HOH:O   | 2.56                     | 0.53              |
| 1:D:424:HIS:CE1  | 3:D:2735:HOH:O   | 2.60                     | 0.53              |
| 1:C:432:ARG:NH2  | 3:C:2753:HOH:O   | 1.72                     | 0.53              |
| 1:D:21:ARG:HD2   | 3:D:2041:HOH:O   | 2.07                     | 0.53              |
| 1:D:13:ARG:NH2   | 3:D:2001:HOH:O   | 2.29                     | 0.53              |
| 1:B:439:GLN:HG2  | 3:B:2789:HOH:O   | 2.07                     | 0.53              |
| 1:A:182:LYS:HD3  | 3:A:2529:HOH:O   | 2.08                     | 0.53              |
| 1:F:338:HIS:HD2  | 3:F:2259:HOH:O   | 1.90                     | 0.53              |
| 2:E:227:ILE:HD11 | 3:E:2332:HOH:O   | 2.09                     | 0.53              |
| 2:E:372:THR:HB   | 2:E:407:MET:HE1  | 1.73                     | 0.53              |
| 1:C:39:GLN:O     | 1:C:458:ASN:HB2  | 2.08                     | 0.53              |
| 1:B:118:LYS:HG3  | 3:B:2314:HOH:O   | 1.94                     | 0.53              |
| 1:B:127:ILE:CG2  | 1:B:180:THR:HG21 | 2.39                     | 0.53              |
| 2:E:164:LYS:NZ   | 3:E:2437:HOH:O   | 2.30                     | 0.53              |
| 1:D:496:GLY:C    | 3:D:2818:HOH:O   | 2.47                     | 0.53              |
| 1:D:315:GLU:HG3  | 3:D:2595:HOH:O   | 2.09                     | 0.53              |
| 1:A:78:TYR:HB3   | 3:A:2213:HOH:O   | 2.09                     | 0.53              |
| 1:D:382:LYS:HE3  | 3:D:2694:HOH:O   | 2.08                     | 0.53              |
| 1:B:21:ARG:HD3   | 3:B:2040:HOH:O   | 2.09                     | 0.52              |
| 1:F:338:HIS:CD2  | 3:F:2259:HOH:O   | 2.62                     | 0.52              |
| 1:D:417:LYS:CE   | 3:D:2731:HOH:O   | 2.55                     | 0.52              |
| 3:A:2571:HOH:O   | 1:B:338:HIS:CE1  | 2.63                     | 0.52              |
| 1:A:343:PRO:HD3  | 1:B:310:TYR:CZ   | 2.45                     | 0.52              |
| 1:D:85:VAL:HG11  | 1:D:129:LEU:HG   | 1.91                     | 0.52              |
| 1:A:317:GLU:CG   | 3:A:2616:HOH:O   | 2.58                     | 0.52              |
| 1:C:66:VAL:HG21  | 3:C:2198:HOH:O   | 2.08                     | 0.52              |
| 1:B:118:LYS:CD   | 3:B:2311:HOH:O   | 2.39                     | 0.52              |
| 2:E:476:ARG:HD2  | 3:E:2234:HOH:O   | 2.10                     | 0.52              |
| 2:E:39:GLN:O     | 2:E:458:ASN:HB2  | 2.09                     | 0.51              |
| 2:E:182:LYS:NZ   | 3:E:2475:HOH:O   | 2.43                     | 0.51              |
| 1:D:314:LYS:CE   | 3:D:2599:HOH:O   | 2.58                     | 0.51              |
| 1:D:345:ASN:ND2  | 3:D:2631:HOH:O   | 2.38                     | 0.51              |
| 2:E:379:MET:HG2  | 2:E:381:PRO:HD3  | 1.91                     | 0.51              |
| 1:F:267:THR:OG1  | 1:F:269:THR:HB   | 2.11                     | 0.51              |
| 1:D:60:ASN:HB3   | 3:D:2160:HOH:O   | 2.09                     | 0.51              |
| 2:E:118:LYS:HG3  | 3:E:2324:HOH:O   | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:227:ILE:HG23 | 3:E:2277:HOH:O   | 2.11                     | 0.51              |
| 2:E:164:LYS:CE   | 3:E:2228:HOH:O   | 2.54                     | 0.51              |
| 1:A:437:LEU:HD21 | 1:A:447:VAL:HG11 | 1.92                     | 0.51              |
| 1:D:269:THR:HG21 | 3:D:2536:HOH:O   | 2.11                     | 0.51              |
| 1:D:193:PHE:HA   | 3:D:2451:HOH:O   | 2.09                     | 0.51              |
| 1:C:337:LYS:NZ   | 3:C:2608:HOH:O   | 2.17                     | 0.51              |
| 1:F:14:LEU:HD21  | 3:F:2026:HOH:O   | 2.11                     | 0.51              |
| 1:D:267:THR:OG1  | 1:D:269:THR:HB   | 2.11                     | 0.51              |
| 2:E:182:LYS:HD3  | 3:E:2470:HOH:O   | 2.10                     | 0.51              |
| 1:F:312:LYS:HE2  | 3:F:2175:HOH:O   | 2.10                     | 0.51              |
| 1:C:227:ILE:HG12 | 3:C:2240:HOH:O   | 1.83                     | 0.50              |
| 1:C:301:ARG:O    | 1:C:305:ARG:HD2  | 2.11                     | 0.50              |
| 1:A:293:ARG:NH2  | 3:A:2571:HOH:O   | 2.44                     | 0.50              |
| 2:E:415:LEU:HD13 | 2:E:420:ALA:HB2  | 1.93                     | 0.50              |
| 1:C:478:ASN:HB3  | 3:C:2804:HOH:O   | 2.10                     | 0.50              |
| 1:C:131:LEU:HD12 | 1:C:180:THR:HG23 | 1.85                     | 0.50              |
| 1:F:301:ARG:O    | 1:F:305:ARG:HD2  | 2.11                     | 0.50              |
| 1:B:301:ARG:O    | 1:B:305:ARG:HD2  | 2.11                     | 0.50              |
| 1:A:39:GLN:O     | 1:A:458:ASN:HB2  | 2.11                     | 0.50              |
| 1:B:414:ASP:HB3  | 3:B:2762:HOH:O   | 2.10                     | 0.50              |
| 1:A:306:ASP:HB2  | 3:A:2312:HOH:O   | 2.12                     | 0.50              |
| 1:F:345:ASN:ND2  | 3:F:2626:HOH:O   | 2.44                     | 0.50              |
| 1:A:317:GLU:CB   | 3:A:2616:HOH:O   | 2.60                     | 0.50              |
| 1:A:269:THR:HG21 | 3:A:2280:HOH:O   | 2.11                     | 0.50              |
| 2:E:342:SER:HB2  | 3:E:2669:HOH:O   | 2.11                     | 0.50              |
| 1:F:171:LYS:HE3  | 3:F:2420:HOH:O   | 2.12                     | 0.50              |
| 1:D:422:GLU:O    | 1:D:422:GLU:HG2  | 2.10                     | 0.50              |
| 1:B:86:ARG:CZ    | 3:B:2247:HOH:O   | 2.59                     | 0.49              |
| 1:D:424:HIS:CG   | 3:D:2735:HOH:O   | 2.65                     | 0.49              |
| 1:A:381:PRO:HB2  | 1:A:436:VAL:HG21 | 1.94                     | 0.49              |
| 1:F:428:ASP:OD1  | 3:F:2748:HOH:O   | 2.20                     | 0.49              |
| 1:D:282:LYS:NZ   | 1:D:350:ASN:HD22 | 2.11                     | 0.49              |
| 1:F:400:MET:CE   | 3:F:2771:HOH:O   | 2.43                     | 0.49              |
| 1:A:476:ARG:NE   | 3:A:2803:HOH:O   | 2.32                     | 0.49              |
| 1:C:476:ARG:HD2  | 3:C:2796:HOH:O   | 2.12                     | 0.49              |
| 1:A:417:LYS:HG2  | 1:A:473:TYR:CZ   | 2.46                     | 0.49              |
| 1:B:267:THR:OG1  | 1:B:269:THR:HB   | 2.11                     | 0.49              |
| 1:A:234:ARG:NE   | 1:A:315:GLU:OE2  | 2.41                     | 0.49              |
| 1:D:131:LEU:CD1  | 1:D:180:THR:HG23 | 2.42                     | 0.49              |
| 1:A:301:ARG:O    | 1:A:305:ARG:HD2  | 2.13                     | 0.49              |
| 1:D:314:LYS:HD3  | 3:D:2592:HOH:O   | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:417:LYS:CB   | 3:B:2410:HOH:O   | 2.60                     | 0.49              |
| 1:D:131:LEU:HD12 | 1:D:180:THR:CG2  | 2.41                     | 0.49              |
| 1:D:476:ARG:HD3  | 3:D:2790:HOH:O   | 2.13                     | 0.49              |
| 1:C:210:PRO:CG   | 3:C:2231:HOH:O   | 2.60                     | 0.49              |
| 1:F:234:ARG:NE   | 1:F:315:GLU:OE2  | 2.35                     | 0.49              |
| 1:F:227:ILE:HD12 | 3:F:2168:HOH:O   | 2.13                     | 0.49              |
| 1:B:227:ILE:HD12 | 3:B:2185:HOH:O   | 2.12                     | 0.49              |
| 1:A:417:LYS:HG2  | 1:A:473:TYR:OH   | 2.12                     | 0.49              |
| 1:B:282:LYS:NZ   | 1:B:350:ASN:HD22 | 2.11                     | 0.49              |
| 2:E:56:HIS:CD2   | 2:E:60:ASN:HD22  | 2.04                     | 0.49              |
| 1:F:372:THR:HB   | 1:F:407:MET:HE1  | 1.94                     | 0.49              |
| 2:E:268:ASN:ND2  | 3:E:2572:HOH:O   | 2.44                     | 0.49              |
| 2:E:171:LYS:NZ   | 2:E:175:GLU:OE2  | 2.42                     | 0.48              |
| 1:A:422:GLU:HG2  | 3:A:2749:HOH:O   | 2.13                     | 0.48              |
| 1:B:361:LYS:HE2  | 1:B:361:LYS:HB3  | 1.67                     | 0.48              |
| 2:E:46:GLU:HG3   | 3:E:2130:HOH:O   | 2.14                     | 0.48              |
| 1:B:417:LYS:N    | 1:B:418:PRO:CD   | 2.75                     | 0.48              |
| 1:F:447:VAL:CG2  | 3:F:2771:HOH:O   | 2.40                     | 0.48              |
| 2:E:460:GLU:HG3  | 2:E:460:GLU:O    | 2.13                     | 0.48              |
| 2:E:178:GLY:O    | 3:E:2468:HOH:O   | 2.20                     | 0.48              |
| 1:F:238:GLU:OE1  | 3:F:2504:HOH:O   | 2.19                     | 0.48              |
| 1:B:227:ILE:CG1  | 3:B:2515:HOH:O   | 1.74                     | 0.48              |
| 1:D:314:LYS:HD2  | 3:D:2599:HOH:O   | 2.13                     | 0.48              |
| 1:C:227:ILE:HD12 | 3:C:2169:HOH:O   | 2.14                     | 0.48              |
| 1:F:477:GLU:CB   | 3:F:2799:HOH:O   | 2.27                     | 0.48              |
| 2:E:381:PRO:HB2  | 2:E:436:VAL:HG21 | 1.96                     | 0.48              |
| 1:D:437:LEU:HD21 | 1:D:447:VAL:HG11 | 1.96                     | 0.48              |
| 1:B:131:LEU:HD11 | 1:B:180:THR:HG23 | 1.84                     | 0.47              |
| 1:A:270:PHE:HA   | 1:A:273:GLN:HE21 | 1.79                     | 0.47              |
| 1:A:313:GLU:HB3  | 3:A:2610:HOH:O   | 2.13                     | 0.47              |
| 2:E:346:SER:CB   | 3:E:2675:HOH:O   | 2.62                     | 0.47              |
| 1:A:76:ASP:OD1   | 1:A:79:HIS:HD2   | 1.98                     | 0.47              |
| 2:E:314:LYS:NZ   | 3:E:2637:HOH:O   | 2.46                     | 0.47              |
| 1:C:210:PRO:HG3  | 3:C:2231:HOH:O   | 2.14                     | 0.47              |
| 1:A:415:LEU:HD13 | 1:A:420:ALA:HB2  | 1.97                     | 0.47              |
| 1:A:127:ILE:HG22 | 1:A:180:THR:HG21 | 1.95                     | 0.47              |
| 1:C:142:PHE:O    | 3:C:2340:HOH:O   | 2.20                     | 0.47              |
| 1:A:13:ARG:HD2   | 3:A:2005:HOH:O   | 2.13                     | 0.47              |
| 1:B:108:LYS:HE2  | 3:B:2138:HOH:O   | 2.13                     | 0.47              |
| 1:C:13:ARG:NH1   | 1:C:13:ARG:CG    | 2.73                     | 0.47              |
| 2:E:76:ASP:OD1   | 2:E:79:HIS:CD2   | 2.60                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:282:LYS:NZ   | 2:E:350:ASN:HD22 | 2.13                     | 0.47              |
| 1:C:131:LEU:HD11 | 1:C:180:THR:HG22 | 1.84                     | 0.47              |
| 1:F:164:LYS:NZ   | 3:F:2405:HOH:O   | 2.47                     | 0.47              |
| 1:C:167:THR:CG2  | 3:C:2405:HOH:O   | 2.62                     | 0.47              |
| 1:B:379:MET:HE2  | 1:B:432:ARG:HD2  | 1.96                     | 0.47              |
| 2:E:161:ARG:CD   | 3:E:2428:HOH:O   | 2.62                     | 0.47              |
| 1:F:282:LYS:NZ   | 1:F:350:ASN:HD22 | 2.12                     | 0.47              |
| 1:C:267:THR:OG1  | 1:C:269:THR:HB   | 2.15                     | 0.47              |
| 1:B:417:LYS:CB   | 3:B:2765:HOH:O   | 2.09                     | 0.47              |
| 2:E:379:MET:CE   | 3:E:2008:HOH:O   | 2.62                     | 0.47              |
| 3:B:2011:HOH:O   | 2:E:269:THR:HG21 | 2.14                     | 0.47              |
| 1:A:127:ILE:CG2  | 1:A:180:THR:HG21 | 2.46                     | 0.46              |
| 1:D:111:LEU:CG   | 3:D:2412:HOH:O   | 2.41                     | 0.46              |
| 1:A:476:ARG:CD   | 3:A:2801:HOH:O   | 2.61                     | 0.46              |
| 1:A:476:ARG:CD   | 3:A:2807:HOH:O   | 2.51                     | 0.46              |
| 1:C:108:LYS:CE   | 3:C:2264:HOH:O   | 2.61                     | 0.46              |
| 1:F:486:ARG:CZ   | 3:F:2821:HOH:O   | 2.63                     | 0.46              |
| 1:F:155:GLY:HA3  | 3:F:2379:HOH:O   | 2.14                     | 0.46              |
| 1:F:381:PRO:HB2  | 1:F:436:VAL:HG21 | 1.98                     | 0.46              |
| 1:C:276:GLN:HE21 | 1:C:276:GLN:HB3  | 1.55                     | 0.46              |
| 2:E:313:GLU:CB   | 3:E:2634:HOH:O   | 2.37                     | 0.46              |
| 1:B:314:LYS:HG2  | 3:B:2623:HOH:O   | 2.15                     | 0.46              |
| 1:D:342:SER:HB2  | 3:D:2624:HOH:O   | 2.16                     | 0.46              |
| 2:E:163:ILE:O    | 2:E:167:THR:HG23 | 2.16                     | 0.46              |
| 1:D:496:GLY:HA2  | 3:D:2819:HOH:O   | 2.15                     | 0.46              |
| 1:F:118:LYS:HE3  | 3:F:2291:HOH:O   | 2.15                     | 0.46              |
| 1:C:238:GLU:CG   | 3:C:2487:HOH:O   | 2.58                     | 0.46              |
| 1:F:62:PRO:HA    | 3:F:2176:HOH:O   | 2.15                     | 0.46              |
| 1:C:270:PHE:HA   | 1:C:273:GLN:HE21 | 1.80                     | 0.46              |
| 1:F:414:ASP:O    | 3:F:2730:HOH:O   | 2.21                     | 0.46              |
| 1:A:415:LEU:HD23 | 3:A:2394:HOH:O   | 2.16                     | 0.46              |
| 1:C:171:LYS:O    | 1:C:175:GLU:CG   | 2.64                     | 0.45              |
| 1:C:62:PRO:HB3   | 3:C:2145:HOH:O   | 2.15                     | 0.45              |
| 1:B:314:LYS:CD   | 3:B:2625:HOH:O   | 2.62                     | 0.45              |
| 2:E:314:LYS:CE   | 3:E:2635:HOH:O   | 2.65                     | 0.45              |
| 1:A:342:SER:HA   | 1:B:310:TYR:OH   | 2.16                     | 0.45              |
| 1:A:379:MET:CE   | 1:A:432:ARG:HD2  | 2.46                     | 0.45              |
| 1:F:238:GLU:OE1  | 1:F:318:LYS:NZ   | 2.36                     | 0.45              |
| 1:F:179:LYS:CD   | 3:F:2199:HOH:O   | 2.60                     | 0.45              |
| 1:D:117:GLU:CB   | 3:D:2299:HOH:O   | 2.09                     | 0.45              |
| 2:E:437:LEU:HD21 | 2:E:447:VAL:HG11 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:117:GLU:OE2  | 3:D:2297:HOH:O   | 2.21                     | 0.45              |
| 2:E:346:SER:HB3  | 3:E:2675:HOH:O   | 2.17                     | 0.45              |
| 1:C:102:TRP:HB3  | 1:C:103:PRO:HD3  | 1.99                     | 0.45              |
| 1:A:315:GLU:HG3  | 3:A:2613:HOH:O   | 2.16                     | 0.45              |
| 2:E:305:ARG:HB3  | 3:E:2616:HOH:O   | 2.16                     | 0.45              |
| 2:E:238:GLU:CG   | 3:E:2541:HOH:O   | 2.46                     | 0.44              |
| 1:F:458:ASN:HD22 | 1:F:458:ASN:C    | 2.20                     | 0.44              |
| 1:C:179:LYS:CE   | 3:C:2434:HOH:O   | 2.24                     | 0.44              |
| 1:B:270:PHE:HA   | 1:B:273:GLN:HE21 | 1.82                     | 0.44              |
| 2:E:13:ARG:HD2   | 3:E:2018:HOH:O   | 2.17                     | 0.44              |
| 1:A:477:GLU:HB2  | 3:A:2810:HOH:O   | 2.07                     | 0.44              |
| 1:C:414:ASP:HB2  | 3:C:2721:HOH:O   | 2.17                     | 0.44              |
| 1:D:270:PHE:HA   | 1:D:273:GLN:HE21 | 1.83                     | 0.44              |
| 1:B:379:MET:HE1  | 1:B:432:ARG:HD2  | 1.98                     | 0.44              |
| 1:B:182:LYS:HE2  | 1:B:182:LYS:HB2  | 1.77                     | 0.44              |
| 2:E:301:ARG:O    | 2:E:305:ARG:HD2  | 2.17                     | 0.44              |
| 1:B:415:LEU:HD13 | 1:B:420:ALA:HB2  | 2.00                     | 0.44              |
| 1:D:39:GLN:O     | 1:D:458:ASN:HB2  | 2.17                     | 0.44              |
| 1:B:13:ARG:HB2   | 3:B:2009:HOH:O   | 2.16                     | 0.44              |
| 1:B:143:HIS:CE1  | 1:B:188:ASN:ND2  | 2.86                     | 0.44              |
| 1:D:407:MET:SD   | 1:D:426:ARG:HA   | 2.58                     | 0.44              |
| 1:D:343:PRO:HA   | 3:D:2628:HOH:O   | 2.18                     | 0.44              |
| 1:D:161:ARG:HD3  | 3:D:2396:HOH:O   | 2.18                     | 0.44              |
| 1:B:179:LYS:HB2  | 3:B:2456:HOH:O   | 2.17                     | 0.44              |
| 1:C:282:LYS:NZ   | 1:C:350:ASN:HD22 | 2.16                     | 0.44              |
| 1:A:102:TRP:HB3  | 1:A:103:PRO:HD3  | 1.99                     | 0.44              |
| 1:C:179:LYS:CA   | 1:C:179:LYS:HZ2  | 2.31                     | 0.43              |
| 1:C:382:LYS:CE   | 3:C:2682:HOH:O   | 2.51                     | 0.43              |
| 1:C:381:PRO:HB2  | 1:C:436:VAL:HG21 | 2.00                     | 0.43              |
| 2:E:372:THR:CB   | 2:E:407:MET:HE1  | 2.37                     | 0.43              |
| 2:E:251:ASP:OD1  | 2:E:251:ASP:N    | 2.50                     | 0.43              |
| 2:E:475:ASP:OD2  | 2:E:477:GLU:CD   | 2.56                     | 0.43              |
| 1:D:131:LEU:HD12 | 1:D:180:THR:HG21 | 2.00                     | 0.43              |
| 1:C:314:LYS:HE3  | 3:C:2590:HOH:O   | 2.17                     | 0.43              |
| 1:B:342:SER:HB2  | 3:B:2164:HOH:O   | 2.18                     | 0.43              |
| 2:E:13:ARG:N     | 3:E:2007:HOH:O   | 2.51                     | 0.43              |
| 1:C:234:ARG:NE   | 1:C:315:GLU:OE2  | 2.47                     | 0.43              |
| 1:C:313:GLU:HB3  | 3:C:2589:HOH:O   | 2.19                     | 0.43              |
| 1:A:394:LYS:HB3  | 3:A:2709:HOH:O   | 2.06                     | 0.43              |
| 1:D:361:LYS:HB3  | 1:D:361:LYS:HE2  | 1.62                     | 0.43              |
| 1:F:476:ARG:NE   | 3:F:2797:HOH:O   | 2.47                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:414:ASP:O    | 1:F:416:PRO:HD3  | 2.19                     | 0.43              |
| 1:F:129:LEU:CA   | 3:F:2314:HOH:O   | 2.31                     | 0.43              |
| 1:F:475:ASP:OD2  | 1:F:477:GLU:CD   | 2.57                     | 0.43              |
| 1:C:437:LEU:HD21 | 1:C:447:VAL:HG11 | 2.00                     | 0.43              |
| 1:C:293:ARG:CZ   | 3:C:2557:HOH:O   | 2.12                     | 0.43              |
| 1:A:182:LYS:HB2  | 1:A:182:LYS:HE2  | 1.82                     | 0.43              |
| 1:A:247:HIS:HD2  | 3:A:2430:HOH:O   | 2.01                     | 0.43              |
| 1:A:422:GLU:HG2  | 1:A:422:GLU:O    | 2.19                     | 0.43              |
| 1:D:234:ARG:NE   | 3:D:2492:HOH:O   | 2.34                     | 0.43              |
| 1:D:460:GLU:HG3  | 1:D:460:GLU:O    | 2.18                     | 0.43              |
| 1:A:476:ARG:HD2  | 3:A:2801:HOH:O   | 2.19                     | 0.43              |
| 1:C:46:GLU:OE2   | 1:C:79:HIS:HE1   | 2.01                     | 0.43              |
| 1:B:437:LEU:HD21 | 1:B:447:VAL:HG11 | 2.00                     | 0.43              |
| 1:F:102:TRP:HB3  | 1:F:103:PRO:HD3  | 2.01                     | 0.43              |
| 1:D:414:ASP:O    | 1:D:416:PRO:HD3  | 2.18                     | 0.43              |
| 1:F:422:GLU:HG3  | 1:F:424:HIS:ND1  | 2.34                     | 0.42              |
| 1:C:363:PRO:HD2  | 3:C:2660:HOH:O   | 2.18                     | 0.42              |
| 1:D:417:LYS:NZ   | 3:D:2731:HOH:O   | 2.52                     | 0.42              |
| 1:B:179:LYS:NZ   | 3:B:2456:HOH:O   | 2.50                     | 0.42              |
| 2:E:177:PHE:C    | 3:E:2468:HOH:O   | 2.57                     | 0.42              |
| 1:F:39:GLN:O     | 1:F:458:ASN:HB2  | 2.18                     | 0.42              |
| 1:C:343:PRO:HA   | 3:C:2620:HOH:O   | 2.18                     | 0.42              |
| 1:F:345:ASN:CG   | 3:F:2626:HOH:O   | 2.54                     | 0.42              |
| 1:C:85:VAL:HG11  | 1:C:129:LEU:HG   | 2.01                     | 0.42              |
| 1:F:251:ASP:N    | 1:F:251:ASP:OD1  | 2.52                     | 0.42              |
| 2:E:361:LYS:HB3  | 2:E:361:LYS:HE2  | 1.25                     | 0.42              |
| 2:E:238:GLU:OE1  | 3:E:2541:HOH:O   | 2.21                     | 0.42              |
| 2:E:63:GLU:HB3   | 3:E:2205:HOH:O   | 2.19                     | 0.42              |
| 1:F:314:LYS:HE3  | 3:F:2604:HOH:O   | 2.13                     | 0.42              |
| 1:B:417:LYS:HB3  | 3:B:2410:HOH:O   | 2.19                     | 0.42              |
| 1:C:337:LYS:CE   | 3:C:2608:HOH:O   | 2.62                     | 0.42              |
| 1:B:412:LYS:NZ   | 3:B:2757:HOH:O   | 2.53                     | 0.42              |
| 1:F:320:VAL:CG2  | 3:F:2600:HOH:O   | 2.65                     | 0.42              |
| 1:F:143:HIS:CE1  | 1:F:188:ASN:ND2  | 2.88                     | 0.42              |
| 1:F:13:ARG:HB3   | 1:F:432:ARG:HH21 | 1.84                     | 0.42              |
| 1:F:314:LYS:HB2  | 3:F:2303:HOH:O   | 2.20                     | 0.42              |
| 1:A:111:LEU:HD22 | 1:A:111:LEU:HA   | 1.91                     | 0.42              |
| 1:F:270:PHE:HA   | 1:F:273:GLN:HE21 | 1.84                     | 0.42              |
| 1:A:361:LYS:HE2  | 1:A:361:LYS:HB3  | 1.74                     | 0.42              |
| 2:E:292:VAL:CG2  | 3:E:2601:HOH:O   | 2.56                     | 0.42              |
| 1:A:476:ARG:HH21 | 1:A:476:ARG:CG   | 2.33                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:314:LYS:HD3  | 3:E:2631:HOH:O   | 2.19                     | 0.42              |
| 1:F:453:TRP:HA   | 1:F:454:SER:HA   | 1.83                     | 0.42              |
| 1:A:439:GLN:CD   | 3:A:2772:HOH:O   | 2.57                     | 0.42              |
| 1:F:422:GLU:CB   | 3:F:2819:HOH:O   | 2.25                     | 0.42              |
| 1:F:417:LYS:CB   | 3:F:2447:HOH:O   | 2.63                     | 0.42              |
| 1:F:412:LYS:NZ   | 3:F:2721:HOH:O   | 2.52                     | 0.42              |
| 1:C:259:ASN:HA   | 1:C:329:ASN:HB2  | 2.02                     | 0.42              |
| 1:D:131:LEU:CD1  | 1:D:180:THR:HG21 | 2.41                     | 0.42              |
| 1:F:462:SER:CB   | 3:F:2782:HOH:O   | 1.63                     | 0.42              |
| 1:D:345:ASN:CG   | 3:D:2631:HOH:O   | 2.58                     | 0.42              |
| 1:C:453:TRP:HA   | 1:C:454:SER:HA   | 1.81                     | 0.42              |
| 1:D:251:ASP:OD1  | 1:D:251:ASP:N    | 2.52                     | 0.42              |
| 1:D:111:LEU:HA   | 1:D:111:LEU:HD22 | 1.83                     | 0.41              |
| 1:D:314:LYS:CD   | 3:D:2599:HOH:O   | 2.67                     | 0.41              |
| 1:D:102:TRP:HB3  | 1:D:103:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:179:LYS:HA   | 1:A:179:LYS:CE   | 2.50                     | 0.41              |
| 1:C:46:GLU:HG3   | 3:C:2115:HOH:O   | 2.20                     | 0.41              |
| 1:A:412:LYS:HE2  | 3:A:2737:HOH:O   | 2.20                     | 0.41              |
| 1:C:412:LYS:HE2  | 3:C:2378:HOH:O   | 2.19                     | 0.41              |
| 1:B:269:THR:HG21 | 3:B:2566:HOH:O   | 2.20                     | 0.41              |
| 1:B:417:LYS:CE   | 3:B:2824:HOH:O   | 2.69                     | 0.41              |
| 1:D:372:THR:HB   | 1:D:407:MET:HE1  | 2.02                     | 0.41              |
| 1:A:13:ARG:HG3   | 3:A:2005:HOH:O   | 2.14                     | 0.41              |
| 1:C:342:SER:HA   | 1:D:310:TYR:OH   | 2.21                     | 0.41              |
| 1:A:117:GLU:HG2  | 3:A:2150:HOH:O   | 2.20                     | 0.41              |
| 1:A:259:ASN:HA   | 1:A:329:ASN:HB2  | 2.02                     | 0.41              |
| 2:E:245:LYS:HE3  | 3:E:2544:HOH:O   | 2.21                     | 0.41              |
| 1:C:131:LEU:HD12 | 1:C:180:THR:CG2  | 2.43                     | 0.41              |
| 2:E:227:ILE:HD13 | 2:E:227:ILE:HA   | 1.83                     | 0.41              |
| 1:C:432:ARG:NE   | 3:C:2753:HOH:O   | 2.52                     | 0.41              |
| 1:C:238:GLU:CD   | 3:C:2487:HOH:O   | 2.56                     | 0.41              |
| 1:B:46:GLU:CD    | 3:B:2129:HOH:O   | 2.52                     | 0.41              |
| 1:C:108:LYS:HE3  | 3:C:2264:HOH:O   | 2.21                     | 0.41              |
| 1:C:143:HIS:HD2  | 3:C:2072:HOH:O   | 2.03                     | 0.41              |
| 1:C:361:LYS:HE2  | 1:C:361:LYS:HB3  | 1.45                     | 0.41              |
| 1:F:293:ARG:HD2  | 3:F:2563:HOH:O   | 2.20                     | 0.41              |
| 1:A:232:LEU:C    | 1:A:232:LEU:HD23 | 2.41                     | 0.41              |
| 2:E:315:GLU:HA   | 3:E:2540:HOH:O   | 2.21                     | 0.41              |
| 1:C:171:LYS:HD3  | 3:C:2418:HOH:O   | 2.21                     | 0.41              |
| 2:E:111:LEU:CD1  | 3:E:2449:HOH:O   | 2.60                     | 0.41              |
| 1:F:171:LYS:HE2  | 3:F:2512:HOH:O   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:179:LYS:NZ   | 1:F:179:LYS:HB3  | 2.35                     | 0.41              |
| 2:E:314:LYS:CG   | 3:E:2647:HOH:O   | 2.69                     | 0.41              |
| 2:E:414:ASP:O    | 2:E:416:PRO:HD3  | 2.21                     | 0.41              |
| 2:E:372:THR:HG21 | 2:E:407:MET:HE3  | 2.02                     | 0.40              |
| 1:C:163:ILE:O    | 1:C:167:THR:HG23 | 2.21                     | 0.40              |
| 1:A:366:ASN:CG   | 3:A:2680:HOH:O   | 2.58                     | 0.40              |
| 1:C:314:LYS:NZ   | 3:C:2590:HOH:O   | 2.54                     | 0.40              |
| 1:B:251:ASP:OD1  | 1:B:251:ASP:N    | 2.54                     | 0.40              |
| 1:F:108:LYS:CE   | 3:F:2263:HOH:O   | 2.65                     | 0.40              |
| 2:E:344:ASN:ND2  | 3:E:2670:HOH:O   | 2.54                     | 0.40              |
| 1:A:58:CYS:HB3   | 1:A:70:ASN:HB3   | 2.02                     | 0.40              |
| 1:F:127:ILE:HG22 | 1:F:180:THR:HG21 | 2.01                     | 0.40              |
| 1:C:76:ASP:OD1   | 1:C:79:HIS:CD2   | 2.61                     | 0.40              |
| 1:C:108:LYS:HE2  | 3:C:2032:HOH:O   | 2.21                     | 0.40              |
| 1:A:417:LYS:HD3  | 3:A:2453:HOH:O   | 2.21                     | 0.40              |
| 1:A:251:ASP:OD1  | 1:A:251:ASP:N    | 2.53                     | 0.40              |
| 2:E:315:GLU:OE1  | 3:E:2641:HOH:O   | 2.04                     | 0.40              |
| 1:F:475:ASP:OD2  | 1:F:477:GLU:CG   | 2.68                     | 0.40              |

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 3:B:2759:HOH:O | 3:D:2088:HOH:O[1_655] | 1.87                     | 0.33              |
| 3:A:2416:HOH:O | 3:C:2368:HOH:O[1_545] | 1.89                     | 0.31              |
| 3:D:2376:HOH:O | 3:F:2409:HOH:O[1_565] | 2.13                     | 0.07              |
| 3:C:2589:HOH:O | 3:E:2173:HOH:O[1_455] | 2.15                     | 0.05              |
| 2:E:314:LYS:CB | 3:A:2168:HOH:O[1_655] | 2.16                     | 0.04              |
| 3:C:2569:HOH:O | 3:E:2518:HOH:O[1_455] | 2.18                     | 0.02              |

## 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     | 482/565 (85%)   | 468 (97%)  | 14 (3%) | 0        | 100         | 100 |
| 1   | B     | 482/565 (85%)   | 467 (97%)  | 15 (3%) | 0        | 100         | 100 |
| 1   | C     | 482/565 (85%)   | 466 (97%)  | 16 (3%) | 0        | 100         | 100 |
| 1   | D     | 482/565 (85%)   | 468 (97%)  | 14 (3%) | 0        | 100         | 100 |
| 1   | F     | 482/565 (85%)   | 469 (97%)  | 13 (3%) | 0        | 100         | 100 |
| 2   | E     | 482/565 (85%)   | 470 (98%)  | 12 (2%) | 0        | 100         | 100 |
| All | All   | 2892/3390 (85%) | 2808 (97%) | 84 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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     | 412/482 (86%)   | 396 (96%)  | 16 (4%)  | 39          | 21 |
| 1   | B     | 412/482 (86%)   | 395 (96%)  | 17 (4%)  | 37          | 19 |
| 1   | C     | 412/482 (86%)   | 393 (95%)  | 19 (5%)  | 33          | 15 |
| 1   | D     | 412/482 (86%)   | 394 (96%)  | 18 (4%)  | 35          | 17 |
| 1   | F     | 412/482 (86%)   | 394 (96%)  | 18 (4%)  | 35          | 17 |
| 2   | E     | 413/482 (86%)   | 395 (96%)  | 18 (4%)  | 35          | 17 |
| All | All   | 2473/2892 (86%) | 2367 (96%) | 106 (4%) | 35          | 17 |

All (106) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 13  | ARG  |
| 1   | A     | 111 | LEU  |
| 1   | A     | 179 | LYS  |
| 1   | A     | 222 | LEU  |
| 1   | A     | 269 | THR  |
| 1   | A     | 276 | GLN  |
| 1   | A     | 325 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 341 | LEU  |
| 1   | A     | 384 | LEU  |
| 1   | A     | 414 | ASP  |
| 1   | A     | 415 | LEU  |
| 1   | A     | 437 | LEU  |
| 1   | A     | 455 | LEU  |
| 1   | A     | 458 | ASN  |
| 1   | A     | 477 | GLU  |
| 1   | A     | 486 | ARG  |
| 1   | B     | 111 | LEU  |
| 1   | B     | 179 | LYS  |
| 1   | B     | 222 | LEU  |
| 1   | B     | 269 | THR  |
| 1   | B     | 276 | GLN  |
| 1   | B     | 319 | LEU  |
| 1   | B     | 325 | MET  |
| 1   | B     | 341 | LEU  |
| 1   | B     | 384 | LEU  |
| 1   | B     | 407 | MET  |
| 1   | B     | 412 | LYS  |
| 1   | B     | 414 | ASP  |
| 1   | B     | 415 | LEU  |
| 1   | B     | 437 | LEU  |
| 1   | B     | 455 | LEU  |
| 1   | B     | 458 | ASN  |
| 1   | B     | 478 | ASN  |
| 1   | C     | 13  | ARG  |
| 1   | C     | 111 | LEU  |
| 1   | C     | 179 | LYS  |
| 1   | C     | 222 | LEU  |
| 1   | C     | 269 | THR  |
| 1   | C     | 276 | GLN  |
| 1   | C     | 319 | LEU  |
| 1   | C     | 325 | MET  |
| 1   | C     | 341 | LEU  |
| 1   | C     | 361 | LYS  |
| 1   | C     | 384 | LEU  |
| 1   | C     | 403 | THR  |
| 1   | C     | 414 | ASP  |
| 1   | C     | 415 | LEU  |
| 1   | C     | 437 | LEU  |
| 1   | C     | 455 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 458 | ASN  |
| 1   | C     | 481 | GLU  |
| 1   | C     | 486 | ARG  |
| 1   | D     | 111 | LEU  |
| 1   | D     | 179 | LYS  |
| 1   | D     | 222 | LEU  |
| 1   | D     | 269 | THR  |
| 1   | D     | 276 | GLN  |
| 1   | D     | 319 | LEU  |
| 1   | D     | 325 | MET  |
| 1   | D     | 341 | LEU  |
| 1   | D     | 361 | LYS  |
| 1   | D     | 384 | LEU  |
| 1   | D     | 407 | MET  |
| 1   | D     | 415 | LEU  |
| 1   | D     | 422 | GLU  |
| 1   | D     | 437 | LEU  |
| 1   | D     | 455 | LEU  |
| 1   | D     | 458 | ASN  |
| 1   | D     | 477 | GLU  |
| 1   | D     | 481 | GLU  |
| 2   | E     | 66  | VAL  |
| 2   | E     | 111 | LEU  |
| 2   | E     | 180 | LYS  |
| 2   | E     | 222 | LEU  |
| 2   | E     | 269 | THR  |
| 2   | E     | 276 | GLN  |
| 2   | E     | 325 | MET  |
| 2   | E     | 341 | LEU  |
| 2   | E     | 361 | LYS  |
| 2   | E     | 384 | LEU  |
| 2   | E     | 407 | MET  |
| 2   | E     | 414 | ASP  |
| 2   | E     | 415 | LEU  |
| 2   | E     | 437 | LEU  |
| 2   | E     | 455 | LEU  |
| 2   | E     | 458 | ASN  |
| 2   | E     | 477 | GLU  |
| 2   | E     | 481 | GLU  |
| 1   | F     | 13  | ARG  |
| 1   | F     | 111 | LEU  |
| 1   | F     | 222 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 269 | THR  |
| 1   | F     | 276 | GLN  |
| 1   | F     | 319 | LEU  |
| 1   | F     | 325 | MET  |
| 1   | F     | 341 | LEU  |
| 1   | F     | 381 | PRO  |
| 1   | F     | 384 | LEU  |
| 1   | F     | 403 | THR  |
| 1   | F     | 407 | MET  |
| 1   | F     | 414 | ASP  |
| 1   | F     | 415 | LEU  |
| 1   | F     | 422 | GLU  |
| 1   | F     | 437 | LEU  |
| 1   | F     | 455 | LEU  |
| 1   | F     | 458 | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 133 | ASN  |
| 1   | A     | 244 | ASN  |
| 1   | A     | 247 | HIS  |
| 1   | A     | 268 | ASN  |
| 1   | A     | 273 | GLN  |
| 1   | A     | 274 | GLN  |
| 1   | A     | 276 | GLN  |
| 1   | A     | 316 | GLN  |
| 1   | A     | 458 | ASN  |
| 1   | A     | 492 | GLN  |
| 1   | B     | 79  | HIS  |
| 1   | B     | 133 | ASN  |
| 1   | B     | 244 | ASN  |
| 1   | B     | 268 | ASN  |
| 1   | B     | 273 | GLN  |
| 1   | B     | 276 | GLN  |
| 1   | B     | 316 | GLN  |
| 1   | B     | 350 | ASN  |
| 1   | B     | 458 | ASN  |
| 1   | B     | 492 | GLN  |
| 1   | C     | 79  | HIS  |
| 1   | C     | 133 | ASN  |
| 1   | C     | 143 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 244 | ASN  |
| 1   | C     | 247 | HIS  |
| 1   | C     | 268 | ASN  |
| 1   | C     | 273 | GLN  |
| 1   | C     | 274 | GLN  |
| 1   | C     | 276 | GLN  |
| 1   | C     | 316 | GLN  |
| 1   | C     | 350 | ASN  |
| 1   | C     | 458 | ASN  |
| 1   | C     | 492 | GLN  |
| 1   | D     | 79  | HIS  |
| 1   | D     | 133 | ASN  |
| 1   | D     | 244 | ASN  |
| 1   | D     | 268 | ASN  |
| 1   | D     | 273 | GLN  |
| 1   | D     | 274 | GLN  |
| 1   | D     | 276 | GLN  |
| 1   | D     | 316 | GLN  |
| 1   | D     | 350 | ASN  |
| 1   | D     | 458 | ASN  |
| 1   | D     | 492 | GLN  |
| 2   | E     | 56  | HIS  |
| 2   | E     | 60  | ASN  |
| 2   | E     | 79  | HIS  |
| 2   | E     | 133 | ASN  |
| 2   | E     | 148 | GLN  |
| 2   | E     | 244 | ASN  |
| 2   | E     | 268 | ASN  |
| 2   | E     | 273 | GLN  |
| 2   | E     | 274 | GLN  |
| 2   | E     | 276 | GLN  |
| 2   | E     | 316 | GLN  |
| 2   | E     | 350 | ASN  |
| 2   | E     | 458 | ASN  |
| 2   | E     | 492 | GLN  |
| 1   | F     | 79  | HIS  |
| 1   | F     | 133 | ASN  |
| 1   | F     | 244 | ASN  |
| 1   | F     | 268 | ASN  |
| 1   | F     | 273 | GLN  |
| 1   | F     | 274 | GLN  |
| 1   | F     | 276 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 316 | GLN  |
| 1   | F     | 350 | ASN  |
| 1   | F     | 458 | ASN  |
| 1   | F     | 492 | 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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|---------------|-----------------------|--------|
| 1   | A     | 484/565 (85%)   | -0.31  | 6 (1%) 81 78  | 20, 26, 37, 53        | 1 (0%) |
| 1   | B     | 484/565 (85%)   | -0.34  | 10 (2%) 67 62 | 20, 26, 37, 52        | 1 (0%) |
| 1   | C     | 484/565 (85%)   | -0.31  | 5 (1%) 84 82  | 20, 26, 37, 52        | 1 (0%) |
| 1   | D     | 484/565 (85%)   | -0.33  | 11 (2%) 64 59 | 20, 26, 37, 54        | 1 (0%) |
| 1   | F     | 484/565 (85%)   | -0.32  | 11 (2%) 64 59 | 19, 25, 36, 54        | 1 (0%) |
| 2   | E     | 484/565 (85%)   | -0.29  | 12 (2%) 61 56 | 19, 25, 37, 51        | 1 (0%) |
| All | All   | 2904/3390 (85%) | -0.32  | 55 (1%) 70 66 | 19, 26, 37, 54        | 6 (0%) |

All (55) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 344 | ASN  | 7.1  |
| 1   | D     | 344 | ASN  | 5.9  |
| 1   | F     | 344 | ASN  | 5.8  |
| 1   | C     | 414 | ASP  | 5.2  |
| 1   | A     | 414 | ASP  | 4.7  |
| 2   | E     | 414 | ASP  | 4.6  |
| 1   | D     | 13  | ARG  | 4.5  |
| 1   | F     | 13  | ARG  | 4.2  |
| 2   | E     | 344 | ASN  | 3.9  |
| 1   | C     | 13  | ARG  | 3.8  |
| 1   | F     | 414 | ASP  | 3.8  |
| 1   | A     | 344 | ASN  | 3.7  |
| 1   | B     | 13  | ARG  | 3.7  |
| 2   | E     | 313 | GLU  | 3.7  |
| 1   | F     | 211 | GLY  | 3.6  |
| 1   | D     | 414 | ASP  | 3.5  |
| 1   | A     | 13  | ARG  | 3.4  |
| 1   | D     | 477 | GLU  | 3.4  |
| 2   | E     | 250 | ALA  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 314 | LYS  | 3.2  |
| 1   | D     | 424 | HIS  | 3.2  |
| 1   | B     | 414 | ASP  | 3.2  |
| 1   | D     | 250 | ALA  | 3.1  |
| 2   | E     | 13  | ARG  | 3.1  |
| 1   | C     | 477 | GLU  | 3.0  |
| 2   | E     | 249 | GLY  | 3.0  |
| 1   | B     | 250 | ALA  | 3.0  |
| 1   | C     | 344 | ASN  | 2.9  |
| 2   | E     | 314 | LYS  | 2.9  |
| 1   | F     | 496 | GLY  | 2.9  |
| 1   | F     | 250 | ALA  | 2.8  |
| 1   | A     | 477 | GLU  | 2.8  |
| 1   | D     | 179 | LYS  | 2.7  |
| 1   | F     | 424 | HIS  | 2.7  |
| 1   | A     | 478 | ASN  | 2.6  |
| 1   | B     | 314 | LYS  | 2.6  |
| 1   | B     | 343 | PRO  | 2.6  |
| 2   | E     | 424 | HIS  | 2.5  |
| 1   | D     | 314 | LYS  | 2.5  |
| 2   | E     | 251 | ASP  | 2.5  |
| 1   | B     | 424 | HIS  | 2.4  |
| 1   | D     | 249 | GLY  | 2.4  |
| 2   | E     | 477 | GLU  | 2.3  |
| 2   | E     | 496 | GLY  | 2.3  |
| 1   | B     | 412 | LYS  | 2.3  |
| 1   | D     | 313 | GLU  | 2.3  |
| 1   | D     | 343 | PRO  | 2.3  |
| 1   | F     | 477 | GLU  | 2.2  |
| 1   | B     | 23  | ASP  | 2.2  |
| 1   | F     | 251 | ASP  | 2.2  |
| 2   | E     | 422 | GLU  | 2.1  |
| 1   | B     | 345 | ASN  | 2.1  |
| 1   | C     | 250 | ALA  | 2.1  |
| 1   | F     | 179 | LYS  | 2.0  |
| 1   | A     | 424 | HIS  | 2.0  |

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.