



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:31 PM UTC

PDB ID : 5ECM / pdb\_00005ecm  
Title : Crystal Structure of FIN219-FIP1 complex with JA and Leu  
Authors : Chen, C.Y.; Cheng, Y.S.  
Deposited on : 2015-10-20  
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

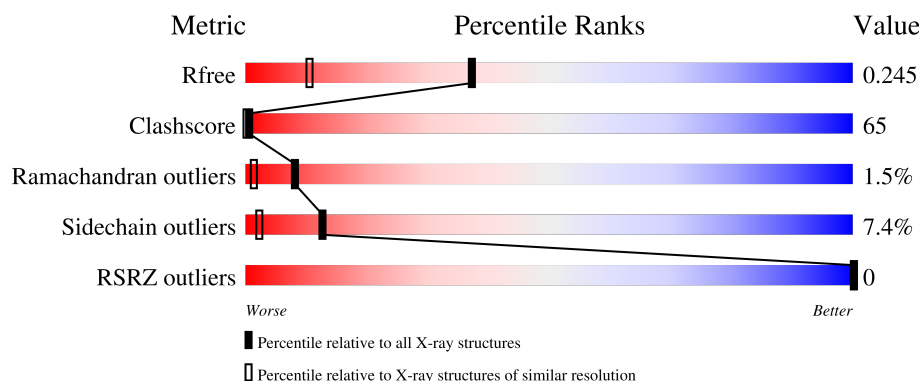
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

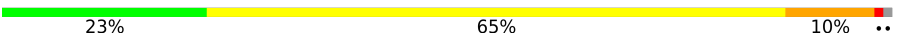
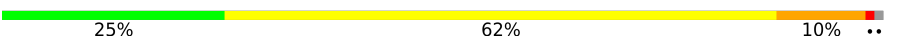
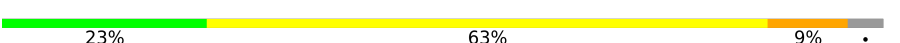
The reported resolution of this entry is 1.60 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 4673 (1.60-1.60)                                      |
| Clashscore            | 190562                      | 4931 (1.60-1.60)                                      |
| Ramachandran outliers | 187476                      | 4831 (1.60-1.60)                                      |
| Sidechain outliers    | 187428                      | 4830 (1.60-1.60)                                      |
| RSRZ outliers         | 180081                      | 4672 (1.60-1.60)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 575    |  |
| 1   | D     | 575    |  |
| 2   | B     | 223    |  |
| 2   | C     | 223    |  |
| 2   | E     | 223    |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 2   | F     | 223    |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | JAA  | A     | 601 | -         | X        | -       | -                |
| 4   | LEU  | A     | 602 | -         | -        | X       | -                |
| 4   | LEU  | D     | 602 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17738 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 Jasmonic acid-amido synthetase JAR1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 569      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4479  | 2859 | 748 | 850 | 22 |         |         |       |
| 1   | D     | 569      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4479  | 2859 | 748 | 850 | 22 |         |         |       |

- Molecule 2 is a protein called Glutathione S-transferase U20.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1748  | 1136 | 284 | 323 | 5 |         |         |       |
| 2   | C     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1748  | 1136 | 284 | 323 | 5 |         |         |       |
| 2   | E     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1748  | 1136 | 284 | 323 | 5 |         |         |       |
| 2   | F     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1748  | 1136 | 284 | 323 | 5 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

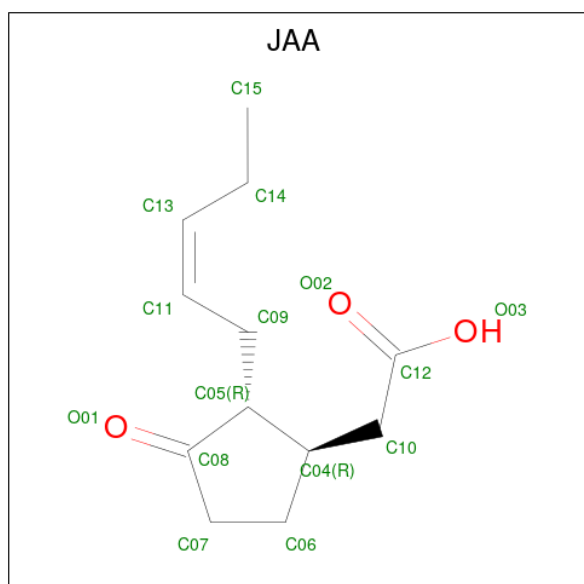
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -5      | HIS      | -      | expression tag | UNP Q8L7C9 |
| B     | -4      | HIS      | -      | expression tag | UNP Q8L7C9 |
| B     | -3      | HIS      | -      | expression tag | UNP Q8L7C9 |
| B     | -2      | HIS      | -      | expression tag | UNP Q8L7C9 |
| B     | -1      | HIS      | -      | expression tag | UNP Q8L7C9 |
| B     | 0       | HIS      | -      | expression tag | UNP Q8L7C9 |
| C     | -5      | HIS      | -      | expression tag | UNP Q8L7C9 |
| C     | -4      | HIS      | -      | expression tag | UNP Q8L7C9 |
| C     | -3      | HIS      | -      | expression tag | UNP Q8L7C9 |
| C     | -2      | HIS      | -      | expression tag | UNP Q8L7C9 |
| C     | -1      | HIS      | -      | expression tag | UNP Q8L7C9 |
| C     | 0       | HIS      | -      | expression tag | UNP Q8L7C9 |

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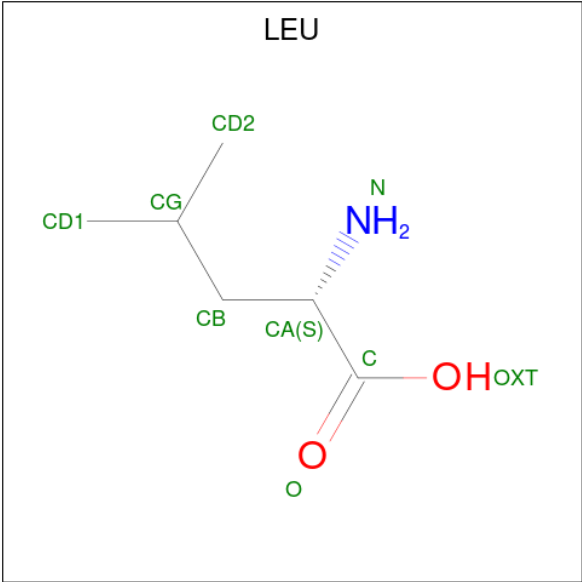
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | -5      | HIS      | -      | expression tag | UNP Q8L7C9 |
| E     | -4      | HIS      | -      | expression tag | UNP Q8L7C9 |
| E     | -3      | HIS      | -      | expression tag | UNP Q8L7C9 |
| E     | -2      | HIS      | -      | expression tag | UNP Q8L7C9 |
| E     | -1      | HIS      | -      | expression tag | UNP Q8L7C9 |
| E     | 0       | HIS      | -      | expression tag | UNP Q8L7C9 |
| F     | -5      | HIS      | -      | expression tag | UNP Q8L7C9 |
| F     | -4      | HIS      | -      | expression tag | UNP Q8L7C9 |
| F     | -3      | HIS      | -      | expression tag | UNP Q8L7C9 |
| F     | -2      | HIS      | -      | expression tag | UNP Q8L7C9 |
| F     | -1      | HIS      | -      | expression tag | UNP Q8L7C9 |
| F     | 0       | HIS      | -      | expression tag | UNP Q8L7C9 |

- Molecule 3 is {(1R,2R)-3-oxo-2-[(2Z)-pent-2-en-1-yl]cyclopentyl}acetic acid (CCD ID: JAA) (formula: C<sub>12</sub>H<sub>18</sub>O<sub>3</sub>).



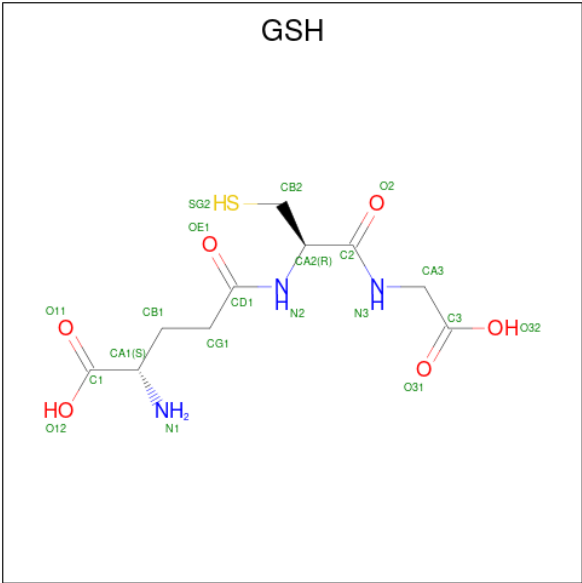
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 3   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 15    | 12 | 3 |         |         |
| 3   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 15    | 12 | 3 |         |         |

- Molecule 4 is LEUCINE (CCD ID: LEU) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 1 | 2 |         |         |
| 4   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 1 | 2 |         |         |

- Molecule 5 is GLUTATHIONE (CCD ID: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 5   | B     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 20    | 10 | 3 | 6 | 1 |         |         |
| 5   | C     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 20    | 10 | 3 | 6 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 5   | E     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 20    | 10 | 3 | 6 | 1 |         |         |
| 5   | F     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 20    | 10 | 3 | 6 | 1 |         |         |

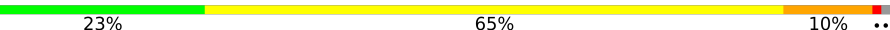
- Molecule 6 is water.

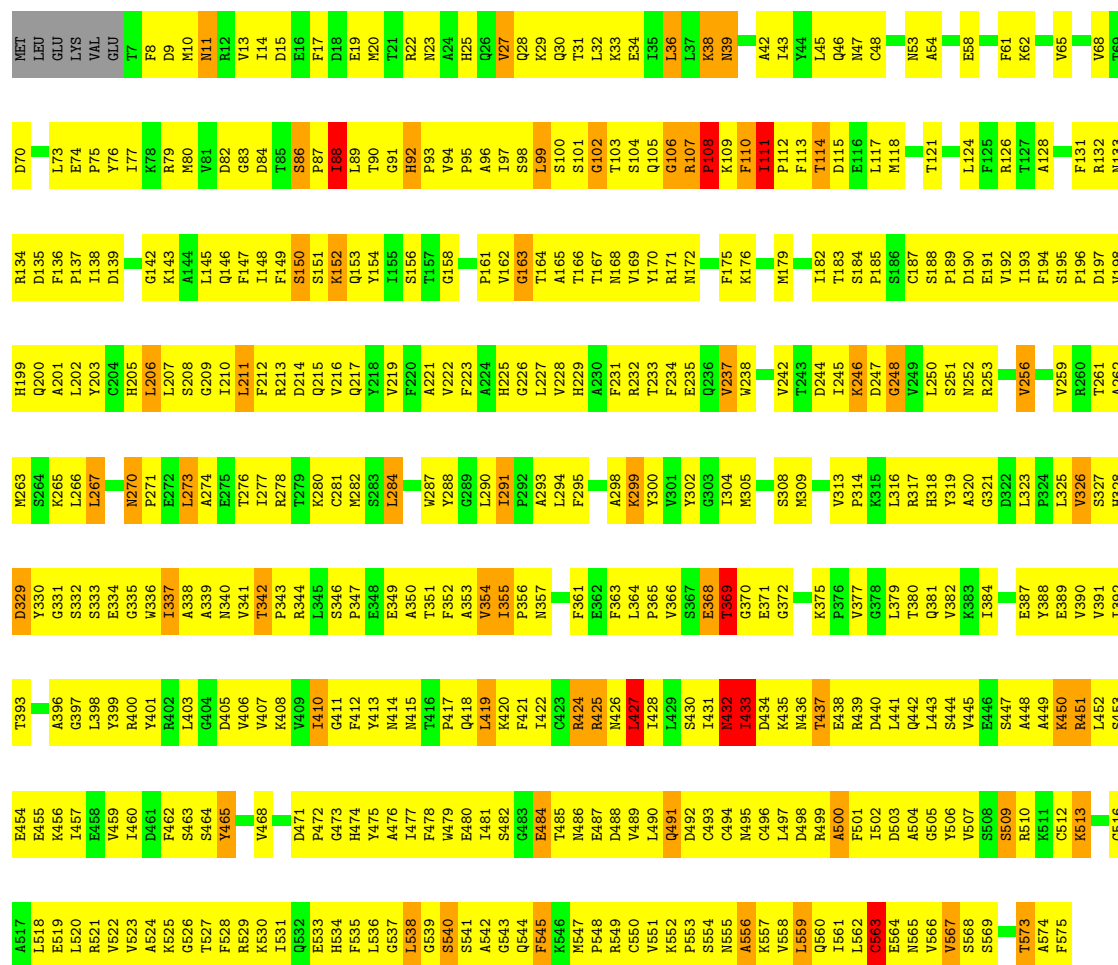
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 6   | A     | 435      | Total | O   | 0       | 0       |
|     |       |          | 435   | 435 |         |         |
| 6   | B     | 185      | Total | O   | 0       | 0       |
|     |       |          | 185   | 185 |         |         |
| 6   | C     | 184      | Total | O   | 0       | 0       |
|     |       |          | 184   | 184 |         |         |
| 6   | D     | 472      | Total | O   | 0       | 0       |
|     |       |          | 472   | 472 |         |         |
| 6   | E     | 215      | Total | O   | 0       | 0       |
|     |       |          | 215   | 215 |         |         |
| 6   | F     | 169      | Total | O   | 0       | 0       |
|     |       |          | 169   | 169 |         |         |

### 3 Residue-property plots

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

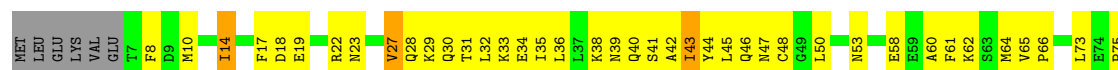
#### • Molecule 1: Jasmonic acid-amido synthetase JAR1

Chain A: 

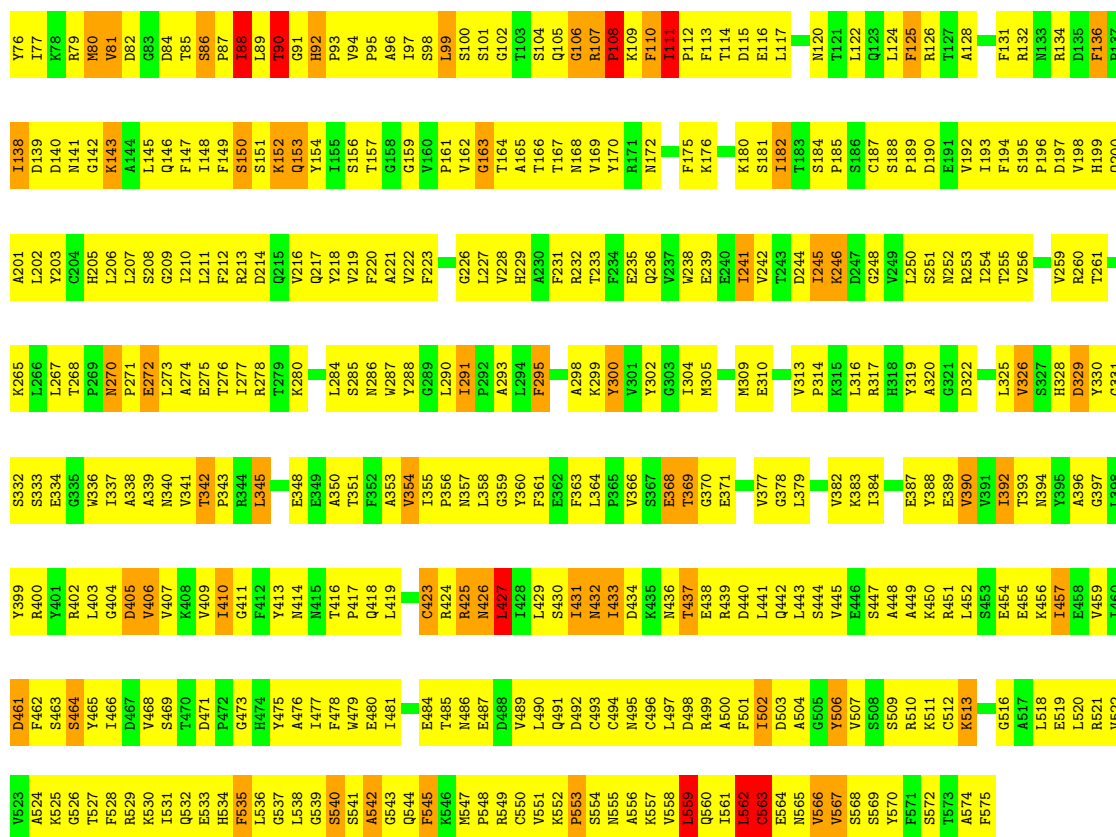


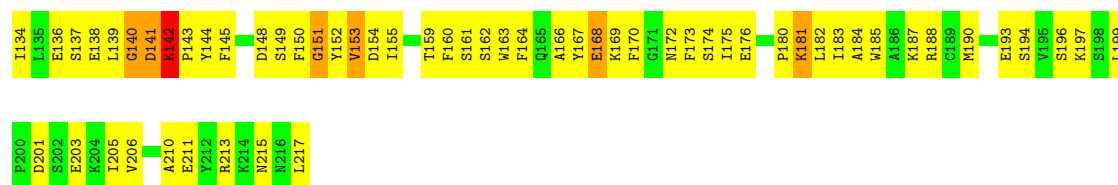
#### • Molecule 1: Jasmonic acid-amido synthetase JAR1

Chain D: 



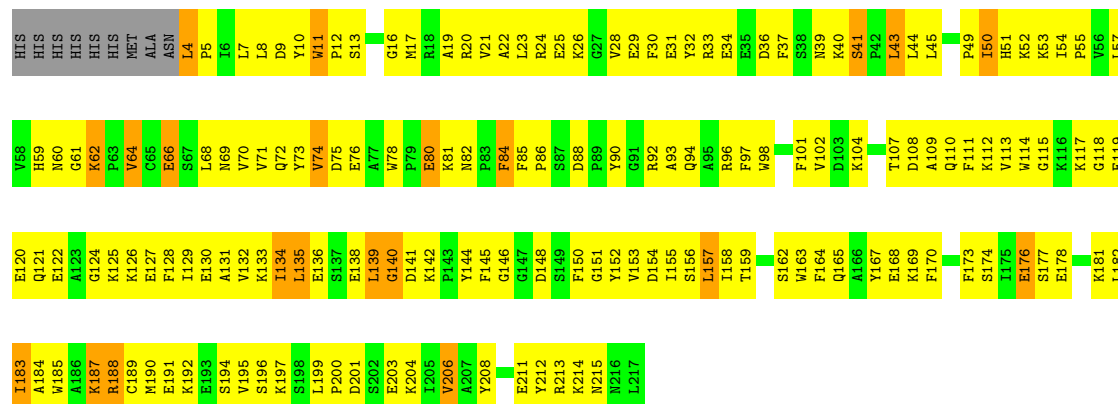






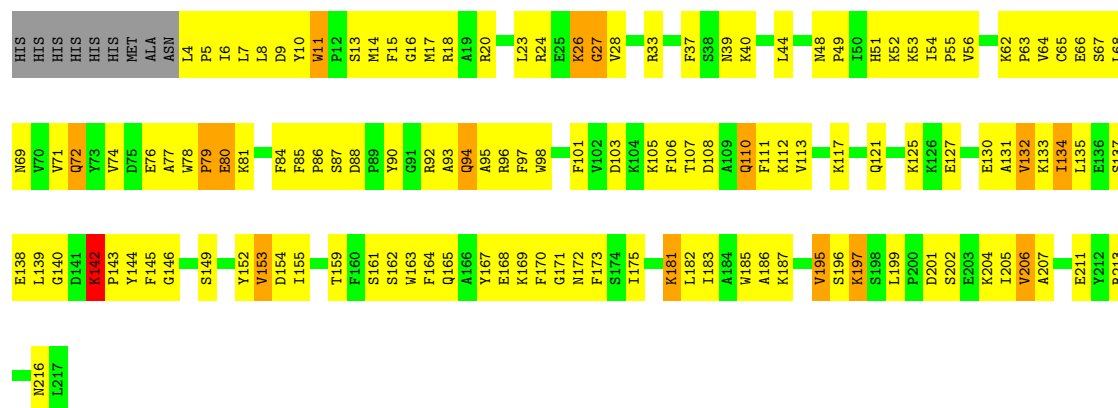
• Molecule 2: Glutathione S-transferase U20

Chain E: 23% 63% 9% .



• Molecule 2: Glutathione S-transferase U20

Chain F: 38% 51% 7% .



## 4 Data and refinement statistics

| Property                                                                | Value                                                              | Source           |
|-------------------------------------------------------------------------|--------------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                                | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 53.82Å 53.90Å 195.81Å<br>97.15° 92.27° 113.64°                     | Depositor        |
| Resolution (Å)                                                          | 24.17 – 1.60<br>24.17 – 1.60                                       | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.9 (24.17-1.60)<br>98.9 (24.17-1.60)                             | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                               | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                    | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.72 (at 1.60Å)                                                    | Xtriage          |
| Refinement program                                                      | PHENIX 1.9_1692                                                    | Depositor        |
| R, $R_{free}$                                                           | 0.232 , 0.245<br>0.232 , 0.245                                     | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 25926 reflections (9.87%)                                          | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 2.8                                                                | Xtriage          |
| Anisotropy                                                              | 0.493                                                              | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.58 , 154.4                                                       | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$        | Xtriage          |
| Estimated twinning fraction                                             | 0.078 for k,h,-h-k-l<br>0.003 for -k,-h,l<br>0.001 for -h,-k,h+k+l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.87                                                               | EDS              |
| Total number of atoms                                                   | 17738                                                              | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 4.0                                                                | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8765e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.70         | 1/4581 (0.0%)  | 1.28        | 44/6219 (0.7%)   |
| 1   | D     | 0.69         | 0/4581         | 1.26        | 48/6219 (0.8%)   |
| 2   | B     | 0.57         | 0/1799         | 1.02        | 5/2428 (0.2%)    |
| 2   | C     | 0.54         | 0/1799         | 1.00        | 9/2428 (0.4%)    |
| 2   | E     | 0.57         | 0/1799         | 1.06        | 11/2428 (0.5%)   |
| 2   | F     | 0.52         | 0/1799         | 0.97        | 5/2428 (0.2%)    |
| All | All   | 0.63         | 1/16358 (0.0%) | 1.16        | 122/22150 (0.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 3                   |
| 1   | D     | 0                   | 3                   |
| 2   | C     | 0                   | 1                   |
| 2   | F     | 0                   | 1                   |
| All | All   | 0                   | 8                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 500 | ALA  | CA-CB | -5.35 | 1.45        | 1.53     |

All (122) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 86  | SER  | CA-C-N | 12.60 | 133.60      | 119.99   |
| 1   | A     | 86  | SER  | C-N-CA | 12.60 | 133.60      | 119.99   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 86  | SER  | CA-C-N    | 11.49 | 133.11      | 120.13   |
| 1   | D     | 86  | SER  | C-N-CA    | 11.49 | 133.11      | 120.13   |
| 1   | D     | 295 | PHE  | CA-C-N    | 11.31 | 130.91      | 119.82   |
| 1   | D     | 295 | PHE  | C-N-CA    | 11.31 | 130.91      | 119.82   |
| 1   | D     | 107 | ARG  | CA-C-N    | 10.98 | 131.07      | 119.76   |
| 1   | D     | 107 | ARG  | C-N-CA    | 10.98 | 131.07      | 119.76   |
| 1   | D     | 270 | ASN  | CA-C-N    | 10.89 | 130.56      | 119.56   |
| 1   | D     | 270 | ASN  | C-N-CA    | 10.89 | 130.56      | 119.56   |
| 1   | A     | 107 | ARG  | CA-C-N    | 10.39 | 130.50      | 119.90   |
| 1   | A     | 107 | ARG  | C-N-CA    | 10.39 | 130.50      | 119.90   |
| 1   | A     | 563 | CYS  | N-CA-C    | 9.65  | 121.56      | 111.14   |
| 1   | A     | 270 | ASN  | CA-C-N    | 8.71  | 128.36      | 119.56   |
| 1   | A     | 270 | ASN  | C-N-CA    | 8.71  | 128.36      | 119.56   |
| 1   | A     | 246 | LYS  | N-CA-C    | 8.40  | 120.36      | 111.03   |
| 1   | A     | 86  | SER  | N-CA-C    | 8.28  | 121.35      | 109.84   |
| 1   | A     | 163 | GLY  | N-CA-C    | 8.20  | 126.36      | 111.03   |
| 1   | D     | 563 | CYS  | N-CA-C    | 7.85  | 120.98      | 111.40   |
| 1   | D     | 246 | LYS  | N-CA-C    | 7.82  | 120.56      | 111.02   |
| 1   | D     | 163 | GLY  | N-CA-C    | 7.63  | 123.86      | 110.80   |
| 1   | D     | 427 | LEU  | N-CA-C    | 7.58  | 121.34      | 107.99   |
| 2   | E     | 188 | ARG  | NE-CZ-NH1 | -7.43 | 114.07      | 121.50   |
| 1   | D     | 111 | ILE  | CA-C-N    | 7.25  | 127.29      | 119.90   |
| 1   | D     | 111 | ILE  | C-N-CA    | 7.25  | 127.29      | 119.90   |
| 1   | A     | 364 | LEU  | CA-C-N    | 7.25  | 127.22      | 119.76   |
| 1   | A     | 364 | LEU  | C-N-CA    | 7.25  | 127.22      | 119.76   |
| 1   | D     | 86  | SER  | N-CA-C    | 7.23  | 119.01      | 109.83   |
| 1   | A     | 111 | ILE  | CA-C-N    | 7.16  | 126.92      | 119.76   |
| 1   | A     | 111 | ILE  | C-N-CA    | 7.16  | 126.92      | 119.76   |
| 1   | A     | 267 | LEU  | N-CA-C    | 7.16  | 120.59      | 109.07   |
| 1   | D     | 267 | LEU  | N-CA-C    | 7.11  | 121.03      | 109.59   |
| 1   | A     | 88  | ILE  | N-CA-C    | 7.02  | 123.95      | 109.34   |
| 1   | D     | 506 | TYR  | N-CA-C    | -7.01 | 103.64      | 111.28   |
| 1   | A     | 354 | VAL  | N-CA-C    | 6.99  | 118.04      | 109.30   |
| 1   | A     | 427 | LEU  | N-CA-C    | 6.99  | 120.16      | 108.20   |
| 1   | A     | 206 | LEU  | N-CA-C    | -6.91 | 102.58      | 111.02   |
| 1   | D     | 106 | GLY  | N-CA-C    | -6.89 | 106.67      | 115.42   |
| 1   | D     | 502 | ILE  | N-CA-C    | 6.87  | 117.62      | 110.62   |
| 1   | A     | 82  | ASP  | N-CA-C    | 6.83  | 119.26      | 110.65   |
| 1   | D     | 136 | PHE  | CA-C-N    | 6.82  | 127.19      | 119.83   |
| 1   | D     | 136 | PHE  | C-N-CA    | 6.82  | 127.19      | 119.83   |
| 1   | A     | 108 | PRO  | N-CA-C    | 6.80  | 121.89      | 111.15   |
| 2   | F     | 142 | LYS  | CA-C-N    | -6.66 | 111.59      | 118.85   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | F     | 142 | LYS  | C-N-CA    | -6.66 | 111.59      | 118.85   |
| 1   | D     | 567 | VAL  | N-CA-C    | -6.63 | 102.77      | 111.05   |
| 2   | E     | 188 | ARG  | NE-CZ-NH2 | 6.47  | 125.03      | 119.20   |
| 1   | A     | 39  | ASN  | N-CA-C    | 6.39  | 119.20      | 110.06   |
| 1   | D     | 457 | ILE  | N-CA-C    | 6.39  | 117.55      | 108.42   |
| 2   | B     | 62  | LYS  | CA-C-N    | 6.33  | 126.67      | 119.83   |
| 2   | B     | 62  | LYS  | C-N-CA    | 6.33  | 126.67      | 119.83   |
| 1   | A     | 106 | GLY  | N-CA-C    | -6.27 | 107.62      | 115.08   |
| 1   | A     | 465 | TYR  | N-CA-C    | 6.24  | 117.88      | 108.46   |
| 2   | C     | 11  | TRP  | CA-C-N    | -6.23 | 113.51      | 121.04   |
| 2   | C     | 11  | TRP  | C-N-CA    | -6.23 | 113.51      | 121.04   |
| 1   | A     | 102 | GLY  | N-CA-C    | -6.22 | 99.38       | 112.45   |
| 1   | A     | 559 | LEU  | N-CA-C    | 6.18  | 117.81      | 111.14   |
| 1   | D     | 108 | PRO  | N-CA-C    | 6.16  | 120.75      | 111.14   |
| 1   | D     | 559 | LEU  | N-CA-C    | 6.13  | 117.76      | 111.14   |
| 1   | A     | 237 | VAL  | N-CA-C    | 6.09  | 117.96      | 112.17   |
| 2   | C     | 142 | LYS  | CA-C-N    | -6.03 | 112.31      | 119.84   |
| 2   | C     | 142 | LYS  | C-N-CA    | -6.03 | 112.31      | 119.84   |
| 1   | A     | 256 | VAL  | CA-C-N    | 6.01  | 125.72      | 119.05   |
| 1   | A     | 256 | VAL  | C-N-CA    | 6.01  | 125.72      | 119.05   |
| 1   | D     | 342 | THR  | CA-C-N    | 6.00  | 125.68      | 119.56   |
| 1   | D     | 342 | THR  | C-N-CA    | 6.00  | 125.68      | 119.56   |
| 1   | D     | 291 | ILE  | CA-C-N    | -5.99 | 113.51      | 119.56   |
| 1   | D     | 291 | ILE  | C-N-CA    | -5.99 | 113.51      | 119.56   |
| 2   | E     | 4   | LEU  | CA-C-N    | 5.95  | 126.25      | 119.83   |
| 2   | E     | 4   | LEU  | C-N-CA    | 5.95  | 126.25      | 119.83   |
| 1   | A     | 248 | GLY  | N-CA-C    | -5.94 | 105.75      | 114.90   |
| 2   | E     | 41  | SER  | CA-C-N    | 5.89  | 126.03      | 119.32   |
| 2   | E     | 41  | SER  | C-N-CA    | 5.89  | 126.03      | 119.32   |
| 2   | F     | 11  | TRP  | CA-C-N    | -5.88 | 113.78      | 120.89   |
| 2   | F     | 11  | TRP  | C-N-CA    | -5.88 | 113.78      | 120.89   |
| 2   | E     | 62  | LYS  | CA-C-N    | 5.77  | 126.06      | 119.83   |
| 2   | E     | 62  | LYS  | C-N-CA    | 5.77  | 126.06      | 119.83   |
| 2   | E     | 11  | TRP  | CA-C-N    | -5.75 | 112.65      | 119.84   |
| 2   | E     | 11  | TRP  | C-N-CA    | -5.75 | 112.65      | 119.84   |
| 1   | D     | 392 | ILE  | N-CA-C    | 5.72  | 116.18      | 108.17   |
| 2   | B     | 11  | TRP  | CA-C-N    | -5.69 | 112.73      | 119.84   |
| 2   | B     | 11  | TRP  | C-N-CA    | -5.69 | 112.73      | 119.84   |
| 1   | A     | 11  | ASN  | N-CA-C    | 5.68  | 117.55      | 111.36   |
| 1   | D     | 90  | THR  | N-CA-C    | -5.66 | 98.74       | 110.80   |
| 1   | D     | 300 | TYR  | N-CA-C    | 5.65  | 117.44      | 108.79   |
| 1   | A     | 567 | VAL  | N-CA-C    | -5.62 | 104.18      | 112.04   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | C     | 4   | LEU  | CA-C-N   | 5.59  | 125.52      | 119.76   |
| 2   | C     | 4   | LEU  | C-N-CA   | 5.59  | 125.52      | 119.76   |
| 1   | D     | 88  | ILE  | N-CA-C   | 5.57  | 120.92      | 109.34   |
| 1   | D     | 81  | VAL  | N-CA-C   | 5.46  | 116.95      | 111.00   |
| 1   | A     | 291 | ILE  | CA-C-N   | -5.46 | 113.99      | 119.56   |
| 1   | A     | 291 | ILE  | C-N-CA   | -5.46 | 113.99      | 119.56   |
| 1   | D     | 406 | VAL  | N-CA-C   | 5.41  | 115.89      | 107.99   |
| 1   | D     | 159 | GLY  | N-CA-C   | -5.37 | 107.86      | 115.43   |
| 1   | D     | 248 | GLY  | N-CA-C   | -5.32 | 106.88      | 115.08   |
| 1   | A     | 355 | ILE  | CA-C-N   | 5.31  | 125.78      | 120.04   |
| 1   | A     | 355 | ILE  | C-N-CA   | 5.31  | 125.78      | 120.04   |
| 2   | C     | 151 | GLY  | N-CA-C   | 5.29  | 118.94      | 111.42   |
| 1   | A     | 211 | LEU  | N-CA-C   | 5.27  | 117.71      | 111.33   |
| 1   | D     | 562 | LEU  | N-CA-C   | 5.27  | 116.83      | 111.14   |
| 1   | A     | 491 | GLN  | CA-CB-CG | -5.26 | 103.57      | 114.10   |
| 1   | D     | 461 | ASP  | N-CA-C   | 5.25  | 115.28      | 107.88   |
| 1   | A     | 300 | TYR  | N-CA-C   | 5.25  | 116.81      | 108.79   |
| 2   | F     | 175 | ILE  | N-CA-C   | -5.23 | 106.44      | 112.98   |
| 1   | A     | 342 | THR  | CA-C-N   | 5.20  | 124.87      | 119.56   |
| 1   | A     | 342 | THR  | C-N-CA   | 5.20  | 124.87      | 119.56   |
| 1   | D     | 390 | VAL  | N-CA-C   | 5.20  | 116.07      | 108.58   |
| 2   | B     | 139 | LEU  | N-CA-C   | -5.19 | 105.63      | 111.28   |
| 1   | D     | 153 | GLN  | CA-CB-CG | 5.18  | 124.46      | 114.10   |
| 1   | D     | 102 | GLY  | N-CA-C   | -5.18 | 101.58      | 112.45   |
| 1   | A     | 556 | ALA  | N-CA-C   | 5.17  | 120.05      | 113.18   |
| 1   | D     | 464 | SER  | N-CA-C   | 5.15  | 115.33      | 108.38   |
| 1   | D     | 535 | PHE  | N-CA-C   | 5.15  | 116.97      | 111.36   |
| 1   | D     | 272 | GLU  | N-CA-C   | 5.15  | 116.70      | 111.14   |
| 1   | A     | 432 | ASN  | N-CA-C   | 5.13  | 117.27      | 109.63   |
| 2   | C     | 88  | ASP  | CA-C-N   | 5.11  | 124.72      | 119.05   |
| 2   | C     | 88  | ASP  | C-N-CA   | 5.11  | 124.72      | 119.05   |
| 1   | D     | 310 | GLU  | CA-C-N   | -5.06 | 114.61      | 119.87   |
| 1   | D     | 310 | GLU  | C-N-CA   | -5.06 | 114.61      | 119.87   |
| 2   | E     | 162 | SER  | N-CA-C   | -5.04 | 107.30      | 113.50   |
| 1   | A     | 451 | ARG  | N-CA-C   | -5.02 | 105.81      | 111.28   |
| 1   | D     | 354 | VAL  | N-CA-C   | 5.00  | 116.12      | 109.37   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 427 | LEU  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 431 | ILE  | Peptide |
| 1   | A     | 432 | ASN  | Peptide |
| 2   | C     | 140 | GLY  | Peptide |
| 1   | D     | 426 | ASN  | Peptide |
| 1   | D     | 427 | LEU  | Peptide |
| 1   | D     | 432 | ASN  | Peptide |
| 2   | F     | 140 | GLY  | Peptide |

## 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     | 4479  | 0        | 4434     | 639     | 4            |
| 1   | D     | 4479  | 0        | 4434     | 673     | 5            |
| 2   | B     | 1748  | 0        | 1704     | 248     | 0            |
| 2   | C     | 1748  | 0        | 1704     | 206     | 0            |
| 2   | E     | 1748  | 0        | 1704     | 297     | 1            |
| 2   | F     | 1748  | 0        | 1704     | 148     | 2            |
| 3   | A     | 15    | 0        | 0        | 5       | 0            |
| 3   | D     | 15    | 0        | 0        | 0       | 0            |
| 4   | A     | 9     | 0        | 10       | 6       | 0            |
| 4   | D     | 9     | 0        | 10       | 6       | 0            |
| 5   | B     | 20    | 0        | 15       | 2       | 0            |
| 5   | C     | 20    | 0        | 15       | 4       | 0            |
| 5   | E     | 20    | 0        | 15       | 2       | 0            |
| 5   | F     | 20    | 0        | 15       | 3       | 0            |
| 6   | A     | 435   | 0        | 0        | 126     | 3            |
| 6   | B     | 185   | 0        | 0        | 54      | 1            |
| 6   | C     | 184   | 0        | 0        | 59      | 1            |
| 6   | D     | 472   | 0        | 0        | 140     | 4            |
| 6   | E     | 215   | 0        | 0        | 98      | 3            |
| 6   | F     | 169   | 0        | 0        | 40      | 2            |
| All | All   | 17738 | 0        | 15764    | 2075    | 18           |

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 65.

All (2075) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:176:LYS:NZ   | 1:A:190:ASP:OD2  | 1.64                     | 1.31              |
| 1:D:499:ARG:O    | 2:E:188:ARG:NH1  | 1.65                     | 1.26              |
| 1:D:176:LYS:NZ   | 1:D:190:ASP:OD2  | 1.69                     | 1.25              |
| 1:A:529:ARG:NH1  | 1:A:533:GLU:OE2  | 1.72                     | 1.23              |
| 1:D:456:LYS:NZ   | 2:E:201:ASP:OD2  | 1.77                     | 1.16              |
| 1:D:529:ARG:NH1  | 1:D:533:GLU:OE2  | 1.77                     | 1.16              |
| 2:F:117:LYS:HG3  | 2:F:213:ARG:HH11 | 1.11                     | 1.15              |
| 1:D:454:GLU:OE2  | 6:D:701:HOH:O    | 1.62                     | 1.14              |
| 2:E:204:LYS:NZ   | 6:E:401:HOH:O    | 1.69                     | 1.13              |
| 1:D:108:PRO:HG2  | 1:D:552:LYS:H    | 1.13                     | 1.11              |
| 1:D:500:ALA:HA   | 2:E:188:ARG:HH12 | 0.94                     | 1.11              |
| 2:E:191:GLU:OE2  | 6:E:402:HOH:O    | 1.71                     | 1.09              |
| 1:D:145:LEU:HD13 | 1:D:209:GLY:HA3  | 1.37                     | 1.07              |
| 1:A:499:ARG:O    | 2:B:188:ARG:NH1  | 1.86                     | 1.06              |
| 2:E:9:ASP:OD1    | 6:E:403:HOH:O    | 1.72                     | 1.04              |
| 2:C:141:ASP:OD2  | 2:C:181:LYS:NZ   | 1.90                     | 1.03              |
| 1:D:152:LYS:HE2  | 1:D:565:ASN:HB2  | 1.43                     | 1.01              |
| 1:D:500:ALA:HA   | 2:E:188:ARG:NH1  | 1.74                     | 1.00              |
| 1:D:445:VAL:HG22 | 1:D:479:TRP:HE1  | 1.26                     | 0.98              |
| 2:E:80:GLU:O     | 6:E:406:HOH:O    | 1.82                     | 0.98              |
| 1:D:152:LYS:NZ   | 1:D:561:ILE:O    | 1.94                     | 0.98              |
| 2:C:125:LYS:NZ   | 6:C:403:HOH:O    | 1.97                     | 0.96              |
| 1:A:48:CYS:SG    | 6:A:960:HOH:O    | 2.22                     | 0.96              |
| 2:B:105:LYS:NZ   | 6:B:407:HOH:O    | 1.99                     | 0.96              |
| 1:D:134:ARG:NH1  | 6:D:711:HOH:O    | 1.98                     | 0.94              |
| 1:D:333:SER:OG   | 1:D:557:LYS:NZ   | 2.00                     | 0.94              |
| 1:A:163:GLY:HA2  | 1:A:560:GLN:HB2  | 1.49                     | 0.94              |
| 1:A:94:VAL:HG11  | 1:A:112:PRO:HB3  | 1.50                     | 0.94              |
| 2:E:165:GLN:NE2  | 6:E:414:HOH:O    | 1.99                     | 0.93              |
| 1:D:492:ASP:OD2  | 6:D:702:HOH:O    | 1.87                     | 0.93              |
| 1:A:199:HIS:HB3  | 1:A:525:LYS:H    | 1.32                     | 0.92              |
| 1:D:500:ALA:CA   | 2:E:188:ARG:HH12 | 1.83                     | 0.92              |
| 2:B:148:ASP:OD1  | 6:B:402:HOH:O    | 1.87                     | 0.92              |
| 1:D:492:ASP:OD2  | 6:D:703:HOH:O    | 1.87                     | 0.92              |
| 1:A:19:GLU:O     | 1:A:23:ASN:ND2   | 2.03                     | 0.92              |
| 1:A:541:SER:O    | 1:A:543:GLY:N    | 2.04                     | 0.91              |
| 2:B:26:LYS:HG2   | 2:B:81:LYS:NZ    | 1.84                     | 0.91              |
| 1:D:541:SER:O    | 1:D:543:GLY:N    | 2.04                     | 0.91              |
| 1:D:447:SER:OG   | 2:E:191:GLU:OE1  | 1.88                     | 0.90              |
| 2:E:66:GLU:OE2   | 6:E:408:HOH:O    | 1.89                     | 0.90              |
| 2:E:112:LYS:NZ   | 6:E:419:HOH:O    | 2.04                     | 0.90              |
| 1:D:436:ASN:ND2  | 6:D:717:HOH:O    | 2.05                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:115:GLY:O    | 6:E:409:HOH:O    | 1.89                     | 0.89              |
| 2:E:176:GLU:OE2  | 6:E:407:HOH:O    | 1.88                     | 0.89              |
| 1:A:299:LYS:NZ   | 6:A:701:HOH:O    | 1.90                     | 0.89              |
| 6:D:701:HOH:O    | 2:E:165:GLN:OE1  | 1.88                     | 0.89              |
| 2:C:145:PHE:HB3  | 2:C:153:VAL:HG13 | 1.54                     | 0.88              |
| 1:A:332:SER:N    | 6:A:711:HOH:O    | 2.01                     | 0.88              |
| 1:D:423:CYS:SG   | 1:D:541:SER:OG   | 2.32                     | 0.88              |
| 2:B:168:GLU:OE2  | 6:B:404:HOH:O    | 1.92                     | 0.88              |
| 2:E:127:GLU:OE1  | 6:E:410:HOH:O    | 1.92                     | 0.88              |
| 1:A:152:LYS:HA   | 1:A:564:GLU:HB2  | 1.57                     | 0.86              |
| 1:A:73:LEU:O     | 6:A:702:HOH:O    | 1.94                     | 0.85              |
| 2:E:78:TRP:O     | 6:E:411:HOH:O    | 1.94                     | 0.85              |
| 2:C:26:LYS:NZ    | 2:C:82:ASN:O     | 2.09                     | 0.85              |
| 2:C:98:TRP:O     | 6:C:401:HOH:O    | 1.93                     | 0.85              |
| 1:D:527:THR:OG1  | 6:D:704:HOH:O    | 1.94                     | 0.85              |
| 2:E:8:LEU:HD22   | 2:E:33:ARG:HH21  | 1.40                     | 0.85              |
| 6:D:846:HOH:O    | 2:E:190:MET:SD   | 2.33                     | 0.84              |
| 2:B:26:LYS:HG2   | 2:B:81:LYS:HZ3   | 1.42                     | 0.84              |
| 2:B:75:ASP:OD1   | 6:B:405:HOH:O    | 1.94                     | 0.84              |
| 2:E:26:LYS:HG2   | 2:E:81:LYS:NZ    | 1.91                     | 0.84              |
| 1:A:499:ARG:NE   | 2:B:184:ALA:HB1  | 1.91                     | 0.84              |
| 1:D:560:GLN:NE2  | 6:D:727:HOH:O    | 2.10                     | 0.84              |
| 2:E:132:VAL:HG23 | 2:E:182:LEU:HD13 | 1.59                     | 0.84              |
| 1:D:94:VAL:HG11  | 1:D:112:PRO:HB3  | 1.59                     | 0.84              |
| 1:D:471:ASP:OD2  | 6:D:707:HOH:O    | 1.96                     | 0.84              |
| 1:D:19:GLU:O     | 1:D:23:ASN:ND2   | 2.11                     | 0.84              |
| 1:D:275:GLU:OE1  | 6:D:706:HOH:O    | 1.95                     | 0.84              |
| 1:A:198:VAL:HA   | 1:A:201:ALA:HB3  | 1.60                     | 0.83              |
| 2:E:156:SER:OG   | 6:E:412:HOH:O    | 1.95                     | 0.83              |
| 2:F:117:LYS:HG3  | 2:F:213:ARG:NH1  | 1.92                     | 0.83              |
| 2:C:124:GLY:O    | 6:C:402:HOH:O    | 1.96                     | 0.83              |
| 1:A:152:LYS:HE2  | 1:A:565:ASN:HB2  | 1.61                     | 0.83              |
| 1:A:53:ASN:O     | 6:A:704:HOH:O    | 1.96                     | 0.82              |
| 1:D:278:ARG:N    | 6:D:708:HOH:O    | 2.08                     | 0.82              |
| 2:F:145:PHE:HB3  | 2:F:153:VAL:HG13 | 1.60                     | 0.82              |
| 1:D:499:ARG:NH2  | 2:E:184:ALA:O    | 2.12                     | 0.82              |
| 2:E:7:LEU:O      | 6:E:403:HOH:O    | 1.97                     | 0.82              |
| 2:E:117:LYS:HE3  | 2:E:213:ARG:NH1  | 1.95                     | 0.82              |
| 2:E:188:ARG:HD2  | 2:E:191:GLU:OE2  | 1.78                     | 0.82              |
| 1:A:447:SER:HB3  | 1:A:496:CYS:SG   | 2.19                     | 0.82              |
| 2:B:8:LEU:HD22   | 2:B:33:ARG:HH21  | 1.42                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:274:ALA:O    | 6:D:708:HOH:O    | 1.97                     | 0.82              |
| 4:D:602:LEU:OXT  | 6:D:709:HOH:O    | 1.97                     | 0.82              |
| 1:D:400:ARG:NH1  | 6:D:735:HOH:O    | 2.12                     | 0.81              |
| 1:D:363:PHE:HD2  | 1:D:382:VAL:HG21 | 1.45                     | 0.81              |
| 1:A:247:ASP:OD1  | 6:A:705:HOH:O    | 1.97                     | 0.81              |
| 2:B:136:GLU:HG3  | 2:B:181:LYS:HD3  | 1.63                     | 0.81              |
| 1:A:228:VAL:O    | 6:A:706:HOH:O    | 1.99                     | 0.81              |
| 2:C:148:ASP:OD2  | 6:C:404:HOH:O    | 1.98                     | 0.81              |
| 1:A:109:LYS:NZ   | 6:A:712:HOH:O    | 2.02                     | 0.81              |
| 2:E:39:ASN:ND2   | 6:E:430:HOH:O    | 2.13                     | 0.81              |
| 2:E:188:ARG:NH1  | 6:E:429:HOH:O    | 2.13                     | 0.81              |
| 2:E:17:MET:HE2   | 2:E:200:PRO:HD2  | 1.63                     | 0.81              |
| 2:E:73:TYR:HE1   | 2:F:96:ARG:HH11  | 1.24                     | 0.81              |
| 2:F:66:GLU:OE1   | 6:F:401:HOH:O    | 1.99                     | 0.80              |
| 1:A:138:ILE:O    | 6:A:708:HOH:O    | 1.99                     | 0.80              |
| 5:F:301:GSH:SG2  | 6:F:472:HOH:O    | 2.33                     | 0.80              |
| 1:A:107:ARG:HD3  | 1:A:433:ILE:HG13 | 1.64                     | 0.80              |
| 1:D:551:VAL:O    | 6:D:712:HOH:O    | 1.98                     | 0.80              |
| 1:A:110:PHE:CE1  | 1:A:556:ALA:HB2  | 2.17                     | 0.80              |
| 1:A:309:MET:HE3  | 1:A:545:PHE:HE2  | 1.47                     | 0.80              |
| 2:E:8:LEU:HD21   | 2:E:43:LEU:HD11  | 1.63                     | 0.80              |
| 2:E:120:GLU:OE1  | 6:E:413:HOH:O    | 1.98                     | 0.80              |
| 1:D:525:LYS:O    | 6:D:713:HOH:O    | 1.99                     | 0.80              |
| 2:E:121:GLN:OE1  | 6:E:415:HOH:O    | 2.00                     | 0.80              |
| 1:A:139:ASP:O    | 6:A:710:HOH:O    | 2.00                     | 0.79              |
| 1:A:331:GLY:N    | 1:A:537:GLY:O    | 2.16                     | 0.79              |
| 2:E:26:LYS:HG2   | 2:E:81:LYS:HZ3   | 1.45                     | 0.79              |
| 2:E:26:LYS:NZ    | 2:E:82:ASN:O     | 2.14                     | 0.79              |
| 2:B:47:SER:O     | 6:B:406:HOH:O    | 1.98                     | 0.79              |
| 1:A:501:PHE:O    | 6:A:709:HOH:O    | 2.00                     | 0.79              |
| 2:B:134:ILE:HD12 | 2:C:50:ILE:HG13  | 1.63                     | 0.79              |
| 2:E:92:ARG:NH2   | 6:E:431:HOH:O    | 2.14                     | 0.79              |
| 1:A:519:GLU:OE2  | 1:A:569:SER:OG   | 2.00                     | 0.79              |
| 1:D:432:ASN:OD1  | 1:D:434:ASP:N    | 2.13                     | 0.79              |
| 1:D:499:ARG:CZ   | 2:E:184:ALA:HB1  | 2.12                     | 0.79              |
| 1:D:511:LYS:O    | 6:D:710:HOH:O    | 1.98                     | 0.79              |
| 2:E:113:VAL:O    | 6:E:416:HOH:O    | 2.00                     | 0.79              |
| 2:C:76:GLU:OE2   | 6:C:405:HOH:O    | 1.99                     | 0.79              |
| 1:D:180:LYS:NZ   | 6:D:739:HOH:O    | 2.14                     | 0.79              |
| 1:A:499:ARG:NH2  | 2:B:184:ALA:O    | 2.16                     | 0.79              |
| 1:A:152:LYS:HD3  | 1:A:561:ILE:HG23 | 1.65                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:149:SER:OG   | 1:D:46:GLN:OE1   | 2.01                     | 0.78              |
| 1:D:53:ASN:OD1   | 6:D:714:HOH:O    | 2.02                     | 0.78              |
| 1:A:445:VAL:HG22 | 1:A:479:TRP:HE1  | 1.47                     | 0.78              |
| 1:D:108:PRO:HG2  | 1:D:552:LYS:N    | 1.97                     | 0.78              |
| 2:C:107:THR:HA   | 2:C:110:GLN:HG2  | 1.64                     | 0.78              |
| 1:A:513:LYS:HZ2  | 1:A:575:PHE:HB3  | 1.48                     | 0.78              |
| 2:F:52:LYS:NZ    | 6:F:413:HOH:O    | 2.16                     | 0.78              |
| 2:B:10:TYR:O     | 6:B:408:HOH:O    | 2.00                     | 0.78              |
| 1:D:351:THR:HG21 | 1:D:410:ILE:HG12 | 1.66                     | 0.78              |
| 1:D:509:SER:O    | 1:D:513:LYS:N    | 2.15                     | 0.78              |
| 1:D:87:PRO:HD3   | 1:D:93:PRO:HG3   | 1.65                     | 0.77              |
| 1:A:98:SER:HB2   | 1:A:111:ILE:HG12 | 1.67                     | 0.77              |
| 2:B:209:ALA:HB3  | 6:B:451:HOH:O    | 1.83                     | 0.77              |
| 2:C:69:ASN:OD1   | 6:C:408:HOH:O    | 2.03                     | 0.77              |
| 1:D:236:GLN:NE2  | 6:D:746:HOH:O    | 2.16                     | 0.77              |
| 2:E:124:GLY:HA2  | 6:E:410:HOH:O    | 1.84                     | 0.77              |
| 1:D:452:LEU:HB3  | 1:D:457:ILE:HD11 | 1.66                     | 0.77              |
| 1:A:132:ARG:HA   | 1:A:343:PRO:HG3  | 1.65                     | 0.77              |
| 1:D:444:SER:O    | 6:D:715:HOH:O    | 2.03                     | 0.77              |
| 2:C:52:LYS:NZ    | 6:C:406:HOH:O    | 2.01                     | 0.77              |
| 1:D:107:ARG:HH12 | 1:D:434:ASP:N    | 1.81                     | 0.77              |
| 1:D:529:ARG:NH2  | 6:D:744:HOH:O    | 2.16                     | 0.76              |
| 1:D:498:ASP:O    | 6:D:716:HOH:O    | 2.03                     | 0.76              |
| 2:C:90:TYR:O     | 2:C:93:ALA:HB3   | 1.86                     | 0.76              |
| 1:D:440:ASP:OD1  | 1:D:501:PHE:HA   | 1.85                     | 0.76              |
| 1:A:150:SER:HB2  | 1:A:167:THR:HA   | 1.68                     | 0.76              |
| 1:A:302:TYR:OH   | 1:A:328:HIS:ND1  | 2.16                     | 0.76              |
| 1:A:432:ASN:OD1  | 1:A:434:ASP:N    | 2.14                     | 0.76              |
| 2:C:159:THR:HA   | 2:C:199:LEU:HD21 | 1.68                     | 0.76              |
| 1:A:424:ARG:HB2  | 6:A:758:HOH:O    | 1.85                     | 0.76              |
| 2:B:23:LEU:HD22  | 2:B:28:VAL:HG11  | 1.67                     | 0.76              |
| 1:A:500:ALA:HB1  | 6:A:924:HOH:O    | 1.86                     | 0.76              |
| 2:C:111:PHE:O    | 6:C:409:HOH:O    | 2.04                     | 0.76              |
| 2:E:148:ASP:OD2  | 6:E:418:HOH:O    | 2.03                     | 0.76              |
| 2:E:145:PHE:O    | 6:E:420:HOH:O    | 2.04                     | 0.75              |
| 1:A:513:LYS:NZ   | 1:A:575:PHE:HB3  | 2.00                     | 0.75              |
| 2:B:80:GLU:OE1   | 6:B:410:HOH:O    | 2.05                     | 0.75              |
| 1:D:152:LYS:HA   | 1:D:564:GLU:HB2  | 1.66                     | 0.75              |
| 2:B:26:LYS:NZ    | 2:B:82:ASN:O     | 2.20                     | 0.75              |
| 1:D:242:VAL:HG12 | 1:D:277:ILE:HD13 | 1.69                     | 0.75              |
| 2:E:125:LYS:NZ   | 6:E:433:HOH:O    | 2.18                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:88:ILE:HD12  | 1:D:89:LEU:H     | 1.50                     | 0.75              |
| 1:A:210:ILE:HD11 | 1:A:294:LEU:HD13 | 1.69                     | 0.75              |
| 2:C:139:LEU:HD22 | 1:D:92:HIS:CD2   | 2.21                     | 0.75              |
| 1:D:400:ARG:NH1  | 6:D:752:HOH:O    | 2.19                     | 0.75              |
| 1:A:535:PHE:O    | 1:A:538:LEU:HB3  | 1.87                     | 0.75              |
| 2:B:8:LEU:HD21   | 2:B:43:LEU:HD11  | 1.69                     | 0.74              |
| 2:C:139:LEU:HD21 | 2:C:142:LYS:O    | 1.87                     | 0.74              |
| 2:F:171:GLY:N    | 6:F:412:HOH:O    | 2.19                     | 0.74              |
| 1:D:547:MET:O    | 6:D:718:HOH:O    | 2.05                     | 0.74              |
| 1:D:499:ARG:C    | 2:E:188:ARG:NH1  | 2.45                     | 0.74              |
| 1:A:150:SER:HB3  | 1:A:170:TYR:CD2  | 2.22                     | 0.74              |
| 1:A:351:THR:HG21 | 1:A:410:ILE:HG12 | 1.67                     | 0.74              |
| 1:A:491:GLN:HE21 | 1:A:573:THR:HG23 | 1.51                     | 0.74              |
| 1:D:10:MET:SD    | 6:D:949:HOH:O    | 2.45                     | 0.74              |
| 1:D:111:ILE:HD13 | 1:D:334:GLU:HG2  | 1.67                     | 0.74              |
| 1:D:445:VAL:HA   | 1:D:479:TRP:CZ2  | 2.23                     | 0.74              |
| 1:A:350:ALA:O    | 6:A:713:HOH:O    | 2.03                     | 0.74              |
| 1:D:332:SER:OG   | 1:D:333:SER:N    | 2.18                     | 0.74              |
| 1:D:454:GLU:HG2  | 6:D:795:HOH:O    | 1.85                     | 0.74              |
| 1:D:528:PHE:HB3  | 1:D:547:MET:HE1  | 1.68                     | 0.74              |
| 1:A:556:ALA:HA   | 1:A:559:LEU:HB2  | 1.70                     | 0.74              |
| 1:A:143:LYS:HD2  | 1:A:212:PHE:HB2  | 1.68                     | 0.74              |
| 1:A:170:TYR:O    | 6:A:715:HOH:O    | 2.06                     | 0.74              |
| 2:B:11:TRP:CD1   | 2:B:12:PRO:HD3   | 2.23                     | 0.74              |
| 2:B:75:ASP:OD2   | 6:B:409:HOH:O    | 2.04                     | 0.74              |
| 1:D:445:VAL:HG22 | 1:D:479:TRP:NE1  | 2.01                     | 0.74              |
| 1:D:480:GLU:HG3  | 1:D:525:LYS:HA   | 1.70                     | 0.74              |
| 2:F:110:GLN:NE2  | 6:F:415:HOH:O    | 2.19                     | 0.74              |
| 1:D:99:LEU:HD13  | 1:D:558:VAL:H    | 1.52                     | 0.73              |
| 1:A:387:GLU:O    | 6:A:714:HOH:O    | 2.05                     | 0.73              |
| 1:D:456:LYS:NZ   | 2:E:204:LYS:HE2  | 2.03                     | 0.73              |
| 2:C:14:MET:SD    | 6:C:418:HOH:O    | 2.45                     | 0.73              |
| 1:A:150:SER:HB3  | 1:A:170:TYR:HD2  | 1.52                     | 0.73              |
| 1:D:389:GLU:N    | 6:D:737:HOH:O    | 2.20                     | 0.73              |
| 2:B:142:LYS:NZ   | 6:B:401:HOH:O    | 1.82                     | 0.73              |
| 1:D:107:ARG:HH21 | 1:D:552:LYS:HD3  | 1.53                     | 0.73              |
| 1:D:138:ILE:HA   | 1:D:217:GLN:HE21 | 1.51                     | 0.73              |
| 2:E:64:VAL:HG23  | 2:E:70:VAL:HG22  | 1.69                     | 0.73              |
| 1:A:246:LYS:HZ2  | 1:A:271:PRO:HA   | 1.54                     | 0.73              |
| 2:B:211:GLU:OE1  | 6:B:412:HOH:O    | 2.06                     | 0.73              |
| 2:C:85:PHE:HB3   | 2:C:92:ARG:HG2   | 1.71                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:322:ASP:O    | 6:D:719:HOH:O    | 2.06                     | 0.73              |
| 2:E:117:LYS:O    | 6:E:417:HOH:O    | 2.07                     | 0.73              |
| 2:F:68:LEU:O     | 6:F:404:HOH:O    | 2.06                     | 0.73              |
| 1:A:154:TYR:O    | 6:A:716:HOH:O    | 2.07                     | 0.73              |
| 1:A:223:PHE:HE2  | 1:A:545:PHE:HZ   | 1.35                     | 0.72              |
| 2:F:127:GLU:OE1  | 6:F:403:HOH:O    | 2.06                     | 0.72              |
| 1:D:552:LYS:C    | 1:D:554:SER:H    | 1.97                     | 0.72              |
| 2:F:159:THR:HA   | 2:F:199:LEU:HD21 | 1.70                     | 0.72              |
| 1:A:538:LEU:O    | 1:A:544:GLN:NE2  | 2.21                     | 0.72              |
| 2:B:150:PHE:O    | 6:B:411:HOH:O    | 2.06                     | 0.72              |
| 2:B:176:GLU:HA   | 6:B:435:HOH:O    | 1.88                     | 0.72              |
| 2:E:203:GLU:OE2  | 6:E:401:HOH:O    | 2.05                     | 0.72              |
| 1:A:142:GLY:HA2  | 1:A:215:GLN:HB2  | 1.70                     | 0.72              |
| 2:C:64:VAL:O     | 6:C:410:HOH:O    | 2.07                     | 0.72              |
| 1:D:198:VAL:HA   | 1:D:201:ALA:HB3  | 1.71                     | 0.72              |
| 1:A:491:GLN:HG2  | 2:B:176:GLU:OE2  | 1.88                     | 0.72              |
| 2:C:139:LEU:HD22 | 1:D:92:HIS:CG    | 2.23                     | 0.72              |
| 1:D:495:ASN:C    | 1:D:499:ARG:NH1  | 2.47                     | 0.72              |
| 2:E:11:TRP:CD1   | 2:E:12:PRO:HD3   | 2.25                     | 0.72              |
| 1:A:199:HIS:H    | 1:A:524:ALA:HB1  | 1.54                     | 0.72              |
| 1:D:100:SER:HB3  | 1:D:109:LYS:HD3  | 1.72                     | 0.72              |
| 1:D:164:THR:HG23 | 1:D:557:LYS:HG3  | 1.70                     | 0.72              |
| 1:A:499:ARG:CZ   | 2:B:184:ALA:HB1  | 2.19                     | 0.72              |
| 1:D:110:PHE:CE1  | 1:D:556:ALA:HB2  | 2.25                     | 0.72              |
| 2:B:13:SER:N     | 6:B:408:HOH:O    | 2.23                     | 0.72              |
| 2:C:215:ASN:O    | 6:C:411:HOH:O    | 2.07                     | 0.72              |
| 1:A:99:LEU:H     | 1:A:557:LYS:HB2  | 1.55                     | 0.72              |
| 1:A:363:PHE:HD2  | 1:A:382:VAL:HG21 | 1.55                     | 0.72              |
| 1:D:423:CYS:O    | 6:D:721:HOH:O    | 2.08                     | 0.72              |
| 2:E:215:ASN:OD1  | 6:E:422:HOH:O    | 2.08                     | 0.72              |
| 1:D:342:THR:OG1  | 1:D:413:TYR:OH   | 2.06                     | 0.72              |
| 2:F:216:ASN:N    | 6:F:402:HOH:O    | 2.03                     | 0.72              |
| 1:A:22:ARG:O     | 6:A:717:HOH:O    | 2.07                     | 0.71              |
| 1:D:445:VAL:HA   | 1:D:479:TRP:HZ2  | 1.53                     | 0.71              |
| 2:F:26:LYS:HE3   | 2:F:28:VAL:CG2   | 2.20                     | 0.71              |
| 1:A:143:LYS:NZ   | 1:A:187:CYS:HA   | 2.05                     | 0.71              |
| 2:C:139:LEU:HD23 | 2:C:142:LYS:H    | 1.53                     | 0.71              |
| 1:D:456:LYS:HB2  | 6:D:810:HOH:O    | 1.89                     | 0.71              |
| 2:E:28:VAL:O     | 6:E:421:HOH:O    | 2.07                     | 0.71              |
| 1:A:232:ARG:NE   | 6:A:746:HOH:O    | 2.21                     | 0.71              |
| 1:A:332:SER:OG   | 1:A:333:SER:N    | 2.18                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:499:ARG:NE   | 2:E:184:ALA:HB1  | 2.06                     | 0.71              |
| 1:A:217:GLN:NE2  | 6:A:755:HOH:O    | 2.23                     | 0.71              |
| 2:E:195:VAL:HG23 | 2:E:199:LEU:HD13 | 1.72                     | 0.71              |
| 1:A:147:PHE:O    | 1:A:529:ARG:NH2  | 2.23                     | 0.71              |
| 1:A:165:ALA:H    | 1:A:557:LYS:HE3  | 1.55                     | 0.71              |
| 1:A:495:ASN:C    | 1:A:499:ARG:NH1  | 2.48                     | 0.71              |
| 1:D:451:ARG:NH1  | 1:D:454:GLU:OE1  | 2.23                     | 0.71              |
| 2:E:22:ALA:HA    | 6:E:455:HOH:O    | 1.89                     | 0.71              |
| 1:A:451:ARG:NH1  | 1:A:454:GLU:OE1  | 2.22                     | 0.71              |
| 1:D:451:ARG:HD3  | 2:E:187:LYS:HG2  | 1.72                     | 0.71              |
| 1:D:504:ALA:O    | 1:D:507:VAL:HB   | 1.91                     | 0.71              |
| 2:F:26:LYS:HE3   | 2:F:28:VAL:HG23  | 1.72                     | 0.71              |
| 2:B:179:SER:O    | 6:B:414:HOH:O    | 2.08                     | 0.71              |
| 1:D:369:THR:OG1  | 6:D:720:HOH:O    | 2.06                     | 0.71              |
| 1:A:132:ARG:O    | 1:A:136:PHE:N    | 2.22                     | 0.71              |
| 1:D:377:VAL:O    | 6:D:722:HOH:O    | 2.08                     | 0.71              |
| 1:A:551:VAL:HG11 | 1:A:559:LEU:HD13 | 1.71                     | 0.71              |
| 1:A:232:ARG:N    | 6:A:706:HOH:O    | 2.23                     | 0.71              |
| 1:D:540:SER:OG   | 1:D:544:GLN:NE2  | 2.23                     | 0.71              |
| 1:A:90:THR:OG1   | 1:A:91:GLY:N     | 2.21                     | 0.70              |
| 1:A:499:ARG:C    | 2:B:188:ARG:HH12 | 1.99                     | 0.70              |
| 1:A:556:ALA:O    | 6:A:718:HOH:O    | 2.09                     | 0.70              |
| 1:D:236:GLN:OE1  | 6:D:723:HOH:O    | 2.09                     | 0.70              |
| 2:E:203:GLU:N    | 6:E:441:HOH:O    | 2.23                     | 0.70              |
| 2:B:7:LEU:HD21   | 2:B:23:LEU:HD12  | 1.72                     | 0.70              |
| 1:D:451:ARG:HE   | 2:E:183:ILE:HD11 | 1.54                     | 0.70              |
| 2:C:115:GLY:N    | 6:C:409:HOH:O    | 2.11                     | 0.70              |
| 1:D:132:ARG:HA   | 1:D:343:PRO:HG3  | 1.70                     | 0.70              |
| 1:D:552:LYS:O    | 1:D:554:SER:N    | 2.23                     | 0.70              |
| 1:A:145:LEU:HD13 | 1:A:209:GLY:HA3  | 1.73                     | 0.70              |
| 1:A:425:ARG:NE   | 6:A:758:HOH:O    | 2.25                     | 0.70              |
| 1:A:540:SER:OG   | 1:A:544:GLN:NE2  | 2.24                     | 0.70              |
| 2:E:32:TYR:HD1   | 2:E:34:GLU:OE2   | 1.73                     | 0.70              |
| 1:A:261:THR:HG22 | 1:A:265:LYS:HE3  | 1.72                     | 0.70              |
| 2:E:178:GLU:OE1  | 6:E:425:HOH:O    | 2.09                     | 0.70              |
| 1:A:559:LEU:O    | 1:A:562:LEU:HB3  | 1.92                     | 0.70              |
| 1:D:47:ASN:ND2   | 6:D:767:HOH:O    | 2.24                     | 0.70              |
| 1:D:495:ASN:CB   | 1:D:499:ARG:HH11 | 2.05                     | 0.70              |
| 1:A:521:ARG:HB3  | 1:A:566:VAL:HG12 | 1.74                     | 0.70              |
| 2:C:125:LYS:HB3  | 2:C:173:PHE:HE2  | 1.56                     | 0.70              |
| 2:E:92:ARG:NE    | 2:F:76:GLU:OE2   | 2.25                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:451:ARG:HB2  | 2:B:187:LYS:HD2  | 1.74                     | 0.70              |
| 2:F:101:PHE:HE1  | 2:F:105:LYS:HE3  | 1.56                     | 0.70              |
| 1:A:451:ARG:HE   | 2:B:183:ILE:HD11 | 1.55                     | 0.69              |
| 2:E:144:TYR:HB3  | 2:E:154:ASP:OD2  | 1.92                     | 0.69              |
| 1:A:252:ASN:O    | 6:A:720:HOH:O    | 2.09                     | 0.69              |
| 1:D:152:LYS:HB3  | 6:D:773:HOH:O    | 1.91                     | 0.69              |
| 1:D:462:PHE:O    | 1:D:549:ARG:NH1  | 2.26                     | 0.69              |
| 2:E:118:GLY:HA3  | 6:E:514:HOH:O    | 1.91                     | 0.69              |
| 2:E:119:GLU:N    | 6:E:443:HOH:O    | 2.24                     | 0.69              |
| 1:A:384:ILE:O    | 6:A:721:HOH:O    | 2.10                     | 0.69              |
| 1:D:442:GLN:HG2  | 1:D:462:PHE:CZ   | 2.28                     | 0.69              |
| 2:B:117:LYS:HE3  | 2:B:213:ARG:NH1  | 2.07                     | 0.69              |
| 1:D:339:ALA:HB2  | 1:D:355:ILE:HD11 | 1.73                     | 0.69              |
| 2:E:168:GLU:OE2  | 6:E:424:HOH:O    | 2.09                     | 0.69              |
| 2:B:203:GLU:N    | 6:B:426:HOH:O    | 2.24                     | 0.69              |
| 2:C:181:LYS:HE3  | 1:D:95:PRO:HD3   | 1.72                     | 0.69              |
| 1:D:150:SER:HB2  | 1:D:167:THR:HA   | 1.73                     | 0.69              |
| 1:A:498:ASP:CG   | 1:A:510:ARG:HH22 | 2.00                     | 0.69              |
| 2:B:64:VAL:HG23  | 2:B:70:VAL:HG22  | 1.74                     | 0.69              |
| 2:F:121:GLN:NE2  | 2:F:170:PHE:O    | 2.26                     | 0.69              |
| 1:A:137:PRO:O    | 6:A:701:HOH:O    | 2.11                     | 0.69              |
| 2:F:125:LYS:HB3  | 2:F:173:PHE:CE2  | 2.28                     | 0.69              |
| 1:A:100:SER:HB3  | 1:A:109:LYS:HD3  | 1.75                     | 0.69              |
| 1:A:295:PHE:HD1  | 1:A:298:ALA:HB2  | 1.58                     | 0.69              |
| 1:A:425:ARG:HB3  | 1:A:427:LEU:HB2  | 1.74                     | 0.69              |
| 2:B:35:GLU:OE1   | 6:B:416:HOH:O    | 2.11                     | 0.69              |
| 2:C:149:SER:O    | 6:C:412:HOH:O    | 2.09                     | 0.69              |
| 2:C:150:PHE:HE1  | 2:C:155:ILE:HG13 | 1.58                     | 0.69              |
| 1:A:407:VAL:HG21 | 1:A:419:LEU:HG   | 1.74                     | 0.69              |
| 2:B:198:SER:N    | 6:B:424:HOH:O    | 2.20                     | 0.69              |
| 1:D:23:ASN:OD1   | 6:D:726:HOH:O    | 2.10                     | 0.69              |
| 1:D:99:LEU:HB2   | 1:D:556:ALA:H    | 1.56                     | 0.69              |
| 1:D:232:ARG:NH2  | 6:D:772:HOH:O    | 2.25                     | 0.69              |
| 1:D:366:VAL:O    | 6:D:728:HOH:O    | 2.10                     | 0.69              |
| 2:F:165:GLN:HA   | 2:F:168:GLU:OE2  | 1.93                     | 0.69              |
| 1:A:235:GLU:OE1  | 6:A:722:HOH:O    | 2.11                     | 0.69              |
| 1:A:445:VAL:HG22 | 1:A:479:TRP:NE1  | 2.07                     | 0.69              |
| 2:C:44:LEU:O     | 6:C:413:HOH:O    | 2.11                     | 0.69              |
| 1:D:143:LYS:NZ   | 1:D:187:CYS:HA   | 2.08                     | 0.69              |
| 2:E:88:ASP:OD2   | 6:E:426:HOH:O    | 2.10                     | 0.69              |
| 1:A:405:ASP:HB3  | 1:A:541:SER:HB3  | 1.75                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:437:THR:HG21 | 1:A:439:ARG:HH21 | 1.58                     | 0.68              |
| 2:B:144:TYR:HB3  | 2:B:154:ASP:OD2  | 1.93                     | 0.68              |
| 1:A:496:CYS:HB2  | 2:B:187:LYS:NZ   | 2.09                     | 0.68              |
| 1:D:53:ASN:OD1   | 6:D:729:HOH:O    | 2.10                     | 0.68              |
| 1:A:379:LEU:HD12 | 1:A:380:THR:HG23 | 1.75                     | 0.68              |
| 2:B:58:VAL:O     | 6:B:415:HOH:O    | 2.10                     | 0.68              |
| 1:A:498:ASP:HB2  | 6:A:757:HOH:O    | 1.94                     | 0.68              |
| 2:B:52:LYS:HD2   | 6:B:525:HOH:O    | 1.93                     | 0.68              |
| 2:B:188:ARG:HD3  | 2:B:191:GLU:OE2  | 1.94                     | 0.68              |
| 2:F:80:GLU:OE1   | 6:F:407:HOH:O    | 2.12                     | 0.68              |
| 2:B:188:ARG:HA   | 2:B:188:ARG:HE   | 1.58                     | 0.68              |
| 1:D:405:ASP:HB2  | 1:D:541:SER:HB3  | 1.76                     | 0.68              |
| 1:A:328:HIS:NE2  | 3:A:601:JAA:O03  | 2.26                     | 0.68              |
| 1:D:532:GLN:NE2  | 6:D:759:HOH:O    | 2.21                     | 0.68              |
| 1:A:19:GLU:OE2   | 6:A:724:HOH:O    | 2.12                     | 0.68              |
| 2:B:206:VAL:HA   | 6:B:451:HOH:O    | 1.94                     | 0.68              |
| 2:C:125:LYS:HB3  | 2:C:173:PHE:CE2  | 2.29                     | 0.68              |
| 1:D:441:LEU:HG   | 6:D:837:HOH:O    | 1.94                     | 0.68              |
| 1:D:132:ARG:O    | 1:D:136:PHE:N    | 2.21                     | 0.68              |
| 1:D:208:SER:HA   | 1:D:211:LEU:HD12 | 1.76                     | 0.68              |
| 1:A:432:ASN:ND2  | 6:A:765:HOH:O    | 2.25                     | 0.68              |
| 1:D:143:LYS:HD2  | 1:D:212:PHE:HB2  | 1.74                     | 0.68              |
| 2:E:39:ASN:OD1   | 6:E:427:HOH:O    | 2.10                     | 0.68              |
| 2:E:117:LYS:HE3  | 2:E:213:ARG:HH11 | 1.56                     | 0.68              |
| 2:F:88:ASP:OD1   | 6:F:405:HOH:O    | 2.10                     | 0.68              |
| 1:A:246:LYS:NZ   | 1:A:271:PRO:HA   | 2.09                     | 0.68              |
| 1:A:491:GLN:NE2  | 1:A:573:THR:HG23 | 2.09                     | 0.68              |
| 1:D:105:GLN:HA   | 1:D:430:SER:HB3  | 1.76                     | 0.68              |
| 2:F:15:PHE:HB3   | 2:F:67:SER:HB3   | 1.76                     | 0.68              |
| 1:D:152:LYS:HD3  | 1:D:561:ILE:HG23 | 1.75                     | 0.67              |
| 1:D:510:ARG:NH1  | 1:D:575:PHE:HE2  | 1.92                     | 0.67              |
| 2:F:161:SER:O    | 6:F:408:HOH:O    | 2.12                     | 0.67              |
| 1:A:199:HIS:N    | 1:A:524:ALA:HB1  | 2.09                     | 0.67              |
| 1:D:147:PHE:N    | 6:D:774:HOH:O    | 2.26                     | 0.67              |
| 1:D:163:GLY:HA2  | 1:D:560:GLN:HB2  | 1.77                     | 0.67              |
| 2:E:114:TRP:HA   | 2:E:170:PHE:HD2  | 1.58                     | 0.67              |
| 1:A:74:GLU:OE1   | 6:A:723:HOH:O    | 2.12                     | 0.67              |
| 1:A:149:PHE:CZ   | 1:A:205:HIS:HD2  | 2.12                     | 0.67              |
| 2:C:188:ARG:HB2  | 1:D:86:SER:HB2   | 1.75                     | 0.67              |
| 1:A:150:SER:CB   | 1:A:167:THR:HA   | 2.25                     | 0.67              |
| 1:A:332:SER:O    | 6:A:711:HOH:O    | 2.12                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:15:PHE:HA    | 2:C:18:ARG:HD2   | 1.75                     | 0.67              |
| 1:D:82:ASP:OD2   | 6:D:730:HOH:O    | 2.11                     | 0.67              |
| 1:D:187:CYS:SG   | 6:D:832:HOH:O    | 2.44                     | 0.67              |
| 1:A:495:ASN:CB   | 1:A:499:ARG:HH11 | 2.08                     | 0.67              |
| 2:B:201:ASP:OD1  | 6:B:417:HOH:O    | 2.11                     | 0.67              |
| 2:C:132:VAL:HG23 | 2:C:182:LEU:HD23 | 1.75                     | 0.67              |
| 2:C:181:LYS:HB2  | 1:D:92:HIS:CD2   | 2.30                     | 0.67              |
| 1:D:39:ASN:HD21  | 1:D:90:THR:C     | 2.03                     | 0.67              |
| 1:D:448:ALA:HB2  | 1:D:496:CYS:HB3  | 1.76                     | 0.67              |
| 1:A:434:ASP:HB2  | 1:A:550:CYS:HB3  | 1.77                     | 0.67              |
| 2:B:90:TYR:CZ    | 2:C:62:LYS:HB3   | 2.29                     | 0.67              |
| 2:E:62:LYS:NZ    | 6:E:437:HOH:O    | 2.20                     | 0.67              |
| 1:A:228:VAL:HG13 | 1:A:319:TYR:HE2  | 1.58                     | 0.67              |
| 2:B:139:LEU:HG   | 2:B:145:PHE:CZ   | 2.30                     | 0.67              |
| 1:D:65:VAL:O     | 6:D:736:HOH:O    | 2.13                     | 0.67              |
| 1:D:216:VAL:O    | 6:D:731:HOH:O    | 2.11                     | 0.67              |
| 2:B:17:MET:HE2   | 2:B:200:PRO:HD2  | 1.75                     | 0.67              |
| 1:D:151:SER:OG   | 1:D:195:SER:O    | 2.12                     | 0.67              |
| 1:D:353:ALA:O    | 6:D:732:HOH:O    | 2.12                     | 0.67              |
| 1:A:108:PRO:HG2  | 1:A:552:LYS:HB3  | 1.76                     | 0.67              |
| 1:A:387:GLU:HG2  | 1:A:408:LYS:HB2  | 1.76                     | 0.67              |
| 1:D:255:THR:O    | 6:D:734:HOH:O    | 2.12                     | 0.67              |
| 2:B:96:ARG:NH1   | 6:C:405:HOH:O    | 2.20                     | 0.67              |
| 1:D:17:PHE:HE1   | 1:D:355:ILE:HG12 | 1.60                     | 0.67              |
| 1:D:286:ASN:ND2  | 6:D:777:HOH:O    | 2.27                     | 0.67              |
| 2:E:190:MET:SD   | 6:E:468:HOH:O    | 2.53                     | 0.67              |
| 1:A:492:ASP:HB3  | 2:B:187:LYS:HD3  | 1.77                     | 0.66              |
| 1:A:500:ALA:HA   | 2:B:188:ARG:HH12 | 1.59                     | 0.66              |
| 2:C:142:LYS:HG3  | 1:D:39:ASN:HA    | 1.78                     | 0.66              |
| 1:D:99:LEU:HB3   | 1:D:557:LYS:HB2  | 1.77                     | 0.66              |
| 1:D:198:VAL:HG12 | 6:D:713:HOH:O    | 1.94                     | 0.66              |
| 1:A:339:ALA:HB2  | 1:A:355:ILE:HD11 | 1.76                     | 0.66              |
| 1:A:492:ASP:CG   | 2:B:183:ILE:HG12 | 2.21                     | 0.66              |
| 2:B:171:GLY:N    | 6:B:418:HOH:O    | 2.15                     | 0.66              |
| 2:C:142:LYS:HG2  | 1:D:41:SER:HB2   | 1.77                     | 0.66              |
| 1:D:429:LEU:O    | 6:D:733:HOH:O    | 2.12                     | 0.66              |
| 1:D:521:ARG:HH11 | 1:D:562:LEU:HD13 | 1.59                     | 0.66              |
| 1:D:389:GLU:O    | 6:D:737:HOH:O    | 2.13                     | 0.66              |
| 1:A:105:GLN:HA   | 1:A:430:SER:HB3  | 1.76                     | 0.66              |
| 2:B:117:LYS:HE3  | 2:B:213:ARG:HH11 | 1.58                     | 0.66              |
| 2:C:166:ALA:HA   | 2:C:169:LYS:HG2  | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:177:SER:OG   | 6:E:407:HOH:O    | 2.10                     | 0.66              |
| 2:F:125:LYS:HB3  | 2:F:173:PHE:HE2  | 1.59                     | 0.66              |
| 1:A:504:ALA:O    | 1:A:507:VAL:HB   | 1.95                     | 0.66              |
| 2:E:53:LYS:HG2   | 5:E:301:GSH:HA31 | 1.77                     | 0.66              |
| 2:E:163:TRP:HB3  | 2:E:167:TYR:CZ   | 2.30                     | 0.66              |
| 1:A:105:GLN:OE1  | 1:A:107:ARG:NH2  | 2.28                     | 0.66              |
| 2:C:133:LYS:O    | 6:C:415:HOH:O    | 2.14                     | 0.66              |
| 2:E:31:GLU:O     | 6:E:428:HOH:O    | 2.12                     | 0.66              |
| 1:A:509:SER:O    | 1:A:513:LYS:N    | 2.21                     | 0.66              |
| 1:D:495:ASN:HB3  | 1:D:499:ARG:HH11 | 1.60                     | 0.66              |
| 2:E:19:ALA:HA    | 6:E:473:HOH:O    | 1.95                     | 0.66              |
| 2:B:139:LEU:O    | 2:B:141:ASP:N    | 2.28                     | 0.66              |
| 2:E:113:VAL:HG22 | 6:E:416:HOH:O    | 1.95                     | 0.66              |
| 1:A:150:SER:O    | 1:A:150:SER:OG   | 2.12                     | 0.66              |
| 2:C:66:GLU:OE1   | 6:C:408:HOH:O    | 2.13                     | 0.65              |
| 1:D:314:PRO:HB3  | 1:D:317:ARG:HH12 | 1.59                     | 0.65              |
| 1:A:432:ASN:OD1  | 1:A:433:ILE:N    | 2.28                     | 0.65              |
| 2:B:75:ASP:HB2   | 2:B:84:PHE:CE2   | 2.31                     | 0.65              |
| 1:D:139:ASP:O    | 6:D:738:HOH:O    | 2.13                     | 0.65              |
| 1:D:199:HIS:HB3  | 1:D:525:LYS:H    | 1.61                     | 0.65              |
| 2:F:195:VAL:O    | 6:F:406:HOH:O    | 2.13                     | 0.65              |
| 1:A:463:SER:HB2  | 1:A:528:PHE:HE1  | 1.62                     | 0.65              |
| 2:B:33:ARG:HH12  | 2:B:41:SER:CB    | 2.09                     | 0.65              |
| 1:A:451:ARG:HH11 | 1:A:454:GLU:CD   | 2.04                     | 0.65              |
| 1:D:233:THR:HA   | 1:D:236:GLN:HE21 | 1.62                     | 0.65              |
| 1:A:223:PHE:HE1  | 1:A:304:ILE:HD12 | 1.61                     | 0.65              |
| 1:A:499:ARG:CZ   | 1:A:499:ARG:HB2  | 2.26                     | 0.65              |
| 1:D:152:LYS:HB2  | 1:D:561:ILE:HA   | 1.78                     | 0.65              |
| 1:A:338:ALA:O    | 6:A:725:HOH:O    | 2.13                     | 0.65              |
| 1:A:341:VAL:N    | 6:A:772:HOH:O    | 2.28                     | 0.65              |
| 1:D:107:ARG:NH1  | 1:D:433:ILE:HG13 | 2.10                     | 0.65              |
| 2:F:74:VAL:HG21  | 6:F:436:HOH:O    | 1.97                     | 0.65              |
| 1:D:358:LEU:O    | 6:D:740:HOH:O    | 2.14                     | 0.65              |
| 2:E:109:ALA:HA   | 6:E:410:HOH:O    | 1.96                     | 0.65              |
| 1:A:151:SER:OG   | 1:A:195:SER:O    | 2.14                     | 0.65              |
| 2:F:167:TYR:O    | 6:F:412:HOH:O    | 2.15                     | 0.65              |
| 1:A:207:LEU:HD11 | 1:A:245:ILE:HD11 | 1.79                     | 0.65              |
| 1:A:138:ILE:HA   | 1:A:217:GLN:HE21 | 1.62                     | 0.65              |
| 1:A:305:MET:HB3  | 1:A:347:PRO:HB3  | 1.79                     | 0.65              |
| 1:D:252:ASN:ND2  | 6:D:787:HOH:O    | 2.30                     | 0.65              |
| 2:E:75:ASP:HB2   | 2:E:84:PHE:CE2   | 2.32                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:99:LEU:HB2   | 1:A:556:ALA:H    | 1.61                     | 0.64              |
| 1:D:200:GLN:HB3  | 1:D:254:ILE:HD12 | 1.79                     | 0.64              |
| 1:D:549:ARG:N    | 6:D:783:HOH:O    | 2.30                     | 0.64              |
| 1:A:485:THR:OG1  | 1:A:486:ASN:N    | 2.31                     | 0.64              |
| 1:A:499:ARG:HE   | 2:B:184:ALA:HB1  | 1.63                     | 0.64              |
| 1:D:108:PRO:HB2  | 1:D:554:SER:OG   | 1.97                     | 0.64              |
| 2:E:33:ARG:HH12  | 2:E:41:SER:CB    | 2.10                     | 0.64              |
| 1:A:153:GLN:HG3  | 1:A:171:ARG:HD2  | 1.79                     | 0.64              |
| 1:A:223:PHE:CZ   | 1:A:536:LEU:HB3  | 2.33                     | 0.64              |
| 2:B:26:LYS:HD2   | 2:B:74:VAL:HG13  | 1.79                     | 0.64              |
| 2:C:91:GLY:O     | 6:C:414:HOH:O    | 2.14                     | 0.64              |
| 1:D:164:THR:HG22 | 6:D:709:HOH:O    | 1.96                     | 0.64              |
| 2:E:33:ARG:NH1   | 2:E:41:SER:OG    | 2.29                     | 0.64              |
| 2:E:122:GLU:HA   | 2:E:125:LYS:HE2  | 1.77                     | 0.64              |
| 1:A:415:ASN:OD1  | 6:A:728:HOH:O    | 2.15                     | 0.64              |
| 2:E:73:TYR:OH    | 6:E:405:HOH:O    | 1.80                     | 0.64              |
| 2:E:168:GLU:HG3  | 6:E:458:HOH:O    | 1.97                     | 0.64              |
| 1:A:47:ASN:OD1   | 6:A:727:HOH:O    | 2.14                     | 0.64              |
| 1:A:418:GLN:OE1  | 6:A:726:HOH:O    | 2.14                     | 0.64              |
| 1:D:535:PHE:O    | 1:D:538:LEU:HB3  | 1.97                     | 0.64              |
| 1:A:198:VAL:HG22 | 1:A:524:ALA:HB3  | 1.80                     | 0.64              |
| 1:D:270:ASN:OD1  | 6:D:741:HOH:O    | 2.15                     | 0.64              |
| 2:F:145:PHE:HB2  | 2:F:154:ASP:OD2  | 1.98                     | 0.64              |
| 2:B:32:TYR:CD1   | 2:B:34:GLU:OE2   | 2.51                     | 0.64              |
| 1:D:345:LEU:HD13 | 1:D:350:ALA:HA   | 1.80                     | 0.64              |
| 1:A:68:VAL:HG13  | 1:A:401:TYR:HD1  | 1.62                     | 0.64              |
| 1:A:203:TYR:HB3  | 6:A:763:HOH:O    | 1.98                     | 0.64              |
| 1:A:411:GLY:O    | 1:A:418:GLN:N    | 2.27                     | 0.64              |
| 1:D:22:ARG:HH11  | 1:D:414:ASN:CG   | 2.05                     | 0.64              |
| 1:D:87:PRO:O     | 6:D:742:HOH:O    | 2.15                     | 0.64              |
| 1:D:199:HIS:N    | 1:D:524:ALA:HB1  | 2.11                     | 0.64              |
| 1:D:364:LEU:N    | 6:D:737:HOH:O    | 2.30                     | 0.64              |
| 2:E:97:PHE:HZ    | 2:F:48:ASN:HD21  | 1.45                     | 0.64              |
| 2:B:82:ASN:ND2   | 6:B:431:HOH:O    | 2.30                     | 0.64              |
| 1:D:314:PRO:HA   | 1:D:317:ARG:NH1  | 2.13                     | 0.64              |
| 1:A:418:GLN:NE2  | 6:A:707:HOH:O    | 2.30                     | 0.63              |
| 1:D:499:ARG:NH1  | 2:E:184:ALA:HB1  | 2.13                     | 0.63              |
| 1:A:110:PHE:HE1  | 1:A:556:ALA:HB2  | 1.61                     | 0.63              |
| 1:D:361:PHE:HE1  | 1:D:392:ILE:HG23 | 1.62                     | 0.63              |
| 1:D:451:ARG:NE   | 2:E:183:ILE:HD11 | 2.14                     | 0.63              |
| 2:E:64:VAL:HB    | 2:E:73:TYR:CD2   | 2.33                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:86:PRO:HB2   | 6:F:405:HOH:O    | 1.98                     | 0.63              |
| 1:A:76:TYR:HB3   | 1:A:88:ILE:HG21  | 1.80                     | 0.63              |
| 1:A:153:GLN:HG2  | 1:A:167:THR:HG21 | 1.80                     | 0.63              |
| 2:E:68:LEU:HA    | 2:E:71:VAL:HG12  | 1.80                     | 0.63              |
| 1:A:574:ALA:HB2  | 2:B:180:PRO:HB2  | 1.81                     | 0.63              |
| 1:D:410:ILE:HG23 | 6:D:812:HOH:O    | 1.99                     | 0.63              |
| 2:B:16:GLY:HA2   | 2:B:55:PRO:HB3   | 1.79                     | 0.63              |
| 2:B:132:VAL:HG23 | 2:B:182:LEU:HD13 | 1.81                     | 0.63              |
| 1:A:168:ASN:O    | 1:A:172:ASN:HB2  | 1.98                     | 0.63              |
| 1:A:248:GLY:HA2  | 1:A:267:LEU:HD22 | 1.80                     | 0.63              |
| 1:D:198:VAL:HG23 | 1:D:565:ASN:HD21 | 1.62                     | 0.63              |
| 2:E:139:LEU:O    | 2:E:141:ASP:N    | 2.31                     | 0.63              |
| 1:A:135:ASP:OD2  | 1:A:343:PRO:HD2  | 1.99                     | 0.63              |
| 2:B:206:VAL:HG23 | 6:B:463:HOH:O    | 1.99                     | 0.63              |
| 1:D:164:THR:OG1  | 1:D:557:LYS:O    | 2.11                     | 0.63              |
| 2:E:215:ASN:ND2  | 6:E:454:HOH:O    | 2.32                     | 0.63              |
| 1:A:73:LEU:HD22  | 1:A:89:LEU:HD13  | 1.81                     | 0.63              |
| 1:A:330:TYR:HE2  | 1:A:540:SER:H    | 1.45                     | 0.63              |
| 2:B:33:ARG:NH1   | 2:B:41:SER:OG    | 2.31                     | 0.63              |
| 2:B:98:TRP:CD1   | 2:B:153:VAL:HG11 | 2.34                     | 0.63              |
| 1:D:84:ASP:C     | 1:D:86:SER:H     | 2.07                     | 0.63              |
| 1:D:480:GLU:CD   | 1:D:526:GLY:H    | 2.07                     | 0.63              |
| 1:A:342:THR:OG1  | 1:A:413:TYR:OH   | 2.11                     | 0.62              |
| 2:C:144:TYR:HB2  | 1:D:41:SER:HB3   | 1.81                     | 0.62              |
| 1:A:164:THR:HA   | 1:A:557:LYS:HG3  | 1.80                     | 0.62              |
| 2:E:23:LEU:HD22  | 2:E:28:VAL:HG11  | 1.80                     | 0.62              |
| 1:A:42:ALA:HB3   | 1:A:45:LEU:HD22  | 1.81                     | 0.62              |
| 1:A:126:ARG:CZ   | 1:A:182:ILE:HD11 | 2.29                     | 0.62              |
| 1:A:447:SER:OG   | 2:B:191:GLU:OE1  | 2.17                     | 0.62              |
| 1:D:149:PHE:HZ   | 1:D:202:LEU:HA   | 1.64                     | 0.62              |
| 1:D:519:GLU:CD   | 1:D:521:ARG:HE   | 2.07                     | 0.62              |
| 2:F:87:SER:N     | 6:F:405:HOH:O    | 2.31                     | 0.62              |
| 2:F:139:LEU:HG   | 2:F:142:LYS:CB   | 2.29                     | 0.62              |
| 1:A:456:LYS:HD2  | 2:B:204:LYS:HZ1  | 1.65                     | 0.62              |
| 2:E:98:TRP:HE3   | 2:E:101:PHE:HB2  | 1.65                     | 0.62              |
| 2:C:141:ASP:OD2  | 1:D:114:THR:HG23 | 2.00                     | 0.62              |
| 1:D:154:TYR:HB2  | 1:D:563:CYS:HB2  | 1.80                     | 0.62              |
| 1:D:384:ILE:HD11 | 1:D:411:GLY:HA2  | 1.81                     | 0.62              |
| 1:A:118:MET:O    | 1:A:121:THR:HB   | 2.00                     | 0.62              |
| 2:C:121:GLN:OE1  | 6:C:416:HOH:O    | 2.15                     | 0.62              |
| 2:C:180:PRO:HD2  | 2:C:181:LYS:HG2  | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:464:SER:HA   | 1:D:476:ALA:O    | 1.98                     | 0.62              |
| 1:D:550:CYS:SG   | 6:D:907:HOH:O    | 2.56                     | 0.62              |
| 2:E:19:ALA:HB3   | 6:E:474:HOH:O    | 1.99                     | 0.62              |
| 1:A:448:ALA:HB2  | 1:A:496:CYS:HB3  | 1.81                     | 0.62              |
| 2:F:132:VAL:HG22 | 2:F:182:LEU:HD23 | 1.82                     | 0.62              |
| 2:E:98:TRP:CD1   | 2:E:153:VAL:HG11 | 2.35                     | 0.62              |
| 1:A:166:THR:HG23 | 4:A:602:LEU:C    | 2.25                     | 0.62              |
| 1:A:309:MET:HE3  | 1:A:545:PHE:CE2  | 2.32                     | 0.62              |
| 1:A:344:ARG:NH1  | 6:A:787:HOH:O    | 2.31                     | 0.62              |
| 1:A:365:PRO:HD2  | 6:A:766:HOH:O    | 2.00                     | 0.61              |
| 1:A:456:LYS:HD2  | 2:B:204:LYS:NZ   | 2.15                     | 0.61              |
| 1:A:492:ASP:OD2  | 6:B:404:HOH:O    | 2.16                     | 0.61              |
| 1:D:88:ILE:HD12  | 1:D:89:LEU:N     | 2.14                     | 0.61              |
| 1:D:99:LEU:HB3   | 1:D:557:LYS:H    | 1.64                     | 0.61              |
| 1:D:162:VAL:HG21 | 1:D:559:LEU:HD23 | 1.82                     | 0.61              |
| 1:D:238:TRP:O    | 1:D:242:VAL:HG13 | 2.00                     | 0.61              |
| 1:A:23:ASN:O     | 1:A:27:VAL:HG12  | 2.00                     | 0.61              |
| 2:C:117:LYS:HE3  | 2:C:213:ARG:HH11 | 1.64                     | 0.61              |
| 1:D:200:GLN:NE2  | 6:D:793:HOH:O    | 2.33                     | 0.61              |
| 2:F:77:ALA:HB2   | 6:F:494:HOH:O    | 2.00                     | 0.61              |
| 1:A:17:PHE:HE1   | 1:A:355:ILE:HG12 | 1.64                     | 0.61              |
| 1:A:424:ARG:C    | 1:A:543:GLY:HA2  | 2.26                     | 0.61              |
| 1:D:231:PHE:O    | 1:D:235:GLU:HG3  | 1.99                     | 0.61              |
| 2:F:18:ARG:HH12  | 2:F:103:ASP:CG   | 2.09                     | 0.61              |
| 1:A:65:VAL:N     | 6:A:792:HOH:O    | 2.33                     | 0.61              |
| 2:B:111:PHE:HB2  | 6:B:477:HOH:O    | 1.99                     | 0.61              |
| 1:D:140:ASP:OD1  | 1:D:140:ASP:N    | 2.31                     | 0.61              |
| 1:D:451:ARG:NH2  | 6:D:703:HOH:O    | 2.33                     | 0.61              |
| 1:D:456:LYS:HZ1  | 2:E:204:LYS:HE2  | 1.63                     | 0.61              |
| 1:D:487:GLU:CD   | 1:D:570:TYR:CE1  | 2.79                     | 0.61              |
| 2:F:162:SER:HB3  | 2:F:199:LEU:HD23 | 1.82                     | 0.61              |
| 1:D:156:SER:N    | 6:D:789:HOH:O    | 2.32                     | 0.61              |
| 1:D:162:VAL:O    | 1:D:560:GLN:HB2  | 2.01                     | 0.61              |
| 1:D:238:TRP:CZ3  | 1:D:278:ARG:HA   | 2.35                     | 0.61              |
| 2:E:5:PRO:O      | 6:E:428:HOH:O    | 2.16                     | 0.61              |
| 1:A:106:GLY:O    | 1:A:432:ASN:ND2  | 2.34                     | 0.61              |
| 2:E:114:TRP:CD1  | 2:E:167:TYR:HE1  | 2.19                     | 0.61              |
| 1:A:223:PHE:HE2  | 1:A:545:PHE:CZ   | 2.18                     | 0.61              |
| 2:E:112:LYS:HB3  | 6:E:457:HOH:O    | 2.01                     | 0.61              |
| 2:B:135:LEU:HD13 | 2:B:182:LEU:HD11 | 1.83                     | 0.61              |
| 1:D:207:LEU:O    | 1:D:211:LEU:HG   | 2.01                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:84:ASP:C     | 1:A:86:SER:H     | 2.09                     | 0.61              |
| 1:A:252:ASN:ND2  | 6:A:767:HOH:O    | 2.26                     | 0.61              |
| 1:A:452:LEU:HB3  | 1:A:457:ILE:HD11 | 1.82                     | 0.61              |
| 2:B:122:GLU:HA   | 2:B:125:LYS:HE2  | 1.81                     | 0.61              |
| 2:C:66:GLU:O     | 2:C:70:VAL:HG23  | 2.01                     | 0.61              |
| 2:C:140:GLY:HA3  | 1:D:38:LYS:HB3   | 1.82                     | 0.61              |
| 1:D:223:PHE:CZ   | 1:D:533:GLU:HA   | 2.36                     | 0.61              |
| 2:E:104:LYS:HD3  | 6:E:517:HOH:O    | 2.01                     | 0.61              |
| 2:E:136:GLU:HG3  | 2:E:181:LYS:HD3  | 1.83                     | 0.61              |
| 2:C:176:GLU:HG3  | 2:C:180:PRO:HA   | 1.82                     | 0.60              |
| 1:D:405:ASP:OD1  | 1:D:405:ASP:N    | 2.33                     | 0.60              |
| 1:A:265:LYS:NZ   | 6:A:747:HOH:O    | 2.21                     | 0.60              |
| 1:A:407:VAL:HB   | 1:A:541:SER:HB2  | 1.82                     | 0.60              |
| 1:A:500:ALA:HA   | 2:B:188:ARG:NH1  | 2.15                     | 0.60              |
| 1:D:432:ASN:OD1  | 1:D:433:ILE:N    | 2.33                     | 0.60              |
| 1:A:113:PHE:HA   | 1:A:117:LEU:HD12 | 1.83                     | 0.60              |
| 1:D:107:ARG:HH21 | 1:D:552:LYS:HB2  | 1.66                     | 0.60              |
| 1:D:278:ARG:NH2  | 6:D:796:HOH:O    | 2.34                     | 0.60              |
| 1:A:15:ASP:OD2   | 6:A:730:HOH:O    | 2.16                     | 0.60              |
| 1:A:25:HIS:NE2   | 1:A:380:THR:OG1  | 2.34                     | 0.60              |
| 1:A:29:LYS:O     | 1:A:33:LYS:HG2   | 2.01                     | 0.60              |
| 1:A:99:LEU:CB    | 1:A:557:LYS:H    | 2.14                     | 0.60              |
| 1:A:165:ALA:N    | 1:A:557:LYS:HE3  | 2.15                     | 0.60              |
| 1:A:223:PHE:CE2  | 1:A:545:PHE:HZ   | 2.18                     | 0.60              |
| 1:A:496:CYS:HA   | 1:A:499:ARG:CZ   | 2.30                     | 0.60              |
| 2:B:163:TRP:HB3  | 2:B:167:TYR:CZ   | 2.36                     | 0.60              |
| 1:D:393:THR:OG1  | 6:D:725:HOH:O    | 2.10                     | 0.60              |
| 1:D:434:ASP:HB2  | 1:D:550:CYS:HB3  | 1.82                     | 0.60              |
| 1:A:28:GLN:HG3   | 1:A:379:LEU:HD21 | 1.82                     | 0.60              |
| 1:A:273:LEU:HA   | 1:A:276:THR:HG23 | 1.82                     | 0.60              |
| 1:A:435:LYS:HZ2  | 1:A:438:GLU:HA   | 1.65                     | 0.60              |
| 1:A:550:CYS:SG   | 6:A:1011:HOH:O   | 2.57                     | 0.60              |
| 2:B:90:TYR:CD2   | 2:C:62:LYS:HD3   | 2.37                     | 0.60              |
| 2:C:150:PHE:CE1  | 2:C:155:ILE:HG13 | 2.36                     | 0.60              |
| 1:D:107:ARG:HG2  | 1:D:107:ARG:HH11 | 1.65                     | 0.60              |
| 1:D:197:ASP:HA   | 1:D:567:VAL:HG12 | 1.84                     | 0.60              |
| 1:D:246:LYS:NZ   | 1:D:271:PRO:HA   | 2.16                     | 0.60              |
| 2:B:73:TYR:HA    | 2:B:76:GLU:OE2   | 2.01                     | 0.60              |
| 2:E:133:LYS:HE2  | 6:E:493:HOH:O    | 2.00                     | 0.60              |
| 2:F:108:ASP:O    | 2:F:112:LYS:HG2  | 2.01                     | 0.60              |
| 1:D:466:ILE:HA   | 6:D:903:HOH:O    | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:493:CYS:HA   | 2:E:187:LYS:HE3  | 1.84                     | 0.60              |
| 2:E:25:GLU:HB3   | 6:E:455:HOH:O    | 2.01                     | 0.60              |
| 1:A:223:PHE:CZ   | 1:A:533:GLU:HA   | 2.36                     | 0.60              |
| 1:A:225:HIS:O    | 6:A:731:HOH:O    | 2.17                     | 0.60              |
| 1:D:331:GLY:HA3  | 1:D:336:TRP:HA   | 1.84                     | 0.60              |
| 2:B:26:LYS:HE2   | 2:B:75:ASP:HA    | 1.83                     | 0.59              |
| 2:C:211:GLU:OE2  | 6:C:417:HOH:O    | 2.16                     | 0.59              |
| 1:D:150:SER:O    | 1:D:150:SER:OG   | 2.19                     | 0.59              |
| 1:D:424:ARG:HB2  | 1:D:425:ARG:HE   | 1.67                     | 0.59              |
| 1:D:492:ASP:HB3  | 2:E:187:LYS:HD3  | 1.84                     | 0.59              |
| 1:A:471:ASP:O    | 6:A:729:HOH:O    | 2.16                     | 0.59              |
| 1:A:219:VAL:HB   | 1:A:295:PHE:CZ   | 2.36                     | 0.59              |
| 1:A:531:ILE:HG13 | 1:A:558:VAL:HG22 | 1.83                     | 0.59              |
| 2:C:121:GLN:O    | 2:C:125:LYS:HG3  | 2.01                     | 0.59              |
| 2:C:142:LYS:C    | 1:D:91:GLY:HA3   | 2.28                     | 0.59              |
| 1:D:110:PHE:HE1  | 1:D:556:ALA:HB2  | 1.66                     | 0.59              |
| 1:D:456:LYS:HE2  | 2:E:204:LYS:HZ1  | 1.68                     | 0.59              |
| 2:B:150:PHE:HB3  | 6:B:468:HOH:O    | 2.02                     | 0.59              |
| 1:D:478:PHE:CZ   | 1:D:562:LEU:HB2  | 2.37                     | 0.59              |
| 1:A:440:ASP:OD1  | 1:A:501:PHE:HA   | 2.01                     | 0.59              |
| 2:B:164:PHE:HD2  | 2:B:183:ILE:HD12 | 1.68                     | 0.59              |
| 2:C:20:ARG:NH2   | 6:C:407:HOH:O    | 2.35                     | 0.59              |
| 1:D:99:LEU:HB3   | 1:D:557:LYS:CB   | 2.30                     | 0.59              |
| 1:D:363:PHE:CD2  | 1:D:382:VAL:HG21 | 2.33                     | 0.59              |
| 2:F:172:ASN:N    | 6:F:412:HOH:O    | 2.32                     | 0.59              |
| 2:B:195:VAL:HG23 | 2:B:199:LEU:HD13 | 1.83                     | 0.59              |
| 2:B:215:ASN:O    | 6:B:419:HOH:O    | 2.16                     | 0.59              |
| 2:C:48:ASN:HB2   | 6:C:501:HOH:O    | 2.03                     | 0.59              |
| 2:C:119:GLU:OE1  | 6:C:419:HOH:O    | 2.17                     | 0.59              |
| 1:D:168:ASN:OD1  | 6:D:743:HOH:O    | 2.15                     | 0.59              |
| 1:A:384:ILE:O    | 6:A:732:HOH:O    | 2.17                     | 0.59              |
| 1:A:496:CYS:N    | 1:A:499:ARG:NH1  | 2.50                     | 0.59              |
| 2:B:28:VAL:O     | 6:B:421:HOH:O    | 2.16                     | 0.59              |
| 2:C:136:GLU:OE2  | 2:C:181:LYS:HD2  | 2.02                     | 0.59              |
| 1:D:442:GLN:HG2  | 1:D:462:PHE:HZ   | 1.67                     | 0.59              |
| 1:D:559:LEU:O    | 1:D:562:LEU:HG   | 2.03                     | 0.59              |
| 2:E:26:LYS:HD2   | 2:E:74:VAL:HG13  | 1.85                     | 0.59              |
| 2:F:98:TRP:CE2   | 2:F:138:GLU:HG2  | 2.38                     | 0.59              |
| 1:D:48:CYS:SG    | 6:D:1005:HOH:O   | 2.48                     | 0.59              |
| 1:D:199:HIS:CE1  | 1:D:200:GLN:HG3  | 2.38                     | 0.59              |
| 1:D:491:GLN:HB2  | 6:D:794:HOH:O    | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:492:ASP:HA   | 1:D:495:ASN:HD22 | 1.67                     | 0.59              |
| 1:A:330:TYR:N    | 6:A:799:HOH:O    | 2.35                     | 0.58              |
| 2:B:33:ARG:HH12  | 2:B:41:SER:HB2   | 1.68                     | 0.58              |
| 2:C:162:SER:HB3  | 2:C:199:LEU:HD23 | 1.85                     | 0.58              |
| 1:D:168:ASN:O    | 1:D:172:ASN:HB2  | 2.02                     | 0.58              |
| 1:D:213:ARG:NH1  | 1:D:214:ASP:OD1  | 2.36                     | 0.58              |
| 1:D:407:VAL:HG21 | 1:D:419:LEU:HB3  | 1.85                     | 0.58              |
| 2:E:153:VAL:O    | 2:E:157:LEU:HD23 | 2.02                     | 0.58              |
| 1:A:101:SER:HB3  | 1:A:535:PHE:CD2  | 2.39                     | 0.58              |
| 1:A:131:PHE:HB2  | 6:A:811:HOH:O    | 2.03                     | 0.58              |
| 1:A:534:HIS:CE1  | 1:A:557:LYS:HG2  | 2.38                     | 0.58              |
| 2:B:153:VAL:O    | 2:B:157:LEU:HD23 | 2.03                     | 0.58              |
| 1:D:90:THR:OG1   | 1:D:397:GLY:HA2  | 2.03                     | 0.58              |
| 1:D:388:TYR:HB3  | 6:D:737:HOH:O    | 2.01                     | 0.58              |
| 1:D:402:ARG:NH1  | 6:D:803:HOH:O    | 2.35                     | 0.58              |
| 1:D:556:ALA:HA   | 1:D:559:LEU:HB2  | 1.85                     | 0.58              |
| 2:F:95:ALA:HB1   | 2:F:152:TYR:HD2  | 1.68                     | 0.58              |
| 2:C:184:ALA:HB3  | 1:D:93:PRO:HG2   | 1.84                     | 0.58              |
| 1:D:330:TYR:HE1  | 1:D:536:LEU:O    | 1.86                     | 0.58              |
| 2:E:5:PRO:HB3    | 2:E:57:LEU:HD11  | 1.85                     | 0.58              |
| 1:A:58:GLU:HG2   | 1:A:62:LYS:HE2   | 1.84                     | 0.58              |
| 1:A:151:SER:HB3  | 1:A:565:ASN:HD21 | 1.67                     | 0.58              |
| 6:A:703:HOH:O    | 2:B:177:SER:HA   | 2.02                     | 0.58              |
| 2:B:114:TRP:CD1  | 2:B:167:TYR:HE1  | 2.22                     | 0.58              |
| 1:D:223:PHE:HE1  | 1:D:304:ILE:HD12 | 1.68                     | 0.58              |
| 1:A:108:PRO:HG2  | 1:A:552:LYS:H    | 1.68                     | 0.58              |
| 1:A:199:HIS:CD2  | 1:A:200:GLN:HG3  | 2.37                     | 0.58              |
| 2:C:172:ASN:ND2  | 6:C:441:HOH:O    | 2.35                     | 0.58              |
| 2:B:64:VAL:HB    | 2:B:73:TYR:CD2   | 2.39                     | 0.58              |
| 1:D:131:PHE:O    | 6:D:711:HOH:O    | 2.17                     | 0.58              |
| 1:D:496:CYS:O    | 6:D:747:HOH:O    | 2.17                     | 0.58              |
| 2:F:121:GLN:O    | 2:F:125:LYS:HG3  | 2.04                     | 0.58              |
| 2:F:183:ILE:HB   | 6:F:432:HOH:O    | 2.04                     | 0.58              |
| 1:A:197:ASP:OD2  | 1:A:200:GLN:NE2  | 2.37                     | 0.58              |
| 1:A:349:GLU:HB2  | 6:A:836:HOH:O    | 2.04                     | 0.58              |
| 1:A:452:LEU:HD23 | 1:A:481:ILE:HG21 | 1.85                     | 0.58              |
| 2:B:201:ASP:HB2  | 2:B:204:LYS:HG3  | 1.85                     | 0.58              |
| 2:C:129:ILE:HA   | 2:C:132:VAL:HG12 | 1.84                     | 0.58              |
| 1:D:143:LYS:HA   | 1:D:184:SER:HB2  | 1.84                     | 0.58              |
| 1:D:496:CYS:HB2  | 2:E:187:LYS:NZ   | 2.17                     | 0.58              |
| 2:E:135:LEU:HD13 | 2:E:182:LEU:HD11 | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:151:GLY:N    | 2:B:154:ASP:OD2  | 2.35                     | 0.58              |
| 1:D:28:GLN:NE2   | 1:D:356:PRO:O    | 2.34                     | 0.58              |
| 1:D:437:THR:OG1  | 1:D:440:ASP:HB2  | 2.03                     | 0.58              |
| 1:D:499:ARG:CZ   | 1:D:499:ARG:HB2  | 2.33                     | 0.58              |
| 2:E:97:PHE:HD1   | 2:F:66:GLU:OE2   | 1.85                     | 0.58              |
| 1:A:98:SER:HB2   | 1:A:111:ILE:CG1  | 2.34                     | 0.58              |
| 1:D:152:LYS:CE   | 1:D:565:ASN:HB2  | 2.26                     | 0.58              |
| 1:D:423:CYS:HB2  | 1:D:543:GLY:N    | 2.19                     | 0.58              |
| 2:C:51:HIS:ND1   | 6:C:437:HOH:O    | 2.31                     | 0.58              |
| 2:C:117:LYS:NZ   | 6:C:440:HOH:O    | 2.33                     | 0.58              |
| 1:D:107:ARG:CZ   | 1:D:433:ILE:HG13 | 2.34                     | 0.58              |
| 1:D:510:ARG:NH1  | 1:D:575:PHE:CE2  | 2.71                     | 0.58              |
| 1:A:32:LEU:HD21  | 1:A:61:PHE:HD2   | 1.68                     | 0.57              |
| 1:A:500:ALA:HB2  | 2:B:188:ARG:HH22 | 1.69                     | 0.57              |
| 1:A:201:ALA:HB1  | 6:A:768:HOH:O    | 2.04                     | 0.57              |
| 1:A:256:VAL:HG13 | 1:A:259:VAL:HG12 | 1.86                     | 0.57              |
| 1:A:284:LEU:HD13 | 1:A:287:TRP:H    | 1.68                     | 0.57              |
| 1:A:352:PHE:HD2  | 1:A:421:PHE:HE2  | 1.52                     | 0.57              |
| 1:D:445:VAL:HG13 | 1:D:479:TRP:CE2  | 2.39                     | 0.57              |
| 2:F:26:LYS:HG3   | 2:F:27:GLY:N     | 2.18                     | 0.57              |
| 2:F:125:LYS:HE2  | 2:F:171:GLY:HA2  | 1.86                     | 0.57              |
| 2:B:117:LYS:O    | 6:B:422:HOH:O    | 2.17                     | 0.57              |
| 2:C:110:GLN:HA   | 6:C:512:HOH:O    | 2.04                     | 0.57              |
| 2:C:121:GLN:HB3  | 6:C:422:HOH:O    | 2.03                     | 0.57              |
| 1:D:498:ASP:OD1  | 1:D:518:LEU:HB3  | 2.03                     | 0.57              |
| 2:E:54:ILE:HB    | 2:E:55:PRO:HA    | 1.86                     | 0.57              |
| 1:A:340:ASN:ND2  | 6:A:807:HOH:O    | 2.37                     | 0.57              |
| 1:D:77:ILE:HD13  | 1:D:111:ILE:HA   | 1.86                     | 0.57              |
| 1:D:479:TRP:CZ2  | 1:D:497:LEU:HD21 | 2.39                     | 0.57              |
| 2:E:36:ASP:O     | 2:E:39:ASN:N     | 2.30                     | 0.57              |
| 1:A:62:LYS:HG2   | 1:A:400:ARG:NH2  | 2.19                     | 0.57              |
| 2:B:98:TRP:HE3   | 2:B:101:PHE:HB2  | 1.68                     | 0.57              |
| 1:D:329:ASP:HB3  | 1:D:339:ALA:HA   | 1.85                     | 0.57              |
| 1:D:452:LEU:HA   | 6:D:916:HOH:O    | 2.03                     | 0.57              |
| 1:D:501:PHE:HB2  | 6:D:716:HOH:O    | 2.04                     | 0.57              |
| 2:E:183:ILE:HG22 | 6:E:432:HOH:O    | 2.04                     | 0.57              |
| 1:A:97:ILE:H     | 1:A:163:GLY:H    | 1.52                     | 0.57              |
| 1:A:99:LEU:HD23  | 1:A:535:PHE:HZ   | 1.69                     | 0.57              |
| 1:A:388:TYR:HA   | 6:A:714:HOH:O    | 2.04                     | 0.57              |
| 1:A:495:ASN:HB2  | 1:A:499:ARG:NH1  | 2.20                     | 0.57              |
| 1:A:498:ASP:CB   | 1:A:510:ARG:HH22 | 2.17                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:85:PHE:CE1   | 2:C:152:TYR:HB2  | 2.39                     | 0.57              |
| 2:C:143:PRO:HG3  | 1:D:42:ALA:HA    | 1.87                     | 0.57              |
| 2:C:167:TYR:OH   | 6:C:418:HOH:O    | 2.17                     | 0.57              |
| 1:D:152:LYS:HE2  | 1:D:565:ASN:CB   | 2.26                     | 0.57              |
| 1:D:152:LYS:HE3  | 6:D:797:HOH:O    | 2.04                     | 0.57              |
| 1:D:336:TRP:HB2  | 1:D:358:LEU:HD13 | 1.85                     | 0.57              |
| 1:A:226:GLY:HA2  | 1:A:529:ARG:HD2  | 1.86                     | 0.57              |
| 2:C:188:ARG:NE   | 1:D:86:SER:HB2   | 2.20                     | 0.57              |
| 1:D:496:CYS:HA   | 1:D:499:ARG:NH2  | 2.20                     | 0.57              |
| 2:E:185:TRP:NE1  | 2:E:189:CYS:SG   | 2.78                     | 0.57              |
| 2:B:24:ARG:HB3   | 2:B:194:SER:HA   | 1.85                     | 0.57              |
| 2:C:24:ARG:HE    | 2:C:197:LYS:HZ2  | 1.51                     | 0.57              |
| 2:C:136:GLU:HG3  | 2:C:181:LYS:HD3  | 1.86                     | 0.57              |
| 5:C:301:GSH:OE1  | 6:C:420:HOH:O    | 2.17                     | 0.57              |
| 1:D:219:VAL:HB   | 1:D:295:PHE:CZ   | 2.39                     | 0.57              |
| 1:D:241:ILE:O    | 1:D:245:ILE:HG12 | 2.04                     | 0.57              |
| 1:D:489:VAL:HA   | 6:D:703:HOH:O    | 2.04                     | 0.57              |
| 2:F:7:LEU:O      | 6:F:414:HOH:O    | 2.17                     | 0.57              |
| 1:D:138:ILE:HA   | 1:D:217:GLN:NE2  | 2.19                     | 0.57              |
| 1:D:273:LEU:O    | 1:D:276:THR:OG1  | 2.21                     | 0.57              |
| 1:D:481:ILE:O    | 1:D:525:LYS:HG2  | 2.05                     | 0.57              |
| 1:A:149:PHE:CE1  | 1:A:205:HIS:HD2  | 2.22                     | 0.57              |
| 1:A:152:LYS:HB2  | 1:A:561:ILE:HA   | 1.87                     | 0.57              |
| 2:B:108:ASP:O    | 2:B:112:LYS:HG2  | 2.05                     | 0.57              |
| 1:D:331:GLY:N    | 1:D:537:GLY:O    | 2.38                     | 0.57              |
| 1:D:425:ARG:HB3  | 1:D:427:LEU:HB2  | 1.87                     | 0.57              |
| 1:D:451:ARG:NH1  | 1:D:454:GLU:CD   | 2.63                     | 0.57              |
| 1:D:563:CYS:N    | 6:D:773:HOH:O    | 2.38                     | 0.57              |
| 2:E:8:LEU:HD13   | 2:E:44:LEU:HB2   | 1.85                     | 0.57              |
| 1:A:439:ARG:O    | 1:A:443:LEU:HB2  | 2.04                     | 0.56              |
| 2:B:86:PRO:HD3   | 2:B:146:GLY:O    | 2.05                     | 0.56              |
| 1:A:103:THR:HG22 | 1:A:548:PRO:HB3  | 1.86                     | 0.56              |
| 1:A:126:ARG:HA   | 1:A:182:ILE:HG21 | 1.86                     | 0.56              |
| 1:A:330:TYR:OH   | 1:A:541:SER:N    | 2.38                     | 0.56              |
| 2:B:98:TRP:CZ2   | 2:B:135:LEU:HD21 | 2.41                     | 0.56              |
| 1:D:35:ILE:HD13  | 1:D:394:ASN:HA   | 1.87                     | 0.56              |
| 1:D:498:ASP:HB3  | 1:D:510:ARG:HH22 | 1.69                     | 0.56              |
| 2:E:98:TRP:CE3   | 2:E:101:PHE:HB2  | 2.40                     | 0.56              |
| 2:E:112:LYS:HD2  | 6:E:413:HOH:O    | 2.04                     | 0.56              |
| 1:A:29:LYS:HG2   | 1:A:33:LYS:HE2   | 1.87                     | 0.56              |
| 1:A:79:ARG:O     | 6:A:733:HOH:O    | 2.17                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:208:SER:HA   | 1:A:211:LEU:HD12 | 1.88                     | 0.56              |
| 1:A:223:PHE:HZ   | 1:A:536:LEU:HB3  | 1.70                     | 0.56              |
| 1:A:363:PHE:CD2  | 1:A:382:VAL:HG21 | 2.39                     | 0.56              |
| 2:C:117:LYS:HG3  | 2:C:213:ARG:NH1  | 2.19                     | 0.56              |
| 2:C:210:ALA:O    | 2:C:213:ARG:HG2  | 2.05                     | 0.56              |
| 1:D:316:LEU:O    | 1:D:320:ALA:N    | 2.39                     | 0.56              |
| 1:D:495:ASN:CB   | 1:D:499:ARG:NH1  | 2.67                     | 0.56              |
| 1:D:510:ARG:NH2  | 6:D:757:HOH:O    | 2.39                     | 0.56              |
| 2:E:139:LEU:HG   | 2:E:145:PHE:CZ   | 2.39                     | 0.56              |
| 1:A:13:VAL:HG23  | 6:A:926:HOH:O    | 2.05                     | 0.56              |
| 1:A:415:ASN:ND2  | 6:A:776:HOH:O    | 2.28                     | 0.56              |
| 1:A:500:ALA:HB2  | 2:B:188:ARG:NH2  | 2.20                     | 0.56              |
| 1:A:111:ILE:HD12 | 1:A:396:ALA:HB1  | 1.86                     | 0.56              |
| 1:A:151:SER:HA   | 1:A:194:PHE:HA   | 1.87                     | 0.56              |
| 1:A:496:CYS:HA   | 1:A:499:ARG:NH2  | 2.20                     | 0.56              |
| 2:B:54:ILE:HB    | 2:B:55:PRO:HA    | 1.88                     | 0.56              |
| 1:D:150:SER:CB   | 1:D:167:THR:HA   | 2.35                     | 0.56              |
| 2:F:164:PHE:CD2  | 2:F:183:ILE:HG13 | 2.40                     | 0.56              |
| 1:A:261:THR:O    | 1:A:265:LYS:HG3  | 2.06                     | 0.56              |
| 1:A:435:LYS:NZ   | 1:A:438:GLU:HA   | 2.19                     | 0.56              |
| 2:C:8:LEU:HD21   | 6:C:479:HOH:O    | 2.05                     | 0.56              |
| 1:D:77:ILE:HG22  | 1:D:110:PHE:HB3  | 1.87                     | 0.56              |
| 1:A:407:VAL:CG2  | 1:A:419:LEU:HG   | 2.34                     | 0.56              |
| 1:D:153:GLN:OE1  | 1:D:560:GLN:NE2  | 2.38                     | 0.56              |
| 2:F:202:SER:O    | 2:F:205:ILE:HG13 | 2.06                     | 0.56              |
| 2:C:169:LYS:HD3  | 2:C:206:VAL:HG13 | 1.88                     | 0.56              |
| 2:C:193:GLU:HA   | 2:C:196:SER:HB3  | 1.87                     | 0.56              |
| 1:D:552:LYS:C    | 1:D:554:SER:N    | 2.64                     | 0.56              |
| 1:A:126:ARG:HA   | 1:A:182:ILE:HD13 | 1.88                     | 0.56              |
| 1:A:499:ARG:NH1  | 2:B:184:ALA:HB1  | 2.20                     | 0.56              |
| 1:A:536:LEU:HB2  | 1:A:545:PHE:CE1  | 2.40                     | 0.56              |
| 2:B:206:VAL:HG11 | 6:B:489:HOH:O    | 2.04                     | 0.56              |
| 2:C:121:GLN:NE2  | 2:C:170:PHE:O    | 2.39                     | 0.56              |
| 1:A:228:VAL:HG12 | 6:A:746:HOH:O    | 2.04                     | 0.56              |
| 1:A:387:GLU:O    | 1:A:388:TYR:HD1  | 1.88                     | 0.56              |
| 2:C:6:ILE:O      | 2:C:57:LEU:HA    | 2.05                     | 0.56              |
| 1:D:526:GLY:HA2  | 1:D:529:ARG:HB3  | 1.88                     | 0.56              |
| 2:E:33:ARG:HH12  | 2:E:41:SER:HB2   | 1.71                     | 0.56              |
| 1:A:246:LYS:HE3  | 6:A:705:HOH:O    | 2.06                     | 0.55              |
| 1:A:363:PHE:HB3  | 1:A:388:TYR:HB3  | 1.87                     | 0.55              |
| 2:C:138:GLU:OE1  | 1:D:38:LYS:NZ    | 2.39                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:188:ARG:HE   | 1:D:86:SER:HB2   | 1.71                     | 0.55              |
| 1:D:64:MET:SD    | 6:D:786:HOH:O    | 2.58                     | 0.55              |
| 1:D:363:PHE:HB3  | 1:D:388:TYR:HB3  | 1.88                     | 0.55              |
| 1:D:437:THR:O    | 1:D:440:ASP:N    | 2.35                     | 0.55              |
| 1:D:529:ARG:NH1  | 1:D:533:GLU:CD   | 2.60                     | 0.55              |
| 2:F:26:LYS:HG3   | 2:F:27:GLY:H     | 1.70                     | 0.55              |
| 1:A:280:LYS:HE2  | 1:A:293:ALA:HB1  | 1.89                     | 0.55              |
| 1:A:451:ARG:NH1  | 1:A:454:GLU:CD   | 2.64                     | 0.55              |
| 2:B:33:ARG:NH1   | 6:B:433:HOH:O    | 2.39                     | 0.55              |
| 1:D:197:ASP:N    | 1:D:197:ASP:OD1  | 2.37                     | 0.55              |
| 1:D:389:GLU:HG3  | 1:D:405:ASP:H    | 1.71                     | 0.55              |
| 1:A:10:MET:HG2   | 6:A:788:HOH:O    | 2.05                     | 0.55              |
| 1:A:203:TYR:HA   | 1:A:206:LEU:HD12 | 1.87                     | 0.55              |
| 2:B:132:VAL:HG23 | 2:B:182:LEU:HD22 | 1.87                     | 0.55              |
| 2:E:8:LEU:HD22   | 2:E:33:ARG:NH2   | 2.16                     | 0.55              |
| 2:E:61:GLY:N     | 6:E:447:HOH:O    | 2.27                     | 0.55              |
| 1:D:378:GLY:O    | 1:D:382:VAL:HG23 | 2.06                     | 0.55              |
| 2:E:185:TRP:NE1  | 2:E:189:CYS:HG   | 2.04                     | 0.55              |
| 1:A:100:SER:HA   | 1:A:535:PHE:CE1  | 2.41                     | 0.55              |
| 1:A:219:VAL:HB   | 1:A:295:PHE:HZ   | 1.70                     | 0.55              |
| 2:E:98:TRP:CZ2   | 2:E:135:LEU:HD21 | 2.42                     | 0.55              |
| 1:A:142:GLY:CA   | 1:A:215:GLN:HB2  | 2.37                     | 0.55              |
| 1:A:143:LYS:HZ2  | 1:A:187:CYS:HA   | 1.71                     | 0.55              |
| 1:D:107:ARG:NH2  | 1:D:552:LYS:HB2  | 2.20                     | 0.55              |
| 1:D:465:TYR:HB3  | 1:D:476:ALA:HB3  | 1.87                     | 0.55              |
| 2:F:139:LEU:HG   | 2:F:142:LYS:HB3  | 1.88                     | 0.55              |
| 2:B:90:TYR:CE2   | 2:C:62:LYS:HD3   | 2.40                     | 0.55              |
| 2:B:92:ARG:NE    | 2:C:76:GLU:OE2   | 2.39                     | 0.55              |
| 2:C:163:TRP:HB3  | 2:C:167:TYR:CZ   | 2.41                     | 0.55              |
| 1:D:45:LEU:HB3   | 1:D:50:LEU:HB2   | 1.88                     | 0.55              |
| 1:D:425:ARG:NH2  | 6:D:813:HOH:O    | 2.39                     | 0.55              |
| 2:F:163:TRP:HB3  | 2:F:167:TYR:CZ   | 2.41                     | 0.55              |
| 1:A:133:ASN:OD1  | 1:A:138:ILE:N    | 2.40                     | 0.55              |
| 1:A:382:VAL:HG13 | 1:A:388:TYR:CD2  | 2.42                     | 0.55              |
| 2:B:73:TYR:CZ    | 2:C:93:ALA:HB1   | 2.41                     | 0.55              |
| 2:B:92:ARG:HE    | 2:B:96:ARG:HH22  | 1.55                     | 0.55              |
| 2:C:24:ARG:HE    | 2:C:197:LYS:NZ   | 2.05                     | 0.55              |
| 2:C:47:SER:HB2   | 6:C:413:HOH:O    | 2.07                     | 0.55              |
| 1:D:44:TYR:HA    | 6:D:767:HOH:O    | 2.06                     | 0.55              |
| 1:A:128:ALA:HA   | 6:A:811:HOH:O    | 2.06                     | 0.55              |
| 1:A:221:ALA:HB3  | 1:A:227:LEU:HG   | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:529:ARG:NH1  | 1:A:533:GLU:CD   | 2.63                     | 0.55              |
| 2:B:211:GLU:HG3  | 6:B:440:HOH:O    | 2.07                     | 0.55              |
| 1:D:154:TYR:O    | 6:D:750:HOH:O    | 2.18                     | 0.55              |
| 1:D:464:SER:O    | 1:D:551:VAL:HG22 | 2.07                     | 0.55              |
| 6:E:405:HOH:O    | 2:F:97:PHE:HB2   | 2.07                     | 0.55              |
| 1:A:143:LYS:HD3  | 1:A:187:CYS:HB3  | 1.88                     | 0.55              |
| 1:A:213:ARG:NH1  | 1:A:214:ASP:OD1  | 2.40                     | 0.55              |
| 2:C:145:PHE:HB2  | 2:C:154:ASP:OD2  | 2.07                     | 0.55              |
| 1:D:23:ASN:O     | 1:D:27:VAL:HG12  | 2.06                     | 0.55              |
| 1:D:29:LYS:HG2   | 1:D:33:LYS:HE2   | 1.88                     | 0.55              |
| 1:D:29:LYS:O     | 1:D:33:LYS:HG2   | 2.07                     | 0.55              |
| 1:A:143:LYS:O    | 1:A:216:VAL:HA   | 2.07                     | 0.54              |
| 1:A:278:ARG:O    | 1:A:282:MET:HE2  | 2.07                     | 0.54              |
| 1:A:521:ARG:NH1  | 1:A:562:LEU:HD21 | 2.22                     | 0.54              |
| 2:C:95:ALA:HB1   | 2:C:152:TYR:HD2  | 1.71                     | 0.54              |
| 1:D:77:ILE:CG2   | 1:D:110:PHE:HB3  | 2.37                     | 0.54              |
| 1:D:106:GLY:O    | 1:D:432:ASN:ND2  | 2.40                     | 0.54              |
| 1:D:166:THR:HG23 | 4:D:602:LEU:OXT  | 2.07                     | 0.54              |
| 2:E:121:GLN:HA   | 6:E:457:HOH:O    | 2.06                     | 0.54              |
| 1:A:246:LYS:HB3  | 6:A:705:HOH:O    | 2.05                     | 0.54              |
| 1:A:491:GLN:HG2  | 2:B:176:GLU:CD   | 2.33                     | 0.54              |
| 1:A:527:THR:HG23 | 1:A:561:ILE:HG21 | 1.88                     | 0.54              |
| 1:D:522:VAL:O    | 1:D:567:VAL:HG22 | 2.07                     | 0.54              |
| 2:E:5:PRO:HG3    | 2:E:59:HIS:CE1   | 2.43                     | 0.54              |
| 2:E:84:PHE:CD1   | 2:E:152:TYR:HB2  | 2.42                     | 0.54              |
| 1:A:46:GLN:NE2   | 6:A:803:HOH:O    | 2.36                     | 0.54              |
| 1:A:193:ILE:HG12 | 1:A:205:HIS:CE1  | 2.43                     | 0.54              |
| 2:B:57:LEU:HB3   | 2:B:64:VAL:HG22  | 1.89                     | 0.54              |
| 1:D:99:LEU:CB    | 1:D:557:LYS:H    | 2.21                     | 0.54              |
| 1:D:107:ARG:NH2  | 1:D:552:LYS:HD3  | 2.22                     | 0.54              |
| 1:D:126:ARG:CZ   | 1:D:182:ILE:HD11 | 2.37                     | 0.54              |
| 1:D:149:PHE:CZ   | 1:D:202:LEU:HA   | 2.42                     | 0.54              |
| 1:D:406:VAL:O    | 1:D:541:SER:OG   | 2.24                     | 0.54              |
| 1:D:496:CYS:HA   | 1:D:499:ARG:CZ   | 2.36                     | 0.54              |
| 1:D:521:ARG:HB3  | 1:D:566:VAL:HG12 | 1.89                     | 0.54              |
| 2:E:86:PRO:HD3   | 2:E:146:GLY:O    | 2.08                     | 0.54              |
| 2:E:98:TRP:CZ2   | 2:E:157:LEU:HD22 | 2.42                     | 0.54              |
| 2:F:205:ILE:HG21 | 6:F:447:HOH:O    | 2.07                     | 0.54              |
| 1:A:77:ILE:N     | 6:A:702:HOH:O    | 2.28                     | 0.54              |
| 1:A:231:PHE:CZ   | 1:A:291:ILE:HG12 | 2.42                     | 0.54              |
| 1:A:276:THR:OG1  | 1:A:277:ILE:N    | 2.38                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:372:GLY:O    | 6:A:736:HOH:O    | 2.19                     | 0.54              |
| 2:C:118:GLY:O    | 6:C:422:HOH:O    | 2.18                     | 0.54              |
| 1:D:426:ASN:OD1  | 6:D:749:HOH:O    | 2.18                     | 0.54              |
| 1:A:495:ASN:HB2  | 1:A:499:ARG:HH11 | 1.72                     | 0.54              |
| 1:A:498:ASP:HB3  | 1:A:510:ARG:HH22 | 1.72                     | 0.54              |
| 1:D:90:THR:HA    | 1:D:399:TYR:HE2  | 1.72                     | 0.54              |
| 1:D:116:GLU:HB2  | 6:D:951:HOH:O    | 2.07                     | 0.54              |
| 1:D:164:THR:HA   | 1:D:557:LYS:HG3  | 1.89                     | 0.54              |
| 1:D:363:PHE:O    | 6:D:722:HOH:O    | 2.19                     | 0.54              |
| 2:F:94:GLN:OE1   | 2:F:94:GLN:HA    | 2.08                     | 0.54              |
| 2:F:159:THR:HG22 | 2:F:199:LEU:HD11 | 1.88                     | 0.54              |
| 1:A:99:LEU:HB3   | 1:A:557:LYS:H    | 1.73                     | 0.54              |
| 1:A:331:GLY:HA3  | 1:A:336:TRP:CE3  | 2.43                     | 0.54              |
| 2:B:40:LYS:HB3   | 2:B:44:LEU:HD23  | 1.90                     | 0.54              |
| 2:B:50:ILE:HD11  | 6:B:483:HOH:O    | 2.08                     | 0.54              |
| 2:C:160:PHE:HB3  | 6:C:470:HOH:O    | 2.08                     | 0.54              |
| 1:D:17:PHE:CE2   | 1:D:341:VAL:HG11 | 2.43                     | 0.54              |
| 1:D:143:LYS:HB2  | 1:D:185:PRO:O    | 2.08                     | 0.54              |
| 1:D:332:SER:CB   | 1:D:538:LEU:HA   | 2.38                     | 0.54              |
| 1:D:399:TYR:N    | 6:D:809:HOH:O    | 2.38                     | 0.54              |
| 1:D:503:ASP:O    | 1:D:507:VAL:HG23 | 2.07                     | 0.54              |
| 2:E:97:PHE:CD1   | 2:F:66:GLU:OE2   | 2.61                     | 0.54              |
| 1:A:25:HIS:CE1   | 1:A:380:THR:HG1  | 2.24                     | 0.54              |
| 1:A:528:PHE:HB3  | 1:A:547:MET:HE1  | 1.90                     | 0.54              |
| 2:C:168:GLU:OE1  | 2:C:175:ILE:HD12 | 2.07                     | 0.54              |
| 1:D:152:LYS:HG2  | 1:D:565:ASN:H    | 1.73                     | 0.54              |
| 1:D:358:LEU:HG   | 6:D:830:HOH:O    | 2.08                     | 0.54              |
| 2:E:24:ARG:HB3   | 2:E:194:SER:HA   | 1.90                     | 0.54              |
| 2:F:107:THR:HG23 | 6:F:415:HOH:O    | 2.08                     | 0.54              |
| 2:F:139:LEU:HG   | 2:F:142:LYS:HB2  | 1.90                     | 0.54              |
| 1:A:476:ALA:HA   | 1:A:519:GLU:O    | 2.08                     | 0.54              |
| 2:B:114:TRP:HA   | 2:B:170:PHE:HD2  | 1.73                     | 0.54              |
| 2:C:35:GLU:HG3   | 2:C:44:LEU:HD22  | 1.90                     | 0.54              |
| 1:D:456:LYS:NZ   | 2:E:204:LYS:CE   | 2.69                     | 0.54              |
| 1:D:143:LYS:CA   | 1:D:184:SER:HB2  | 2.38                     | 0.53              |
| 1:D:309:MET:HE3  | 1:D:545:PHE:CE2  | 2.43                     | 0.53              |
| 1:D:342:THR:O    | 1:D:345:LEU:HG   | 2.08                     | 0.53              |
| 1:D:521:ARG:NH1  | 1:D:562:LEU:HD13 | 2.22                     | 0.53              |
| 2:E:158:ILE:HG13 | 6:E:500:HOH:O    | 2.08                     | 0.53              |
| 2:E:197:LYS:HE2  | 6:E:536:HOH:O    | 2.08                     | 0.53              |
| 1:A:88:ILE:N     | 6:A:741:HOH:O    | 2.21                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:295:PHE:CD1  | 1:A:298:ALA:HB2  | 2.41                     | 0.53              |
| 1:A:363:PHE:CE1  | 1:A:390:VAL:HG22 | 2.43                     | 0.53              |
| 1:A:412:PHE:N    | 6:A:726:HOH:O    | 2.35                     | 0.53              |
| 1:A:441:LEU:HD13 | 6:A:1007:HOH:O   | 2.07                     | 0.53              |
| 1:A:444:SER:HA   | 1:A:500:ALA:CB   | 2.37                     | 0.53              |
| 1:A:496:CYS:HB2  | 2:B:187:LYS:CE   | 2.38                     | 0.53              |
| 1:A:512:CYS:SG   | 1:A:513:LYS:N    | 2.81                     | 0.53              |
| 2:C:56:VAL:HG21  | 6:C:501:HOH:O    | 2.08                     | 0.53              |
| 2:E:40:LYS:HD2   | 2:E:52:LYS:HB3   | 1.91                     | 0.53              |
| 2:B:102:VAL:O    | 2:B:107:THR:HG23 | 2.08                     | 0.53              |
| 1:D:101:SER:HB3  | 1:D:535:PHE:CD2  | 2.43                     | 0.53              |
| 1:D:456:LYS:HZ3  | 2:E:204:LYS:HE2  | 1.74                     | 0.53              |
| 1:D:535:PHE:HB3  | 1:D:544:GLN:O    | 2.07                     | 0.53              |
| 2:B:58:VAL:HG12  | 6:B:441:HOH:O    | 2.09                     | 0.53              |
| 1:D:390:VAL:O    | 6:D:753:HOH:O    | 2.19                     | 0.53              |
| 1:D:439:ARG:O    | 1:D:443:LEU:HB2  | 2.08                     | 0.53              |
| 1:D:491:GLN:O    | 1:D:495:ASN:ND2  | 2.41                     | 0.53              |
| 2:C:142:LYS:HE3  | 1:D:40:GLN:N     | 2.24                     | 0.53              |
| 1:D:496:CYS:N    | 1:D:499:ARG:NH1  | 2.57                     | 0.53              |
| 2:E:122:GLU:HB3  | 6:E:488:HOH:O    | 2.08                     | 0.53              |
| 1:A:496:CYS:HB2  | 2:B:187:LYS:HZ3  | 1.73                     | 0.53              |
| 1:A:510:ARG:NH1  | 1:A:575:PHE:HE2  | 2.07                     | 0.53              |
| 2:B:117:LYS:N    | 6:B:422:HOH:O    | 2.34                     | 0.53              |
| 2:C:98:TRP:CE2   | 2:C:138:GLU:HG2  | 2.42                     | 0.53              |
| 2:F:28:VAL:HG22  | 6:F:457:HOH:O    | 2.09                     | 0.53              |
| 2:F:101:PHE:HZ   | 2:F:131:ALA:HB1  | 1.74                     | 0.53              |
| 1:A:472:PRO:O    | 6:A:737:HOH:O    | 2.19                     | 0.53              |
| 1:A:535:PHE:HB3  | 1:A:544:GLN:O    | 2.07                     | 0.53              |
| 1:D:199:HIS:H    | 1:D:524:ALA:HB1  | 1.73                     | 0.53              |
| 2:C:188:ARG:HB2  | 1:D:87:PRO:HD2   | 1.89                     | 0.53              |
| 1:D:450:LYS:HB2  | 6:D:846:HOH:O    | 2.08                     | 0.53              |
| 2:E:7:LEU:HD21   | 2:E:23:LEU:HD12  | 1.91                     | 0.53              |
| 1:A:377:VAL:HG12 | 1:A:381:GLN:CB   | 2.39                     | 0.53              |
| 1:A:510:ARG:NH1  | 1:A:575:PHE:CE2  | 2.77                     | 0.53              |
| 2:C:109:ALA:O    | 6:C:402:HOH:O    | 2.18                     | 0.53              |
| 2:C:184:ALA:HB1  | 1:D:85:THR:O     | 2.08                     | 0.53              |
| 1:D:353:ALA:HB2  | 1:D:413:TYR:CD2  | 2.44                     | 0.53              |
| 2:E:185:TRP:O    | 2:E:188:ARG:HB3  | 2.09                     | 0.53              |
| 1:A:152:LYS:CB   | 1:A:561:ILE:HA   | 2.39                     | 0.53              |
| 1:A:206:LEU:HB3  | 1:A:234:PHE:CE1  | 2.44                     | 0.53              |
| 1:A:519:GLU:CD   | 1:A:521:ARG:HE   | 2.17                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:162:VAL:N    | 6:D:789:HOH:O    | 2.42                     | 0.53              |
| 1:D:250:LEU:HD21 | 1:D:260:ARG:HG2  | 1.91                     | 0.53              |
| 1:D:494:CYS:HA   | 1:D:497:LEU:HD12 | 1.90                     | 0.53              |
| 2:B:90:TYR:O     | 2:B:94:GLN:HG3   | 2.10                     | 0.52              |
| 2:B:170:PHE:CD2  | 2:B:213:ARG:HD2  | 2.44                     | 0.52              |
| 2:C:142:LYS:HB2  | 1:D:38:LYS:O     | 2.08                     | 0.52              |
| 1:D:62:LYS:HG2   | 1:D:400:ARG:NH2  | 2.24                     | 0.52              |
| 1:D:490:LEU:HD22 | 1:D:522:VAL:HG21 | 1.90                     | 0.52              |
| 1:D:526:GLY:O    | 1:D:530:LYS:HG3  | 2.09                     | 0.52              |
| 1:A:187:CYS:SG   | 6:A:802:HOH:O    | 2.58                     | 0.52              |
| 1:A:199:HIS:HA   | 1:A:525:LYS:HB2  | 1.90                     | 0.52              |
| 1:A:387:GLU:OE1  | 6:A:738:HOH:O    | 2.19                     | 0.52              |
| 1:A:442:GLN:NE2  | 6:A:814:HOH:O    | 2.40                     | 0.52              |
| 2:C:148:ASP:HA   | 1:D:41:SER:HA    | 1.91                     | 0.52              |
| 1:D:238:TRP:CH2  | 1:D:278:ARG:HA   | 2.44                     | 0.52              |
| 2:C:102:VAL:N    | 6:C:401:HOH:O    | 2.18                     | 0.52              |
| 2:C:145:PHE:HB2  | 2:C:154:ASP:CG   | 2.34                     | 0.52              |
| 1:D:195:SER:OG   | 1:D:197:ASP:OD1  | 2.27                     | 0.52              |
| 1:D:406:VAL:HG22 | 6:D:860:HOH:O    | 2.09                     | 0.52              |
| 2:E:125:LYS:HA   | 2:E:128:PHE:CD2  | 2.43                     | 0.52              |
| 2:F:23:LEU:N     | 6:F:436:HOH:O    | 2.42                     | 0.52              |
| 1:D:108:PRO:HB3  | 1:D:555:ASN:CB   | 2.39                     | 0.52              |
| 1:D:229:HIS:HA   | 1:D:232:ARG:HE   | 1.73                     | 0.52              |
| 2:C:145:PHE:N    | 2:C:154:ASP:OD2  | 2.42                     | 0.52              |
| 2:C:181:LYS:HB2  | 1:D:92:HIS:CG    | 2.45                     | 0.52              |
| 1:A:207:LEU:O    | 1:A:211:LEU:HG   | 2.09                     | 0.52              |
| 1:A:478:PHE:HA   | 6:A:748:HOH:O    | 2.09                     | 0.52              |
| 1:A:506:TYR:HB3  | 6:A:709:HOH:O    | 2.10                     | 0.52              |
| 2:B:185:TRP:O    | 2:B:188:ARG:HB3  | 2.10                     | 0.52              |
| 1:D:146:GLN:HB3  | 1:D:148:ILE:HG12 | 1.92                     | 0.52              |
| 1:A:287:TRP:CE3  | 1:A:290:LEU:HD12 | 2.45                     | 0.52              |
| 1:A:522:VAL:HA   | 6:A:748:HOH:O    | 2.10                     | 0.52              |
| 2:B:65:CYS:SG    | 6:B:445:HOH:O    | 2.35                     | 0.52              |
| 2:C:139:LEU:HD12 | 2:C:145:PHE:CE1  | 2.44                     | 0.52              |
| 1:D:494:CYS:SG   | 1:D:572:SER:HA   | 2.50                     | 0.52              |
| 1:A:102:GLY:HA3  | 1:A:426:ASN:HD21 | 1.74                     | 0.52              |
| 1:A:137:PRO:O    | 1:A:299:LYS:NZ   | 2.41                     | 0.52              |
| 1:A:149:PHE:CE1  | 1:A:205:HIS:CD2  | 2.97                     | 0.52              |
| 1:A:304:ILE:HG13 | 1:A:328:HIS:HB3  | 1.90                     | 0.52              |
| 2:B:181:LYS:HA   | 2:B:184:ALA:HB3  | 1.90                     | 0.52              |
| 1:D:339:ALA:N    | 1:D:353:ALA:O    | 2.37                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:73:TYR:HD1   | 2:E:76:GLU:OE2   | 1.93                     | 0.52              |
| 1:A:163:GLY:O    | 6:A:735:HOH:O    | 2.18                     | 0.52              |
| 1:A:328:HIS:CG   | 1:A:329:ASP:N    | 2.77                     | 0.52              |
| 1:D:76:TYR:O     | 1:D:79:ARG:HB2   | 2.09                     | 0.52              |
| 1:D:384:ILE:HG23 | 6:D:849:HOH:O    | 2.09                     | 0.52              |
| 1:D:530:LYS:HB3  | 6:D:769:HOH:O    | 2.10                     | 0.52              |
| 2:E:73:TYR:HE1   | 2:F:96:ARG:NH1   | 2.01                     | 0.52              |
| 1:A:22:ARG:HH11  | 1:A:414:ASN:CG   | 2.17                     | 0.52              |
| 1:A:131:PHE:O    | 1:A:134:ARG:HB3  | 2.10                     | 0.52              |
| 1:A:407:VAL:HG23 | 1:A:420:LYS:O    | 2.10                     | 0.52              |
| 2:B:10:TYR:HH    | 2:B:208:TYR:HH   | 1.58                     | 0.52              |
| 2:C:143:PRO:HA   | 1:D:87:PRO:HB2   | 1.92                     | 0.52              |
| 1:D:559:LEU:HA   | 1:D:562:LEU:HD23 | 1.90                     | 0.52              |
| 2:E:73:TYR:HA    | 2:E:76:GLU:OE2   | 2.09                     | 0.52              |
| 2:F:26:LYS:HE2   | 2:F:78:TRP:CG    | 2.45                     | 0.52              |
| 2:F:90:TYR:O     | 2:F:93:ALA:HB3   | 2.10                     | 0.52              |
| 1:A:121:THR:HG23 | 3:A:601:JAA:C13  | 2.40                     | 0.51              |
| 1:A:193:ILE:HG12 | 1:A:205:HIS:HE1  | 1.75                     | 0.51              |
| 1:A:544:GLN:HA   | 6:A:743:HOH:O    | 2.10                     | 0.51              |
| 1:D:389:GLU:OE2  | 1:D:404:GLY:HA2  | 2.10                     | 0.51              |
| 1:D:400:ARG:N    | 6:D:725:HOH:O    | 2.43                     | 0.51              |
| 1:A:328:HIS:CE1  | 1:A:329:ASP:OD2  | 2.64                     | 0.51              |
| 1:A:492:ASP:C    | 2:B:187:LYS:HE3  | 2.35                     | 0.51              |
| 1:D:96:ALA:HB3   | 1:D:113:PHE:CD2  | 2.45                     | 0.51              |
| 1:D:98:SER:HB2   | 1:D:111:ILE:HG23 | 1.92                     | 0.51              |
| 1:D:322:ASP:HB2  | 6:D:1010:HOH:O   | 2.09                     | 0.51              |
| 1:D:491:GLN:HG2  | 2:E:176:GLU:OE2  | 2.10                     | 0.51              |
| 1:A:96:ALA:HB3   | 1:A:113:PHE:CD2  | 2.46                     | 0.51              |
| 1:A:330:TYR:HB3  | 6:A:725:HOH:O    | 2.09                     | 0.51              |
| 1:A:337:ILE:O    | 1:A:354:VAL:HA   | 2.09                     | 0.51              |
| 1:A:516:GLY:HA3  | 6:A:737:HOH:O    | 2.09                     | 0.51              |
| 1:D:114:THR:HG22 | 1:D:115:ASP:H    | 1.74                     | 0.51              |
| 1:D:424:ARG:HG3  | 6:D:791:HOH:O    | 2.10                     | 0.51              |
| 1:D:477:ILE:HG12 | 1:D:518:LEU:HD11 | 1.91                     | 0.51              |
| 2:E:11:TRP:CG    | 2:E:12:PRO:HD3   | 2.44                     | 0.51              |
| 2:F:145:PHE:N    | 2:F:154:ASP:OD2  | 2.42                     | 0.51              |
| 1:A:213:ARG:HG3  | 1:A:214:ASP:N    | 2.25                     | 0.51              |
| 1:D:107:ARG:NH1  | 1:D:107:ARG:HG2  | 2.25                     | 0.51              |
| 2:E:96:ARG:NH2   | 6:E:431:HOH:O    | 2.24                     | 0.51              |
| 2:E:127:GLU:HB2  | 6:E:410:HOH:O    | 2.10                     | 0.51              |
| 2:F:77:ALA:HB3   | 2:F:78:TRP:CE3   | 2.46                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:99:LEU:HA    | 1:A:109:LYS:O    | 2.11                     | 0.51              |
| 1:A:377:VAL:HG23 | 6:A:820:HOH:O    | 2.10                     | 0.51              |
| 1:A:480:GLU:HA   | 6:A:850:HOH:O    | 2.10                     | 0.51              |
| 1:A:512:CYS:O    | 1:A:513:LYS:HB2  | 2.10                     | 0.51              |
| 1:A:574:ALA:HB2  | 2:B:180:PRO:CB   | 2.41                     | 0.51              |
| 2:C:139:LEU:HG   | 2:C:142:LYS:HB3  | 1.93                     | 0.51              |
| 1:D:284:LEU:HD13 | 1:D:287:TRP:H    | 1.75                     | 0.51              |
| 1:A:143:LYS:CD   | 1:A:212:PHE:HB2  | 2.39                     | 0.51              |
| 1:A:523:VAL:HG23 | 6:A:778:HOH:O    | 2.09                     | 0.51              |
| 2:B:21:VAL:HG12  | 2:B:155:ILE:HG12 | 1.93                     | 0.51              |
| 2:C:138:GLU:CD   | 1:D:38:LYS:HZ1   | 2.18                     | 0.51              |
| 1:D:31:THR:OG1   | 1:D:357:ASN:HA   | 2.11                     | 0.51              |
| 1:D:84:ASP:OD1   | 1:D:86:SER:HB3   | 2.11                     | 0.51              |
| 1:D:166:THR:HG23 | 4:D:602:LEU:C    | 2.36                     | 0.51              |
| 1:D:384:ILE:N    | 6:D:821:HOH:O    | 2.43                     | 0.51              |
| 1:D:76:TYR:O     | 1:D:88:ILE:HG12  | 2.10                     | 0.51              |
| 1:D:208:SER:O    | 1:D:211:LEU:HB2  | 2.10                     | 0.51              |
| 1:D:542:ALA:O    | 6:D:755:HOH:O    | 2.19                     | 0.51              |
| 2:E:7:LEU:HD11   | 2:E:23:LEU:CD1   | 2.41                     | 0.51              |
| 2:E:10:TYR:O     | 2:E:20:ARG:NH2   | 2.38                     | 0.51              |
| 1:A:165:ALA:HB3  | 4:A:602:LEU:OXT  | 2.11                     | 0.51              |
| 1:A:481:ILE:HG13 | 6:A:764:HOH:O    | 2.10                     | 0.51              |
| 2:B:64:VAL:HB    | 2:B:73:TYR:CE2   | 2.45                     | 0.51              |
| 2:C:80:GLU:OE1   | 6:C:423:HOH:O    | 2.18                     | 0.51              |
| 1:D:111:ILE:HG13 | 1:D:396:ALA:O    | 2.10                     | 0.51              |
| 2:E:141:ASP:N    | 2:E:141:ASP:OD1  | 2.44                     | 0.51              |
| 2:E:142:LYS:NZ   | 6:E:404:HOH:O    | 1.77                     | 0.51              |
| 2:F:23:LEU:HG    | 6:F:436:HOH:O    | 2.10                     | 0.51              |
| 2:F:130:GLU:O    | 2:F:134:ILE:HD12 | 2.10                     | 0.51              |
| 1:A:87:PRO:HD3   | 1:A:93:PRO:HG3   | 1.92                     | 0.51              |
| 3:A:601:JAA:C05  | 4:A:602:LEU:HB2  | 2.40                     | 0.51              |
| 1:D:330:TYR:OH   | 1:D:541:SER:N    | 2.44                     | 0.51              |
| 1:D:534:HIS:CE1  | 1:D:557:LYS:HG2  | 2.46                     | 0.51              |
| 2:F:146:GLY:HA2  | 6:F:417:HOH:O    | 2.09                     | 0.51              |
| 1:A:99:LEU:HD13  | 1:A:558:VAL:H    | 1.76                     | 0.51              |
| 1:A:263:MET:HG3  | 6:A:1064:HOH:O   | 2.11                     | 0.51              |
| 1:A:490:LEU:HD13 | 1:A:522:VAL:HG21 | 1.92                     | 0.51              |
| 1:D:81:VAL:HG22  | 1:D:97:ILE:HG13  | 1.93                     | 0.51              |
| 1:D:218:TYR:HD2  | 6:D:818:HOH:O    | 1.94                     | 0.51              |
| 1:D:228:VAL:HG13 | 1:D:319:TYR:HE2  | 1.76                     | 0.51              |
| 1:D:360:TYR:O    | 1:D:393:THR:HB   | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:432:ASN:O    | 1:D:433:ILE:HG23 | 2.11                     | 0.51              |
| 2:E:124:GLY:HA3  | 6:E:457:HOH:O    | 2.11                     | 0.51              |
| 2:E:130:GLU:OE1  | 6:E:434:HOH:O    | 2.19                     | 0.51              |
| 1:A:478:PHE:CZ   | 1:A:562:LEU:HG   | 2.45                     | 0.50              |
| 2:B:20:ARG:NH2   | 6:B:408:HOH:O    | 2.38                     | 0.50              |
| 2:B:57:LEU:O     | 2:B:64:VAL:HG22  | 2.11                     | 0.50              |
| 2:B:79:PRO:HG2   | 6:B:537:HOH:O    | 2.11                     | 0.50              |
| 1:D:107:ARG:NH1  | 1:D:433:ILE:H    | 2.09                     | 0.50              |
| 2:E:203:GLU:HG2  | 6:E:441:HOH:O    | 2.10                     | 0.50              |
| 2:F:24:ARG:HD3   | 2:F:197:LYS:HZ3  | 1.76                     | 0.50              |
| 1:A:538:LEU:HD12 | 1:A:539:GLY:N    | 2.27                     | 0.50              |
| 1:D:139:ASP:OD2  | 1:D:142:GLY:HA3  | 2.10                     | 0.50              |
| 1:D:309:MET:HE3  | 1:D:545:PHE:HE2  | 1.76                     | 0.50              |
| 2:E:90:TYR:HE1   | 2:F:63:PRO:O     | 1.94                     | 0.50              |
| 1:A:198:VAL:HG13 | 1:A:565:ASN:HD21 | 1.76                     | 0.50              |
| 1:A:302:TYR:HD1  | 1:A:326:VAL:HG13 | 1.76                     | 0.50              |
| 1:A:338:ALA:HA   | 1:A:354:VAL:HA   | 1.92                     | 0.50              |
| 1:A:366:VAL:HG13 | 6:A:714:HOH:O    | 2.10                     | 0.50              |
| 1:A:526:GLY:O    | 1:A:530:LYS:N    | 2.42                     | 0.50              |
| 2:B:68:LEU:HA    | 2:B:71:VAL:HG12  | 1.92                     | 0.50              |
| 2:C:43:LEU:HD21  | 2:C:58:VAL:HG21  | 1.93                     | 0.50              |
| 2:C:130:GLU:O    | 2:C:134:ILE:HG13 | 2.11                     | 0.50              |
| 1:D:552:LYS:HD2  | 1:D:553:PRO:HD2  | 1.94                     | 0.50              |
| 2:E:57:LEU:HB3   | 2:E:64:VAL:HG22  | 1.92                     | 0.50              |
| 2:F:24:ARG:HD3   | 2:F:197:LYS:NZ   | 2.27                     | 0.50              |
| 1:A:406:VAL:O    | 1:A:541:SER:OG   | 2.25                     | 0.50              |
| 1:A:526:GLY:HA2  | 1:A:529:ARG:HB3  | 1.93                     | 0.50              |
| 2:B:129:ILE:HA   | 2:B:132:VAL:HG12 | 1.93                     | 0.50              |
| 2:C:40:LYS:HB3   | 2:C:44:LEU:HD23  | 1.93                     | 0.50              |
| 1:D:280:LYS:HE2  | 1:D:293:ALA:HB1  | 1.92                     | 0.50              |
| 1:D:495:ASN:HB2  | 1:D:499:ARG:NH1  | 2.27                     | 0.50              |
| 1:A:36:LEU:HD13  | 1:A:61:PHE:CZ    | 2.46                     | 0.50              |
| 1:A:108:PRO:HB2  | 1:A:554:SER:OG   | 2.11                     | 0.50              |
| 1:A:363:PHE:O    | 1:A:365:PRO:HD3  | 2.12                     | 0.50              |
| 1:A:451:ARG:NH1  | 1:A:454:GLU:OE2  | 2.44                     | 0.50              |
| 1:D:169:VAL:O    | 1:D:175:PHE:HB2  | 2.11                     | 0.50              |
| 1:D:413:TYR:CE2  | 1:D:418:GLN:HG2  | 2.46                     | 0.50              |
| 1:A:238:TRP:HZ3  | 1:A:278:ARG:HA   | 1.76                     | 0.50              |
| 2:B:8:LEU:HD13   | 2:B:44:LEU:HB2   | 1.93                     | 0.50              |
| 2:C:110:GLN:HG3  | 2:C:111:PHE:N    | 2.27                     | 0.50              |
| 1:D:164:THR:HG23 | 1:D:557:LYS:CG   | 2.41                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:448:ALA:HB3  | 1:D:479:TRP:HH2  | 1.77                     | 0.50              |
| 2:E:32:TYR:HA    | 6:E:403:HOH:O    | 2.10                     | 0.50              |
| 1:A:148:ILE:HD12 | 1:A:170:TYR:CZ   | 2.47                     | 0.50              |
| 1:A:442:GLN:HG3  | 1:A:462:PHE:HZ   | 1.77                     | 0.50              |
| 2:C:125:LYS:O    | 2:C:129:ILE:HG13 | 2.11                     | 0.50              |
| 1:D:97:ILE:H     | 1:D:163:GLY:H    | 1.60                     | 0.50              |
| 1:D:383:LYS:HG3  | 6:D:861:HOH:O    | 2.10                     | 0.50              |
| 1:D:491:GLN:NE2  | 1:D:570:TYR:HD2  | 2.10                     | 0.50              |
| 2:E:29:GLU:OE1   | 6:E:436:HOH:O    | 2.20                     | 0.50              |
| 2:E:50:ILE:HD12  | 2:E:51:HIS:CD2   | 2.46                     | 0.50              |
| 2:E:117:LYS:HA   | 2:E:121:GLN:HB2  | 1.92                     | 0.50              |
| 1:A:223:PHE:CE2  | 1:A:533:GLU:HA   | 2.47                     | 0.50              |
| 1:A:329:ASP:HB3  | 1:A:339:ALA:HA   | 1.93                     | 0.50              |
| 2:B:98:TRP:CE3   | 2:B:101:PHE:HB2  | 2.46                     | 0.50              |
| 2:F:18:ARG:NH1   | 2:F:103:ASP:OD1  | 2.45                     | 0.50              |
| 2:F:49:PRO:HG3   | 6:F:466:HOH:O    | 2.11                     | 0.50              |
| 1:D:143:LYS:HD3  | 1:D:187:CYS:HB3  | 1.93                     | 0.50              |
| 2:E:9:ASP:HB2    | 2:E:20:ARG:HH21  | 1.76                     | 0.50              |
| 2:E:113:VAL:HG21 | 2:E:128:PHE:CE2  | 2.47                     | 0.50              |
| 1:A:94:VAL:HG21  | 1:A:112:PRO:HA   | 1.94                     | 0.49              |
| 1:A:288:TYR:HB2  | 1:A:318:HIS:CE1  | 2.47                     | 0.49              |
| 1:A:478:PHE:O    | 1:A:479:TRP:HD1  | 1.95                     | 0.49              |
| 1:A:496:CYS:N    | 1:A:499:ARG:HH12 | 2.09                     | 0.49              |
| 2:C:118:GLY:N    | 6:C:416:HOH:O    | 2.38                     | 0.49              |
| 1:D:235:GLU:HG2  | 1:D:287:TRP:CG   | 2.47                     | 0.49              |
| 1:D:423:CYS:HB2  | 1:D:542:ALA:C    | 2.36                     | 0.49              |
| 2:E:111:PHE:HB2  | 6:E:478:HOH:O    | 2.11                     | 0.49              |
| 2:E:164:PHE:HD2  | 2:E:183:ILE:HD12 | 1.77                     | 0.49              |
| 1:A:90:THR:CG2   | 1:A:397:GLY:HA2  | 2.42                     | 0.49              |
| 1:A:377:VAL:HG12 | 1:A:381:GLN:HB2  | 1.93                     | 0.49              |
| 1:A:391:VAL:HG23 | 6:A:818:HOH:O    | 2.11                     | 0.49              |
| 2:B:118:GLY:N    | 6:B:429:HOH:O    | 2.28                     | 0.49              |
| 2:C:5:PRO:HB3    | 2:C:57:LEU:HD21  | 1.94                     | 0.49              |
| 1:D:507:VAL:HG13 | 1:D:511:LYS:HE2  | 1.93                     | 0.49              |
| 2:E:108:ASP:O    | 2:E:112:LYS:HG2  | 2.12                     | 0.49              |
| 2:E:169:LYS:HD3  | 2:E:206:VAL:HG13 | 1.94                     | 0.49              |
| 1:A:143:LYS:HZ3  | 1:A:187:CYS:HA   | 1.75                     | 0.49              |
| 1:A:212:PHE:HD2  | 1:A:215:GLN:HE21 | 1.59                     | 0.49              |
| 1:A:232:ARG:HB3  | 6:A:885:HOH:O    | 2.10                     | 0.49              |
| 1:A:442:GLN:HG3  | 1:A:462:PHE:CZ   | 2.47                     | 0.49              |
| 1:A:445:VAL:HG23 | 6:A:794:HOH:O    | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:450:LYS:HD3  | 2:B:190:MET:CB   | 2.43                     | 0.49              |
| 1:A:494:CYS:SG   | 1:A:495:ASN:N    | 2.85                     | 0.49              |
| 1:A:534:HIS:HA   | 4:A:602:LEU:N    | 2.26                     | 0.49              |
| 2:B:73:TYR:HE1   | 2:C:96:ARG:HH11  | 1.58                     | 0.49              |
| 2:C:10:TYR:HA    | 2:C:34:GLU:OE2   | 2.12                     | 0.49              |
| 2:C:70:VAL:HG22  | 6:C:410:HOH:O    | 2.12                     | 0.49              |
| 2:C:141:ASP:C    | 1:D:92:HIS:H     | 2.20                     | 0.49              |
| 1:D:138:ILE:HG12 | 1:D:217:GLN:HG3  | 1.93                     | 0.49              |
| 1:D:473:GLY:O    | 1:D:516:GLY:N    | 2.30                     | 0.49              |
| 2:E:71:VAL:O     | 2:E:74:VAL:HB    | 2.12                     | 0.49              |
| 1:A:131:PHE:HD2  | 6:A:811:HOH:O    | 1.94                     | 0.49              |
| 1:A:354:VAL:HG21 | 6:A:1090:HOH:O   | 2.12                     | 0.49              |
| 1:A:413:TYR:CD2  | 1:A:418:GLN:HG2  | 2.47                     | 0.49              |
| 1:A:450:LYS:HD3  | 2:B:190:MET:HB3  | 1.94                     | 0.49              |
| 2:B:141:ASP:N    | 2:B:141:ASP:OD1  | 2.42                     | 0.49              |
| 2:E:10:TYR:HH    | 2:E:208:TYR:HH   | 1.56                     | 0.49              |
| 2:E:101:PHE:CE1  | 2:F:51:HIS:NE2   | 2.80                     | 0.49              |
| 1:A:152:LYS:HE3  | 1:A:527:THR:OG1  | 2.12                     | 0.49              |
| 1:A:152:LYS:NZ   | 1:A:561:ILE:O    | 2.30                     | 0.49              |
| 1:A:410:ILE:HD11 | 6:A:707:HOH:O    | 2.12                     | 0.49              |
| 1:D:443:LEU:HD11 | 6:E:557:HOH:O    | 2.11                     | 0.49              |
| 1:D:512:CYS:O    | 1:D:513:LYS:HB2  | 2.12                     | 0.49              |
| 1:A:454:GLU:HG3  | 2:B:202:SER:HB2  | 1.94                     | 0.49              |
| 1:A:573:THR:OG1  | 2:B:177:SER:HA   | 2.12                     | 0.49              |
| 2:B:22:ALA:HA    | 2:B:155:ILE:HD13 | 1.94                     | 0.49              |
| 2:B:185:TRP:NE1  | 2:B:189:CYS:HG   | 2.10                     | 0.49              |
| 1:D:338:ALA:HA   | 1:D:354:VAL:HA   | 1.93                     | 0.49              |
| 1:D:438:GLU:O    | 1:D:442:GLN:HG3  | 2.13                     | 0.49              |
| 2:E:90:TYR:CD2   | 2:F:62:LYS:HD3   | 2.48                     | 0.49              |
| 2:E:102:VAL:O    | 2:E:107:THR:HG23 | 2.11                     | 0.49              |
| 2:F:15:PHE:HA    | 2:F:18:ARG:HD2   | 1.95                     | 0.49              |
| 2:F:65:CYS:O     | 2:F:69:ASN:HB3   | 2.13                     | 0.49              |
| 1:A:273:LEU:HD12 | 1:A:276:THR:HG21 | 1.95                     | 0.49              |
| 2:C:139:LEU:O    | 2:C:141:ASP:N    | 2.45                     | 0.49              |
| 1:D:389:GLU:HA   | 1:D:405:ASP:O    | 2.13                     | 0.49              |
| 2:E:85:PHE:HE2   | 6:E:431:HOH:O    | 1.95                     | 0.49              |
| 1:A:352:PHE:CD2  | 1:A:421:PHE:HE2  | 2.31                     | 0.49              |
| 1:D:219:VAL:HB   | 1:D:295:PHE:CE2  | 2.48                     | 0.49              |
| 2:E:64:VAL:HB    | 2:E:73:TYR:CE2   | 2.47                     | 0.49              |
| 1:A:100:SER:HA   | 1:A:535:PHE:HE1  | 1.77                     | 0.49              |
| 2:B:7:LEU:HD13   | 2:B:30:PHE:CD2   | 2.48                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:11:TRP:CG    | 2:B:12:PRO:HD3   | 2.46                     | 0.49              |
| 1:D:448:ALA:HB3  | 1:D:479:TRP:CH2  | 2.47                     | 0.49              |
| 1:D:492:ASP:CG   | 2:E:183:ILE:HG12 | 2.38                     | 0.49              |
| 2:F:37:PHE:CE1   | 5:F:301:GSH:HA32 | 2.48                     | 0.49              |
| 1:A:31:THR:OG1   | 1:A:357:ASN:HA   | 2.12                     | 0.49              |
| 1:A:225:HIS:NE2  | 1:A:529:ARG:HG3  | 2.27                     | 0.49              |
| 1:A:531:ILE:HA   | 1:A:534:HIS:ND1  | 2.28                     | 0.49              |
| 1:D:299:LYS:HB2  | 1:D:300:TYR:HD1  | 1.78                     | 0.49              |
| 2:E:26:LYS:HE2   | 2:E:75:ASP:HA    | 1.94                     | 0.49              |
| 2:E:196:SER:HA   | 6:E:468:HOH:O    | 2.13                     | 0.49              |
| 1:A:34:GLU:O     | 1:A:38:LYS:HG2   | 2.13                     | 0.48              |
| 1:A:206:LEU:O    | 1:A:210:ILE:HG12 | 2.13                     | 0.48              |
| 1:A:340:ASN:HB2  | 1:A:352:PHE:HD1  | 1.78                     | 0.48              |
| 1:A:522:VAL:O    | 1:A:567:VAL:HG22 | 2.13                     | 0.48              |
| 2:B:36:ASP:O     | 2:B:39:ASN:N     | 2.45                     | 0.48              |
| 2:B:84:PHE:CD1   | 2:B:152:TYR:HB2  | 2.48                     | 0.48              |
| 2:C:169:LYS:HG3  | 2:C:170:PHE:N    | 2.28                     | 0.48              |
| 1:D:275:GLU:C    | 6:D:708:HOH:O    | 2.56                     | 0.48              |
| 1:D:489:VAL:HG13 | 6:E:471:HOH:O    | 2.12                     | 0.48              |
| 1:D:531:ILE:HA   | 1:D:534:HIS:ND1  | 2.28                     | 0.48              |
| 1:D:562:LEU:HD12 | 1:D:563:CYS:N    | 2.28                     | 0.48              |
| 1:A:107:ARG:HD3  | 1:A:433:ILE:CG1  | 2.40                     | 0.48              |
| 1:A:340:ASN:HB2  | 1:A:352:PHE:CD1  | 2.48                     | 0.48              |
| 2:C:9:ASP:OD1    | 2:C:16:GLY:HA3   | 2.13                     | 0.48              |
| 1:D:100:SER:HA   | 1:D:535:PHE:CE1  | 2.48                     | 0.48              |
| 1:D:107:ARG:HH11 | 1:D:433:ILE:H    | 1.61                     | 0.48              |
| 1:D:153:GLN:NE2  | 6:D:780:HOH:O    | 2.29                     | 0.48              |
| 1:D:542:ALA:HB1  | 6:D:721:HOH:O    | 2.13                     | 0.48              |
| 2:F:110:GLN:HG3  | 2:F:111:PHE:N    | 2.27                     | 0.48              |
| 2:B:8:LEU:HD22   | 2:B:33:ARG:NH2   | 2.21                     | 0.48              |
| 2:B:12:PRO:O     | 2:B:163:TRP:CZ2  | 2.67                     | 0.48              |
| 6:B:434:HOH:O    | 2:C:73:TYR:HA    | 2.13                     | 0.48              |
| 1:D:527:THR:O    | 1:D:530:LYS:HB2  | 2.12                     | 0.48              |
| 1:A:77:ILE:CG2   | 1:A:110:PHE:HB3  | 2.44                     | 0.48              |
| 1:A:287:TRP:HE3  | 1:A:290:LEU:HD12 | 1.78                     | 0.48              |
| 1:A:327:SER:N    | 6:A:807:HOH:O    | 2.46                     | 0.48              |
| 1:A:435:LYS:HZ3  | 1:A:441:LEU:HD23 | 1.78                     | 0.48              |
| 2:B:57:LEU:HB3   | 2:B:64:VAL:CG2   | 2.43                     | 0.48              |
| 2:B:70:VAL:O     | 2:B:73:TYR:HB2   | 2.13                     | 0.48              |
| 2:C:15:PHE:O     | 2:C:18:ARG:HB2   | 2.14                     | 0.48              |
| 2:C:188:ARG:HH22 | 1:D:88:ILE:HG23  | 1.78                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:451:ARG:NH1  | 6:E:445:HOH:O    | 2.46                     | 0.48              |
| 1:D:456:LYS:HZ1  | 2:E:204:LYS:CE   | 2.27                     | 0.48              |
| 1:D:486:ASN:CG   | 1:D:487:GLU:H    | 2.20                     | 0.48              |
| 2:E:12:PRO:O     | 2:E:163:TRP:CZ2  | 2.66                     | 0.48              |
| 2:E:70:VAL:O     | 2:E:73:TYR:HB2   | 2.13                     | 0.48              |
| 2:E:114:TRP:CZ3  | 2:E:212:TYR:HD2  | 2.31                     | 0.48              |
| 1:A:87:PRO:HB3   | 1:A:93:PRO:HD3   | 1.96                     | 0.48              |
| 1:A:111:ILE:O    | 1:A:111:ILE:HG13 | 2.07                     | 0.48              |
| 1:A:444:SER:HB3  | 6:A:864:HOH:O    | 2.13                     | 0.48              |
| 1:A:479:TRP:CZ2  | 1:A:497:LEU:HD11 | 2.49                     | 0.48              |
| 2:B:26:LYS:HE3   | 2:B:78:TRP:O     | 2.13                     | 0.48              |
| 2:C:181:LYS:HB3  | 1:D:93:PRO:O     | 2.12                     | 0.48              |
| 1:D:19:GLU:OE1   | 6:D:756:HOH:O    | 2.20                     | 0.48              |
| 1:D:157:THR:HG22 | 1:D:469:SER:HB3  | 1.96                     | 0.48              |
| 1:D:524:ALA:N    | 6:D:704:HOH:O    | 2.47                     | 0.48              |
| 2:E:76:GLU:OE2   | 2:F:96:ARG:NH1   | 2.46                     | 0.48              |
| 2:F:196:SER:HB2  | 6:F:421:HOH:O    | 2.14                     | 0.48              |
| 1:A:150:SER:HB2  | 1:A:167:THR:CA   | 2.41                     | 0.48              |
| 1:A:198:VAL:HG13 | 1:A:565:ASN:ND2  | 2.28                     | 0.48              |
| 1:A:217:GLN:HA   | 1:A:217:GLN:OE1  | 2.13                     | 0.48              |
| 1:A:368:GLU:HG3  | 1:A:369:THR:HG22 | 1.95                     | 0.48              |
| 2:C:56:VAL:HG11  | 6:C:501:HOH:O    | 2.14                     | 0.48              |
| 1:D:124:LEU:HD12 | 1:D:355:ILE:HD12 | 1.96                     | 0.48              |
| 2:E:9:ASP:HB2    | 2:E:20:ARG:NH2   | 2.28                     | 0.48              |
| 2:E:49:PRO:HB3   | 6:E:522:HOH:O    | 2.14                     | 0.48              |
| 1:A:363:PHE:CD1  | 1:A:390:VAL:HA   | 2.49                     | 0.48              |
| 1:A:393:THR:HA   | 1:A:398:LEU:O    | 2.13                     | 0.48              |
| 2:B:10:TYR:CD2   | 2:B:12:PRO:HD2   | 2.48                     | 0.48              |
| 2:C:139:LEU:CD2  | 2:C:142:LYS:H    | 2.22                     | 0.48              |
| 1:D:117:LEU:HD23 | 1:D:120:ASN:HD22 | 1.78                     | 0.48              |
| 2:E:45:LEU:HD12  | 6:E:487:HOH:O    | 2.12                     | 0.48              |
| 1:A:313:VAL:HB   | 1:A:314:PRO:HD3  | 1.96                     | 0.48              |
| 1:A:495:ASN:CB   | 1:A:499:ARG:NH1  | 2.74                     | 0.48              |
| 2:B:120:GLU:HB2  | 6:B:422:HOH:O    | 2.11                     | 0.48              |
| 2:B:125:LYS:HD2  | 2:B:173:PHE:CE1  | 2.48                     | 0.48              |
| 2:B:174:SER:C    | 2:B:176:GLU:H    | 2.21                     | 0.48              |
| 1:D:97:ILE:H     | 1:D:162:VAL:HA   | 1.78                     | 0.48              |
| 1:D:146:GLN:O    | 1:D:148:ILE:N    | 2.45                     | 0.48              |
| 1:D:332:SER:HB3  | 1:D:538:LEU:HA   | 1.95                     | 0.48              |
| 1:D:449:ALA:O    | 1:D:452:LEU:HB2  | 2.13                     | 0.48              |
| 2:E:10:TYR:HB3   | 2:E:13:SER:HB2   | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:37:PHE:HD1   | 2:E:40:LYS:HG2   | 1.79                     | 0.48              |
| 2:F:84:PHE:C     | 2:F:85:PHE:HD1   | 2.22                     | 0.48              |
| 1:A:494:CYS:HA   | 1:A:497:LEU:HD12 | 1.96                     | 0.48              |
| 2:C:169:LYS:HG3  | 2:C:170:PHE:H    | 1.79                     | 0.48              |
| 1:D:42:ALA:HB3   | 1:D:45:LEU:HD22  | 1.95                     | 0.48              |
| 1:D:141:ASN:ND2  | 6:D:827:HOH:O    | 2.46                     | 0.48              |
| 1:D:189:PRO:O    | 1:D:192:VAL:HG12 | 2.13                     | 0.48              |
| 1:D:213:ARG:HG3  | 1:D:214:ASP:N    | 2.28                     | 0.48              |
| 1:D:246:LYS:HZ2  | 1:D:271:PRO:HA   | 1.77                     | 0.48              |
| 1:D:331:GLY:HA2  | 1:D:539:GLY:CA   | 2.44                     | 0.48              |
| 2:E:33:ARG:HH22  | 2:E:41:SER:HB2   | 1.78                     | 0.48              |
| 2:E:125:LYS:HA   | 2:E:128:PHE:CE2  | 2.49                     | 0.48              |
| 2:E:215:ASN:O    | 6:E:435:HOH:O    | 2.19                     | 0.48              |
| 2:F:145:PHE:HB2  | 2:F:154:ASP:CG   | 2.39                     | 0.48              |
| 2:F:183:ILE:O    | 2:F:187:LYS:HG3  | 2.14                     | 0.48              |
| 2:F:204:LYS:HB2  | 6:F:420:HOH:O    | 2.14                     | 0.48              |
| 1:A:164:THR:HG23 | 1:A:557:LYS:HG3  | 1.96                     | 0.48              |
| 1:A:191:GLU:O    | 1:A:195:SER:N    | 2.47                     | 0.48              |
| 1:A:426:ASN:HB3  | 1:A:543:GLY:O    | 2.14                     | 0.48              |
| 1:D:465:TYR:HD1  | 1:D:551:VAL:HG23 | 1.79                     | 0.48              |
| 2:E:24:ARG:HG3   | 2:E:30:PHE:CE1   | 2.49                     | 0.48              |
| 2:E:26:LYS:HD2   | 2:E:74:VAL:CG1   | 2.43                     | 0.48              |
| 1:A:188:SER:OG   | 1:A:205:HIS:ND1  | 2.47                     | 0.47              |
| 1:A:231:PHE:HA   | 1:A:234:PHE:HB2  | 1.95                     | 0.47              |
| 1:A:244:ASP:OD1  | 1:A:251:SER:HB2  | 2.14                     | 0.47              |
| 2:B:185:TRP:NE1  | 2:B:189:CYS:SG   | 2.87                     | 0.47              |
| 2:E:17:MET:SD    | 2:E:199:LEU:HG   | 2.54                     | 0.47              |
| 2:F:199:LEU:N    | 6:F:406:HOH:O    | 2.10                     | 0.47              |
| 1:A:58:GLU:O     | 1:A:62:LYS:HG3   | 2.13                     | 0.47              |
| 1:A:341:VAL:HG22 | 6:A:761:HOH:O    | 2.14                     | 0.47              |
| 1:A:444:SER:HA   | 1:A:500:ALA:HB1  | 1.96                     | 0.47              |
| 1:D:143:LYS:HZ3  | 1:D:187:CYS:HA   | 1.76                     | 0.47              |
| 1:D:382:VAL:HG13 | 1:D:388:TYR:CD2  | 2.50                     | 0.47              |
| 2:E:57:LEU:O     | 2:E:64:VAL:HG22  | 2.15                     | 0.47              |
| 2:E:110:GLN:O    | 2:E:113:VAL:HG12 | 2.14                     | 0.47              |
| 2:E:112:LYS:NZ   | 6:E:440:HOH:O    | 2.23                     | 0.47              |
| 1:A:234:PHE:HD1  | 6:A:867:HOH:O    | 1.98                     | 0.47              |
| 1:A:337:ILE:HG13 | 1:A:539:GLY:CA   | 2.45                     | 0.47              |
| 1:A:441:LEU:O    | 1:A:444:SER:HB2  | 2.14                     | 0.47              |
| 2:B:98:TRP:CZ2   | 2:B:157:LEU:HD22 | 2.49                     | 0.47              |
| 2:B:201:ASP:OD2  | 2:B:204:LYS:HE2  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:102:VAL:HB   | 6:C:401:HOH:O    | 2.15                     | 0.47              |
| 1:D:451:ARG:CZ   | 6:D:703:HOH:O    | 2.61                     | 0.47              |
| 1:D:455:GLU:OE1  | 1:D:485:THR:HB   | 2.14                     | 0.47              |
| 1:A:320:ALA:O    | 1:A:323:LEU:HB2  | 2.14                     | 0.47              |
| 1:D:100:SER:CB   | 1:D:109:LYS:HD3  | 2.43                     | 0.47              |
| 1:D:328:HIS:CG   | 1:D:329:ASP:N    | 2.81                     | 0.47              |
| 1:D:384:ILE:HG13 | 1:D:409:VAL:HG12 | 1.96                     | 0.47              |
| 1:A:30:GLN:HG2   | 6:A:944:HOH:O    | 2.15                     | 0.47              |
| 1:A:417:PRO:HB2  | 6:A:849:HOH:O    | 2.13                     | 0.47              |
| 1:A:424:ARG:HD3  | 6:A:946:HOH:O    | 2.14                     | 0.47              |
| 1:A:450:LYS:H    | 1:A:450:LYS:HG2  | 1.34                     | 0.47              |
| 2:B:17:MET:SD    | 2:B:199:LEU:HG   | 2.55                     | 0.47              |
| 2:C:102:VAL:HA   | 2:C:106:PHE:CB   | 2.44                     | 0.47              |
| 2:C:163:TRP:CD1  | 2:C:205:ILE:HD13 | 2.50                     | 0.47              |
| 1:D:29:LYS:NZ    | 1:D:33:LYS:NZ    | 2.63                     | 0.47              |
| 1:D:203:TYR:CZ   | 1:D:241:ILE:HG13 | 2.50                     | 0.47              |
| 1:D:288:TYR:HB3  | 6:D:931:HOH:O    | 2.13                     | 0.47              |
| 1:D:313:VAL:O    | 1:D:317:ARG:N    | 2.35                     | 0.47              |
| 1:D:450:LYS:HE2  | 1:D:450:LYS:HB3  | 1.63                     | 0.47              |
| 2:E:181:LYS:HA   | 2:E:184:ALA:HB3  | 1.95                     | 0.47              |
| 2:E:187:LYS:HE2  | 2:E:187:LYS:HB2  | 1.59                     | 0.47              |
| 1:A:91:GLY:O     | 1:A:92:HIS:C     | 2.58                     | 0.47              |
| 1:A:454:GLU:HB2  | 2:B:202:SER:OG   | 2.13                     | 0.47              |
| 1:A:555:ASN:O    | 1:A:559:LEU:HD22 | 2.15                     | 0.47              |
| 2:B:5:PRO:HB3    | 2:B:57:LEU:HD11  | 1.96                     | 0.47              |
| 1:D:164:THR:HG21 | 1:D:561:ILE:HD12 | 1.96                     | 0.47              |
| 1:D:305:MET:HE3  | 1:D:325:LEU:HB3  | 1.97                     | 0.47              |
| 1:D:361:PHE:CE1  | 1:D:392:ILE:HG23 | 2.46                     | 0.47              |
| 1:D:479:TRP:HZ2  | 1:D:497:LEU:HD21 | 1.80                     | 0.47              |
| 2:E:128:PHE:O    | 2:E:132:VAL:HG12 | 2.14                     | 0.47              |
| 2:E:204:LYS:HG3  | 6:E:441:HOH:O    | 2.15                     | 0.47              |
| 1:A:222:VAL:HG12 | 1:A:223:PHE:CD1  | 2.49                     | 0.47              |
| 1:A:229:HIS:HA   | 1:A:232:ARG:HE   | 1.80                     | 0.47              |
| 1:A:346:SER:N    | 6:A:836:HOH:O    | 2.47                     | 0.47              |
| 1:A:436:ASN:O    | 1:A:437:THR:O    | 2.32                     | 0.47              |
| 2:B:7:LEU:HD13   | 2:B:30:PHE:HD2   | 1.80                     | 0.47              |
| 2:C:190:MET:HE1  | 6:C:546:HOH:O    | 2.14                     | 0.47              |
| 1:D:32:LEU:HD21  | 1:D:61:PHE:HD2   | 1.79                     | 0.47              |
| 1:D:104:SER:N    | 6:D:823:HOH:O    | 2.47                     | 0.47              |
| 2:E:169:LYS:HA   | 6:E:504:HOH:O    | 2.14                     | 0.47              |
| 2:E:170:PHE:CD2  | 2:E:213:ARG:HD2  | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:412:PHE:HB3  | 1:A:414:ASN:O    | 2.15                     | 0.47              |
| 2:B:91:GLY:N     | 6:B:439:HOH:O    | 2.46                     | 0.47              |
| 1:D:34:GLU:O     | 1:D:38:LYS:HG2   | 2.15                     | 0.47              |
| 1:D:149:PHE:HA   | 1:D:193:ILE:HG23 | 1.96                     | 0.47              |
| 2:E:10:TYR:CD2   | 2:E:12:PRO:HD2   | 2.50                     | 0.47              |
| 2:E:97:PHE:HD1   | 2:F:66:GLU:CD    | 2.23                     | 0.47              |
| 2:F:130:GLU:O    | 2:F:133:LYS:HB3  | 2.15                     | 0.47              |
| 2:F:169:LYS:HG3  | 2:F:170:PHE:N    | 2.30                     | 0.47              |
| 1:A:334:GLU:O    | 1:A:398:LEU:HD12 | 2.15                     | 0.47              |
| 1:A:445:VAL:HA   | 1:A:479:TRP:HZ2  | 1.79                     | 0.47              |
| 1:A:451:ARG:NE   | 2:B:183:ILE:HD11 | 2.25                     | 0.47              |
| 1:D:223:PHE:CE2  | 1:D:545:PHE:HZ   | 2.32                     | 0.47              |
| 1:D:383:LYS:NZ   | 6:D:751:HOH:O    | 2.18                     | 0.47              |
| 1:D:451:ARG:HH11 | 1:D:454:GLU:CD   | 2.23                     | 0.47              |
| 2:E:127:GLU:HG3  | 6:E:464:HOH:O    | 2.14                     | 0.47              |
| 1:A:233:THR:O    | 1:A:237:VAL:HG22 | 2.15                     | 0.47              |
| 2:B:108:ASP:O    | 2:B:111:PHE:HB3  | 2.15                     | 0.47              |
| 1:D:223:PHE:CZ   | 1:D:536:LEU:HB2  | 2.49                     | 0.47              |
| 2:E:144:TYR:HB3  | 2:E:154:ASP:CG   | 2.40                     | 0.47              |
| 2:E:199:LEU:N    | 6:E:451:HOH:O    | 2.30                     | 0.47              |
| 1:A:152:LYS:CE   | 1:A:565:ASN:HB2  | 2.37                     | 0.46              |
| 1:D:104:SER:N    | 1:D:107:ARG:O    | 2.38                     | 0.46              |
| 2:E:57:LEU:HB3   | 2:E:64:VAL:CG2   | 2.45                     | 0.46              |
| 2:F:101:PHE:HE2  | 2:F:135:LEU:HG   | 1.79                     | 0.46              |
| 2:C:139:LEU:HD23 | 2:C:142:LYS:N    | 2.27                     | 0.46              |
| 2:C:211:GLU:HB3  | 6:C:450:HOH:O    | 2.14                     | 0.46              |
| 1:D:246:LYS:O    | 1:D:270:ASN:N    | 2.41                     | 0.46              |
| 1:D:368:GLU:HG3  | 1:D:369:THR:HG22 | 1.95                     | 0.46              |
| 1:D:424:ARG:HB2  | 1:D:425:ARG:NE   | 2.30                     | 0.46              |
| 1:D:463:SER:HB2  | 1:D:528:PHE:HE1  | 1.80                     | 0.46              |
| 1:A:88:ILE:HG22  | 1:A:89:LEU:N     | 2.30                     | 0.46              |
| 1:A:97:ILE:H     | 1:A:162:VAL:HA   | 1.80                     | 0.46              |
| 1:A:153:GLN:HG2  | 1:A:167:THR:CG2  | 2.45                     | 0.46              |
| 1:A:156:SER:HB2  | 6:A:974:HOH:O    | 2.15                     | 0.46              |
| 1:A:349:GLU:OE2  | 6:A:739:HOH:O    | 2.20                     | 0.46              |
| 2:C:53:LYS:HG2   | 5:C:301:GSH:HA31 | 1.97                     | 0.46              |
| 1:D:95:PRO:HD2   | 1:D:113:PHE:O    | 2.16                     | 0.46              |
| 1:D:198:VAL:O    | 1:D:202:LEU:N    | 2.48                     | 0.46              |
| 1:D:231:PHE:CD1  | 1:D:290:LEU:HD11 | 2.50                     | 0.46              |
| 2:E:7:LEU:HD11   | 2:E:23:LEU:HD13  | 1.97                     | 0.46              |
| 2:E:16:GLY:HA2   | 2:E:55:PRO:HB3   | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:150:PHE:CD1  | 2:E:192:LYS:HG3  | 2.49                     | 0.46              |
| 1:A:150:SER:OG   | 1:A:167:THR:HA   | 2.15                     | 0.46              |
| 1:A:290:LEU:O    | 1:A:293:ALA:HB3  | 2.16                     | 0.46              |
| 2:C:144:TYR:HB3  | 2:C:154:ASP:OD2  | 2.15                     | 0.46              |
| 2:E:26:LYS:HE3   | 2:E:78:TRP:O     | 2.15                     | 0.46              |
| 2:F:17:MET:HG2   | 2:F:20:ARG:NH1   | 2.31                     | 0.46              |
| 2:F:39:ASN:OD1   | 6:F:416:HOH:O    | 2.21                     | 0.46              |
| 2:F:101:PHE:CE1  | 2:F:105:LYS:HE3  | 2.43                     | 0.46              |
| 1:A:104:SER:N    | 1:A:107:ARG:O    | 2.39                     | 0.46              |
| 1:A:331:GLY:C    | 1:A:538:LEU:HA   | 2.41                     | 0.46              |
| 1:A:369:THR:OG1  | 1:A:370:GLY:N    | 2.48                     | 0.46              |
| 2:B:165:GLN:HA   | 2:B:168:GLU:OE1  | 2.15                     | 0.46              |
| 2:C:188:ARG:NH2  | 1:D:86:SER:OG    | 2.49                     | 0.46              |
| 1:D:487:GLU:HG3  | 6:D:794:HOH:O    | 2.15                     | 0.46              |
| 1:D:496:CYS:HB2  | 2:E:187:LYS:HZ3  | 1.78                     | 0.46              |
| 1:D:521:ARG:NH1  | 1:D:562:LEU:CD1  | 2.78                     | 0.46              |
| 1:A:238:TRP:CZ3  | 1:A:278:ARG:HA   | 2.50                     | 0.46              |
| 2:C:188:ARG:HH22 | 1:D:88:ILE:CG2   | 2.29                     | 0.46              |
| 1:D:105:GLN:C    | 1:D:107:ARG:H    | 2.24                     | 0.46              |
| 1:D:405:ASP:CG   | 1:D:540:SER:HB2  | 2.40                     | 0.46              |
| 1:D:498:ASP:CB   | 1:D:510:ARG:HH22 | 2.27                     | 0.46              |
| 1:D:566:VAL:HB   | 1:D:569:SER:HB2  | 1.96                     | 0.46              |
| 2:E:92:ARG:HE    | 2:E:96:ARG:HH22  | 1.64                     | 0.46              |
| 2:F:26:LYS:HE3   | 2:F:28:VAL:HG22  | 1.97                     | 0.46              |
| 2:F:52:LYS:HD2   | 6:F:497:HOH:O    | 2.15                     | 0.46              |
| 1:A:263:MET:SD   | 1:A:266:LEU:HD12 | 2.56                     | 0.46              |
| 1:A:353:ALA:HB2  | 1:A:413:TYR:CD2  | 2.50                     | 0.46              |
| 1:A:473:GLY:O    | 1:A:516:GLY:N    | 2.42                     | 0.46              |
| 2:B:5:PRO:HB3    | 2:B:59:HIS:NE2   | 2.31                     | 0.46              |
| 2:B:5:PRO:HG3    | 2:B:59:HIS:CE1   | 2.50                     | 0.46              |
| 2:B:153:VAL:HA   | 2:B:156:SER:HG   | 1.80                     | 0.46              |
| 2:C:142:LYS:CG   | 1:D:41:SER:HB2   | 2.43                     | 0.46              |
| 1:D:29:LYS:NZ    | 1:D:33:LYS:HZ1   | 2.13                     | 0.46              |
| 1:D:73:LEU:HD22  | 1:D:89:LEU:CD2   | 2.46                     | 0.46              |
| 1:D:99:LEU:HD23  | 1:D:535:PHE:HZ   | 1.81                     | 0.46              |
| 1:D:212:PHE:O    | 1:D:216:VAL:HG23 | 2.16                     | 0.46              |
| 1:D:246:LYS:HE3  | 1:D:246:LYS:HB3  | 1.67                     | 0.46              |
| 1:D:465:TYR:CD1  | 1:D:551:VAL:HG23 | 2.51                     | 0.46              |
| 1:D:534:HIS:HA   | 4:D:602:LEU:N    | 2.31                     | 0.46              |
| 2:E:26:LYS:HG2   | 2:E:81:LYS:HZ1   | 1.75                     | 0.46              |
| 2:F:51:HIS:O     | 2:F:53:LYS:HG3   | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:67:SER:O     | 2:F:71:VAL:HG23  | 2.16                     | 0.46              |
| 2:F:110:GLN:CD   | 2:F:167:TYR:HH   | 2.11                     | 0.46              |
| 1:A:448:ALA:CB   | 1:A:496:CYS:HB3  | 2.45                     | 0.46              |
| 1:A:499:ARG:C    | 2:B:188:ARG:NH1  | 2.68                     | 0.46              |
| 1:D:75:PRO:O     | 1:D:79:ARG:HG3   | 2.15                     | 0.46              |
| 1:D:126:ARG:HB3  | 6:D:839:HOH:O    | 2.14                     | 0.46              |
| 1:D:170:TYR:HB3  | 1:D:194:PHE:CZ   | 2.51                     | 0.46              |
| 2:E:93:ALA:HB1   | 2:F:64:VAL:HG13  | 1.98                     | 0.46              |
| 2:F:183:ILE:O    | 2:F:186:ALA:HB3  | 2.15                     | 0.46              |
| 1:A:70:ASP:HB2   | 1:A:104:SER:HB2  | 1.98                     | 0.46              |
| 1:A:107:ARG:HB3  | 1:A:108:PRO:HD2  | 1.97                     | 0.46              |
| 1:A:281:CYS:HA   | 6:A:995:HOH:O    | 2.15                     | 0.46              |
| 1:A:363:PHE:HD1  | 1:A:390:VAL:HA   | 1.81                     | 0.46              |
| 2:B:33:ARG:HH22  | 2:B:41:SER:HB2   | 1.80                     | 0.46              |
| 2:B:187:LYS:NZ   | 2:B:187:LYS:HB2  | 2.30                     | 0.46              |
| 1:D:76:TYR:HB3   | 1:D:88:ILE:HB    | 1.96                     | 0.46              |
| 1:D:95:PRO:O     | 1:D:161:PRO:HB2  | 2.16                     | 0.46              |
| 1:D:125:PHE:HD1  | 1:D:125:PHE:HA   | 1.62                     | 0.46              |
| 1:D:363:PHE:HE1  | 1:D:390:VAL:HG13 | 1.81                     | 0.46              |
| 1:D:477:ILE:CG1  | 1:D:518:LEU:HD11 | 2.46                     | 0.46              |
| 1:D:486:ASN:CG   | 1:D:487:GLU:N    | 2.74                     | 0.46              |
| 2:F:88:ASP:N     | 6:F:405:HOH:O    | 2.09                     | 0.46              |
| 1:A:84:ASP:C     | 1:A:86:SER:N     | 2.74                     | 0.46              |
| 2:B:98:TRP:HD1   | 2:B:153:VAL:HG11 | 1.80                     | 0.46              |
| 1:D:117:LEU:HD23 | 1:D:120:ASN:ND2  | 2.31                     | 0.46              |
| 1:D:387:GLU:O    | 1:D:388:TYR:HD1  | 1.98                     | 0.46              |
| 1:D:466:ILE:N    | 6:D:712:HOH:O    | 2.41                     | 0.46              |
| 2:F:11:TRP:NE1   | 6:F:425:HOH:O    | 2.29                     | 0.46              |
| 1:A:75:PRO:O     | 1:A:79:ARG:HG3   | 2.16                     | 0.45              |
| 1:A:242:VAL:HG22 | 1:A:277:ILE:HD13 | 1.96                     | 0.45              |
| 1:A:434:ASP:O    | 1:A:435:LYS:HG3  | 2.16                     | 0.45              |
| 1:A:562:LEU:HD23 | 1:A:563:CYS:N    | 2.31                     | 0.45              |
| 2:B:125:LYS:HA   | 2:B:128:PHE:CE2  | 2.51                     | 0.45              |
| 2:C:188:ARG:CB   | 1:D:87:PRO:HD2   | 2.46                     | 0.45              |
| 2:C:201:ASP:HB3  | 2:C:203:GLU:HG2  | 1.98                     | 0.45              |
| 1:D:43:ILE:N     | 6:D:762:HOH:O    | 2.50                     | 0.45              |
| 1:D:153:GLN:HA   | 1:D:560:GLN:CG   | 2.46                     | 0.45              |
| 1:D:295:PHE:HD2  | 1:D:298:ALA:HB2  | 1.81                     | 0.45              |
| 1:D:531:ILE:HG13 | 1:D:558:VAL:HG22 | 1.97                     | 0.45              |
| 2:F:164:PHE:CE2  | 2:F:183:ILE:HG13 | 2.52                     | 0.45              |
| 1:A:143:LYS:HB2  | 1:A:185:PRO:O    | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:253:ARG:O    | 1:A:484:GLU:HG3  | 2.16                     | 0.45              |
| 1:A:336:TRP:HA   | 6:A:711:HOH:O    | 2.15                     | 0.45              |
| 2:B:73:TYR:HD1   | 2:B:76:GLU:OE2   | 1.99                     | 0.45              |
| 2:B:121:GLN:O    | 2:B:125:LYS:HG3  | 2.16                     | 0.45              |
| 1:D:188:SER:HB3  | 1:D:192:VAL:HG13 | 1.99                     | 0.45              |
| 1:D:223:PHE:CZ   | 1:D:536:LEU:CB   | 3.00                     | 0.45              |
| 1:D:261:THR:HG22 | 1:D:265:LYS:HE3  | 1.98                     | 0.45              |
| 2:E:4:LEU:HA     | 2:E:5:PRO:HD3    | 1.72                     | 0.45              |
| 2:E:98:TRP:HD1   | 2:E:153:VAL:HG11 | 1.81                     | 0.45              |
| 2:E:142:LYS:HG2  | 2:E:144:TYR:H    | 1.81                     | 0.45              |
| 2:F:26:LYS:HE2   | 2:F:78:TRP:CD1   | 2.51                     | 0.45              |
| 2:F:40:LYS:HB3   | 2:F:44:LEU:HD23  | 1.97                     | 0.45              |
| 2:F:139:LEU:O    | 2:F:142:LYS:HB2  | 2.17                     | 0.45              |
| 1:A:88:ILE:HG22  | 1:A:89:LEU:HG    | 1.98                     | 0.45              |
| 1:A:109:LYS:HA   | 6:A:762:HOH:O    | 2.15                     | 0.45              |
| 1:A:192:VAL:HA   | 1:A:195:SER:HB2  | 1.97                     | 0.45              |
| 1:A:477:ILE:O    | 1:A:520:LEU:HD12 | 2.16                     | 0.45              |
| 2:C:143:PRO:HB2  | 6:D:742:HOH:O    | 2.15                     | 0.45              |
| 1:D:96:ALA:HA    | 1:D:161:PRO:O    | 2.16                     | 0.45              |
| 1:D:162:VAL:HB   | 1:D:556:ALA:HB1  | 1.98                     | 0.45              |
| 1:D:206:LEU:O    | 1:D:210:ILE:HG12 | 2.16                     | 0.45              |
| 2:E:169:LYS:HB2  | 2:E:169:LYS:HE3  | 1.74                     | 0.45              |
| 2:C:139:LEU:HD23 | 2:C:141:ASP:HA   | 1.98                     | 0.45              |
| 1:D:99:LEU:HA    | 1:D:109:LYS:O    | 2.17                     | 0.45              |
| 1:D:101:SER:HB3  | 1:D:535:PHE:CE2  | 2.52                     | 0.45              |
| 2:E:173:PHE:HB3  | 2:E:174:SER:H    | 1.62                     | 0.45              |
| 2:F:213:ARG:C    | 6:F:402:HOH:O    | 2.60                     | 0.45              |
| 4:A:602:LEU:HD12 | 4:A:602:LEU:HA   | 1.84                     | 0.45              |
| 2:B:45:LEU:N     | 6:B:428:HOH:O    | 2.48                     | 0.45              |
| 1:D:108:PRO:CG   | 1:D:552:LYS:H    | 2.04                     | 0.45              |
| 1:D:114:THR:HG22 | 1:D:115:ASP:N    | 2.30                     | 0.45              |
| 1:D:357:ASN:ND2  | 6:D:815:HOH:O    | 2.40                     | 0.45              |
| 1:D:489:VAL:HG11 | 6:D:892:HOH:O    | 2.16                     | 0.45              |
| 1:D:496:CYS:N    | 1:D:499:ARG:HH12 | 2.14                     | 0.45              |
| 1:D:519:GLU:OE2  | 1:D:569:SER:OG   | 2.35                     | 0.45              |
| 2:E:197:LYS:HA   | 6:E:502:HOH:O    | 2.17                     | 0.45              |
| 2:F:154:ASP:OD1  | 2:F:185:TRP:NE1  | 2.43                     | 0.45              |
| 1:A:527:THR:HG23 | 1:A:561:ILE:CG2  | 2.46                     | 0.45              |
| 2:B:153:VAL:HG23 | 2:B:156:SER:HB2  | 1.99                     | 0.45              |
| 1:D:221:ALA:HB3  | 1:D:227:LEU:HG   | 1.98                     | 0.45              |
| 1:D:242:VAL:HG21 | 1:D:278:ARG:HH21 | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:125:LYS:HD2  | 2:E:173:PHE:CE1  | 2.51                     | 0.45              |
| 1:A:353:ALA:HB2  | 1:A:413:TYR:HD2  | 1.82                     | 0.45              |
| 1:A:449:ALA:O    | 1:A:452:LEU:HB2  | 2.17                     | 0.45              |
| 2:C:168:GLU:HA   | 6:C:447:HOH:O    | 2.15                     | 0.45              |
| 1:D:198:VAL:CG2  | 1:D:565:ASN:HD21 | 2.29                     | 0.45              |
| 2:F:205:ILE:HG23 | 6:F:420:HOH:O    | 2.17                     | 0.45              |
| 1:A:97:ILE:HD13  | 1:A:112:PRO:HA   | 1.99                     | 0.45              |
| 1:D:355:ILE:HG22 | 6:D:830:HOH:O    | 2.17                     | 0.45              |
| 1:D:475:TYR:CE1  | 1:D:506:TYR:HE1  | 2.35                     | 0.45              |
| 1:D:499:ARG:C    | 2:E:188:ARG:HH12 | 2.19                     | 0.45              |
| 1:A:245:ILE:HD13 | 1:A:245:ILE:HA   | 1.75                     | 0.45              |
| 1:A:375:LYS:C    | 6:A:766:HOH:O    | 2.60                     | 0.45              |
| 1:A:551:VAL:HG13 | 1:A:555:ASN:CB   | 2.46                     | 0.45              |
| 2:C:121:GLN:NE2  | 6:C:424:HOH:O    | 2.50                     | 0.45              |
| 2:C:182:LEU:HD22 | 6:C:449:HOH:O    | 2.17                     | 0.45              |
| 1:D:60:ALA:HB1   | 1:D:64:MET:HE3   | 1.98                     | 0.45              |
| 2:E:68:LEU:HB2   | 2:E:152:TYR:OH   | 2.16                     | 0.45              |
| 2:F:69:ASN:ND2   | 6:F:428:HOH:O    | 2.50                     | 0.45              |
| 1:A:288:TYR:CZ   | 1:A:321:GLY:HA2  | 2.52                     | 0.45              |
| 2:B:27:GLY:O     | 6:B:425:HOH:O    | 2.21                     | 0.45              |
| 2:B:128:PHE:O    | 2:B:132:VAL:HG12 | 2.16                     | 0.45              |
| 2:B:205:ILE:HG23 | 6:B:478:HOH:O    | 2.17                     | 0.45              |
| 1:D:10:MET:O     | 1:D:14:ILE:HG23  | 2.17                     | 0.45              |
| 1:D:77:ILE:HD13  | 1:D:112:PRO:HD3  | 1.99                     | 0.45              |
| 1:D:340:ASN:O    | 6:D:760:HOH:O    | 2.21                     | 0.45              |
| 1:D:494:CYS:SG   | 1:D:495:ASN:N    | 2.90                     | 0.45              |
| 2:E:25:GLU:CB    | 6:E:455:HOH:O    | 2.64                     | 0.45              |
| 2:E:93:ALA:O     | 2:F:69:ASN:ND2   | 2.48                     | 0.45              |
| 2:E:159:THR:HA   | 2:E:199:LEU:HD21 | 1.98                     | 0.45              |
| 2:F:17:MET:SD    | 2:F:199:LEU:HG   | 2.57                     | 0.45              |
| 1:A:488:ASP:OD2  | 2:B:168:GLU:CD   | 2.60                     | 0.44              |
| 1:A:552:LYS:CD   | 1:A:553:PRO:HD2  | 2.47                     | 0.44              |
| 2:C:117:LYS:CD   | 2:C:213:ARG:HH11 | 2.29                     | 0.44              |
| 1:D:222:VAL:HG12 | 1:D:223:PHE:CD1  | 2.53                     | 0.44              |
| 1:D:403:LEU:HD23 | 1:D:540:SER:HG   | 1.82                     | 0.44              |
| 1:D:455:GLU:HG3  | 6:E:541:HOH:O    | 2.17                     | 0.44              |
| 2:E:140:GLY:N    | 2:E:181:LYS:HZ1  | 2.15                     | 0.44              |
| 2:F:152:TYR:O    | 2:F:155:ILE:HB   | 2.17                     | 0.44              |
| 2:F:169:LYS:NZ   | 2:F:206:VAL:HG13 | 2.33                     | 0.44              |
| 1:A:231:PHE:CD1  | 1:A:290:LEU:HD22 | 2.51                     | 0.44              |
| 1:A:325:LEU:O    | 6:A:742:HOH:O    | 2.21                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:98:TRP:CD1   | 2:B:153:VAL:HG21 | 2.52                     | 0.44              |
| 2:C:21:VAL:HG22  | 2:C:194:SER:O    | 2.17                     | 0.44              |
| 1:D:314:PRO:CB   | 1:D:317:ARG:HH12 | 2.26                     | 0.44              |
| 2:E:133:LYS:HB2  | 6:E:493:HOH:O    | 2.17                     | 0.44              |
| 2:E:145:PHE:CD2  | 2:E:157:LEU:HD21 | 2.53                     | 0.44              |
| 2:F:13:SER:O     | 2:F:17:MET:HG3   | 2.18                     | 0.44              |
| 1:A:162:VAL:HG21 | 1:A:559:LEU:HD23 | 1.98                     | 0.44              |
| 1:A:179:MET:HE3  | 1:A:183:THR:HG21 | 2.00                     | 0.44              |
| 1:A:331:GLY:HA2  | 1:A:539:GLY:N    | 2.33                     | 0.44              |
| 1:A:365:PRO:HG3  | 1:A:388:TYR:CZ   | 2.53                     | 0.44              |
| 2:B:4:LEU:HA     | 2:B:5:PRO:HD3    | 1.69                     | 0.44              |
| 2:C:11:TRP:CG    | 2:C:12:PRO:HD3   | 2.52                     | 0.44              |
| 2:C:17:MET:HE1   | 2:C:205:ILE:HD11 | 1.98                     | 0.44              |
| 1:D:330:TYR:CE1  | 1:D:536:LEU:O    | 2.68                     | 0.44              |
| 2:E:34:GLU:CD    | 2:E:34:GLU:N     | 2.75                     | 0.44              |
| 2:E:81:LYS:HD2   | 6:E:456:HOH:O    | 2.17                     | 0.44              |
| 2:E:130:GLU:O    | 2:E:134:ILE:HG22 | 2.17                     | 0.44              |
| 1:A:9:ASP:OD1    | 6:A:744:HOH:O    | 2.21                     | 0.44              |
| 1:A:338:ALA:N    | 6:A:725:HOH:O    | 2.48                     | 0.44              |
| 1:A:370:GLY:HA2  | 1:A:371:GLU:HA   | 1.70                     | 0.44              |
| 1:A:389:GLU:HA   | 1:A:405:ASP:O    | 2.18                     | 0.44              |
| 2:B:9:ASP:HB2    | 2:B:20:ARG:NH2   | 2.32                     | 0.44              |
| 2:B:73:TYR:CE1   | 2:C:93:ALA:CB    | 3.01                     | 0.44              |
| 1:D:80:MET:HG2   | 1:D:86:SER:O     | 2.17                     | 0.44              |
| 1:D:101:SER:N    | 1:D:535:PHE:CZ   | 2.85                     | 0.44              |
| 1:D:440:ASP:OD2  | 1:D:502:ILE:HG12 | 2.17                     | 0.44              |
| 1:D:490:LEU:HD13 | 1:D:568:SER:OG   | 2.16                     | 0.44              |
| 1:A:208:SER:O    | 1:A:211:LEU:HB2  | 2.18                     | 0.44              |
| 1:A:500:ALA:CA   | 2:B:188:ARG:HH12 | 2.29                     | 0.44              |
| 2:B:15:PHE:CE1   | 5:B:301:GSH:HB12 | 2.52                     | 0.44              |
| 2:B:26:LYS:HD2   | 2:B:74:VAL:CG1   | 2.48                     | 0.44              |
| 2:B:169:LYS:HD3  | 2:B:206:VAL:HG13 | 1.99                     | 0.44              |
| 1:D:491:GLN:NE2  | 1:D:570:TYR:CD2  | 2.86                     | 0.44              |
| 1:A:169:VAL:O    | 1:A:175:PHE:HB2  | 2.18                     | 0.44              |
| 1:A:454:GLU:HG3  | 6:B:426:HOH:O    | 2.16                     | 0.44              |
| 1:A:495:ASN:HB3  | 1:A:499:ARG:HH11 | 1.81                     | 0.44              |
| 2:C:129:ILE:HG13 | 2:C:129:ILE:H    | 1.70                     | 0.44              |
| 2:C:132:VAL:HG21 | 2:C:175:ILE:CG2  | 2.47                     | 0.44              |
| 1:D:35:ILE:HD11  | 1:D:359:GLY:HA2  | 1.99                     | 0.44              |
| 1:D:478:PHE:CE2  | 1:D:562:LEU:HB2  | 2.52                     | 0.44              |
| 2:E:131:ALA:O    | 2:E:135:LEU:HB2  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:137:SER:HB2  | 6:F:453:HOH:O    | 2.17                     | 0.44              |
| 1:A:392:ILE:HD11 | 1:A:539:GLY:O    | 2.17                     | 0.44              |
| 1:A:403:LEU:HD23 | 1:A:403:LEU:HA   | 1.81                     | 0.44              |
| 1:D:270:ASN:HA   | 1:D:271:PRO:HD2  | 1.83                     | 0.44              |
| 1:D:492:ASP:OD1  | 2:E:176:GLU:HG3  | 2.18                     | 0.44              |
| 1:D:499:ARG:NH1  | 2:E:184:ALA:CB   | 2.79                     | 0.44              |
| 2:E:73:TYR:CZ    | 2:F:93:ALA:HB1   | 2.53                     | 0.44              |
| 2:E:129:ILE:HA   | 2:E:132:VAL:HG12 | 1.99                     | 0.44              |
| 2:F:7:LEU:O      | 2:F:33:ARG:HB2   | 2.18                     | 0.44              |
| 1:A:452:LEU:HD13 | 1:A:493:CYS:SG   | 2.58                     | 0.44              |
| 1:A:525:LYS:HG3  | 6:A:816:HOH:O    | 2.18                     | 0.44              |
| 2:B:60:ASN:O     | 2:B:60:ASN:ND2   | 2.50                     | 0.44              |
| 2:C:117:LYS:CE   | 2:C:213:ARG:HH11 | 2.28                     | 0.44              |
| 1:D:285:SER:HB2  | 6:D:931:HOH:O    | 2.17                     | 0.44              |
| 1:A:149:PHE:CZ   | 1:A:205:HIS:CD2  | 3.00                     | 0.44              |
| 1:A:226:GLY:CA   | 1:A:529:ARG:HD2  | 2.48                     | 0.44              |
| 1:A:330:TYR:HE1  | 1:A:536:LEU:O    | 2.01                     | 0.44              |
| 2:B:23:LEU:CD2   | 2:B:28:VAL:HG11  | 2.42                     | 0.44              |
| 2:B:97:PHE:CZ    | 2:C:65:CYS:HB2   | 2.53                     | 0.44              |
| 2:C:11:TRP:HB3   | 2:C:34:GLU:OE1   | 2.18                     | 0.44              |
| 2:C:59:HIS:HB3   | 2:C:73:TYR:OH    | 2.17                     | 0.44              |
| 1:D:18:ASP:OD1   | 1:D:414:ASN:ND2  | 2.51                     | 0.44              |
| 1:D:143:LYS:NZ   | 1:D:212:PHE:CD1  | 2.86                     | 0.44              |
| 1:D:196:PRO:HA   | 1:D:565:ASN:OD1  | 2.18                     | 0.44              |
| 1:D:223:PHE:HZ   | 1:D:536:LEU:HB2  | 1.83                     | 0.44              |
| 1:D:252:ASN:N    | 6:D:801:HOH:O    | 2.35                     | 0.44              |
| 1:D:477:ILE:HG12 | 1:D:518:LEU:HD21 | 2.00                     | 0.44              |
| 1:D:477:ILE:HG21 | 1:D:497:LEU:HD22 | 1.99                     | 0.44              |
| 2:E:113:VAL:HG23 | 2:E:125:LYS:HG2  | 2.00                     | 0.44              |
| 1:A:25:HIS:CE1   | 1:A:380:THR:HG21 | 2.52                     | 0.43              |
| 1:A:167:THR:HB   | 1:A:560:GLN:OE1  | 2.18                     | 0.43              |
| 1:A:170:TYR:OH   | 4:A:602:LEU:HD23 | 2.18                     | 0.43              |
| 1:A:245:ILE:HG23 | 1:A:245:ILE:HD12 | 1.72                     | 0.43              |
| 1:A:465:TYR:HA   | 1:A:551:VAL:O    | 2.18                     | 0.43              |
| 1:A:474:HIS:HB3  | 6:A:737:HOH:O    | 2.17                     | 0.43              |
| 1:A:486:ASN:HB3  | 6:B:459:HOH:O    | 2.17                     | 0.43              |
| 2:B:98:TRP:CE3   | 2:B:98:TRP:O     | 2.70                     | 0.43              |
| 1:D:114:THR:HB   | 6:D:951:HOH:O    | 2.18                     | 0.43              |
| 1:D:272:GLU:O    | 1:D:275:GLU:HB3  | 2.17                     | 0.43              |
| 1:D:351:THR:HG21 | 1:D:410:ILE:CG1  | 2.43                     | 0.43              |
| 2:E:5:PRO:HG2    | 2:E:28:VAL:CG2   | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:9:ASP:OD1    | 2:F:10:TYR:N     | 2.37                     | 0.43              |
| 2:F:106:PHE:CZ   | 2:F:132:VAL:HG23 | 2.53                     | 0.43              |
| 1:A:99:LEU:HB3   | 1:A:557:LYS:CB   | 2.47                     | 0.43              |
| 1:A:124:LEU:HB3  | 3:A:601:JAA:C15  | 2.48                     | 0.43              |
| 1:A:197:ASP:O    | 6:A:745:HOH:O    | 2.21                     | 0.43              |
| 1:A:253:ARG:HA   | 1:A:484:GLU:OE2  | 2.18                     | 0.43              |
| 1:A:330:TYR:CZ   | 1:A:538:LEU:O    | 2.70                     | 0.43              |
| 1:A:464:SER:O    | 1:A:551:VAL:N    | 2.44                     | 0.43              |
| 2:B:84:PHE:HD1   | 2:B:85:PHE:N     | 2.15                     | 0.43              |
| 1:D:73:LEU:HD22  | 1:D:89:LEU:HD21  | 1.99                     | 0.43              |
| 1:D:91:GLY:O     | 1:D:92:HIS:C     | 2.61                     | 0.43              |
| 1:D:205:HIS:HA   | 1:D:208:SER:HB2  | 2.00                     | 0.43              |
| 2:E:71:VAL:HB    | 6:E:473:HOH:O    | 2.19                     | 0.43              |
| 2:E:72:GLN:HE21  | 2:F:96:ARG:HD2   | 1.83                     | 0.43              |
| 2:E:81:LYS:HG3   | 6:E:411:HOH:O    | 2.18                     | 0.43              |
| 2:E:188:ARG:HA   | 2:E:188:ARG:HD3  | 1.70                     | 0.43              |
| 1:A:143:LYS:HG3  | 1:A:216:VAL:HG22 | 2.00                     | 0.43              |
| 1:A:463:SER:HB2  | 1:A:528:PHE:CE1  | 2.47                     | 0.43              |
| 2:B:70:VAL:HA    | 2:B:73:TYR:CD2   | 2.54                     | 0.43              |
| 2:B:140:GLY:N    | 2:B:181:LYS:NZ   | 2.67                     | 0.43              |
| 2:F:4:LEU:HA     | 2:F:5:PRO:HD3    | 1.83                     | 0.43              |
| 2:F:145:PHE:O    | 6:F:417:HOH:O    | 2.21                     | 0.43              |
| 1:A:222:VAL:HB   | 1:A:533:GLU:HB3  | 2.00                     | 0.43              |
| 1:A:342:THR:N    | 6:A:772:HOH:O    | 2.38                     | 0.43              |
| 1:A:393:THR:HG23 | 1:A:399:TYR:CD1  | 2.53                     | 0.43              |
| 2:B:72:GLN:O     | 2:B:76:GLU:HG2   | 2.18                     | 0.43              |
| 1:D:107:ARG:HA   | 1:D:108:PRO:HD3  | 1.83                     | 0.43              |
| 1:D:239:GLU:O    | 1:D:242:VAL:HG22 | 2.17                     | 0.43              |
| 1:D:459:VAL:HG22 | 1:D:481:ILE:HG22 | 2.01                     | 0.43              |
| 2:E:98:TRP:O     | 2:E:102:VAL:HG23 | 2.19                     | 0.43              |
| 2:E:178:GLU:HG2  | 6:E:449:HOH:O    | 2.18                     | 0.43              |
| 2:E:201:ASP:C    | 6:E:441:HOH:O    | 2.61                     | 0.43              |
| 2:F:54:ILE:HB    | 2:F:55:PRO:HA    | 2.00                     | 0.43              |
| 2:F:106:PHE:HZ   | 2:F:132:VAL:HG23 | 1.83                     | 0.43              |
| 1:A:53:ASN:HB3   | 1:A:54:ALA:H     | 1.43                     | 0.43              |
| 1:A:131:PHE:HD1  | 1:A:134:ARG:NH2  | 2.16                     | 0.43              |
| 1:A:425:ARG:HG3  | 6:A:758:HOH:O    | 2.19                     | 0.43              |
| 1:A:464:SER:HA   | 1:A:476:ALA:O    | 2.17                     | 0.43              |
| 1:A:488:ASP:OD2  | 2:B:168:GLU:OE2  | 2.36                     | 0.43              |
| 1:A:499:ARG:NH1  | 2:B:184:ALA:CB   | 2.80                     | 0.43              |
| 1:A:549:ARG:HG2  | 6:A:863:HOH:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:116:LYS:HB3  | 2:B:116:LYS:HE3  | 1.85                     | 0.43              |
| 2:C:37:PHE:CZ    | 5:C:301:GSH:HA32 | 2.54                     | 0.43              |
| 2:C:87:SER:N     | 6:C:434:HOH:O    | 2.51                     | 0.43              |
| 2:C:102:VAL:HA   | 2:C:106:PHE:HB3  | 2.00                     | 0.43              |
| 1:D:199:HIS:CE1  | 1:D:200:GLN:HE21 | 2.37                     | 0.43              |
| 1:D:291:ILE:HD12 | 1:D:320:ALA:HA   | 1.99                     | 0.43              |
| 1:D:295:PHE:HB2  | 6:D:731:HOH:O    | 2.19                     | 0.43              |
| 1:D:451:ARG:NH1  | 1:D:454:GLU:OE2  | 2.51                     | 0.43              |
| 1:D:477:ILE:O    | 1:D:520:LEU:HD12 | 2.19                     | 0.43              |
| 2:E:114:TRP:HA   | 2:E:170:PHE:CD2  | 2.44                     | 0.43              |
| 1:A:450:LYS:NZ   | 2:B:191:GLU:HA   | 2.33                     | 0.43              |
| 2:B:170:PHE:HB3  | 6:B:418:HOH:O    | 2.19                     | 0.43              |
| 2:C:130:GLU:O    | 2:C:133:LYS:HB3  | 2.19                     | 0.43              |
| 2:C:142:LYS:CA   | 1:D:91:GLY:HA3   | 2.48                     | 0.43              |
| 2:C:201:ASP:CB   | 2:C:203:GLU:HG2  | 2.48                     | 0.43              |
| 1:D:223:PHE:HZ   | 1:D:536:LEU:CB   | 2.32                     | 0.43              |
| 1:D:389:GLU:OE2  | 1:D:402:ARG:HG3  | 2.19                     | 0.43              |
| 2:E:98:TRP:CD1   | 2:E:153:VAL:HG21 | 2.53                     | 0.43              |
| 1:A:223:PHE:CZ   | 1:A:536:LEU:CB   | 3.01                     | 0.43              |
| 1:A:332:SER:HB3  | 1:A:538:LEU:HD13 | 2.01                     | 0.43              |
| 2:C:65:CYS:O     | 2:C:66:GLU:HB2   | 2.19                     | 0.43              |
| 1:D:58:GLU:OE2   | 1:D:360:TYR:OH   | 2.27                     | 0.43              |
| 1:D:304:ILE:HG13 | 1:D:328:HIS:HB3  | 2.01                     | 0.43              |
| 1:D:417:PRO:HD2  | 6:D:888:HOH:O    | 2.18                     | 0.43              |
| 1:D:448:ALA:CB   | 1:D:496:CYS:HB3  | 2.46                     | 0.43              |
| 1:D:569:SER:C    | 1:D:570:TYR:CD1  | 2.97                     | 0.43              |
| 2:F:54:ILE:HG13  | 5:F:301:GSH:HB23 | 2.01                     | 0.43              |
| 1:A:77:ILE:CG2   | 1:A:97:ILE:HD12  | 2.49                     | 0.43              |
| 1:A:401:TYR:HE2  | 1:A:403:LEU:HD23 | 1.83                     | 0.43              |
| 1:A:499:ARG:HH12 | 2:B:187:LYS:HZ1  | 1.67                     | 0.43              |
| 2:B:144:TYR:HB3  | 2:B:154:ASP:CG   | 2.43                     | 0.43              |
| 2:B:202:SER:HA   | 2:B:205:ILE:HB   | 2.00                     | 0.43              |
| 1:D:253:ARG:NH1  | 1:D:484:GLU:H    | 2.16                     | 0.43              |
| 2:E:31:GLU:N     | 6:E:428:HOH:O    | 2.52                     | 0.43              |
| 2:E:70:VAL:HA    | 2:E:73:TYR:CD2   | 2.54                     | 0.43              |
| 1:A:198:VAL:CG2  | 1:A:524:ALA:HB3  | 2.48                     | 0.43              |
| 1:A:363:PHE:HD2  | 1:A:382:VAL:CG2  | 2.29                     | 0.43              |
| 1:A:442:GLN:NE2  | 6:A:847:HOH:O    | 2.51                     | 0.43              |
| 1:A:489:VAL:O    | 1:A:492:ASP:HB2  | 2.19                     | 0.43              |
| 1:A:534:HIS:NE2  | 1:A:535:PHE:CE1  | 2.87                     | 0.43              |
| 2:B:179:SER:HA   | 2:B:180:PRO:HD3  | 1.74                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:114:TRP:CG   | 6:C:409:HOH:O    | 2.72                     | 0.43              |
| 2:C:141:ASP:CB   | 1:D:92:HIS:HB2   | 2.49                     | 0.43              |
| 1:D:17:PHE:HZ    | 6:D:732:HOH:O    | 2.02                     | 0.43              |
| 1:D:199:HIS:H    | 1:D:199:HIS:CD2  | 2.37                     | 0.43              |
| 2:F:181:LYS:H    | 2:F:181:LYS:HG3  | 1.40                     | 0.43              |
| 1:A:355:ILE:HA   | 1:A:356:PRO:HD3  | 1.89                     | 0.43              |
| 2:B:68:LEU:O     | 2:B:72:GLN:HG3   | 2.19                     | 0.43              |
| 1:D:156:SER:HB3  | 1:D:162:VAL:HG13 | 2.00                     | 0.43              |
| 1:D:256:VAL:O    | 1:D:259:VAL:HG12 | 2.19                     | 0.43              |
| 1:D:370:GLY:HA2  | 1:D:371:GLU:HA   | 1.68                     | 0.43              |
| 2:E:84:PHE:HD1   | 2:E:85:PHE:N     | 2.17                     | 0.43              |
| 2:E:104:LYS:HD2  | 2:E:104:LYS:C    | 2.44                     | 0.43              |
| 2:E:121:GLN:O    | 2:E:125:LYS:HG3  | 2.18                     | 0.43              |
| 2:E:130:GLU:HA   | 6:E:493:HOH:O    | 2.19                     | 0.43              |
| 1:A:17:PHE:CE2   | 1:A:341:VAL:HG11 | 2.54                     | 0.42              |
| 2:B:50:ILE:HG13  | 2:B:51:HIS:H     | 1.83                     | 0.42              |
| 2:B:92:ARG:HB2   | 6:C:405:HOH:O    | 2.20                     | 0.42              |
| 2:B:93:ALA:O     | 2:B:97:PHE:HB2   | 2.18                     | 0.42              |
| 2:C:101:PHE:HE1  | 2:C:105:LYS:HE3  | 1.84                     | 0.42              |
| 2:C:151:GLY:N    | 6:C:412:HOH:O    | 2.51                     | 0.42              |
| 1:D:84:ASP:O     | 1:D:86:SER:N     | 2.52                     | 0.42              |
| 1:D:128:ALA:HB2  | 1:D:329:ASP:OD2  | 2.19                     | 0.42              |
| 1:D:198:VAL:HB   | 1:D:524:ALA:HB3  | 2.00                     | 0.42              |
| 4:D:602:LEU:HD12 | 4:D:602:LEU:HA   | 1.85                     | 0.42              |
| 1:A:11:ASN:O     | 1:A:14:ILE:HG13  | 2.19                     | 0.42              |
| 1:A:20:MET:HE2   | 1:A:356:PRO:HD2  | 2.01                     | 0.42              |
| 1:A:149:PHE:HZ   | 1:A:202:LEU:HA   | 1.83                     | 0.42              |
| 1:A:151:SER:O    | 1:A:171:ARG:NH2  | 2.52                     | 0.42              |
| 1:A:503:ASP:CG   | 1:A:505:GLY:H    | 2.25                     | 0.42              |
| 2:B:71:VAL:O     | 2:B:74:VAL:HB    | 2.18                     | 0.42              |
| 1:D:28:GLN:NE2   | 1:D:359:GLY:O    | 2.52                     | 0.42              |
| 1:D:107:ARG:NH1  | 1:D:434:ASP:N    | 2.57                     | 0.42              |
| 1:D:111:ILE:HD11 | 1:D:334:GLU:HA   | 2.01                     | 0.42              |
| 1:D:193:ILE:HG12 | 1:D:205:HIS:CE1  | 2.54                     | 0.42              |
| 1:D:363:PHE:CE1  | 1:D:390:VAL:HG22 | 2.54                     | 0.42              |
| 1:D:478:PHE:CZ   | 1:D:562:LEU:HD22 | 2.53                     | 0.42              |
| 2:E:84:PHE:HB2   | 2:E:152:TYR:N    | 2.33                     | 0.42              |
| 1:A:28:GLN:CG    | 1:A:379:LEU:HD21 | 2.49                     | 0.42              |
| 1:A:114:THR:HG22 | 1:A:115:ASP:H    | 1.85                     | 0.42              |
| 1:A:175:PHE:HE2  | 6:A:996:HOH:O    | 2.02                     | 0.42              |
| 1:A:475:TYR:CE2  | 1:A:506:TYR:HE1  | 2.37                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:477:ILE:HG12 | 1:A:518:LEU:HD21 | 2.00                     | 0.42              |
| 1:A:552:LYS:HD2  | 1:A:553:PRO:HD2  | 2.01                     | 0.42              |
| 2:B:182:LEU:HB3  | 6:B:414:HOH:O    | 2.19                     | 0.42              |
| 2:B:211:GLU:O    | 2:B:214:LYS:HG2  | 2.19                     | 0.42              |
| 2:C:114:TRP:N    | 6:C:409:HOH:O    | 2.52                     | 0.42              |
| 2:C:148:ASP:N    | 2:C:148:ASP:OD1  | 2.51                     | 0.42              |
| 1:D:198:VAL:HG23 | 1:D:565:ASN:ND2  | 2.31                     | 0.42              |
| 2:E:93:ALA:O     | 2:E:97:PHE:HB2   | 2.18                     | 0.42              |
| 1:A:97:ILE:N     | 6:A:735:HOH:O    | 2.52                     | 0.42              |
| 1:A:189:PRO:O    | 1:A:192:VAL:HG12 | 2.19                     | 0.42              |
| 1:A:534:HIS:CD2  | 1:A:557:LYS:HE2  | 2.54                     | 0.42              |
| 1:A:551:VAL:HG11 | 1:A:559:LEU:CD1  | 2.44                     | 0.42              |
| 2:B:9:ASP:HB2    | 2:B:20:ARG:HH21  | 1.84                     | 0.42              |
| 2:B:10:TYR:HB3   | 2:B:13:SER:HB2   | 2.01                     | 0.42              |
| 2:C:16:GLY:O     | 2:C:20:ARG:HG3   | 2.19                     | 0.42              |
| 2:C:18:ARG:HH21  | 2:C:160:PHE:HE1  | 1.66                     | 0.42              |
| 2:C:40:LYS:HE3   | 2:C:40:LYS:HB2   | 1.92                     | 0.42              |
| 2:C:137:SER:O    | 6:C:426:HOH:O    | 2.22                     | 0.42              |
| 2:C:183:ILE:HD12 | 2:C:183:ILE:N    | 2.34                     | 0.42              |
| 1:D:223:PHE:HE2  | 1:D:545:PHE:HZ   | 1.68                     | 0.42              |
| 1:D:244:ASP:OD1  | 1:D:251:SER:HB2  | 2.19                     | 0.42              |
| 1:D:407:VAL:CG2  | 1:D:419:LEU:HB3  | 2.48                     | 0.42              |
| 2:E:53:LYS:HG2   | 5:E:301:GSH:CA3  | 2.46                     | 0.42              |
| 2:E:181:LYS:C    | 2:E:184:ALA:HB3  | 2.45                     | 0.42              |
| 1:A:32:LEU:HD21  | 1:A:61:PHE:CD2   | 2.51                     | 0.42              |
| 1:A:77:ILE:HA    | 1:A:80:MET:SD    | 2.59                     | 0.42              |
| 1:A:121:THR:HA   | 3:A:601:JAA:C15  | 2.50                     | 0.42              |
| 1:A:152:LYS:HG2  | 1:A:565:ASN:H    | 1.85                     | 0.42              |
| 1:A:316:LEU:O    | 1:A:320:ALA:N    | 2.50                     | 0.42              |
| 1:A:438:GLU:O    | 1:A:442:GLN:HB2  | 2.19                     | 0.42              |
| 1:A:450:LYS:HA   | 1:A:453:SER:HB3  | 2.01                     | 0.42              |
| 2:B:98:TRP:O     | 2:B:102:VAL:HG23 | 2.19                     | 0.42              |
| 2:B:114:TRP:HA   | 2:B:170:PHE:CD2  | 2.53                     | 0.42              |
| 2:C:116:LYS:O    | 6:C:424:HOH:O    | 2.20                     | 0.42              |
| 2:C:175:ILE:HG22 | 2:C:183:ILE:HD11 | 2.01                     | 0.42              |
| 1:D:334:GLU:HB2  | 1:D:538:LEU:CD1  | 2.49                     | 0.42              |
| 1:D:499:ARG:CZ   | 2:E:184:ALA:CB   | 2.93                     | 0.42              |
| 2:E:21:VAL:HG12  | 2:E:155:ILE:HG12 | 2.02                     | 0.42              |
| 2:E:97:PHE:CE1   | 2:F:65:CYS:HB2   | 2.55                     | 0.42              |
| 2:F:170:PHE:N    | 6:F:412:HOH:O    | 2.52                     | 0.42              |
| 1:A:39:ASN:ND2   | 1:A:90:THR:O     | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:101:SER:N    | 1:A:535:PHE:CE1  | 2.88                     | 0.42              |
| 1:A:361:PHE:CE1  | 1:A:392:ILE:HG23 | 2.55                     | 0.42              |
| 2:B:107:THR:HG22 | 2:B:160:PHE:CZ   | 2.55                     | 0.42              |
| 1:D:152:LYS:CB   | 1:D:561:ILE:HA   | 2.47                     | 0.42              |
| 1:D:265:LYS:HG3  | 6:D:845:HOH:O    | 2.19                     | 0.42              |
| 1:D:487:GLU:HG2  | 1:D:570:TYR:OH   | 2.19                     | 0.42              |
| 2:E:126:LYS:O    | 2:E:129:ILE:HG13 | 2.20                     | 0.42              |
| 2:E:184:ALA:HA   | 2:E:187:LYS:NZ   | 2.34                     | 0.42              |
| 2:F:77:ALA:C     | 2:F:79:PRO:HD3   | 2.44                     | 0.42              |
| 1:A:38:LYS:HB2   | 6:A:770:HOH:O    | 2.19                     | 0.42              |
| 1:A:339:ALA:N    | 1:A:353:ALA:O    | 2.51                     | 0.42              |
| 1:A:460:ILE:HD11 | 1:A:482:SER:HB3  | 2.00                     | 0.42              |
| 1:A:527:THR:O    | 1:A:530:LYS:HB2  | 2.20                     | 0.42              |
| 2:B:34:GLU:CD    | 2:B:34:GLU:N     | 2.77                     | 0.42              |
| 1:D:461:ASP:HA   | 6:D:841:HOH:O    | 2.20                     | 0.42              |
| 1:D:536:LEU:HD11 | 6:D:721:HOH:O    | 2.20                     | 0.42              |
| 2:E:5:PRO:HG2    | 2:E:28:VAL:HG21  | 2.01                     | 0.42              |
| 2:E:23:LEU:CD2   | 2:E:28:VAL:HG11  | 2.48                     | 0.42              |
| 2:E:98:TRP:HH2   | 2:E:135:LEU:HD11 | 1.84                     | 0.42              |
| 2:E:120:GLU:HB3  | 6:E:413:HOH:O    | 2.19                     | 0.42              |
| 2:F:9:ASP:OD1    | 2:F:16:GLY:HA3   | 2.20                     | 0.42              |
| 2:F:110:GLN:O    | 2:F:113:VAL:HB   | 2.20                     | 0.42              |
| 2:F:117:LYS:CG   | 2:F:213:ARG:HH11 | 2.02                     | 0.42              |
| 1:A:19:GLU:C     | 1:A:23:ASN:HD22  | 2.18                     | 0.42              |
| 1:A:242:VAL:HG11 | 1:A:278:ARG:HH21 | 1.85                     | 0.42              |
| 1:A:284:LEU:HD22 | 1:A:287:TRP:HA   | 2.01                     | 0.42              |
| 1:A:434:ASP:O    | 1:A:550:CYS:HB3  | 2.20                     | 0.42              |
| 1:D:475:TYR:CZ   | 1:D:506:TYR:HE1  | 2.38                     | 0.42              |
| 1:D:563:CYS:O    | 1:D:566:VAL:HG13 | 2.18                     | 0.42              |
| 2:E:167:TYR:HB2  | 6:E:458:HOH:O    | 2.20                     | 0.42              |
| 1:A:43:ILE:HD11  | 1:A:88:ILE:HG23  | 2.02                     | 0.42              |
| 1:A:222:VAL:HG12 | 1:A:223:PHE:CE1  | 2.55                     | 0.42              |
| 1:A:246:LYS:HD2  | 1:A:274:ALA:CB   | 2.49                     | 0.42              |
| 1:A:314:PRO:HB3  | 1:A:317:ARG:HH12 | 1.84                     | 0.42              |
| 1:A:335:GLY:C    | 6:A:711:HOH:O    | 2.63                     | 0.42              |
| 2:B:5:PRO:HG2    | 2:B:28:VAL:CG2   | 2.50                     | 0.42              |
| 2:B:89:PRO:HD3   | 6:B:484:HOH:O    | 2.20                     | 0.42              |
| 2:C:53:LYS:HD2   | 5:C:301:GSH:HB13 | 2.02                     | 0.42              |
| 1:D:222:VAL:HB   | 1:D:533:GLU:CD   | 2.44                     | 0.42              |
| 1:D:302:TYR:HD1  | 1:D:326:VAL:HG13 | 1.83                     | 0.42              |
| 1:D:336:TRP:CB   | 1:D:358:LEU:HD13 | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:450:LYS:HD3  | 2:E:190:MET:O    | 2.20                     | 0.42              |
| 2:E:96:ARG:NH1   | 2:F:69:ASN:OD1   | 2.53                     | 0.42              |
| 2:E:97:PHE:HZ    | 2:F:48:ASN:ND2   | 2.13                     | 0.42              |
| 2:F:8:LEU:HB2    | 2:F:56:VAL:HB    | 2.02                     | 0.42              |
| 1:A:83:GLY:N     | 1:A:158:GLY:HA3  | 2.35                     | 0.42              |
| 1:A:84:ASP:O     | 1:A:86:SER:N     | 2.52                     | 0.42              |
| 1:A:212:PHE:HB3  | 1:A:215:GLN:HE21 | 1.85                     | 0.42              |
| 1:A:242:VAL:HG22 | 1:A:277:ILE:HG21 | 2.02                     | 0.42              |
| 2:B:68:LEU:HB2   | 2:B:152:TYR:OH   | 2.20                     | 0.42              |
| 2:C:154:ASP:HA   | 2:C:185:TRP:HZ2  | 1.85                     | 0.42              |
| 1:D:36:LEU:HD22  | 1:D:61:PHE:CZ    | 2.55                     | 0.42              |
| 1:D:80:MET:HE2   | 1:D:88:ILE:H     | 1.84                     | 0.42              |
| 2:E:90:TYR:O     | 2:E:94:GLN:HG3   | 2.20                     | 0.42              |
| 2:E:113:VAL:HG21 | 2:E:128:PHE:HE2  | 1.84                     | 0.42              |
| 1:A:377:VAL:HG12 | 1:A:381:GLN:HB3  | 2.02                     | 0.41              |
| 1:A:393:THR:HG23 | 1:A:399:TYR:HD1  | 1.85                     | 0.41              |
| 2:B:76:GLU:HG3   | 2:C:89:PRO:HB3   | 2.01                     | 0.41              |
| 2:B:131:ALA:O    | 2:B:135:LEU:HB2  | 2.20                     | 0.41              |
| 1:D:149:PHE:CG   | 1:D:198:VAL:HG13 | 2.55                     | 0.41              |
| 1:D:223:PHE:HE2  | 1:D:545:PHE:CZ   | 2.38                     | 0.41              |
| 1:D:413:TYR:O    | 1:D:416:THR:HG22 | 2.20                     | 0.41              |
| 1:D:498:ASP:HA   | 6:D:757:HOH:O    | 2.19                     | 0.41              |
| 1:A:108:PRO:HG2  | 1:A:552:LYS:CB   | 2.47                     | 0.41              |
| 1:A:252:ASN:HD22 | 1:A:252:ASN:N    | 2.18                     | 0.41              |
| 1:A:448:ALA:HB3  | 1:A:479:TRP:CH2  | 2.55                     | 0.41              |
| 1:A:492:ASP:O    | 2:B:187:LYS:HE3  | 2.20                     | 0.41              |
| 2:B:14:MET:HG3   | 2:B:163:TRP:CH2  | 2.56                     | 0.41              |
| 2:B:150:PHE:CD1  | 2:B:192:LYS:HG3  | 2.54                     | 0.41              |
| 1:D:22:ARG:HH11  | 1:D:414:ASN:CB   | 2.33                     | 0.41              |
| 1:D:22:ARG:HG2   | 1:D:414:ASN:HB3  | 2.03                     | 0.41              |
| 1:D:81:VAL:HG21  | 1:D:110:PHE:CE2  | 2.55                     | 0.41              |
| 1:D:143:LYS:NZ   | 1:D:212:PHE:CG   | 2.82                     | 0.41              |
| 1:D:153:GLN:HA   | 1:D:560:GLN:HG3  | 2.03                     | 0.41              |
| 1:D:451:ARG:HG2  | 2:E:187:LYS:HD2  | 2.02                     | 0.41              |
| 1:D:521:ARG:HH11 | 1:D:562:LEU:CD1  | 2.30                     | 0.41              |
| 2:E:98:TRP:CE3   | 2:E:98:TRP:O     | 2.73                     | 0.41              |
| 2:E:119:GLU:CD   | 6:E:466:HOH:O    | 2.63                     | 0.41              |
| 2:F:201:ASP:OD2  | 2:F:204:LYS:HE2  | 2.20                     | 0.41              |
| 2:F:207:ALA:O    | 2:F:211:GLU:HB2  | 2.19                     | 0.41              |
| 1:A:111:ILE:HA   | 1:A:112:PRO:HD3  | 1.87                     | 0.41              |
| 1:A:338:ALA:HB1  | 1:A:353:ALA:C    | 2.45                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:37:PHE:HD1   | 2:B:40:LYS:HG2   | 1.85                     | 0.41              |
| 2:B:69:ASN:HB2   | 6:B:438:HOH:O    | 2.20                     | 0.41              |
| 2:B:125:LYS:HA   | 2:B:128:PHE:CD2  | 2.54                     | 0.41              |
| 2:C:143:PRO:HD3  | 1:D:90:THR:O     | 2.20                     | 0.41              |
| 1:D:405:ASP:OD2  | 1:D:540:SER:HB2  | 2.20                     | 0.41              |
| 1:D:499:ARG:HB3  | 6:D:747:HOH:O    | 2.19                     | 0.41              |
| 2:E:72:GLN:HE21  | 2:F:96:ARG:CD    | 2.34                     | 0.41              |
| 2:E:114:TRP:CD1  | 2:E:167:TYR:CE1  | 3.04                     | 0.41              |
| 2:E:200:PRO:HD3  | 6:E:479:HOH:O    | 2.20                     | 0.41              |
| 2:F:6:ILE:N      | 2:F:6:ILE:HD12   | 2.35                     | 0.41              |
| 2:B:199:LEU:HA   | 2:B:200:PRO:HD2  | 1.87                     | 0.41              |
| 2:C:18:ARG:HH12  | 2:C:103:ASP:CG   | 2.28                     | 0.41              |
| 1:D:148:ILE:HB   | 1:D:170:TYR:HE2  | 1.86                     | 0.41              |
| 1:D:284:LEU:H    | 1:D:284:LEU:HG   | 1.78                     | 0.41              |
| 1:D:329:ASP:N    | 1:D:329:ASP:OD1  | 2.51                     | 0.41              |
| 2:E:151:GLY:N    | 2:E:154:ASP:OD2  | 2.52                     | 0.41              |
| 1:A:246:LYS:HD2  | 1:A:274:ALA:HB2  | 2.01                     | 0.41              |
| 1:A:365:PRO:HA   | 1:A:388:TYR:CD1  | 2.56                     | 0.41              |
| 1:A:410:ILE:HG13 | 1:A:411:GLY:N    | 2.35                     | 0.41              |
| 1:A:472:PRO:HG2  | 1:A:516:GLY:CA   | 2.51                     | 0.41              |
| 2:B:15:PHE:CD2   | 5:B:301:GSH:HG13 | 2.56                     | 0.41              |
| 2:B:26:LYS:HG2   | 2:B:81:LYS:HZ1   | 1.79                     | 0.41              |
| 1:D:30:GLN:OE1   | 1:D:30:GLN:HA    | 2.21                     | 0.41              |
| 1:D:165:ALA:HB3  | 6:D:709:HOH:O    | 2.21                     | 0.41              |
| 1:D:549:ARG:HD3  | 1:D:549:ARG:HA   | 1.70                     | 0.41              |
| 1:A:8:PHE:CD1    | 1:A:182:ILE:HG23 | 2.56                     | 0.41              |
| 1:A:8:PHE:CE1    | 1:A:182:ILE:HG23 | 2.55                     | 0.41              |
| 1:A:77:ILE:CD1   | 1:A:112:PRO:HD3  | 2.50                     | 0.41              |
| 1:A:464:SER:C    | 1:A:551:VAL:H    | 2.25                     | 0.41              |
| 1:A:551:VAL:HG13 | 1:A:555:ASN:HB2  | 2.03                     | 0.41              |
| 2:B:84:PHE:CD1   | 2:B:85:PHE:N     | 2.89                     | 0.41              |
| 2:C:80:GLU:HB2   | 6:C:503:HOH:O    | 2.19                     | 0.41              |
| 1:D:143:LYS:CD   | 1:D:187:CYS:HB3  | 2.51                     | 0.41              |
| 1:D:151:SER:HA   | 1:D:194:PHE:HA   | 2.03                     | 0.41              |
| 1:D:403:LEU:HD23 | 1:D:540:SER:OG   | 2.20                     | 0.41              |
| 1:D:478:PHE:O    | 1:D:479:TRP:HD1  | 2.03                     | 0.41              |
| 1:D:492:ASP:C    | 2:E:187:LYS:HE3  | 2.45                     | 0.41              |
| 2:E:199:LEU:HA   | 2:E:200:PRO:HD2  | 1.85                     | 0.41              |
| 2:F:143:PRO:O    | 2:F:185:TRP:HD1  | 2.03                     | 0.41              |
| 1:A:76:TYR:O     | 1:A:79:ARG:HB2   | 2.21                     | 0.41              |
| 1:A:97:ILE:HB    | 1:A:162:VAL:HB   | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:351:THR:HA   | 6:A:713:HOH:O    | 2.20                     | 0.41              |
| 1:A:479:TRP:N    | 6:A:748:HOH:O    | 2.54                     | 0.41              |
| 2:B:24:ARG:NE    | 6:B:420:HOH:O    | 2.16                     | 0.41              |
| 2:B:145:PHE:HB3  | 2:B:153:VAL:HG13 | 2.01                     | 0.41              |
| 2:B:169:LYS:HB2  | 2:B:169:LYS:HE3  | 1.81                     | 0.41              |
| 2:C:138:GLU:OE1  | 6:C:425:HOH:O    | 2.21                     | 0.41              |
| 2:C:139:LEU:CD2  | 1:D:92:HIS:CG    | 2.97                     | 0.41              |
| 1:D:81:VAL:CG2   | 1:D:97:ILE:HG13  | 2.50                     | 0.41              |
| 1:D:122:LEU:HD23 | 1:D:122:LEU:HA   | 1.90                     | 0.41              |
| 1:D:170:TYR:HA   | 1:D:175:PHE:CD2  | 2.56                     | 0.41              |
| 2:E:60:ASN:HB2   | 6:E:492:HOH:O    | 2.20                     | 0.41              |
| 2:E:142:LYS:HE3  | 2:E:142:LYS:HB2  | 1.75                     | 0.41              |
| 2:F:14:MET:HG2   | 2:F:163:TRP:CD1  | 2.56                     | 0.41              |
| 2:F:85:PHE:N     | 2:F:85:PHE:CD1   | 2.88                     | 0.41              |
| 1:A:262:ALA:O    | 1:A:265:LYS:HB2  | 2.21                     | 0.41              |
| 1:A:487:GLU:OE1  | 1:A:568:SER:OG   | 2.33                     | 0.41              |
| 1:A:498:ASP:CG   | 1:A:510:ARG:NH2  | 2.74                     | 0.41              |
| 2:B:12:PRO:O     | 2:B:163:TRP:HZ2  | 2.03                     | 0.41              |
| 2:C:68:LEU:O     | 2:C:72:GLN:NE2   | 2.49                     | 0.41              |
| 1:D:66:PRO:HG2   | 6:D:896:HOH:O    | 2.20                     | 0.41              |
| 1:D:406:VAL:C    | 1:D:541:SER:HG   | 2.26                     | 0.41              |
| 1:D:495:ASN:O    | 1:D:498:ASP:HB2  | 2.21                     | 0.41              |
| 1:D:548:PRO:HB2  | 6:D:928:HOH:O    | 2.20                     | 0.41              |
| 2:E:12:PRO:O     | 2:E:163:TRP:HZ2  | 2.03                     | 0.41              |
| 1:A:22:ARG:NH1   | 1:A:414:ASN:HB3  | 2.36                     | 0.41              |
| 1:A:95:PRO:O     | 1:A:161:PRO:HB2  | 2.21                     | 0.41              |
| 1:A:97:ILE:O     | 1:A:163:GLY:N    | 2.54                     | 0.41              |
| 1:A:227:LEU:HD13 | 1:A:316:LEU:HD21 | 2.02                     | 0.41              |
| 1:A:252:ASN:HD22 | 1:A:252:ASN:H    | 1.69                     | 0.41              |
| 1:A:308:SER:HB2  | 6:A:825:HOH:O    | 2.21                     | 0.41              |
| 1:A:415:ASN:HD22 | 1:A:415:ASN:HA   | 1.66                     | 0.41              |
| 2:B:76:GLU:CG    | 2:C:89:PRO:HB3   | 2.51                     | 0.41              |
| 2:C:141:ASP:CG   | 1:D:92:HIS:HB2   | 2.46                     | 0.41              |
| 2:C:161:SER:HA   | 2:C:164:PHE:CG   | 2.55                     | 0.41              |
| 2:C:181:LYS:O    | 1:D:93:PRO:HD2   | 2.21                     | 0.41              |
| 1:D:8:PHE:CE1    | 1:D:181:SER:HB2  | 2.55                     | 0.41              |
| 1:D:108:PRO:HB3  | 1:D:555:ASN:HB2  | 2.03                     | 0.41              |
| 1:D:197:ASP:OD2  | 1:D:200:GLN:OE1  | 2.38                     | 0.41              |
| 1:D:314:PRO:CA   | 1:D:317:ARG:NH1  | 2.82                     | 0.41              |
| 1:D:463:SER:OG   | 1:D:464:SER:N    | 2.54                     | 0.41              |
| 1:D:566:VAL:HG23 | 1:D:566:VAL:O    | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:119:GLU:N    | 6:E:417:HOH:O    | 2.53                     | 0.41              |
| 2:E:138:GLU:HG3  | 2:E:145:PHE:HE1  | 1.85                     | 0.41              |
| 2:E:153:VAL:HG23 | 2:E:156:SER:HB2  | 2.02                     | 0.41              |
| 1:A:210:ILE:HD12 | 1:A:210:ILE:HG23 | 1.90                     | 0.41              |
| 1:A:455:GLU:HB2  | 6:A:878:HOH:O    | 2.19                     | 0.41              |
| 2:C:36:ASP:OD2   | 2:C:38:SER:HB2   | 2.21                     | 0.41              |
| 2:C:103:ASP:O    | 2:C:107:THR:HB   | 2.21                     | 0.41              |
| 1:D:116:GLU:HG3  | 6:D:843:HOH:O    | 2.21                     | 0.41              |
| 1:D:120:ASN:CG   | 1:D:358:LEU:HD22 | 2.46                     | 0.41              |
| 1:D:150:SER:HB3  | 1:D:170:TYR:CD2  | 2.56                     | 0.41              |
| 1:D:222:VAL:HB   | 1:D:533:GLU:CG   | 2.51                     | 0.41              |
| 2:E:24:ARG:NH1   | 2:E:30:PHE:HZ    | 2.19                     | 0.41              |
| 1:A:196:PRO:HA   | 1:A:565:ASN:OD1  | 2.21                     | 0.40              |
| 2:B:145:PHE:CE2  | 2:B:157:LEU:HD21 | 2.57                     | 0.40              |
| 2:C:4:LEU:HA     | 2:C:5:PRO:HD3    | 1.88                     | 0.40              |
| 2:C:142:LYS:CG   | 1:D:39:ASN:HA    | 2.50                     | 0.40              |
| 1:D:29:LYS:HZ1   | 1:D:33:LYS:HZ1   | 1.67                     | 0.40              |
| 1:D:99:LEU:H     | 1:D:557:LYS:HB2  | 1.86                     | 0.40              |
| 1:D:290:LEU:O    | 1:D:293:ALA:HB3  | 2.21                     | 0.40              |
| 1:D:353:ALA:HB2  | 1:D:413:TYR:CE2  | 2.56                     | 0.40              |
| 1:D:455:GLU:HB2  | 6:D:795:HOH:O    | 2.21                     | 0.40              |
| 1:D:538:LEU:HG   | 1:D:544:GLN:NE2  | 2.37                     | 0.40              |
| 1:A:223:PHE:CG   | 1:A:533:GLU:HG2  | 2.56                     | 0.40              |
| 2:B:110:GLN:HA   | 2:B:113:VAL:HG12 | 2.04                     | 0.40              |
| 2:C:8:LEU:O      | 2:C:55:PRO:HA    | 2.21                     | 0.40              |
| 1:D:166:THR:HA   | 4:D:602:LEU:HG   | 2.03                     | 0.40              |
| 1:D:226:GLY:HA2  | 1:D:529:ARG:HD2  | 2.03                     | 0.40              |
| 2:E:10:TYR:CG    | 2:E:12:PRO:HD2   | 2.56                     | 0.40              |
| 2:E:66:GLU:HB2   | 2:E:69:ASN:HB2   | 2.03                     | 0.40              |
| 2:E:140:GLY:N    | 2:E:181:LYS:NZ   | 2.70                     | 0.40              |
| 2:F:72:GLN:HG3   | 2:F:85:PHE:HZ    | 1.86                     | 0.40              |
| 2:F:169:LYS:HD3  | 2:F:206:VAL:HG13 | 2.03                     | 0.40              |
| 1:A:79:ARG:HB2   | 1:A:88:ILE:CD1   | 2.51                     | 0.40              |
| 1:A:187:CYS:HB2  | 1:A:208:SER:O    | 2.20                     | 0.40              |
| 1:A:452:LEU:HD11 | 1:A:490:LEU:HD23 | 2.02                     | 0.40              |
| 2:C:217:LEU:HG   | 6:C:440:HOH:O    | 2.20                     | 0.40              |
| 1:D:574:ALA:O    | 1:D:575:PHE:HB2  | 2.21                     | 0.40              |
| 1:A:10:MET:O     | 1:A:14:ILE:HG23  | 2.21                     | 0.40              |
| 1:A:222:VAL:C    | 1:A:223:PHE:HD1  | 2.30                     | 0.40              |
| 1:A:281:CYS:O    | 1:A:284:LEU:HG   | 2.21                     | 0.40              |
| 1:A:284:LEU:HD13 | 1:A:287:TRP:N    | 2.34                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:346:SER:O    | 1:A:350:ALA:N    | 2.55                     | 0.40              |
| 1:A:503:ASP:O    | 1:A:507:VAL:HG23 | 2.22                     | 0.40              |
| 2:B:145:PHE:CD2  | 2:B:157:LEU:HD21 | 2.56                     | 0.40              |
| 2:C:7:LEU:O      | 6:C:427:HOH:O    | 2.22                     | 0.40              |
| 2:C:183:ILE:O    | 2:C:187:LYS:HG3  | 2.22                     | 0.40              |
| 1:D:145:LEU:O    | 1:D:220:PHE:N    | 2.53                     | 0.40              |
| 1:D:244:ASP:OD2  | 1:D:251:SER:CB   | 2.69                     | 0.40              |
| 1:D:332:SER:HB2  | 1:D:538:LEU:HA   | 2.02                     | 0.40              |
| 1:D:440:ASP:CG   | 1:D:501:PHE:HA   | 2.46                     | 0.40              |
| 2:E:145:PHE:HB3  | 2:E:153:VAL:HG13 | 2.02                     | 0.40              |
| 2:E:197:LYS:HB3  | 2:E:197:LYS:HE3  | 1.84                     | 0.40              |
| 1:A:17:PHE:CE1   | 1:A:355:ILE:HG12 | 2.51                     | 0.40              |
| 1:A:126:ARG:NH1  | 6:A:719:HOH:O    | 2.09                     | 0.40              |
| 2:B:10:TYR:CG    | 2:B:12:PRO:HD2   | 2.56                     | 0.40              |
| 2:B:98:TRP:HH2   | 2:B:135:LEU:HD11 | 1.86                     | 0.40              |
| 2:C:67:SER:O     | 2:C:70:VAL:HB    | 2.22                     | 0.40              |
| 2:C:81:LYS:NZ    | 6:C:463:HOH:O    | 2.54                     | 0.40              |
| 2:C:132:VAL:HG23 | 2:C:182:LEU:CD2  | 2.45                     | 0.40              |
| 2:C:168:GLU:OE2  | 2:C:174:SER:HA   | 2.21                     | 0.40              |
| 1:D:143:LYS:CD   | 1:D:212:PHE:HB2  | 2.45                     | 0.40              |
| 2:E:165:GLN:HA   | 2:E:168:GLU:OE1  | 2.22                     | 0.40              |
| 2:E:211:GLU:O    | 2:E:214:LYS:HG2  | 2.21                     | 0.40              |
| 2:F:139:LEU:HD11 | 2:F:144:TYR:O    | 2.21                     | 0.40              |
| 2:F:139:LEU:HD12 | 2:F:139:LEU:HA   | 1.91                     | 0.40              |

All (18) 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) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:D:270:ASN:O   | 1:D:511:LYS:NZ[1_455]  | 1.93                     | 0.27              |
| 2:E:215:ASN:O   | 2:F:33:ARG:NH2[1_455]  | 1.99                     | 0.21              |
| 1:A:46:GLN:OE1  | 2:F:149:SER:OG[1_566]  | 2.01                     | 0.19              |
| 1:D:299:LYS:NZ  | 1:D:431:ILE:O[1_455]   | 2.01                     | 0.19              |
| 1:A:270:ASN:ND2 | 1:A:510:ARG:O[1_455]   | 2.02                     | 0.18              |
| 6:C:441:HOH:O   | 6:D:936:HOH:O[1_545]   | 2.02                     | 0.18              |
| 6:E:430:HOH:O   | 6:F:502:HOH:O[1_455]   | 2.07                     | 0.13              |
| 6:E:470:HOH:O   | 6:F:521:HOH:O[1_455]   | 2.07                     | 0.13              |
| 1:A:211:LEU:O   | 1:A:509:SER:OG[1_455]  | 2.10                     | 0.10              |
| 1:A:213:ARG:NE  | 1:A:503:ASP:OD2[1_455] | 2.11                     | 0.09              |
| 6:D:849:HOH:O   | 6:D:945:HOH:O[1_565]   | 2.12                     | 0.08              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:D:213:ARG:NE  | 1:D:503:ASP:OD2[1_455] | 2.13                     | 0.07              |
| 1:D:270:ASN:ND2 | 1:D:510:ARG:O[1_455]   | 2.13                     | 0.07              |
| 6:A:895:HOH:O   | 6:A:1024:HOH:O[1_455]  | 2.15                     | 0.05              |
| 6:D:998:HOH:O   | 6:D:1018:HOH:O[1_655]  | 2.16                     | 0.04              |
| 6:A:1119:HOH:O  | 6:E:560:HOH:O[1_566]   | 2.17                     | 0.03              |
| 6:A:1112:HOH:O  | 6:B:582:HOH:O[1_565]   | 2.19                     | 0.01              |
| 1:D:268:THR:N   | 6:D:710:HOH:O[1_455]   | 2.19                     | 0.01              |

## 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     | 567/575 (99%)   | 523 (92%)  | 34 (6%)  | 10 (2%)  | 6           | 1  |
| 1   | D     | 567/575 (99%)   | 520 (92%)  | 38 (7%)  | 9 (2%)   | 7           | 1  |
| 2   | B     | 212/223 (95%)   | 191 (90%)  | 15 (7%)  | 6 (3%)   | 4           | 0  |
| 2   | C     | 212/223 (95%)   | 199 (94%)  | 12 (6%)  | 1 (0%)   | 24          | 10 |
| 2   | E     | 212/223 (95%)   | 194 (92%)  | 16 (8%)  | 2 (1%)   | 14          | 3  |
| 2   | F     | 212/223 (95%)   | 198 (93%)  | 12 (6%)  | 2 (1%)   | 14          | 3  |
| All | All   | 1982/2042 (97%) | 1825 (92%) | 127 (6%) | 30 (2%)  | 8           | 1  |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 433 | ILE  |
| 1   | A     | 437 | THR  |
| 1   | A     | 513 | LYS  |
| 1   | A     | 540 | SER  |
| 1   | A     | 542 | ALA  |
| 1   | D     | 369 | THR  |
| 1   | D     | 513 | LYS  |
| 1   | D     | 540 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 542 | ALA  |
| 2   | E     | 140 | GLY  |
| 1   | A     | 369 | THR  |
| 2   | B     | 140 | GLY  |
| 2   | C     | 141 | ASP  |
| 1   | D     | 368 | GLU  |
| 1   | D     | 433 | ILE  |
| 1   | A     | 368 | GLU  |
| 1   | A     | 88  | ILE  |
| 2   | B     | 66  | GLU  |
| 1   | D     | 437 | THR  |
| 2   | E     | 66  | GLU  |
| 2   | B     | 141 | ASP  |
| 1   | D     | 553 | PRO  |
| 1   | A     | 424 | ARG  |
| 2   | B     | 27  | GLY  |
| 2   | B     | 180 | PRO  |
| 2   | F     | 27  | GLY  |
| 1   | A     | 92  | HIS  |
| 2   | B     | 175 | ILE  |
| 1   | D     | 566 | VAL  |
| 2   | F     | 79  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|----------|-------------|---|
| 1   | A     | 499/505 (99%)   | 463 (93%)  | 36 (7%)  | 13          | 2 |
| 1   | D     | 499/505 (99%)   | 464 (93%)  | 35 (7%)  | 14          | 2 |
| 2   | B     | 187/195 (96%)   | 169 (90%)  | 18 (10%) | 8           | 1 |
| 2   | C     | 187/195 (96%)   | 175 (94%)  | 12 (6%)  | 16          | 3 |
| 2   | E     | 187/195 (96%)   | 173 (92%)  | 14 (8%)  | 12          | 2 |
| 2   | F     | 187/195 (96%)   | 172 (92%)  | 15 (8%)  | 11          | 2 |
| All | All   | 1746/1790 (98%) | 1616 (93%) | 130 (7%) | 13          | 2 |

All (130) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 27  | VAL  |
| 1   | A     | 36  | LEU  |
| 1   | A     | 38  | LYS  |
| 1   | A     | 99  | LEU  |
| 1   | A     | 108 | PRO  |
| 1   | A     | 110 | PHE  |
| 1   | A     | 111 | ILE  |
| 1   | A     | 114 | THR  |
| 1   | A     | 146 | GLN  |
| 1   | A     | 150 | SER  |
| 1   | A     | 152 | LYS  |
| 1   | A     | 184 | SER  |
| 1   | A     | 250 | LEU  |
| 1   | A     | 273 | LEU  |
| 1   | A     | 284 | LEU  |
| 1   | A     | 299 | LYS  |
| 1   | A     | 326 | VAL  |
| 1   | A     | 329 | ASP  |
| 1   | A     | 337 | ILE  |
| 1   | A     | 369 | THR  |
| 1   | A     | 410 | ILE  |
| 1   | A     | 419 | LEU  |
| 1   | A     | 422 | ILE  |
| 1   | A     | 425 | ARG  |
| 1   | A     | 428 | ILE  |
| 1   | A     | 433 | ILE  |
| 1   | A     | 450 | LYS  |
| 1   | A     | 459 | VAL  |
| 1   | A     | 468 | VAL  |
| 1   | A     | 484 | GLU  |
| 1   | A     | 502 | ILE  |
| 1   | A     | 509 | SER  |
| 1   | A     | 538 | LEU  |
| 1   | A     | 545 | PHE  |
| 1   | A     | 563 | CYS  |
| 1   | A     | 573 | THR  |
| 2   | B     | 43  | LEU  |
| 2   | B     | 50  | ILE  |
| 2   | B     | 64  | VAL  |
| 2   | B     | 68  | LEU  |
| 2   | B     | 71  | VAL  |
| 2   | B     | 74  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 84  | PHE  |
| 2   | B     | 133 | LYS  |
| 2   | B     | 134 | ILE  |
| 2   | B     | 135 | LEU  |
| 2   | B     | 139 | LEU  |
| 2   | B     | 157 | LEU  |
| 2   | B     | 176 | GLU  |
| 2   | B     | 183 | ILE  |
| 2   | B     | 187 | LYS  |
| 2   | B     | 193 | GLU  |
| 2   | B     | 206 | VAL  |
| 2   | B     | 211 | GLU  |
| 2   | C     | 54  | ILE  |
| 2   | C     | 57  | LEU  |
| 2   | C     | 69  | ASN  |
| 2   | C     | 80  | GLU  |
| 2   | C     | 81  | LYS  |
| 2   | C     | 103 | ASP  |
| 2   | C     | 110 | GLN  |
| 2   | C     | 129 | ILE  |
| 2   | C     | 142 | LYS  |
| 2   | C     | 153 | VAL  |
| 2   | C     | 168 | GLU  |
| 2   | C     | 181 | LYS  |
| 1   | D     | 14  | ILE  |
| 1   | D     | 27  | VAL  |
| 1   | D     | 43  | ILE  |
| 1   | D     | 80  | MET  |
| 1   | D     | 88  | ILE  |
| 1   | D     | 90  | THR  |
| 1   | D     | 92  | HIS  |
| 1   | D     | 99  | LEU  |
| 1   | D     | 108 | PRO  |
| 1   | D     | 110 | PHE  |
| 1   | D     | 111 | ILE  |
| 1   | D     | 125 | PHE  |
| 1   | D     | 138 | ILE  |
| 1   | D     | 143 | LYS  |
| 1   | D     | 150 | SER  |
| 1   | D     | 152 | LYS  |
| 1   | D     | 182 | ILE  |
| 1   | D     | 241 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 245 | ILE  |
| 1   | D     | 326 | VAL  |
| 1   | D     | 329 | ASP  |
| 1   | D     | 337 | ILE  |
| 1   | D     | 345 | LEU  |
| 1   | D     | 348 | GLU  |
| 1   | D     | 379 | LEU  |
| 1   | D     | 405 | ASP  |
| 1   | D     | 410 | ILE  |
| 1   | D     | 423 | CYS  |
| 1   | D     | 425 | ARG  |
| 1   | D     | 431 | ILE  |
| 1   | D     | 468 | VAL  |
| 1   | D     | 545 | PHE  |
| 1   | D     | 559 | LEU  |
| 1   | D     | 562 | LEU  |
| 1   | D     | 563 | CYS  |
| 2   | E     | 43  | LEU  |
| 2   | E     | 50  | ILE  |
| 2   | E     | 64  | VAL  |
| 2   | E     | 74  | VAL  |
| 2   | E     | 80  | GLU  |
| 2   | E     | 84  | PHE  |
| 2   | E     | 134 | ILE  |
| 2   | E     | 135 | LEU  |
| 2   | E     | 139 | LEU  |
| 2   | E     | 157 | LEU  |
| 2   | E     | 176 | GLU  |
| 2   | E     | 183 | ILE  |
| 2   | E     | 187 | LYS  |
| 2   | E     | 206 | VAL  |
| 2   | F     | 26  | LYS  |
| 2   | F     | 72  | GLN  |
| 2   | F     | 80  | GLU  |
| 2   | F     | 81  | LYS  |
| 2   | F     | 92  | ARG  |
| 2   | F     | 94  | GLN  |
| 2   | F     | 110 | GLN  |
| 2   | F     | 132 | VAL  |
| 2   | F     | 134 | ILE  |
| 2   | F     | 142 | LYS  |
| 2   | F     | 153 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 181 | LYS  |
| 2   | F     | 195 | VAL  |
| 2   | F     | 197 | LYS  |
| 2   | F     | 206 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 28  | GLN  |
| 1   | A     | 146 | GLN  |
| 1   | A     | 205 | HIS  |
| 1   | A     | 215 | GLN  |
| 1   | A     | 217 | GLN  |
| 1   | A     | 394 | ASN  |
| 1   | A     | 415 | ASN  |
| 1   | A     | 544 | GLN  |
| 1   | A     | 565 | ASN  |
| 2   | C     | 69  | ASN  |
| 2   | C     | 94  | GLN  |
| 1   | D     | 120 | ASN  |
| 1   | D     | 199 | HIS  |
| 1   | D     | 217 | GLN  |
| 1   | D     | 236 | GLN  |
| 1   | D     | 286 | ASN  |
| 1   | D     | 544 | GLN  |
| 1   | D     | 560 | GLN  |
| 1   | D     | 565 | ASN  |
| 2   | E     | 48  | ASN  |
| 2   | E     | 110 | GLN  |
| 2   | E     | 165 | GLN  |
| 2   | E     | 216 | ASN  |
| 2   | F     | 39  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | GSH  | F     | 301 | -    | 18,19,19     | 1.61 | 4 (22%)  | 21,24,24    | 2.86 | 7 (33%)  |
| 5   | GSH  | C     | 301 | -    | 18,19,19     | 1.57 | 4 (22%)  | 21,24,24    | 2.53 | 8 (38%)  |
| 5   | GSH  | E     | 301 | -    | 18,19,19     | 1.52 | 4 (22%)  | 21,24,24    | 2.76 | 7 (33%)  |
| 4   | LEU  | D     | 602 | -    | 6,8,8        | 1.31 | 1 (16%)  | 5,10,10     | 1.26 | 1 (20%)  |
| 4   | LEU  | A     | 602 | -    | 6,8,8        | 1.25 | 1 (16%)  | 5,10,10     | 1.49 | 1 (20%)  |
| 5   | GSH  | B     | 301 | -    | 18,19,19     | 1.44 | 3 (16%)  | 21,24,24    | 2.56 | 5 (23%)  |
| 3   | JAA  | A     | 601 | -    | 15,15,15     | 5.35 | 7 (46%)  | 14,19,19    | 3.32 | 10 (71%) |
| 3   | JAA  | D     | 601 | -    | 15,15,15     | 5.44 | 6 (40%)  | 14,19,19    | 3.38 | 9 (64%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | GSH  | F     | 301 | -    | -       | 2/24/24/24 | -       |
| 5   | GSH  | C     | 301 | -    | -       | 6/24/24/24 | -       |
| 5   | GSH  | E     | 301 | -    | -       | 4/24/24/24 | -       |
| 4   | LEU  | D     | 602 | -    | -       | 4/8/8/8    | -       |
| 4   | LEU  | A     | 602 | -    | -       | 4/8/8/8    | -       |
| 5   | GSH  | B     | 301 | -    | -       | 4/24/24/24 | -       |
| 3   | JAA  | A     | 601 | -    | -       | 7/9/22/22  | 0/1/1/1 |
| 3   | JAA  | D     | 601 | -    | -       | 7/9/22/22  | 0/1/1/1 |

All (30) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3   | D     | 601 | JAA  | C05-C08 | -13.28 | 1.30        | 1.52     |
| 3   | A     | 601 | JAA  | C05-C08 | -13.11 | 1.31        | 1.52     |
| 3   | A     | 601 | JAA  | C06-C04 | -11.77 | 1.24        | 1.53     |
| 3   | D     | 601 | JAA  | C06-C04 | -11.76 | 1.24        | 1.53     |
| 3   | A     | 601 | JAA  | C07-C08 | 6.38   | 1.61        | 1.51     |
| 3   | D     | 601 | JAA  | C07-C08 | 5.90   | 1.60        | 1.51     |
| 3   | D     | 601 | JAA  | C10-C04 | -5.80  | 1.44        | 1.53     |
| 3   | D     | 601 | JAA  | C09-C05 | -5.10  | 1.47        | 1.54     |
| 3   | A     | 601 | JAA  | C10-C04 | -5.01  | 1.45        | 1.53     |
| 3   | D     | 601 | JAA  | C05-C04 | 4.68   | 1.66        | 1.54     |
| 3   | A     | 601 | JAA  | C05-C04 | 4.66   | 1.65        | 1.54     |
| 3   | A     | 601 | JAA  | C09-C05 | -4.51  | 1.48        | 1.54     |
| 5   | E     | 301 | GSH  | CA2-N2  | -3.29  | 1.39        | 1.45     |
| 4   | D     | 602 | LEU  | OXT-C   | -3.01  | 1.21        | 1.30     |
| 5   | B     | 301 | GSH  | CA2-N2  | -2.98  | 1.39        | 1.45     |
| 4   | A     | 602 | LEU  | OXT-C   | -2.84  | 1.21        | 1.30     |
| 5   | F     | 301 | GSH  | CA2-N2  | -2.83  | 1.40        | 1.45     |
| 5   | C     | 301 | GSH  | CA2-N2  | -2.75  | 1.40        | 1.45     |
| 5   | C     | 301 | GSH  | C2-N3   | 2.73   | 1.40        | 1.33     |
| 5   | F     | 301 | GSH  | C2-N3   | 2.69   | 1.40        | 1.33     |
| 5   | B     | 301 | GSH  | C2-N3   | 2.69   | 1.40        | 1.33     |
| 5   | F     | 301 | GSH  | CD1-N2  | 2.62   | 1.39        | 1.34     |
| 5   | B     | 301 | GSH  | CD1-N2  | 2.61   | 1.39        | 1.34     |
| 5   | C     | 301 | GSH  | CD1-N2  | 2.49   | 1.39        | 1.34     |
| 5   | F     | 301 | GSH  | CB2-CA2 | -2.47  | 1.50        | 1.53     |
| 5   | E     | 301 | GSH  | CD1-N2  | 2.42   | 1.39        | 1.34     |
| 5   | C     | 301 | GSH  | CB2-CA2 | -2.33  | 1.50        | 1.53     |
| 5   | E     | 301 | GSH  | C2-N3   | 2.28   | 1.39        | 1.33     |
| 5   | E     | 301 | GSH  | CB2-CA2 | -2.12  | 1.50        | 1.53     |
| 3   | A     | 601 | JAA  | O03-C12 | -2.07  | 1.24        | 1.30     |

All (48) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 5   | B     | 301 | GSH  | CA2-CB2-SG2 | -10.00 | 102.89      | 114.16   |
| 5   | F     | 301 | GSH  | CA2-CB2-SG2 | -9.17  | 103.82      | 114.16   |
| 5   | E     | 301 | GSH  | CA2-CB2-SG2 | -9.05  | 103.95      | 114.16   |
| 5   | C     | 301 | GSH  | CA2-CB2-SG2 | -7.81  | 105.35      | 114.16   |
| 3   | D     | 601 | JAA  | C07-C06-C04 | -6.55  | 97.53       | 104.45   |
| 3   | A     | 601 | JAA  | C07-C06-C04 | -6.18  | 97.92       | 104.45   |
| 3   | A     | 601 | JAA  | C09-C11-C13 | -5.95  | 104.34      | 126.21   |
| 3   | D     | 601 | JAA  | C09-C11-C13 | -5.62  | 105.55      | 126.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | F     | 301 | GSH  | CB2-CA2-N2  | -5.12 | 103.99      | 111.28   |
| 5   | E     | 301 | GSH  | CB2-CA2-N2  | -4.66 | 104.64      | 111.28   |
| 3   | D     | 601 | JAA  | C06-C07-C08 | -4.25 | 101.18      | 105.39   |
| 3   | D     | 601 | JAA  | C06-C04-C10 | -3.98 | 106.01      | 113.41   |
| 5   | C     | 301 | GSH  | CB2-CA2-N2  | -3.74 | 105.94      | 111.28   |
| 5   | F     | 301 | GSH  | CG1-CD1-N2  | -3.69 | 109.37      | 115.86   |
| 5   | C     | 301 | GSH  | CB1-CG1-CD1 | 3.68  | 121.28      | 113.06   |
| 3   | A     | 601 | JAA  | O03-C12-C10 | 3.63  | 125.30      | 114.00   |
| 3   | A     | 601 | JAA  | O01-C08-C05 | 3.61  | 130.21      | 125.60   |
| 5   | F     | 301 | GSH  | CB1-CG1-CD1 | 3.61  | 121.10      | 113.06   |
| 5   | E     | 301 | GSH  | CG1-CD1-N2  | -3.58 | 109.56      | 115.86   |
| 3   | D     | 601 | JAA  | O02-C12-C10 | -3.53 | 112.01      | 122.84   |
| 5   | C     | 301 | GSH  | CG1-CD1-N2  | -3.48 | 109.74      | 115.86   |
| 3   | D     | 601 | JAA  | O03-C12-C10 | 3.45  | 124.73      | 114.00   |
| 3   | A     | 601 | JAA  | C07-C08-C05 | -3.44 | 103.40      | 109.06   |
| 3   | A     | 601 | JAA  | C06-C07-C08 | -3.40 | 102.02      | 105.39   |
| 5   | E     | 301 | GSH  | C2-CA2-N2   | -3.22 | 102.40      | 111.11   |
| 5   | E     | 301 | GSH  | C3-CA3-N3   | -3.15 | 103.27      | 113.06   |
| 3   | A     | 601 | JAA  | C06-C04-C10 | -3.13 | 107.58      | 113.41   |
| 5   | F     | 301 | GSH  | CG1-CB1-CA1 | -3.12 | 106.70      | 113.86   |
| 3   | D     | 601 | JAA  | C07-C08-C05 | -3.07 | 104.01      | 109.06   |
| 3   | A     | 601 | JAA  | O02-C12-C10 | -3.00 | 113.64      | 122.84   |
| 4   | A     | 602 | LEU  | OXT-C-O     | -2.99 | 117.28      | 124.08   |
| 5   | B     | 301 | GSH  | CB2-CA2-N2  | -2.89 | 107.17      | 111.28   |
| 5   | C     | 301 | GSH  | OE1-CD1-CG1 | 2.56  | 126.65      | 122.02   |
| 5   | B     | 301 | GSH  | C3-CA3-N3   | -2.48 | 105.36      | 113.06   |
| 5   | F     | 301 | GSH  | CB2-CA2-C2  | -2.45 | 104.16      | 109.50   |
| 4   | D     | 602 | LEU  | OXT-C-O     | -2.44 | 118.54      | 124.08   |
| 3   | A     | 601 | JAA  | C14-C13-C11 | -2.43 | 111.80      | 126.42   |
| 5   | E     | 301 | GSH  | OE1-CD1-CG1 | 2.41  | 126.38      | 122.02   |
| 3   | D     | 601 | JAA  | O01-C08-C05 | 2.38  | 128.65      | 125.60   |
| 5   | C     | 301 | GSH  | C2-CA2-N2   | -2.28 | 104.94      | 111.11   |
| 5   | E     | 301 | GSH  | CB1-CG1-CD1 | 2.26  | 118.11      | 113.06   |
| 5   | C     | 301 | GSH  | CB2-CA2-C2  | -2.22 | 104.67      | 109.50   |
| 5   | B     | 301 | GSH  | CG1-CD1-N2  | -2.22 | 111.96      | 115.86   |
| 5   | F     | 301 | GSH  | OE1-CD1-CG1 | 2.21  | 126.03      | 122.02   |
| 3   | D     | 601 | JAA  | C14-C13-C11 | -2.19 | 113.22      | 126.42   |
| 3   | A     | 601 | JAA  | C04-C10-C12 | -2.16 | 108.95      | 113.33   |
| 5   | B     | 301 | GSH  | CG1-CB1-CA1 | -2.11 | 109.02      | 113.86   |
| 5   | C     | 301 | GSH  | CG1-CB1-CA1 | -2.09 | 109.07      | 113.86   |

There are no chirality outliers.

All (38) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | B     | 301 | GSH  | N2-CA2-CB2-SG2  |
| 5   | B     | 301 | GSH  | C2-CA2-CB2-SG2  |
| 5   | C     | 301 | GSH  | N1-CA1-CB1-CG1  |
| 5   | C     | 301 | GSH  | C1-CA1-CB1-CG1  |
| 5   | C     | 301 | GSH  | N2-CA2-CB2-SG2  |
| 5   | C     | 301 | GSH  | C2-CA2-CB2-SG2  |
| 5   | E     | 301 | GSH  | N2-CA2-CB2-SG2  |
| 5   | E     | 301 | GSH  | C2-CA2-CB2-SG2  |
| 4   | D     | 602 | LEU  | C-CA-CB-CG      |
| 3   | A     | 601 | JAA  | C09-C11-C13-C14 |
| 4   | D     | 602 | LEU  | OXT-C-CA-N      |
| 5   | F     | 301 | GSH  | O12-C1-CA1-N1   |
| 4   | A     | 602 | LEU  | OXT-C-CA-N      |
| 4   | A     | 602 | LEU  | C-CA-CB-CG      |
| 3   | D     | 601 | JAA  | C09-C11-C13-C14 |
| 4   | D     | 602 | LEU  | O-C-CA-N        |
| 5   | F     | 301 | GSH  | O11-C1-CA1-N1   |
| 3   | D     | 601 | JAA  | C04-C05-C09-C11 |
| 4   | A     | 602 | LEU  | N-CA-CB-CG      |
| 3   | D     | 601 | JAA  | C08-C05-C09-C11 |
| 3   | A     | 601 | JAA  | C05-C04-C10-C12 |
| 5   | B     | 301 | GSH  | CA1-CB1-CG1-CD1 |
| 3   | A     | 601 | JAA  | C05-C09-C11-C13 |
| 5   | C     | 301 | GSH  | CA1-CB1-CG1-CD1 |
| 3   | A     | 601 | JAA  | C11-C13-C14-C15 |
| 3   | D     | 601 | JAA  | C11-C13-C14-C15 |
| 3   | D     | 601 | JAA  | C05-C09-C11-C13 |
| 4   | A     | 602 | LEU  | O-C-CA-N        |
| 4   | D     | 602 | LEU  | N-CA-CB-CG      |
| 3   | A     | 601 | JAA  | C06-C04-C10-C12 |
| 3   | A     | 601 | JAA  | C04-C10-C12-O03 |
| 5   | B     | 301 | GSH  | C3-CA3-N3-C2    |
| 3   | A     | 601 | JAA  | C04-C10-C12-O02 |
| 3   | D     | 601 | JAA  | C04-C10-C12-O02 |
| 5   | C     | 301 | GSH  | O12-C1-CA1-N1   |
| 5   | E     | 301 | GSH  | CA1-CB1-CG1-CD1 |
| 3   | D     | 601 | JAA  | C04-C10-C12-O03 |
| 5   | E     | 301 | GSH  | O12-C1-CA1-N1   |

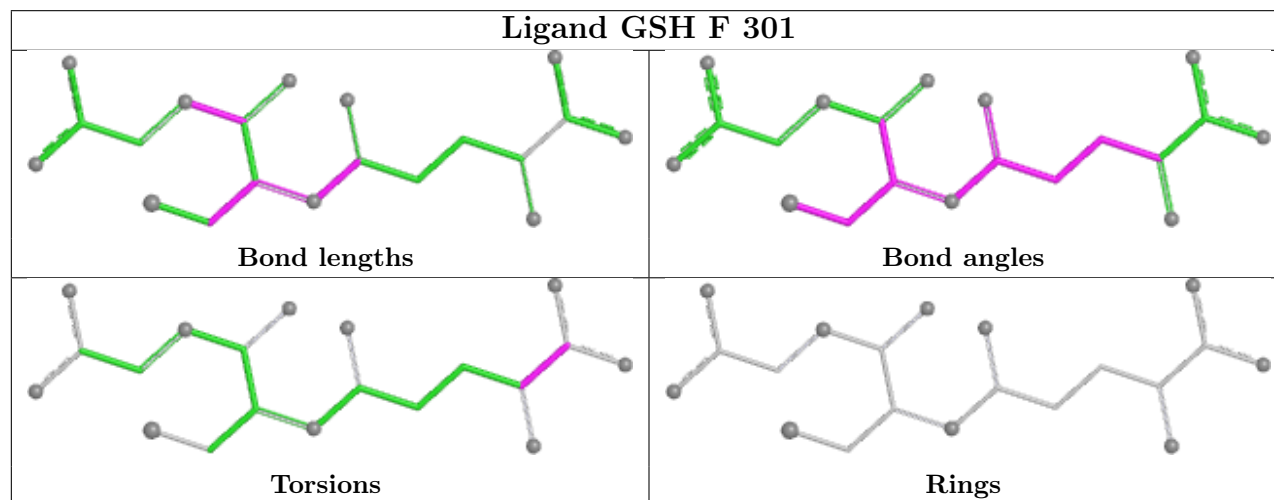
There are no ring outliers.

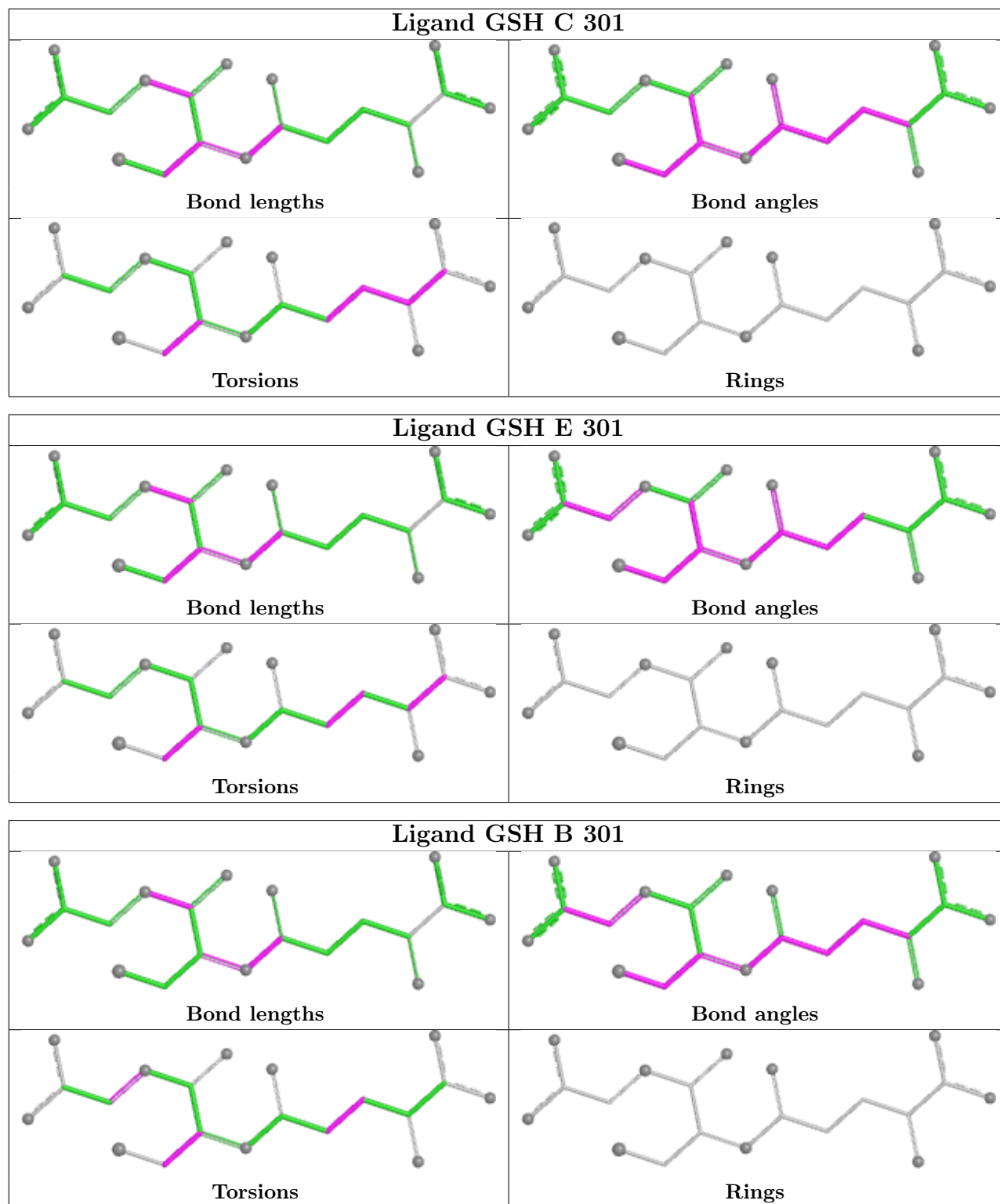
7 monomers are involved in 27 short contacts:



| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | F     | 301 | GSH  | 3       | 0            |
| 5   | C     | 301 | GSH  | 4       | 0            |
| 5   | E     | 301 | GSH  | 2       | 0            |
| 4   | D     | 602 | LEU  | 6       | 0            |
| 4   | A     | 602 | LEU  | 6       | 0            |
| 5   | B     | 301 | GSH  | 2       | 0            |
| 3   | A     | 601 | JAA  | 5       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------|-----------------------|-------|
| 1   | A     | 569/575 (98%)   | -1.42  | 0 100 100 | 3, 5, 5, 30           | 0     |
| 1   | D     | 569/575 (98%)   | -1.46  | 0 100 100 | 3, 5, 5, 16           | 0     |
| 2   | B     | 214/223 (95%)   | -1.50  | 0 100 100 | 2, 3, 7, 11           | 0     |
| 2   | C     | 214/223 (95%)   | -1.50  | 0 100 100 | 3, 4, 5, 5            | 0     |
| 2   | E     | 214/223 (95%)   | -1.51  | 0 100 100 | 2, 3, 7, 11           | 0     |
| 2   | F     | 214/223 (95%)   | -1.52  | 0 100 100 | 4, 4, 5, 6            | 0     |
| All | All   | 1994/2042 (97%) | -1.47  | 0 100 100 | 2, 5, 5, 30           | 0     |

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | JAA  | A     | 601 | 15/15 | 0.99 | 0.03 | 3,3,4,4                    | 0     |

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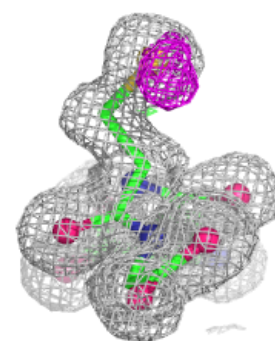
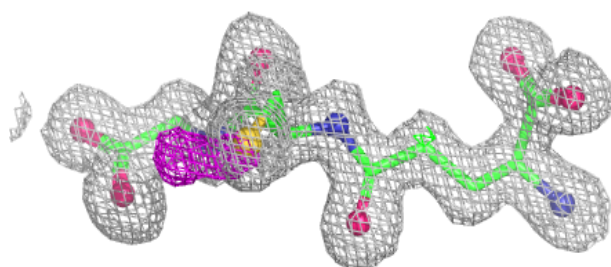
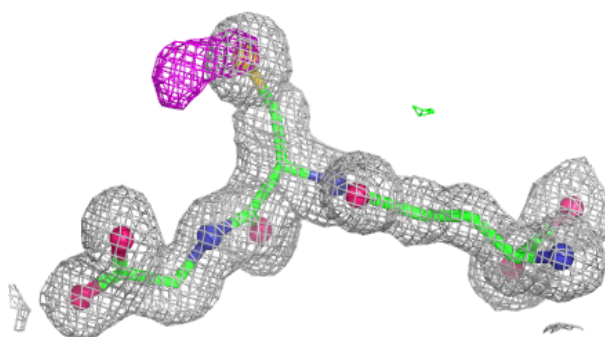
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | JAA  | D     | 601 | 15/15 | 0.99 | 0.04 | 3,4,4,5                     | 0     |
| 4   | LEU  | A     | 602 | 9/9   | 0.99 | 0.02 | 3,3,4,5                     | 0     |
| 4   | LEU  | D     | 602 | 9/9   | 0.99 | 0.03 | 4,5,5,5                     | 0     |
| 5   | GSH  | E     | 301 | 20/20 | 0.99 | 0.02 | 3,4,4,5                     | 0     |
| 5   | GSH  | C     | 301 | 20/20 | 1.00 | 0.02 | 3,4,4,4                     | 0     |
| 5   | GSH  | B     | 301 | 20/20 | 1.00 | 0.02 | 3,4,4,4                     | 0     |
| 5   | GSH  | F     | 301 | 20/20 | 1.00 | 0.02 | 3,4,5,5                     | 0     |

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

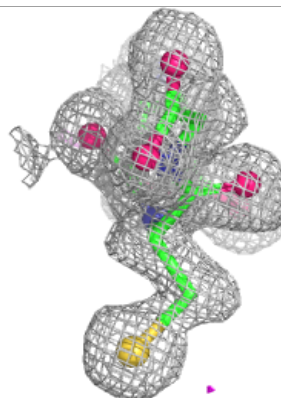
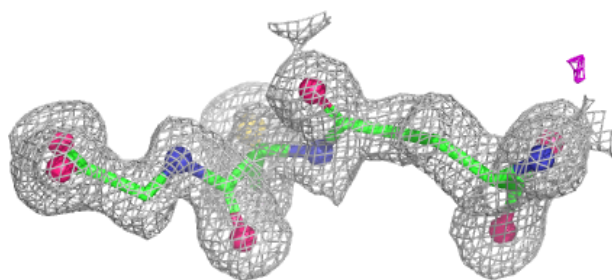
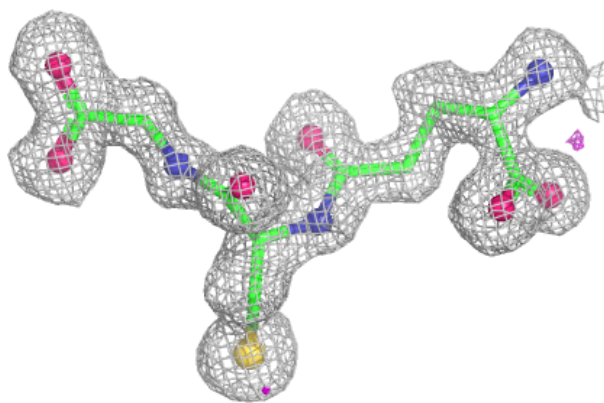
#### Electron density around GSH E 301:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

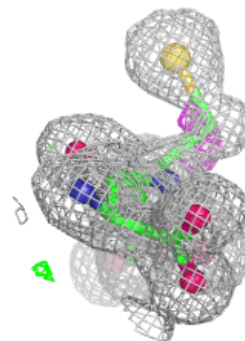
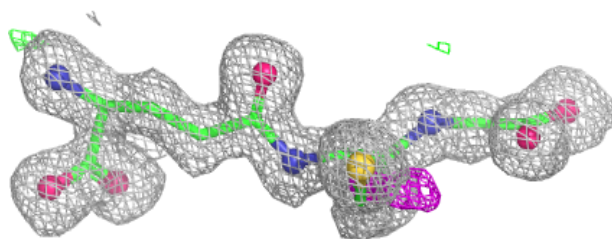
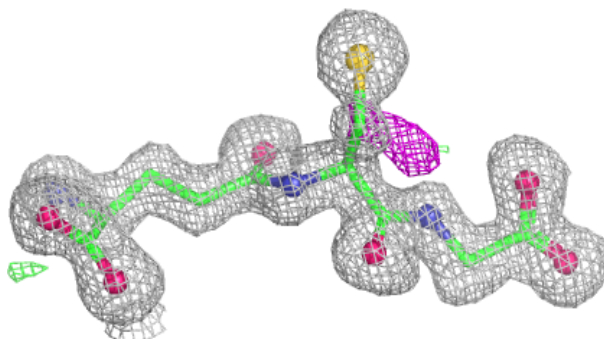


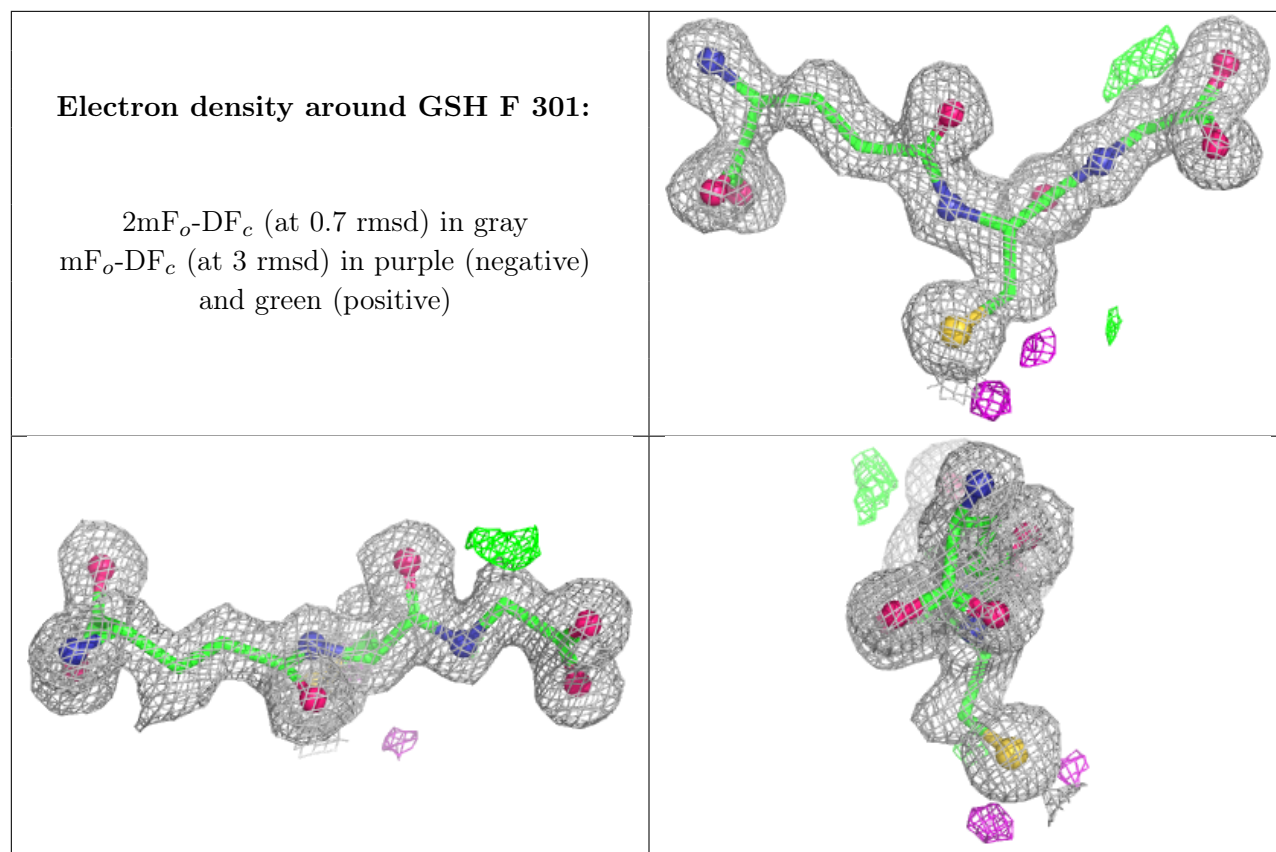
**Electron density around GSH C 301:**

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

**Electron density around GSH B 301:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.