



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 12:17 PM BST

PDB ID : 3PCO  
Title : crystal structure of E. coli phenylalanine-tRNA synthetase complexed with phenylalanine and AMP  
Authors : Mermershtain, I.; Finarov, I.; Klipcan, L.; Kessler, N.; Rozenberg, H.; Safro, M.G.  
Deposited on : 2010-10-21  
Resolution : 3.02 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

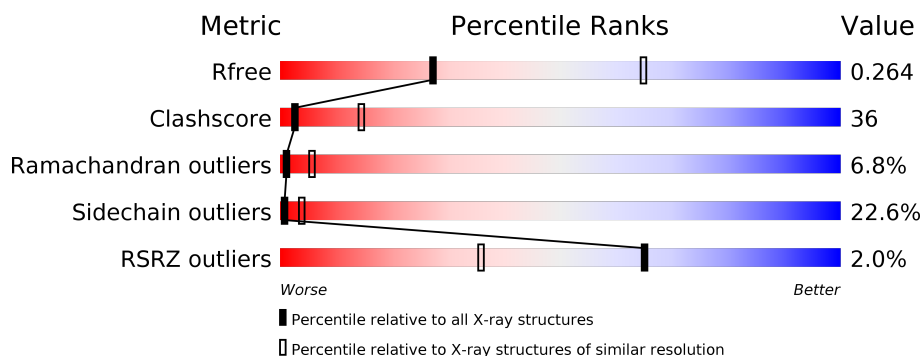
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.02 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 2399 (3.04-3.00)                                      |
| Clashscore            | 141614                      | 2734 (3.04-3.00)                                      |
| Ramachandran outliers | 138981                      | 2640 (3.04-3.00)                                      |
| Sidechain outliers    | 138945                      | 2643 (3.04-3.00)                                      |
| RSRZ outliers         | 127900                      | 2287 (3.04-3.00)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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     | 327    | <div> <div>29%</div> <div>32%</div> <div>11%</div> <div>•</div> <div>26%</div> </div>  |
| 1   | C     | 327    | <div> <div>9%</div> <div>43%</div> <div>40%</div> <div>13%</div> <div>• •</div> </div> |
| 2   | B     | 795    | <div> <div>45%</div> <div>40%</div> <div>13%</div> <div>•</div> </div>                 |
| 2   | D     | 795    | <div> <div>46%</div> <div>38%</div> <div>14%</div> <div>•</div> </div>                 |

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 crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | AMP  | A     | 992 | -         | -        | X       | -                |
| 4   | AMP  | C     | 999 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16724 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.

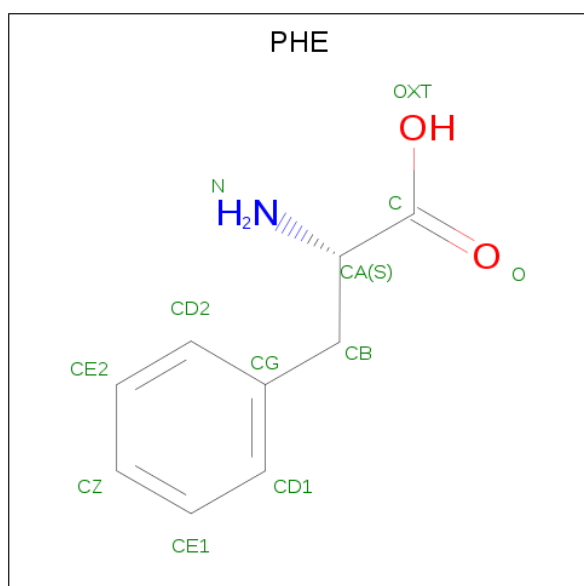
- Molecule 1 is a protein called Phenylalanyl-tRNA synthetase, alpha subunit.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 242      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1964  | 1250 | 347 | 358 | 9 |         |         |       |
| 1   | C     | 323      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2462  | 1552 | 445 | 456 | 9 |         |         |       |

- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase, beta chain.

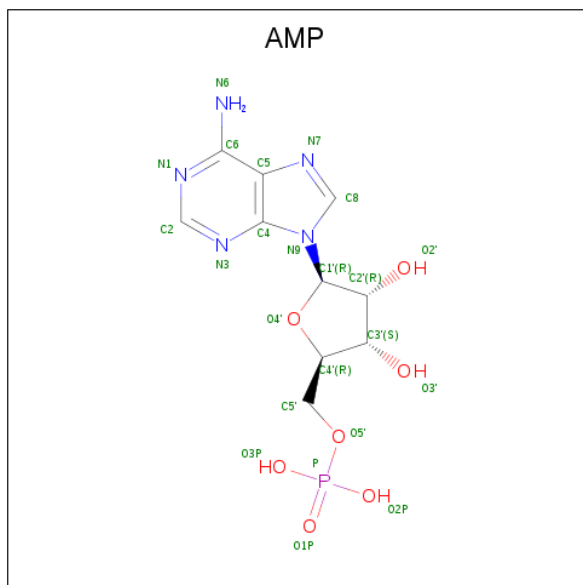
| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | B     | 795      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6111  | 3845 | 1081 | 1158 | 27 |         |         |       |
| 2   | D     | 795      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6117  | 3848 | 1081 | 1161 | 27 |         |         |       |

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula:  $C_9H_{11}NO_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).

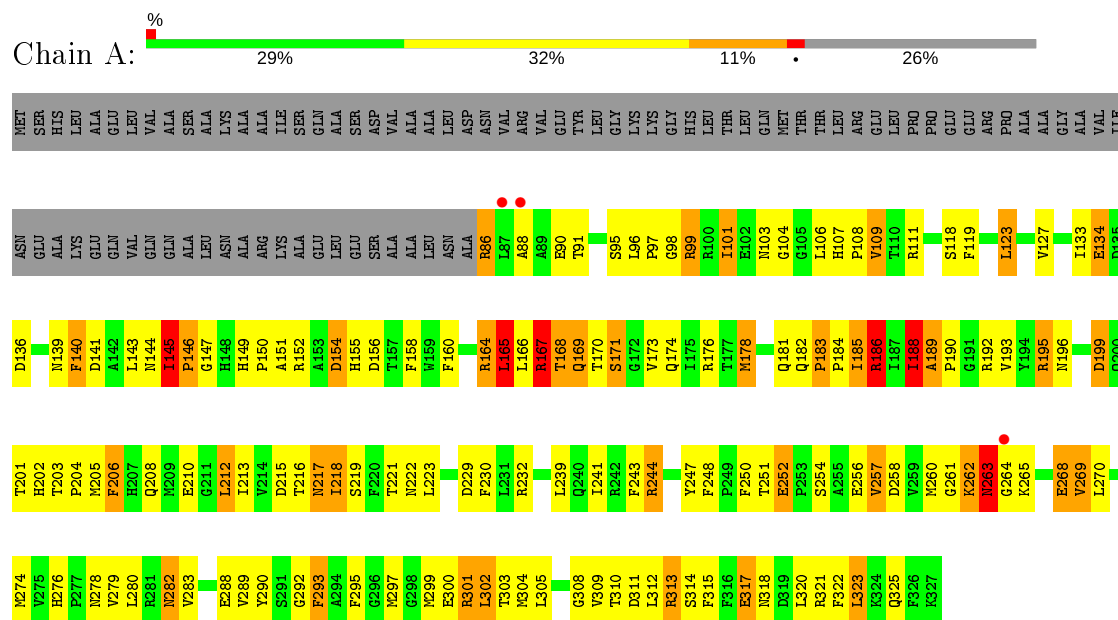


| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 4   | A     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 23    | 10 | 5 | 7 | 1 |         |         |
| 4   | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 23    | 10 | 5 | 7 | 1 |         |         |

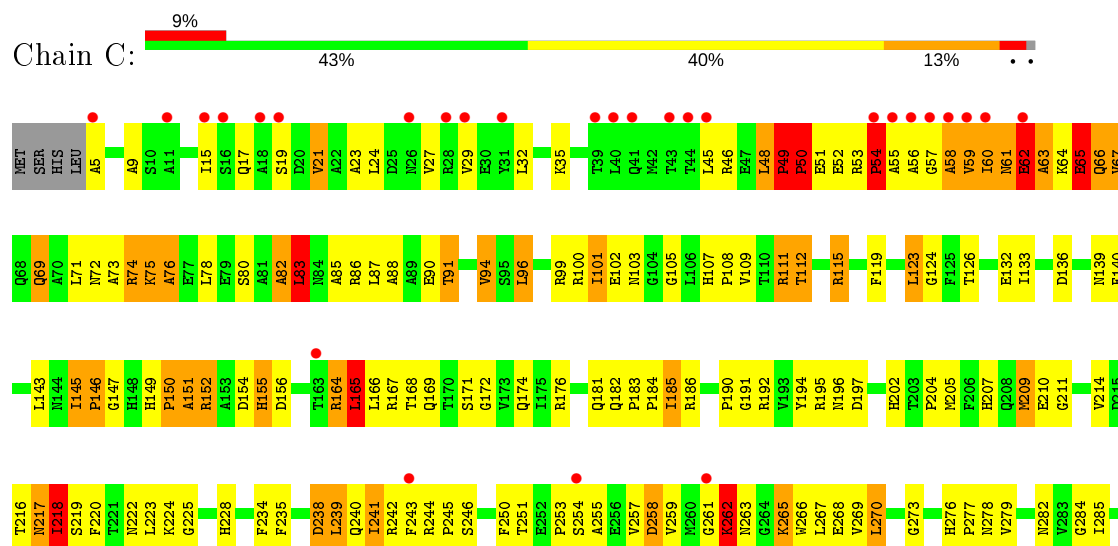
### 3 Residue-property plots

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: Phenylalanyl-tRNA synthetase, alpha subunit



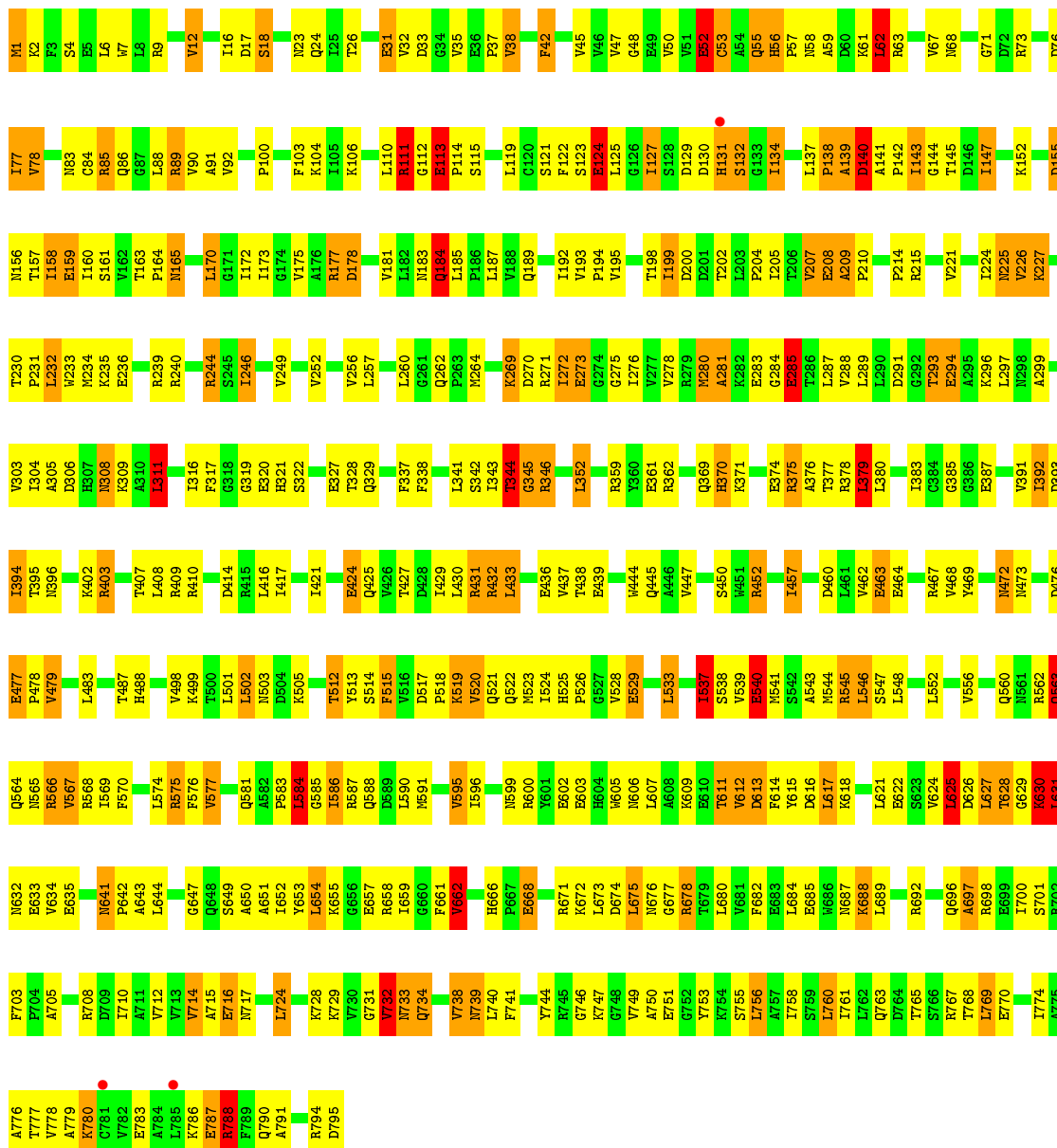
- Molecule 1: Phenylalanyl-tRNA synthetase, alpha subunit





• Molecule 2: Phenylalanyl-tRNA synthetase, beta chain

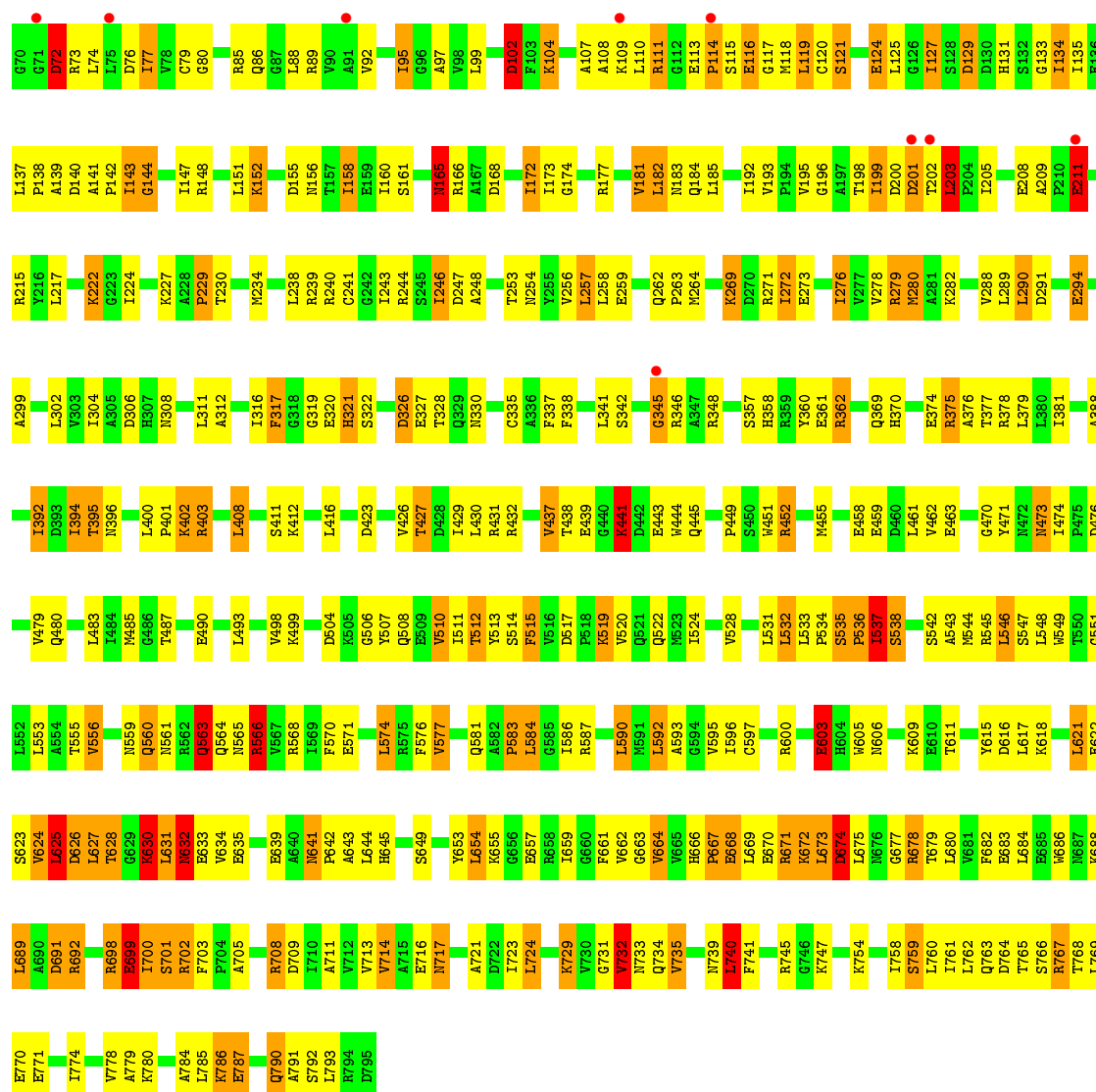
Chain B: 45% 40% 13%



• Molecule 2: Phenylalanyl-tRNA synthetase, beta chain

Chain D: 46% 38% 14%





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 65.55Å 178.94Å 254.42Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)  | 38.71 – 3.02<br>38.71 – 3.02                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.4 (38.71-3.02)<br>98.4 (38.71-3.02)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.11  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.67 (at 3.01Å)   | Xtriage          |
| Refinement program  | REFMAC  | Depositor        |
| R, $R_{free}$   | 0.232 , 0.300<br>0.267 , 0.264                              | Depositor<br>DCC |
| $R_{free}$ test set   | 2981 reflections (5.06%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 75.4  | Xtriage          |
| Anisotropy  | 0.080   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 58.9   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 16724   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 91.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.76         | 0/2016         | 0.98        | 5/2730 (0.2%)   |
| 1   | C     | 0.65         | 0/2516         | 0.88        | 8/3412 (0.2%)   |
| 2   | B     | 0.69         | 2/6212 (0.0%)  | 0.90        | 10/8432 (0.1%)  |
| 2   | D     | 0.63         | 0/6218         | 0.84        | 4/8440 (0.0%)   |
| All | All   | 0.67         | 2/16962 (0.0%) | 0.89        | 27/23014 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | C     | 0                   | 3                   |
| 2   | B     | 0                   | 9                   |
| 2   | D     | 0                   | 6                   |
| All | All   | 0                   | 19                  |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | B     | 463 | GLU  | CB-CG | 5.87 | 1.63        | 1.52     |
| 2   | B     | 540 | GLU  | CG-CD | 5.10 | 1.59        | 1.51     |

All (27) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 563 | GLN  | N-CA-C  | -5.99 | 94.82       | 111.00   |
| 1   | C     | 54  | PRO  | N-CA-CB | 5.99  | 110.48      | 103.30   |
| 1   | C     | 49  | PRO  | N-CA-CB | 5.96  | 110.46      | 103.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 270 | LEU  | CA-CB-CG  | 5.90  | 128.87      | 115.30   |
| 1   | C     | 50  | PRO  | N-CA-CB   | 5.82  | 110.29      | 103.30   |
| 1   | A     | 140 | PHE  | CB-CA-C   | -5.75 | 98.89       | 110.40   |
| 1   | A     | 215 | ASP  | CB-CA-C   | -5.62 | 99.16       | 110.40   |
| 2   | B     | 533 | LEU  | CA-CB-CG  | 5.61  | 128.20      | 115.30   |
| 1   | C     | 165 | LEU  | CA-CB-CG  | 5.60  | 128.17      | 115.30   |
| 2   | B     | 595 | VAL  | CB-CA-C   | -5.43 | 101.08      | 111.40   |
| 2   | B     | 311 | LEU  | CA-CB-CG  | 5.39  | 127.71      | 115.30   |
| 2   | B     | 379 | LEU  | CA-CB-CG  | 5.34  | 127.59      | 115.30   |
| 1   | A     | 165 | LEU  | CA-CB-CG  | 5.32  | 127.54      | 115.30   |
| 1   | C     | 96  | LEU  | CA-CB-CG  | 5.31  | 127.52      | 115.30   |
| 2   | B     | 627 | LEU  | CA-CB-CG  | -5.29 | 103.13      | 115.30   |
| 2   | B     | 662 | VAL  | CB-CA-C   | -5.28 | 101.36      | 111.40   |
| 2   | D     | 724 | LEU  | CA-CB-CG  | 5.24  | 127.36      | 115.30   |
| 2   | D     | 740 | LEU  | CA-CB-CG  | 5.24  | 127.36      | 115.30   |
| 2   | D     | 119 | LEU  | CA-CB-CG  | 5.21  | 127.28      | 115.30   |
| 1   | C     | 312 | LEU  | CA-CB-CG  | 5.20  | 127.25      | 115.30   |
| 2   | B     | 654 | LEU  | CA-CB-CG  | 5.19  | 127.23      | 115.30   |
| 1   | C     | 302 | LEU  | N-CA-CB   | 5.17  | 120.74      | 110.40   |
| 1   | A     | 301 | ARG  | NE-CZ-NH2 | -5.12 | 117.74      | 120.30   |
| 1   | A     | 167 | ARG  | NE-CZ-NH1 | -5.07 | 117.76      | 120.30   |
| 2   | B     | 625 | LEU  | CA-CB-CG  | -5.04 | 103.71      | 115.30   |
| 2   | B     | 537 | ILE  | CB-CA-C   | -5.01 | 101.59      | 111.60   |
| 2   | D     | 641 | ASN  | C-N-CD    | -5.00 | 109.60      | 120.60   |

There are no chirality outliers.

All (19) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 183 | PRO  | Peptide |
| 2   | B     | 113 | GLU  | Peptide |
| 2   | B     | 42  | PHE  | Peptide |
| 2   | B     | 472 | ASN  | Peptide |
| 2   | B     | 529 | GLU  | Peptide |
| 2   | B     | 55  | GLN  | Peptide |
| 2   | B     | 61  | LYS  | Peptide |
| 2   | B     | 62  | LEU  | Peptide |
| 2   | B     | 625 | LEU  | Peptide |
| 2   | B     | 631 | LEU  | Peptide |
| 1   | C     | 182 | GLN  | Peptide |
| 1   | C     | 183 | PRO  | Peptide |
| 1   | C     | 262 | LYS  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | D     | 246 | ILE  | Peptide |
| 2   | D     | 345 | GLY  | Peptide |
| 2   | D     | 55  | GLN  | Peptide |
| 2   | D     | 58  | ASN  | Peptide |
| 2   | D     | 672 | LYS  | Peptide |
| 2   | D     | 72  | ASP  | 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     | 1964  | 0        | 1900     | 213     | 0            |
| 1   | C     | 2462  | 0        | 2307     | 217     | 0            |
| 2   | B     | 6111  | 0        | 6166     | 419     | 0            |
| 2   | D     | 6117  | 0        | 6169     | 430     | 0            |
| 3   | A     | 12    | 0        | 8        | 2       | 0            |
| 3   | C     | 12    | 0        | 8        | 1       | 0            |
| 4   | A     | 23    | 0        | 12       | 9       | 0            |
| 4   | C     | 23    | 0        | 12       | 9       | 0            |
| All | All   | 16724 | 0        | 16582    | 1211    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (1211) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:55:GLN:HB2   | 2:D:56:HIS:CA    | 1.37                     | 1.46              |
| 1:C:58:ALA:C     | 1:C:60:ILE:HB    | 1.48                     | 1.34              |
| 1:C:58:ALA:HB1   | 1:C:60:ILE:CG2   | 1.58                     | 1.33              |
| 2:D:631:LEU:HD12 | 2:D:632:ASN:N    | 1.47                     | 1.27              |
| 2:D:55:GLN:HB2   | 2:D:56:HIS:C     | 1.56                     | 1.24              |
| 1:A:155:HIS:CD2  | 1:A:168:THR:HG21 | 1.76                     | 1.19              |
| 1:A:185:ILE:CD1  | 1:A:212:LEU:HD13 | 1.72                     | 1.19              |
| 1:C:58:ALA:O     | 1:C:59:VAL:HG12  | 1.43                     | 1.18              |
| 1:C:239:LEU:HB3  | 1:C:240:GLN:HA   | 1.24                     | 1.17              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:158:PHE:CE2  | 1:A:195:ARG:O    | 1.97                     | 1.17              |
| 2:D:56:HIS:HB3   | 2:D:57:PRO:HA    | 1.17                     | 1.16              |
| 1:A:170:THR:O    | 1:A:210:GLU:HG3  | 1.42                     | 1.16              |
| 1:C:62:GLU:HG3   | 1:C:63:ALA:H     | 1.05                     | 1.15              |
| 1:A:140:PHE:O    | 1:A:145:ILE:HG12 | 1.47                     | 1.14              |
| 2:D:56:HIS:CE1   | 2:D:58:ASN:HB3   | 1.82                     | 1.14              |
| 2:D:115:SER:O    | 2:D:116:GLU:O    | 1.65                     | 1.13              |
| 1:C:60:ILE:HG22  | 1:C:61:ASN:H     | 0.97                     | 1.13              |
| 2:D:375:ARG:HG3  | 2:D:375:ARG:HH11 | 1.02                     | 1.12              |
| 1:A:104:GLY:O    | 2:B:503:ASN:CG   | 1.88                     | 1.12              |
| 2:D:631:LEU:CD1  | 2:D:632:ASN:H    | 1.62                     | 1.12              |
| 2:B:522:GLN:NE2  | 2:B:529:GLU:HG3  | 1.65                     | 1.12              |
| 2:B:537:ILE:HD12 | 2:B:537:ILE:H    | 0.98                     | 1.12              |
| 1:A:145:ILE:HB   | 1:A:146:PRO:HA   | 1.31                     | 1.11              |
| 1:C:59:VAL:N     | 1:C:60:ILE:HB    | 1.63                     | 1.11              |
| 1:A:185:ILE:HD11 | 1:A:212:LEU:HD13 | 1.26                     | 1.09              |
| 1:A:88:ALA:O     | 1:A:91:THR:HG23  | 1.49                     | 1.09              |
| 1:C:58:ALA:CB    | 1:C:60:ILE:CG2   | 2.30                     | 1.09              |
| 2:D:55:GLN:HB2   | 2:D:56:HIS:HA    | 1.20                     | 1.09              |
| 2:D:55:GLN:CB    | 2:D:56:HIS:CA    | 2.30                     | 1.08              |
| 2:B:452:ARG:HG2  | 2:B:452:ARG:HH11 | 1.00                     | 1.07              |
| 1:C:60:ILE:CG2   | 1:C:61:ASN:H     | 1.66                     | 1.07              |
| 1:C:62:GLU:HG3   | 1:C:63:ALA:N     | 1.62                     | 1.07              |
| 1:A:166:LEU:O    | 1:A:167:ARG:O    | 1.70                     | 1.07              |
| 1:C:60:ILE:HG22  | 1:C:61:ASN:N     | 1.64                     | 1.06              |
| 1:A:166:LEU:HD11 | 2:B:544:MET:CE   | 1.83                     | 1.05              |
| 2:B:522:GLN:HE22 | 2:B:529:GLU:CG   | 1.67                     | 1.05              |
| 2:D:452:ARG:HH11 | 2:D:452:ARG:HG2  | 1.18                     | 1.04              |
| 2:B:631:LEU:HG   | 2:B:632:ASN:H    | 1.17                     | 1.04              |
| 2:D:55:GLN:CB    | 2:D:56:HIS:O     | 2.06                     | 1.04              |
| 1:C:59:VAL:HA    | 1:C:60:ILE:O     | 1.59                     | 1.03              |
| 2:B:787:GLU:O    | 2:B:788:ARG:HD2  | 1.58                     | 1.03              |
| 2:D:56:HIS:CB    | 2:D:57:PRO:HA    | 1.88                     | 1.03              |
| 2:D:449:PRO:HD2  | 2:D:455:MET:HE1  | 1.40                     | 1.02              |
| 1:C:58:ALA:CA    | 1:C:60:ILE:HB    | 1.90                     | 1.01              |
| 2:B:522:GLN:HE22 | 2:B:529:GLU:HG3  | 0.88                     | 1.01              |
| 2:B:537:ILE:CD1  | 2:B:537:ILE:H    | 1.73                     | 1.00              |
| 1:A:136:ASP:OD1  | 1:A:152:ARG:NH2  | 1.95                     | 1.00              |
| 2:B:600:ARG:NH1  | 2:B:616:ASP:OD2  | 1.94                     | 1.00              |
| 1:A:164:ARG:NH1  | 2:B:585:GLY:H    | 1.58                     | 0.99              |
| 1:C:58:ALA:HB1   | 1:C:60:ILE:HG22  | 0.98                     | 0.98              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:279:VAL:HA   | 1:A:282:ASN:HD21 | 1.26                     | 0.98              |
| 1:A:164:ARG:HH12 | 2:B:585:GLY:H    | 1.05                     | 0.98              |
| 2:D:625:LEU:O    | 2:D:626:ASP:CB   | 2.12                     | 0.97              |
| 1:A:139:ASN:HD21 | 1:A:168:THR:HB   | 1.27                     | 0.97              |
| 2:D:55:GLN:CB    | 2:D:56:HIS:C     | 2.31                     | 0.97              |
| 2:D:732:VAL:HG13 | 2:D:733:ASN:H    | 1.26                     | 0.97              |
| 2:D:269:LYS:O    | 2:D:272:ILE:HD12 | 1.65                     | 0.97              |
| 1:A:140:PHE:C    | 1:A:145:ILE:HG12 | 1.84                     | 0.96              |
| 2:D:375:ARG:CG   | 2:D:375:ARG:HH11 | 1.78                     | 0.96              |
| 2:B:244:ARG:HE   | 2:B:244:ARG:H    | 1.10                     | 0.96              |
| 1:A:166:LEU:HD11 | 2:B:544:MET:HE3  | 1.48                     | 0.96              |
| 1:C:58:ALA:CB    | 1:C:60:ILE:HG22  | 1.92                     | 0.95              |
| 1:A:222:ASN:HB3  | 2:B:479:VAL:HG12 | 1.47                     | 0.95              |
| 2:B:630:LYS:HB3  | 2:B:631:LEU:O    | 1.66                     | 0.95              |
| 2:D:631:LEU:HD12 | 2:D:632:ASN:H    | 0.79                     | 0.94              |
| 2:D:716:GLU:OE1  | 2:D:745:ARG:NH1  | 2.00                     | 0.94              |
| 1:A:188:ILE:O    | 1:A:189:ALA:HB2  | 1.65                     | 0.94              |
| 1:A:168:THR:HG22 | 1:A:169:GLN:HG3  | 1.47                     | 0.94              |
| 2:B:644:LEU:HD13 | 2:B:649:SER:HB2  | 1.50                     | 0.94              |
| 2:D:253:THR:HG22 | 2:D:264:MET:HB2  | 1.48                     | 0.94              |
| 1:C:59:VAL:N     | 1:C:60:ILE:CB    | 2.30                     | 0.93              |
| 2:B:631:LEU:CG   | 2:B:632:ASN:H    | 1.81                     | 0.93              |
| 2:B:600:ARG:NH1  | 2:B:616:ASP:OD1  | 2.02                     | 0.93              |
| 1:C:276:HIS:HD2  | 1:C:278:ASN:HB2  | 1.33                     | 0.93              |
| 2:D:26:THR:HG22  | 2:D:32:VAL:H     | 1.34                     | 0.93              |
| 1:C:202:HIS:CE1  | 1:C:301:ARG:HH22 | 1.85                     | 0.93              |
| 2:B:452:ARG:HG2  | 2:B:452:ARG:NH1  | 1.76                     | 0.92              |
| 1:C:75:LYS:O     | 1:C:75:LYS:HG3   | 1.67                     | 0.92              |
| 2:D:632:ASN:OD1  | 2:D:633:GLU:HG2  | 1.68                     | 0.92              |
| 2:D:499:LYS:HD3  | 2:D:570:PHE:HE1  | 1.33                     | 0.91              |
| 2:D:55:GLN:CB    | 2:D:56:HIS:HA    | 1.98                     | 0.91              |
| 2:B:537:ILE:HD12 | 2:B:537:ILE:N    | 1.84                     | 0.91              |
| 2:D:577:VAL:HG13 | 2:D:587:ARG:HB3  | 1.52                     | 0.91              |
| 2:D:626:ASP:O    | 2:D:628:THR:N    | 2.05                     | 0.90              |
| 2:B:586:ILE:H    | 2:B:586:ILE:HD12 | 1.35                     | 0.90              |
| 2:D:53:CYS:SG    | 2:D:53:CYS:O     | 2.30                     | 0.90              |
| 2:B:78:VAL:HG12  | 2:B:115:SER:HB3  | 1.52                     | 0.90              |
| 1:A:203:THR:H    | 4:A:992:AMP:HN61 | 1.20                     | 0.89              |
| 2:D:786:LYS:HD2  | 2:D:791:ALA:HB3  | 1.53                     | 0.89              |
| 2:B:596:ILE:HD12 | 2:B:612:VAL:HG21 | 1.53                     | 0.88              |
| 1:A:145:ILE:CB   | 1:A:146:PRO:HA   | 2.02                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:155:HIS:HD2  | 1:A:168:THR:HG21 | 1.29                     | 0.88              |
| 2:B:111:ARG:N    | 2:B:112:GLY:HA2  | 1.89                     | 0.88              |
| 2:B:600:ARG:NH1  | 2:B:616:ASP:CG   | 2.27                     | 0.88              |
| 2:B:668:GLU:OE1  | 2:B:668:GLU:N    | 2.06                     | 0.88              |
| 2:D:517:ASP:HB3  | 2:D:520:VAL:HB   | 1.55                     | 0.87              |
| 2:B:344:THR:HA   | 2:B:361:GLU:OE1  | 1.75                     | 0.87              |
| 2:B:625:LEU:O    | 2:B:627:LEU:N    | 2.08                     | 0.87              |
| 2:B:205:ILE:HG22 | 2:B:276:ILE:HB   | 1.54                     | 0.87              |
| 2:D:375:ARG:NH1  | 2:D:375:ARG:HG3  | 1.84                     | 0.87              |
| 2:D:634:VAL:HG22 | 2:D:654:LEU:HB2  | 1.55                     | 0.87              |
| 1:A:166:LEU:O    | 1:A:167:ARG:C    | 2.12                     | 0.86              |
| 1:C:54:PRO:N     | 1:C:55:ALA:HA    | 1.89                     | 0.86              |
| 1:A:104:GLY:O    | 2:B:503:ASN:CB   | 2.23                     | 0.86              |
| 1:C:58:ALA:CB    | 1:C:60:ILE:HG21  | 2.04                     | 0.85              |
| 2:B:710:ILE:HD13 | 2:B:712:VAL:HG23 | 1.55                     | 0.85              |
| 1:C:195:ARG:O    | 1:C:204:PRO:HA   | 1.77                     | 0.85              |
| 1:A:95:SER:HB2   | 2:D:721:ALA:HB2  | 1.59                     | 0.85              |
| 1:A:145:ILE:HB   | 1:A:146:PRO:CA   | 2.06                     | 0.84              |
| 2:B:165:ASN:H    | 2:B:165:ASN:HD22 | 1.24                     | 0.84              |
| 2:D:701:SER:HA   | 2:D:702:ARG:HH21 | 1.42                     | 0.84              |
| 2:D:177:ARG:O    | 2:D:181:VAL:HG12 | 1.77                     | 0.84              |
| 2:D:700:ILE:O    | 2:D:701:SER:HB3  | 1.77                     | 0.84              |
| 1:C:107:HIS:HE1  | 1:C:109:VAL:HG13 | 1.43                     | 0.84              |
| 2:D:113:GLU:HB3  | 2:D:114:PRO:HD2  | 1.58                     | 0.83              |
| 1:A:140:PHE:CA   | 1:A:145:ILE:HG12 | 2.07                     | 0.83              |
| 1:C:202:HIS:CE1  | 1:C:301:ARG:NH2  | 2.45                     | 0.83              |
| 2:D:627:LEU:HD11 | 2:D:631:LEU:HD23 | 1.61                     | 0.83              |
| 1:C:62:GLU:CG    | 1:C:63:ALA:N     | 2.42                     | 0.83              |
| 2:D:205:ILE:HG22 | 2:D:276:ILE:HB   | 1.60                     | 0.82              |
| 1:A:300:GLU:HB3  | 1:A:312:LEU:CD1  | 2.10                     | 0.82              |
| 1:C:59:VAL:N     | 1:C:60:ILE:C     | 2.33                     | 0.82              |
| 2:D:626:ASP:C    | 2:D:628:THR:H    | 1.80                     | 0.82              |
| 1:C:224:LYS:HE2  | 2:D:474:ILE:O    | 1.78                     | 0.82              |
| 2:B:343:ILE:O    | 2:B:346:ARG:HG2  | 1.80                     | 0.81              |
| 2:D:85:ARG:HB3   | 2:D:88:LEU:HD13  | 1.62                     | 0.81              |
| 2:B:432:ARG:HG2  | 2:B:432:ARG:HH11 | 1.44                     | 0.81              |
| 2:D:515:PHE:HD1  | 2:D:544:MET:HE1  | 1.46                     | 0.81              |
| 1:A:166:LEU:HD11 | 2:B:544:MET:HE1  | 1.60                     | 0.81              |
| 1:A:140:PHE:O    | 1:A:145:ILE:CG1  | 2.27                     | 0.81              |
| 1:C:59:VAL:H     | 1:C:60:ILE:C     | 1.84                     | 0.81              |
| 1:C:59:VAL:O     | 1:C:59:VAL:HG13  | 1.80                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:181:VAL:HG22 | 2:B:432:ARG:HG3  | 1.63                     | 0.80              |
| 2:B:631:LEU:HG   | 2:B:632:ASN:N    | 1.96                     | 0.80              |
| 2:D:45:VAL:HB    | 2:D:147:ILE:HD11 | 1.62                     | 0.80              |
| 2:D:55:GLN:HB3   | 2:D:56:HIS:O     | 1.80                     | 0.80              |
| 2:B:429:ILE:HG23 | 2:B:468:VAL:HG21 | 1.63                     | 0.80              |
| 1:C:59:VAL:HG23  | 1:C:62:GLU:HG2   | 1.61                     | 0.80              |
| 1:C:59:VAL:CA    | 1:C:60:ILE:C     | 2.50                     | 0.80              |
| 2:D:510:VAL:O    | 2:D:571:GLU:HG3  | 1.80                     | 0.80              |
| 2:D:626:ASP:C    | 2:D:628:THR:N    | 2.32                     | 0.80              |
| 2:B:651:ALA:HB1  | 2:B:658:ARG:HD3  | 1.64                     | 0.79              |
| 2:D:644:LEU:HD13 | 2:D:649:SER:HB2  | 1.64                     | 0.79              |
| 1:A:185:ILE:HD12 | 1:A:212:LEU:HD13 | 1.64                     | 0.79              |
| 2:D:790:GLN:HE21 | 2:D:791:ALA:H    | 1.29                     | 0.79              |
| 1:C:58:ALA:CA    | 1:C:60:ILE:CB    | 2.61                     | 0.79              |
| 2:D:56:HIS:HB3   | 2:D:57:PRO:CA    | 2.07                     | 0.79              |
| 2:B:244:ARG:HE   | 2:B:244:ARG:N    | 1.79                     | 0.79              |
| 2:D:733:ASN:HA   | 2:D:734:GLN:HB2  | 1.63                     | 0.79              |
| 2:D:357:SER:O    | 2:D:361:GLU:HG2  | 1.82                     | 0.79              |
| 2:B:285:GLU:HB2  | 2:B:297:LEU:HB2  | 1.65                     | 0.78              |
| 1:C:59:VAL:CA    | 1:C:60:ILE:O     | 2.31                     | 0.78              |
| 2:D:56:HIS:CE1   | 2:D:58:ASN:CB    | 2.64                     | 0.78              |
| 1:A:203:THR:H    | 4:A:992:AMP:N6   | 1.81                     | 0.78              |
| 1:A:149:HIS:CG   | 1:A:150:PRO:HD2  | 2.18                     | 0.78              |
| 1:A:300:GLU:HB3  | 1:A:312:LEU:HD13 | 1.66                     | 0.78              |
| 2:D:85:ARG:HB3   | 2:D:88:LEU:CD1   | 2.13                     | 0.78              |
| 1:A:155:HIS:CD2  | 1:A:168:THR:CG2  | 2.63                     | 0.77              |
| 2:B:85:ARG:NH2   | 2:B:88:LEU:HD11  | 1.99                     | 0.77              |
| 1:C:107:HIS:CE1  | 1:C:109:VAL:HG13 | 2.20                     | 0.77              |
| 2:D:209:ALA:HB1  | 2:D:211:GLU:OE2  | 1.84                     | 0.77              |
| 2:B:198:THR:O    | 2:B:199:ILE:HG23 | 1.84                     | 0.77              |
| 1:A:147:GLY:HA2  | 1:A:152:ARG:NE   | 2.00                     | 0.77              |
| 1:A:270:LEU:HB3  | 1:A:297:MET:HB3  | 1.66                     | 0.77              |
| 1:A:139:ASN:O    | 1:A:143:LEU:HD12 | 1.84                     | 0.77              |
| 2:B:560:GLN:HE22 | 2:B:675:LEU:HA   | 1.49                     | 0.77              |
| 2:D:32:VAL:HB    | 2:D:158:ILE:HD11 | 1.66                     | 0.77              |
| 2:B:56:HIS:HB3   | 2:B:63:ARG:H     | 1.51                     | 0.76              |
| 2:D:641:ASN:O    | 2:D:643:ALA:N    | 2.18                     | 0.76              |
| 2:B:272:ILE:HG12 | 2:B:273:GLU:N    | 2.00                     | 0.76              |
| 1:A:164:ARG:HH12 | 2:B:585:GLY:N    | 1.83                     | 0.76              |
| 2:B:272:ILE:HG12 | 2:B:273:GLU:H    | 1.51                     | 0.76              |
| 2:B:9:ARG:HA     | 2:B:12:VAL:O     | 1.86                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:319:GLY:O    | 2:D:321:HIS:N    | 2.18                     | 0.76              |
| 1:C:239:LEU:HB3  | 1:C:240:GLN:CA   | 2.13                     | 0.75              |
| 2:B:600:ARG:HH11 | 2:B:616:ASP:CG   | 1.89                     | 0.75              |
| 1:A:188:ILE:O    | 1:A:189:ALA:CB   | 2.33                     | 0.75              |
| 2:D:618:LYS:O    | 2:D:622:GLU:HB2  | 1.86                     | 0.75              |
| 2:B:38:VAL:HG21  | 2:B:240:ARG:HD3  | 1.69                     | 0.74              |
| 1:C:58:ALA:O     | 1:C:59:VAL:CG1   | 2.30                     | 0.74              |
| 1:C:59:VAL:N     | 1:C:60:ILE:CA    | 2.49                     | 0.74              |
| 1:A:276:HIS:HD2  | 1:A:278:ASN:H    | 1.35                     | 0.74              |
| 2:D:784:ALA:O    | 2:D:787:GLU:HB3  | 1.87                     | 0.74              |
| 1:A:304:MET:HG2  | 1:A:309:VAL:O    | 1.88                     | 0.74              |
| 2:B:202:THR:HG21 | 2:B:392:ILE:HD11 | 1.69                     | 0.74              |
| 2:D:473:ASN:ND2  | 2:D:473:ASN:H    | 1.86                     | 0.74              |
| 2:B:425:GLN:O    | 2:B:429:ILE:HG12 | 1.88                     | 0.74              |
| 1:C:62:GLU:O     | 1:C:64:LYS:N     | 2.21                     | 0.74              |
| 2:B:393:ASP:OD2  | 2:B:395:THR:HG23 | 1.87                     | 0.74              |
| 2:D:499:LYS:HD3  | 2:D:570:PHE:CE1  | 2.20                     | 0.74              |
| 1:A:145:ILE:CB   | 1:A:146:PRO:CA   | 2.61                     | 0.73              |
| 2:B:710:ILE:CD1  | 2:B:712:VAL:HG23 | 2.17                     | 0.73              |
| 3:A:980:PHE:N    | 4:A:992:AMP:HO3' | 1.86                     | 0.73              |
| 2:B:341:LEU:HD12 | 2:B:341:LEU:H    | 1.53                     | 0.73              |
| 2:D:624:VAL:HG12 | 2:D:625:LEU:N    | 2.02                     | 0.73              |
| 1:A:263:ASN:HB3  | 1:A:264:GLY:CA   | 2.18                     | 0.73              |
| 1:C:276:HIS:CD2  | 1:C:278:ASN:HB2  | 2.22                     | 0.73              |
| 2:D:168:ASP:O    | 2:D:174:GLY:HA3  | 1.88                     | 0.73              |
| 2:B:515:PHE:HD1  | 2:B:544:MET:HE1  | 1.54                     | 0.73              |
| 2:B:631:LEU:CG   | 2:B:632:ASN:N    | 2.51                     | 0.73              |
| 1:C:146:PRO:O    | 1:C:152:ARG:NE   | 2.21                     | 0.73              |
| 1:A:136:ASP:CG   | 1:A:152:ARG:HH22 | 1.91                     | 0.72              |
| 1:A:216:THR:O    | 1:A:217:ASN:HB2  | 1.88                     | 0.72              |
| 1:C:239:LEU:CB   | 1:C:240:GLN:HA   | 2.12                     | 0.72              |
| 1:C:87:LEU:O     | 1:C:91:THR:HG22  | 1.89                     | 0.72              |
| 1:A:95:SER:HB2   | 2:D:721:ALA:CB   | 2.18                     | 0.72              |
| 1:A:104:GLY:O    | 2:B:503:ASN:HB3  | 1.89                     | 0.72              |
| 2:D:631:LEU:CD1  | 2:D:632:ASN:N    | 2.35                     | 0.72              |
| 2:D:273:GLU:HG3  | 2:D:306:ASP:OD1  | 1.90                     | 0.72              |
| 2:D:626:ASP:CB   | 2:D:631:LEU:HD22 | 2.19                     | 0.72              |
| 2:D:127:ILE:HD13 | 2:D:127:ILE:C    | 2.10                     | 0.72              |
| 2:D:702:ARG:H    | 2:D:702:ARG:NE   | 1.88                     | 0.72              |
| 2:B:47:VAL:HG21  | 2:B:141:ALA:HB1  | 1.70                     | 0.71              |
| 2:B:432:ARG:CG   | 2:B:432:ARG:HH11 | 2.01                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:69:GLN:HA    | 1:C:69:GLN:HE21  | 1.55                     | 0.71              |
| 2:D:596:ILE:HG13 | 2:D:680:LEU:HB2  | 1.72                     | 0.71              |
| 2:D:57:PRO:HB3   | 2:D:59:ALA:O     | 1.90                     | 0.71              |
| 2:B:111:ARG:H    | 2:B:112:GLY:HA2  | 1.56                     | 0.71              |
| 1:A:218:ILE:HD13 | 1:A:293:PHE:CD1  | 2.26                     | 0.71              |
| 2:D:699:GLU:HA   | 2:D:699:GLU:OE1  | 1.90                     | 0.71              |
| 2:D:338:PHE:HD2  | 2:D:360:TYR:CE1  | 2.09                     | 0.70              |
| 1:C:299:MET:HA   | 1:C:299:MET:HE2  | 1.73                     | 0.70              |
| 2:D:47:VAL:HG23  | 2:D:142:PRO:O    | 1.91                     | 0.70              |
| 1:A:170:THR:OG1  | 1:A:210:GLU:HG2  | 1.91                     | 0.70              |
| 2:B:626:ASP:CA   | 2:B:629:GLY:H    | 2.05                     | 0.70              |
| 2:D:22:ALA:HB1   | 2:D:32:VAL:HG21  | 1.72                     | 0.70              |
| 2:D:193:VAL:O    | 2:D:378:ARG:NH1  | 2.24                     | 0.70              |
| 2:B:119:LEU:HB3  | 2:B:134:ILE:HG21 | 1.73                     | 0.70              |
| 2:D:243:ILE:HG13 | 2:D:258:LEU:HD11 | 1.73                     | 0.70              |
| 1:C:66:GLN:HG2   | 1:C:67:VAL:N     | 2.06                     | 0.70              |
| 2:D:119:LEU:HB3  | 2:D:134:ILE:HD11 | 1.72                     | 0.70              |
| 2:D:394:ILE:HG13 | 2:D:394:ILE:O    | 1.92                     | 0.70              |
| 2:D:534:PRO:O    | 2:D:535:SER:HB3  | 1.92                     | 0.70              |
| 2:D:732:VAL:HG13 | 2:D:733:ASN:N    | 2.05                     | 0.70              |
| 1:A:145:ILE:HG22 | 1:A:146:PRO:C    | 2.13                     | 0.69              |
| 1:C:58:ALA:CA    | 1:C:60:ILE:CG2   | 2.70                     | 0.69              |
| 2:D:195:VAL:HG21 | 2:D:377:THR:HB   | 1.74                     | 0.69              |
| 2:B:522:GLN:NE2  | 2:B:529:GLU:CG   | 2.41                     | 0.69              |
| 1:C:185:ILE:HD13 | 1:C:186:ARG:N    | 2.08                     | 0.69              |
| 1:A:263:ASN:HB3  | 1:A:264:GLY:HA2  | 1.74                     | 0.69              |
| 1:A:158:PHE:HZ   | 2:B:537:ILE:HG13 | 1.58                     | 0.69              |
| 1:A:145:ILE:CG2  | 1:A:146:PRO:O    | 2.40                     | 0.69              |
| 1:A:140:PHE:CD1  | 1:A:145:ILE:HG13 | 2.29                     | 0.68              |
| 2:B:205:ILE:CG2  | 2:B:276:ILE:HB   | 2.24                     | 0.68              |
| 1:C:60:ILE:CG2   | 1:C:61:ASN:N     | 2.34                     | 0.68              |
| 2:B:605:TRP:HB3  | 2:D:740:LEU:HD12 | 1.76                     | 0.68              |
| 2:D:791:ALA:HB1  | 2:D:792:SER:CB   | 2.23                     | 0.68              |
| 2:B:429:ILE:HG22 | 2:B:433:LEU:CD2  | 2.24                     | 0.68              |
| 2:B:215:ARG:HE   | 2:B:395:THR:HG22 | 1.58                     | 0.68              |
| 2:D:253:THR:HG22 | 2:D:264:MET:CB   | 2.22                     | 0.68              |
| 2:B:272:ILE:CG1  | 2:B:273:GLU:H    | 2.05                     | 0.68              |
| 2:B:609:LYS:O    | 2:B:609:LYS:HG2  | 1.93                     | 0.68              |
| 1:A:279:VAL:HA   | 1:A:282:ASN:ND2  | 2.06                     | 0.68              |
| 2:B:165:ASN:N    | 2:B:165:ASN:HD22 | 1.90                     | 0.68              |
| 2:B:56:HIS:HB3   | 2:B:63:ARG:N     | 2.09                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:158:PHE:CZ   | 2:B:537:ILE:HG13 | 2.29                     | 0.67              |
| 2:B:429:ILE:HG22 | 2:B:433:LEU:HD22 | 1.76                     | 0.67              |
| 2:B:596:ILE:HD12 | 2:B:612:VAL:CG2  | 2.25                     | 0.67              |
| 2:D:345:GLY:H    | 2:D:346:ARG:HH11 | 1.43                     | 0.67              |
| 2:D:427:THR:HG22 | 2:D:444:TRP:HE1  | 1.59                     | 0.67              |
| 2:D:512:THR:HG21 | 2:D:551:GLY:HA3  | 1.75                     | 0.67              |
| 2:B:617:LEU:HD12 | 2:B:680:LEU:HB3  | 1.76                     | 0.67              |
| 2:D:512:THR:HB   | 2:D:571:GLU:OE1  | 1.94                     | 0.67              |
| 1:A:169:GLN:HA   | 1:A:193:VAL:HG11 | 1.76                     | 0.67              |
| 2:B:403:ARG:HH21 | 2:B:450:SER:HB3  | 1.61                     | 0.67              |
| 1:A:311:ASP:OD1  | 1:A:313:ARG:HG3  | 1.95                     | 0.66              |
| 2:B:763:GLN:HA   | 2:B:769:LEU:HD11 | 1.77                     | 0.66              |
| 1:C:61:ASN:O     | 1:C:62:GLU:C     | 2.33                     | 0.66              |
| 2:D:57:PRO:HG3   | 2:D:63:ARG:HH12  | 1.59                     | 0.66              |
| 2:D:673:LEU:O    | 2:D:674:ASP:O    | 2.13                     | 0.66              |
| 2:B:24:GLN:HE22  | 2:B:183:ASN:CG   | 1.98                     | 0.66              |
| 2:B:647:GLY:CA   | 1:C:91:THR:HB    | 2.25                     | 0.66              |
| 2:B:42:PHE:HB3   | 2:B:100:PRO:HD3  | 1.77                     | 0.66              |
| 2:D:701:SER:HA   | 2:D:702:ARG:NH2  | 2.11                     | 0.66              |
| 1:C:58:ALA:HA    | 1:C:60:ILE:CB    | 2.25                     | 0.66              |
| 2:D:116:GLU:OE1  | 2:D:117:GLY:HA3  | 1.96                     | 0.66              |
| 1:A:166:LEU:C    | 1:A:167:ARG:O    | 2.34                     | 0.66              |
| 2:D:703:PHE:CE2  | 2:D:766:SER:O    | 2.49                     | 0.65              |
| 1:A:107:HIS:CD2  | 1:A:109:VAL:H    | 2.15                     | 0.65              |
| 1:C:214:VAL:HG22 | 1:C:292:GLY:HA3  | 1.77                     | 0.65              |
| 2:B:701:SER:HB3  | 2:B:765:THR:HA   | 1.77                     | 0.65              |
| 1:A:134:GLU:HA   | 1:A:134:GLU:OE2  | 1.96                     | 0.65              |
| 2:D:596:ILE:HG12 | 2:D:617:LEU:HD13 | 1.78                     | 0.65              |
| 1:A:170:THR:O    | 1:A:210:GLU:CG   | 2.33                     | 0.65              |
| 2:D:64:VAL:CG2   | 2:D:114:PRO:HG2  | 2.26                     | 0.65              |
| 2:D:770:GLU:O    | 2:D:774:ILE:HG12 | 1.96                     | 0.65              |
| 1:A:178:MET:CE   | 1:A:280:LEU:HD23 | 2.26                     | 0.65              |
| 2:D:32:VAL:HA    | 2:D:160:ILE:HG22 | 1.78                     | 0.65              |
| 1:A:260:MET:SD   | 1:A:265:LYS:HE3  | 2.37                     | 0.65              |
| 2:B:139:ALA:C    | 2:B:141:ALA:H    | 2.00                     | 0.65              |
| 1:C:61:ASN:O     | 1:C:63:ALA:N     | 2.30                     | 0.65              |
| 1:C:299:MET:HA   | 1:C:299:MET:CE   | 2.27                     | 0.65              |
| 1:C:59:VAL:H     | 1:C:61:ASN:N     | 1.95                     | 0.65              |
| 2:D:259:GLU:OE1  | 2:D:375:ARG:NH1  | 2.29                     | 0.65              |
| 1:A:229:ASP:OD1  | 1:A:232:ARG:NH2  | 2.31                     | 0.64              |
| 2:D:624:VAL:CG1  | 2:D:625:LEU:H    | 2.05                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:59:VAL:HA    | 1:C:60:ILE:C     | 2.16                     | 0.64              |
| 2:D:64:VAL:HG23  | 2:D:114:PRO:HG2  | 1.80                     | 0.64              |
| 2:B:139:ALA:O    | 2:B:141:ALA:N    | 2.30                     | 0.64              |
| 1:A:133:ILE:HD12 | 2:B:576:PHE:CD1  | 2.32                     | 0.64              |
| 2:B:225:ASN:H    | 2:B:385:GLY:H    | 1.45                     | 0.64              |
| 2:B:586:ILE:HD12 | 2:B:586:ILE:N    | 2.05                     | 0.64              |
| 2:D:624:VAL:HG12 | 2:D:625:LEU:H    | 1.58                     | 0.64              |
| 2:B:305:ALA:HA   | 2:B:311:LEU:HD13 | 1.79                     | 0.64              |
| 2:B:62:LEU:HB2   | 2:B:63:ARG:HD2   | 1.79                     | 0.64              |
| 1:C:192:ARG:HG3  | 1:C:207:HIS:CE1  | 2.33                     | 0.64              |
| 2:D:717:ASN:ND2  | 2:D:717:ASN:O    | 2.30                     | 0.64              |
| 2:B:311:LEU:O    | 2:B:319:GLY:HA3  | 1.98                     | 0.64              |
| 2:B:452:ARG:CG   | 2:B:452:ARG:HH11 | 1.92                     | 0.64              |
| 2:D:166:ARG:HG3  | 2:D:166:ARG:O    | 1.96                     | 0.64              |
| 2:D:192:ILE:HG12 | 2:D:375:ARG:HG2  | 1.80                     | 0.64              |
| 2:B:427:THR:HG21 | 2:B:439:GLU:CD   | 2.18                     | 0.64              |
| 2:B:462:VAL:O    | 2:B:463:GLU:C    | 2.35                     | 0.64              |
| 2:B:55:GLN:O     | 2:B:56:HIS:ND1   | 2.31                     | 0.64              |
| 2:D:624:VAL:CG1  | 2:D:625:LEU:N    | 2.60                     | 0.64              |
| 2:D:120:CYS:O    | 2:D:134:ILE:HD12 | 1.99                     | 0.63              |
| 2:D:641:ASN:O    | 2:D:641:ASN:ND2  | 2.30                     | 0.63              |
| 2:D:653:TYR:O    | 2:D:654:LEU:HB3  | 1.99                     | 0.63              |
| 2:B:192:ILE:HG12 | 2:B:375:ARG:HG2  | 1.80                     | 0.63              |
| 1:A:312:LEU:HD12 | 1:A:315:PHE:HD1  | 1.63                     | 0.63              |
| 2:B:626:ASP:CB   | 2:B:630:LYS:N    | 2.62                     | 0.63              |
| 2:D:273:GLU:CG   | 2:D:306:ASP:OD1  | 2.46                     | 0.63              |
| 2:B:562:ARG:N    | 2:B:563:GLN:HA   | 2.14                     | 0.63              |
| 2:D:449:PRO:CD   | 2:D:455:MET:HE1  | 2.24                     | 0.63              |
| 2:D:729:LYS:C    | 2:D:731:GLY:H    | 2.01                     | 0.63              |
| 2:B:626:ASP:CB   | 2:B:630:LYS:H    | 2.12                     | 0.62              |
| 2:D:113:GLU:HB3  | 2:D:114:PRO:CD   | 2.29                     | 0.62              |
| 2:D:627:LEU:CD1  | 2:D:631:LEU:HD23 | 2.28                     | 0.62              |
| 2:B:122:PHE:CD1  | 2:B:127:ILE:HD13 | 2.34                     | 0.62              |
| 2:D:537:ILE:N    | 2:D:537:ILE:HD12 | 2.15                     | 0.62              |
| 1:C:155:HIS:O    | 1:C:195:ARG:HD3  | 1.99                     | 0.62              |
| 1:C:166:LEU:HD11 | 2:D:544:MET:HE1  | 1.81                     | 0.62              |
| 1:C:66:GLN:HG2   | 1:C:67:VAL:H     | 1.64                     | 0.62              |
| 1:C:58:ALA:HA    | 1:C:60:ILE:HD12  | 1.80                     | 0.62              |
| 1:A:104:GLY:O    | 2:B:503:ASN:ND2  | 2.32                     | 0.62              |
| 2:B:429:ILE:HG23 | 2:B:468:VAL:CG2  | 2.28                     | 0.62              |
| 2:B:729:LYS:O    | 2:B:732:VAL:HG22 | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:268:GLU:OE2  | 4:C:999:AMP:H3'  | 2.00                     | 0.62              |
| 1:C:23:ALA:HA    | 1:C:74:ARG:HG3   | 1.81                     | 0.62              |
| 2:B:740:LEU:HD21 | 2:B:756:LEU:HB2  | 1.82                     | 0.62              |
| 2:B:226:VAL:O    | 2:B:226:VAL:HG22 | 2.00                     | 0.62              |
| 2:D:256:VAL:HG21 | 2:D:376:ALA:HB2  | 1.81                     | 0.62              |
| 1:A:155:HIS:CG   | 1:A:168:THR:HG21 | 2.34                     | 0.61              |
| 1:A:251:THR:O    | 1:A:252:GLU:HB2  | 2.00                     | 0.61              |
| 2:B:672:LYS:O    | 2:B:673:LEU:HB2  | 2.00                     | 0.61              |
| 2:B:272:ILE:CG1  | 2:B:273:GLU:N    | 2.63                     | 0.61              |
| 2:D:26:THR:HG22  | 2:D:32:VAL:N     | 2.10                     | 0.61              |
| 2:D:451:TRP:CD1  | 2:D:452:ARG:HG3  | 2.35                     | 0.61              |
| 1:C:65:GLU:HA    | 1:C:66:GLN:C     | 2.20                     | 0.61              |
| 2:D:786:LYS:HD2  | 2:D:791:ALA:CB   | 2.27                     | 0.61              |
| 1:A:145:ILE:CG2  | 1:A:146:PRO:C    | 2.68                     | 0.61              |
| 1:A:185:ILE:HD11 | 1:A:212:LEU:CD1  | 2.16                     | 0.61              |
| 2:B:205:ILE:HG22 | 2:B:276:ILE:CB   | 2.30                     | 0.61              |
| 2:D:111:ARG:C    | 2:D:113:GLU:H    | 2.03                     | 0.61              |
| 2:D:253:THR:CG2  | 2:D:264:MET:HB2  | 2.28                     | 0.61              |
| 2:D:56:HIS:HE1   | 2:D:58:ASN:HB3   | 1.55                     | 0.61              |
| 1:A:205:MET:O    | 1:A:206:PHE:HB3  | 1.99                     | 0.61              |
| 1:A:269:VAL:HG13 | 1:A:302:LEU:CD1  | 2.31                     | 0.61              |
| 1:C:225:GLY:HA2  | 2:D:476:ASP:HB3  | 1.83                     | 0.61              |
| 2:D:626:ASP:O    | 2:D:627:LEU:C    | 2.37                     | 0.61              |
| 1:C:124:GLY:HA3  | 1:C:186:ARG:HH11 | 1.66                     | 0.61              |
| 2:B:78:VAL:CG1   | 2:B:115:SER:HB3  | 2.28                     | 0.61              |
| 2:B:427:THR:HG23 | 2:B:444:TRP:HE1  | 1.66                     | 0.61              |
| 2:D:115:SER:C    | 2:D:116:GLU:O    | 2.38                     | 0.61              |
| 2:D:452:ARG:CG   | 2:D:452:ARG:HH11 | 2.05                     | 0.61              |
| 2:D:121:SER:HA   | 2:D:135:ILE:HG13 | 1.82                     | 0.61              |
| 2:B:734:GLN:HG3  | 2:B:777:THR:HG21 | 1.83                     | 0.61              |
| 2:B:68:ASN:ND2   | 2:B:143:ILE:HG21 | 2.15                     | 0.60              |
| 2:B:271:ARG:HH21 | 2:B:321:HIS:HD2  | 1.47                     | 0.60              |
| 2:B:31:GLU:HG2   | 2:B:161:SER:HB2  | 1.83                     | 0.60              |
| 2:D:119:LEU:HB3  | 2:D:134:ILE:CD1  | 2.31                     | 0.60              |
| 2:D:634:VAL:HG12 | 2:D:635:GLU:N    | 2.16                     | 0.60              |
| 1:C:166:LEU:HD11 | 2:D:544:MET:CE   | 2.31                     | 0.60              |
| 2:D:631:LEU:C    | 2:D:633:GLU:H    | 2.05                     | 0.60              |
| 2:D:56:HIS:CG    | 2:D:57:PRO:HA    | 2.35                     | 0.60              |
| 1:A:202:HIS:CE1  | 4:A:992:AMP:O2P  | 2.55                     | 0.60              |
| 2:B:24:GLN:NE2   | 2:B:183:ASN:OD1  | 2.31                     | 0.60              |
| 2:D:659:ILE:HD12 | 2:D:684:LEU:HD22 | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:644:LEU:HD13 | 2:B:649:SER:CB   | 2.27                     | 0.60              |
| 2:B:576:PHE:CD1  | 2:B:588:GLN:HG2  | 2.37                     | 0.60              |
| 2:B:630:LYS:HB3  | 2:B:631:LEU:C    | 2.22                     | 0.60              |
| 2:D:56:HIS:CB    | 2:D:57:PRO:CA    | 2.72                     | 0.60              |
| 2:D:55:GLN:CA    | 2:D:56:HIS:O     | 2.48                     | 0.60              |
| 2:B:269:LYS:O    | 2:B:272:ILE:HD12 | 2.01                     | 0.60              |
| 1:C:242:ARG:HB2  | 1:C:257:VAL:O    | 2.01                     | 0.60              |
| 2:D:499:LYS:CD   | 2:D:570:PHE:HE1  | 2.10                     | 0.60              |
| 2:B:137:LEU:O    | 2:B:139:ALA:N    | 2.33                     | 0.60              |
| 2:D:47:VAL:CG2   | 2:D:142:PRO:O    | 2.49                     | 0.60              |
| 2:D:76:ASP:OD2   | 2:D:114:PRO:HB3  | 2.02                     | 0.59              |
| 2:B:209:ALA:H    | 2:B:210:PRO:HD3  | 1.68                     | 0.59              |
| 2:B:627:LEU:HD22 | 1:C:100:ARG:HH12 | 1.67                     | 0.59              |
| 1:C:61:ASN:O     | 1:C:64:LYS:N     | 2.32                     | 0.59              |
| 2:D:473:ASN:H    | 2:D:473:ASN:HD22 | 1.48                     | 0.59              |
| 2:D:566:ARG:HG3  | 2:D:566:ARG:HH11 | 1.68                     | 0.59              |
| 2:B:633:GLU:HB3  | 2:B:655:LYS:H    | 1.66                     | 0.59              |
| 1:C:300:GLU:H    | 1:C:300:GLU:CD   | 2.05                     | 0.59              |
| 2:D:643:ALA:HB1  | 2:D:669:LEU:CD2  | 2.33                     | 0.59              |
| 1:A:140:PHE:HA   | 1:A:145:ILE:HG12 | 1.81                     | 0.59              |
| 1:A:149:HIS:ND1  | 1:A:150:PRO:HD2  | 2.17                     | 0.59              |
| 2:D:19:ASP:OD1   | 2:D:19:ASP:N     | 2.35                     | 0.59              |
| 2:D:127:ILE:HG12 | 2:D:239:ARG:CZ   | 2.32                     | 0.59              |
| 1:A:133:ILE:CD1  | 2:B:576:PHE:CD1  | 2.85                     | 0.59              |
| 2:B:787:GLU:HG3  | 2:B:787:GLU:O    | 2.03                     | 0.59              |
| 2:D:263:PRO:HB2  | 2:D:360:TYR:CE2  | 2.38                     | 0.59              |
| 2:D:26:THR:CG2   | 2:D:32:VAL:H     | 2.12                     | 0.59              |
| 2:D:205:ILE:HD11 | 2:D:392:ILE:HB   | 1.83                     | 0.59              |
| 2:D:634:VAL:CG1  | 2:D:635:GLU:N    | 2.66                     | 0.59              |
| 1:A:300:GLU:CB   | 1:A:312:LEU:CD1  | 2.79                     | 0.59              |
| 2:B:257:LEU:HA   | 2:B:262:GLN:O    | 2.03                     | 0.59              |
| 2:B:666:HIS:ND1  | 2:B:668:GLU:OE1  | 2.35                     | 0.59              |
| 1:C:108:PRO:HG3  | 1:C:326:PHE:CD2  | 2.37                     | 0.59              |
| 2:B:750:ALA:HB3  | 2:B:753:TYR:HD1  | 1.68                     | 0.59              |
| 1:A:140:PHE:HD1  | 1:A:145:ILE:HG13 | 1.66                     | 0.59              |
| 1:A:314:SER:HA   | 1:A:317:GLU:HG3  | 1.85                     | 0.59              |
| 1:A:143:LEU:HD11 | 1:A:171:SER:HB3  | 1.84                     | 0.58              |
| 2:D:49:GLU:HB3   | 2:D:89:ARG:HD3   | 1.85                     | 0.58              |
| 2:D:689:LEU:O    | 2:D:689:LEU:HG   | 2.02                     | 0.58              |
| 2:D:711:ALA:HB3  | 2:D:793:LEU:O    | 2.03                     | 0.58              |
| 2:B:90:VAL:HG13  | 2:B:91:ALA:N     | 2.17                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:62:GLU:C     | 1:C:64:LYS:H     | 2.05                     | 0.58              |
| 2:D:515:PHE:HA   | 2:D:543:ALA:O    | 2.03                     | 0.58              |
| 1:A:107:HIS:CG   | 1:A:108:PRO:HD2  | 2.38                     | 0.58              |
| 2:D:142:PRO:O    | 2:D:144:GLY:N    | 2.36                     | 0.58              |
| 2:D:272:ILE:O    | 2:D:306:ASP:HB2  | 2.03                     | 0.58              |
| 2:D:735:VAL:HA   | 2:D:762:LEU:HD23 | 1.86                     | 0.58              |
| 1:C:218:ILE:HG12 | 1:C:222:ASN:HD22 | 1.67                     | 0.58              |
| 1:C:62:GLU:C     | 1:C:64:LYS:N     | 2.57                     | 0.58              |
| 2:D:32:VAL:HB    | 2:D:158:ILE:CD1  | 2.32                     | 0.58              |
| 2:D:473:ASN:N    | 2:D:473:ASN:ND2  | 2.49                     | 0.58              |
| 2:D:306:ASP:OD2  | 2:D:306:ASP:C    | 2.42                     | 0.58              |
| 2:D:713:VAL:O    | 2:D:714:VAL:HG23 | 2.04                     | 0.58              |
| 1:C:60:ILE:O     | 1:C:61:ASN:C     | 2.42                     | 0.58              |
| 2:D:370:HIS:O    | 2:D:374:GLU:HG2  | 2.04                     | 0.58              |
| 2:D:762:LEU:HD12 | 2:D:774:ILE:HG23 | 1.85                     | 0.58              |
| 1:A:156:ASP:CB   | 1:A:196:ASN:HB3  | 2.34                     | 0.58              |
| 2:B:652:ILE:HD11 | 2:B:662:VAL:HG22 | 1.85                     | 0.58              |
| 2:B:629:GLY:HA2  | 2:B:692:ARG:HB2  | 1.85                     | 0.58              |
| 1:C:139:ASN:HD21 | 1:C:168:THR:H    | 1.51                     | 0.58              |
| 1:C:17:GLN:C     | 1:C:19:SER:H     | 2.06                     | 0.58              |
| 2:B:111:ARG:HH11 | 2:B:111:ARG:HG3  | 1.69                     | 0.58              |
| 1:C:65:GLU:HG2   | 1:C:65:GLU:O     | 2.04                     | 0.58              |
| 1:A:107:HIS:HE1  | 1:A:315:PHE:O    | 1.87                     | 0.58              |
| 1:A:166:LEU:CD1  | 2:B:544:MET:HE1  | 2.32                     | 0.58              |
| 2:B:287:LEU:O    | 2:B:294:GLU:HA   | 2.04                     | 0.57              |
| 2:B:698:ARG:H    | 1:C:325:GLN:HE22 | 1.50                     | 0.57              |
| 2:B:644:LEU:HA   | 2:B:666:HIS:H    | 1.68                     | 0.57              |
| 1:C:251:THR:OG1  | 1:C:254:SER:HB3  | 2.05                     | 0.57              |
| 2:B:214:PRO:HD2  | 2:B:337:PHE:HD2  | 1.69                     | 0.57              |
| 2:B:750:ALA:O    | 2:B:753:TYR:HB2  | 2.04                     | 0.57              |
| 1:A:145:ILE:HG21 | 1:A:146:PRO:O    | 2.03                     | 0.57              |
| 2:D:319:GLY:C    | 2:D:321:HIS:H    | 2.05                     | 0.57              |
| 2:D:626:ASP:CB   | 2:D:627:LEU:HD12 | 2.35                     | 0.57              |
| 2:B:621:LEU:O    | 2:B:625:LEU:N    | 2.31                     | 0.57              |
| 1:C:258:ASP:HA   | 1:C:267:LEU:O    | 2.04                     | 0.57              |
| 1:C:304:MET:HA   | 1:C:309:VAL:HB   | 1.85                     | 0.57              |
| 2:D:732:VAL:CG1  | 2:D:733:ASN:H    | 2.09                     | 0.57              |
| 1:A:202:HIS:HE1  | 4:A:992:AMP:O2P  | 1.86                     | 0.57              |
| 2:B:195:VAL:HG21 | 2:B:377:THR:HG22 | 1.87                     | 0.57              |
| 2:B:577:VAL:HG23 | 2:B:587:ARG:HB3  | 1.87                     | 0.57              |
| 1:C:301:ARG:HD2  | 4:C:999:AMP:C2   | 2.39                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:735:VAL:HB   | 2:D:762:LEU:HD23 | 1.87                     | 0.57              |
| 2:B:767:ARG:HH11 | 2:B:767:ARG:HB3  | 1.68                     | 0.57              |
| 1:C:253:PRO:HB3  | 2:D:463:GLU:HA   | 1.87                     | 0.57              |
| 2:D:533:LEU:HD23 | 2:D:536:PRO:HB3  | 1.87                     | 0.57              |
| 2:D:626:ASP:CB   | 2:D:631:LEU:CD2  | 2.82                     | 0.57              |
| 1:A:203:THR:N    | 4:A:992:AMP:N6   | 2.52                     | 0.56              |
| 2:B:436:GLU:HB3  | 2:B:447:VAL:HB   | 1.86                     | 0.56              |
| 1:A:134:GLU:HB3  | 1:A:165:LEU:CD2  | 2.34                     | 0.56              |
| 1:C:88:ALA:O     | 1:C:91:THR:HG23  | 2.04                     | 0.56              |
| 2:D:92:VAL:HG13  | 2:D:119:LEU:HD23 | 1.87                     | 0.56              |
| 1:C:277:PRO:HG3  | 2:D:459:GLU:CD   | 2.25                     | 0.56              |
| 2:B:644:LEU:CD1  | 2:B:649:SER:HB2  | 2.32                     | 0.56              |
| 2:D:115:SER:O    | 2:D:116:GLU:C    | 2.43                     | 0.56              |
| 1:A:145:ILE:HG22 | 1:A:146:PRO:N    | 2.19                     | 0.56              |
| 1:A:243:PHE:HD2  | 1:A:257:VAL:HG12 | 1.69                     | 0.56              |
| 1:C:257:VAL:HG23 | 1:C:269:VAL:HG23 | 1.86                     | 0.56              |
| 2:B:2:LYS:HB3    | 2:B:159:GLU:HB2  | 1.86                     | 0.56              |
| 2:B:376:ALA:HA   | 2:B:379:LEU:HD22 | 1.86                     | 0.56              |
| 2:D:38:VAL:HG11  | 2:D:240:ARG:HD3  | 1.88                     | 0.56              |
| 1:A:136:ASP:OD1  | 1:A:152:ARG:CZ   | 2.54                     | 0.56              |
| 2:B:50:VAL:HA    | 2:B:67:VAL:HG12  | 1.88                     | 0.56              |
| 2:B:650:ALA:O    | 2:B:661:PHE:HD1  | 1.88                     | 0.56              |
| 1:C:167:ARG:NH2  | 1:C:191:GLY:HA3  | 2.21                     | 0.56              |
| 2:D:205:ILE:O    | 2:D:394:ILE:HD13 | 2.06                     | 0.56              |
| 1:A:210:GLU:HA   | 1:A:295:PHE:O    | 2.06                     | 0.56              |
| 2:B:256:VAL:HG13 | 2:B:260:LEU:HD12 | 1.87                     | 0.56              |
| 2:B:626:ASP:C    | 2:B:629:GLY:H    | 2.09                     | 0.56              |
| 2:D:555:THR:O    | 2:D:559:ASN:ND2  | 2.38                     | 0.56              |
| 1:A:178:MET:SD   | 1:A:212:LEU:HD11 | 2.46                     | 0.56              |
| 2:B:741:PHE:CB   | 2:D:603:GLU:HG3  | 2.36                     | 0.56              |
| 1:A:156:ASP:HB3  | 1:A:196:ASN:HB3  | 1.87                     | 0.56              |
| 1:A:139:ASN:ND2  | 1:A:168:THR:HB   | 2.09                     | 0.56              |
| 2:D:7:TRP:O      | 2:D:10:GLU:HB2   | 2.06                     | 0.56              |
| 2:B:283:GLU:HG2  | 2:B:299:ALA:HB2  | 1.88                     | 0.56              |
| 2:B:477:GLU:OE1  | 2:B:478:PRO:HD2  | 2.06                     | 0.56              |
| 2:B:575:ARG:O    | 2:B:588:GLN:HA   | 2.06                     | 0.56              |
| 2:B:121:SER:OG   | 2:B:124:GLU:HG2  | 2.06                     | 0.55              |
| 2:B:488:HIS:CD2  | 2:B:488:HIS:H    | 2.23                     | 0.55              |
| 1:C:241:ILE:H    | 1:C:241:ILE:HD13 | 1.71                     | 0.55              |
| 2:B:708:ARG:O    | 2:B:760:LEU:HD12 | 2.06                     | 0.55              |
| 1:C:58:ALA:CA    | 1:C:60:ILE:HG21  | 2.35                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:87:LEU:O     | 1:C:91:THR:CG2   | 2.54                     | 0.55              |
| 1:A:252:GLU:OE2  | 2:B:463:GLU:CD   | 2.45                     | 0.55              |
| 2:B:562:ARG:H    | 2:B:563:GLN:HA   | 1.71                     | 0.55              |
| 2:B:576:PHE:CE1  | 2:B:588:GLN:HG2  | 2.41                     | 0.55              |
| 1:C:62:GLU:O     | 1:C:65:GLU:N     | 2.35                     | 0.55              |
| 2:D:280:MET:HG2  | 2:D:299:ALA:O    | 2.07                     | 0.55              |
| 2:B:202:THR:CG2  | 2:B:392:ILE:HD11 | 2.36                     | 0.55              |
| 2:D:470:GLY:HA3  | 2:D:473:ASN:HD21 | 1.71                     | 0.55              |
| 2:B:783:GLU:HA   | 2:B:786:LYS:HB2  | 1.88                     | 0.55              |
| 1:C:228:HIS:HB2  | 1:C:243:PHE:HZ   | 1.70                     | 0.55              |
| 2:D:338:PHE:CD2  | 2:D:360:TYR:CE1  | 2.94                     | 0.55              |
| 2:D:553:LEU:HA   | 2:D:556:VAL:CG1  | 2.37                     | 0.55              |
| 2:B:127:ILE:HG13 | 2:B:239:ARG:CZ   | 2.37                     | 0.55              |
| 2:B:209:ALA:N    | 2:B:210:PRO:HD3  | 2.22                     | 0.55              |
| 2:D:408:LEU:HD23 | 2:D:458:GLU:HG3  | 1.89                     | 0.55              |
| 1:A:158:PHE:CD2  | 1:A:195:ARG:O    | 2.54                     | 0.55              |
| 2:B:53:CYS:SG    | 2:B:63:ARG:HG2   | 2.47                     | 0.55              |
| 2:D:729:LYS:HB3  | 2:D:729:LYS:NZ   | 2.21                     | 0.55              |
| 2:B:139:ALA:C    | 2:B:141:ALA:N    | 2.59                     | 0.55              |
| 2:B:483:LEU:HB3  | 1:C:123:LEU:HG   | 1.88                     | 0.55              |
| 1:C:301:ARG:CD   | 4:C:999:AMP:C2   | 2.89                     | 0.55              |
| 2:D:375:ARG:CG   | 2:D:375:ARG:NH1  | 2.47                     | 0.55              |
| 2:B:631:LEU:CD2  | 2:B:632:ASN:H    | 2.20                     | 0.54              |
| 2:D:617:LEU:HD23 | 2:D:662:VAL:HG23 | 1.89                     | 0.54              |
| 1:C:171:SER:HA   | 1:C:210:GLU:CD   | 2.28                     | 0.54              |
| 2:D:723:ILE:HG23 | 2:D:785:LEU:HD22 | 1.89                     | 0.54              |
| 2:D:764:ASP:OD2  | 2:D:765:THR:N    | 2.40                     | 0.54              |
| 1:A:218:ILE:HD12 | 1:A:219:SER:N    | 2.22                     | 0.54              |
| 2:B:294:GLU:CD   | 2:B:294:GLU:H    | 2.10                     | 0.54              |
| 2:B:641:ASN:O    | 2:B:643:ALA:N    | 2.40                     | 0.54              |
| 2:B:134:ILE:N    | 2:B:134:ILE:HD12 | 2.23                     | 0.54              |
| 2:B:524:ILE:O    | 2:B:643:ALA:HB2  | 2.07                     | 0.54              |
| 2:B:662:VAL:HG13 | 2:B:682:PHE:HB3  | 1.89                     | 0.54              |
| 1:C:58:ALA:HB1   | 1:C:61:ASN:N     | 2.23                     | 0.54              |
| 2:D:606:ASN:CG   | 2:D:606:ASN:O    | 2.46                     | 0.54              |
| 2:D:698:ARG:O    | 2:D:699:GLU:O    | 2.26                     | 0.54              |
| 2:B:256:VAL:HG21 | 2:B:376:ALA:HB2  | 1.90                     | 0.54              |
| 2:B:272:ILE:O    | 2:B:273:GLU:HB2  | 2.08                     | 0.54              |
| 2:B:59:ALA:HB2   | 2:B:111:ARG:HG2  | 1.89                     | 0.54              |
| 2:B:7:TRP:HD1    | 2:B:7:TRP:O      | 1.91                     | 0.54              |
| 2:B:7:TRP:CD1    | 2:B:7:TRP:O      | 2.61                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:641:ASN:HB2  | 2:D:661:PHE:CE1  | 2.41                     | 0.54              |
| 2:D:733:ASN:HA   | 2:D:734:GLN:CB   | 2.30                     | 0.54              |
| 2:B:522:GLN:O    | 2:B:526:PRO:HA   | 2.07                     | 0.54              |
| 2:B:724:LEU:HD12 | 2:B:738:VAL:HB   | 1.90                     | 0.54              |
| 1:C:140:PHE:HD1  | 1:C:145:ILE:HD13 | 1.72                     | 0.54              |
| 1:C:220:PHE:O    | 1:C:223:LEU:N    | 2.40                     | 0.54              |
| 2:D:76:ASP:OD2   | 2:D:114:PRO:CB   | 2.56                     | 0.54              |
| 1:A:192:ARG:NH2  | 2:B:512:THR:O    | 2.41                     | 0.54              |
| 2:B:521:GLN:NE2  | 2:B:546:LEU:H    | 2.06                     | 0.54              |
| 1:C:21:VAL:HA    | 1:C:24:LEU:HB2   | 1.90                     | 0.54              |
| 2:B:641:ASN:C    | 2:B:643:ALA:H    | 2.10                     | 0.54              |
| 2:D:127:ILE:C    | 2:D:127:ILE:CD1  | 2.76                     | 0.54              |
| 1:A:160:PHE:CE1  | 1:A:166:LEU:HG   | 2.43                     | 0.54              |
| 2:D:560:GLN:HG2  | 2:D:675:LEU:HB3  | 1.89                     | 0.54              |
| 2:B:338:PHE:CB   | 2:B:343:ILE:HD11 | 2.39                     | 0.53              |
| 2:B:457:ILE:HG22 | 2:B:460:ASP:CG   | 2.27                     | 0.53              |
| 2:B:517:ASP:CA   | 2:B:540:GLU:O    | 2.56                     | 0.53              |
| 2:B:647:GLY:HA3  | 1:C:91:THR:HB    | 1.90                     | 0.53              |
| 1:C:257:VAL:CG2  | 1:C:269:VAL:HG23 | 2.38                     | 0.53              |
| 2:D:109:LYS:HA   | 2:D:115:SER:HA   | 1.90                     | 0.53              |
| 2:D:55:GLN:CG    | 2:D:56:HIS:HA    | 2.36                     | 0.53              |
| 1:A:151:ALA:O    | 1:A:154:ASP:N    | 2.41                     | 0.53              |
| 1:A:164:ARG:NH1  | 2:B:585:GLY:N    | 2.42                     | 0.53              |
| 2:B:304:ILE:O    | 2:B:311:LEU:HD22 | 2.09                     | 0.53              |
| 2:B:630:LYS:HB3  | 2:B:631:LEU:CA   | 2.38                     | 0.53              |
| 2:B:674:ASP:O    | 2:B:675:LEU:CB   | 2.55                     | 0.53              |
| 2:D:205:ILE:CG2  | 2:D:276:ILE:HB   | 2.36                     | 0.53              |
| 1:C:58:ALA:HA    | 1:C:60:ILE:HG21  | 1.89                     | 0.53              |
| 1:A:270:LEU:C    | 1:A:270:LEU:HD12 | 2.29                     | 0.53              |
| 1:A:218:ILE:CD1  | 1:A:293:PHE:CD1  | 2.92                     | 0.53              |
| 2:D:630:LYS:NZ   | 2:D:691:ASP:OD2  | 2.42                     | 0.53              |
| 1:A:312:LEU:HD12 | 1:A:315:PHE:CD1  | 2.44                     | 0.53              |
| 2:B:370:HIS:CE1  | 2:B:393:ASP:OD1  | 2.62                     | 0.53              |
| 1:C:82:ALA:O     | 1:C:85:ALA:N     | 2.41                     | 0.53              |
| 2:B:565:ASN:OD1  | 2:B:566:ARG:N    | 2.34                     | 0.53              |
| 2:D:312:ALA:HB1  | 2:D:317:PHE:O    | 2.09                     | 0.53              |
| 2:D:729:LYS:C    | 2:D:731:GLY:N    | 2.63                     | 0.53              |
| 1:C:5:ALA:O      | 1:C:9:ALA:HB3    | 2.09                     | 0.53              |
| 2:D:498:VAL:HG13 | 2:D:624:VAL:HG13 | 1.90                     | 0.53              |
| 2:D:57:PRO:CB    | 2:D:59:ALA:O     | 2.57                     | 0.53              |
| 2:B:45:VAL:HG13  | 2:B:92:VAL:O     | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:202:HIS:ND1  | 1:C:301:ARG:NH2  | 2.56                     | 0.53              |
| 2:B:32:VAL:HG12  | 2:B:160:ILE:HG22 | 1.91                     | 0.52              |
| 2:B:376:ALA:HA   | 2:B:379:LEU:CD2  | 2.40                     | 0.52              |
| 1:C:71:LEU:C     | 1:C:73:ALA:H     | 2.13                     | 0.52              |
| 2:D:549:TRP:O    | 2:D:553:LEU:HG   | 2.10                     | 0.52              |
| 2:D:634:VAL:HG23 | 2:D:654:LEU:HD13 | 1.91                     | 0.52              |
| 1:A:185:ILE:CG1  | 1:A:186:ARG:N    | 2.72                     | 0.52              |
| 1:A:244:ARG:NH1  | 1:A:256:GLU:OE2  | 2.42                     | 0.52              |
| 1:C:218:ILE:O    | 1:C:218:ILE:HG23 | 2.09                     | 0.52              |
| 2:D:263:PRO:HB2  | 2:D:360:TYR:HE2  | 1.74                     | 0.52              |
| 2:D:653:TYR:O    | 2:D:654:LEU:CB   | 2.57                     | 0.52              |
| 1:A:86:ARG:HG2   | 1:A:90:GLU:OE1   | 2.08                     | 0.52              |
| 2:B:165:ASN:H    | 2:B:165:ASN:ND2  | 2.01                     | 0.52              |
| 2:B:4:SER:HB3    | 2:B:7:TRP:HB2    | 1.91                     | 0.52              |
| 1:C:56:ALA:N     | 1:C:57:GLY:HA3   | 2.24                     | 0.52              |
| 2:D:199:ILE:HD13 | 2:D:222:LYS:HG2  | 1.90                     | 0.52              |
| 2:D:358:HIS:O    | 2:D:362:ARG:HD3  | 2.08                     | 0.52              |
| 1:C:194:TYR:OH   | 2:D:514:SER:HB2  | 2.09                     | 0.52              |
| 1:A:145:ILE:HG22 | 1:A:146:PRO:CA   | 2.39                     | 0.52              |
| 2:B:123:SER:O    | 2:B:125:LEU:N    | 2.42                     | 0.52              |
| 2:B:603:GLU:HA   | 2:B:603:GLU:OE1  | 2.10                     | 0.52              |
| 2:B:739:ASN:ND2  | 2:B:740:LEU:H    | 2.08                     | 0.52              |
| 1:C:190:PRO:N    | 1:C:209:MET:HE3  | 2.25                     | 0.52              |
| 1:C:211:GLY:HA3  | 1:C:295:PHE:CZ   | 2.44                     | 0.52              |
| 2:D:624:VAL:O    | 2:D:625:LEU:C    | 2.46                     | 0.52              |
| 2:D:735:VAL:HB   | 2:D:762:LEU:CD2  | 2.39                     | 0.52              |
| 1:C:255:ALA:HB2  | 2:D:471:TYR:HE2  | 1.75                     | 0.52              |
| 1:C:58:ALA:HA    | 1:C:60:ILE:HB    | 1.79                     | 0.52              |
| 1:A:247:TYR:CE1  | 2:B:165:ASN:HB3  | 2.45                     | 0.52              |
| 2:D:672:LYS:O    | 2:D:674:ASP:CB   | 2.58                     | 0.52              |
| 2:D:631:LEU:CG   | 2:D:632:ASN:H    | 2.21                     | 0.52              |
| 1:A:218:ILE:CD1  | 1:A:293:PHE:HD1  | 2.23                     | 0.52              |
| 1:A:201:THR:C    | 1:A:312:LEU:HD23 | 2.29                     | 0.52              |
| 2:B:344:THR:HA   | 2:B:361:GLU:CD   | 2.31                     | 0.52              |
| 2:B:205:ILE:O    | 2:B:394:ILE:HD13 | 2.10                     | 0.52              |
| 2:B:521:GLN:HE22 | 2:B:545:ARG:HA   | 1.74                     | 0.52              |
| 1:C:241:ILE:CD1  | 1:C:241:ILE:H    | 2.22                     | 0.52              |
| 2:D:548:LEU:HD23 | 2:D:571:GLU:HB3  | 1.91                     | 0.52              |
| 2:D:731:GLY:HA2  | 2:D:735:VAL:HG13 | 1.92                     | 0.52              |
| 1:C:322:PHE:O    | 1:C:325:GLN:HG2  | 2.10                     | 0.51              |
| 1:C:59:VAL:O     | 1:C:59:VAL:CG1   | 2.53                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:288:VAL:HA   | 2:D:294:GLU:HA   | 1.91                     | 0.51              |
| 2:D:43:HIS:O     | 2:D:97:ALA:HB1   | 2.09                     | 0.51              |
| 2:D:702:ARG:N    | 2:D:702:ARG:NE   | 2.55                     | 0.51              |
| 1:A:318:ASN:HD22 | 1:A:323:LEU:HD21 | 1.74                     | 0.51              |
| 1:A:86:ARG:O     | 1:A:90:GLU:HB2   | 2.10                     | 0.51              |
| 2:B:38:VAL:HB    | 2:B:155:ASP:O    | 2.09                     | 0.51              |
| 2:B:264:MET:CE   | 2:B:376:ALA:HB2  | 2.41                     | 0.51              |
| 2:B:626:ASP:C    | 2:B:628:THR:N    | 2.62                     | 0.51              |
| 1:C:257:VAL:O    | 1:C:258:ASP:HB2  | 2.10                     | 0.51              |
| 1:A:269:VAL:HG13 | 1:A:302:LEU:HD13 | 1.91                     | 0.51              |
| 2:B:264:MET:HE1  | 2:B:376:ALA:HB2  | 1.91                     | 0.51              |
| 1:C:132:GLU:HA   | 1:C:167:ARG:HD3  | 1.92                     | 0.51              |
| 1:C:185:ILE:C    | 1:C:185:ILE:HD13 | 2.30                     | 0.51              |
| 1:C:23:ALA:HA    | 1:C:74:ARG:CG    | 2.40                     | 0.51              |
| 2:D:142:PRO:C    | 2:D:144:GLY:H    | 2.13                     | 0.51              |
| 2:D:24:GLN:HG3   | 2:D:182:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:218:ILE:HD13 | 1:A:293:PHE:HD1  | 1.74                     | 0.51              |
| 2:B:17:ASP:OD1   | 2:B:18:SER:N     | 2.44                     | 0.51              |
| 2:B:630:LYS:CB   | 2:B:631:LEU:O    | 2.50                     | 0.51              |
| 2:B:631:LEU:HD23 | 2:B:632:ASN:N    | 2.26                     | 0.51              |
| 1:C:211:GLY:HA3  | 1:C:295:PHE:CE2  | 2.45                     | 0.51              |
| 2:D:55:GLN:C     | 2:D:56:HIS:O     | 2.48                     | 0.51              |
| 2:D:593:ALA:HB2  | 2:D:683:GLU:HG3  | 1.91                     | 0.51              |
| 2:D:709:ASP:HA   | 2:D:759:SER:HA   | 1.91                     | 0.51              |
| 1:A:270:LEU:CB   | 1:A:297:MET:HB3  | 2.38                     | 0.51              |
| 1:C:119:PHE:N    | 1:C:119:PHE:CD1  | 2.78                     | 0.51              |
| 2:B:48:GLY:HA2   | 2:B:143:ILE:HG23 | 1.93                     | 0.51              |
| 2:B:501:LEU:HA   | 2:D:504:ASP:OD2  | 2.11                     | 0.51              |
| 2:B:517:ASP:HA   | 2:B:540:GLU:O    | 2.10                     | 0.51              |
| 2:B:55:GLN:C     | 2:B:56:HIS:CG    | 2.84                     | 0.51              |
| 2:B:90:VAL:O     | 2:B:137:LEU:HD22 | 2.11                     | 0.51              |
| 2:B:790:GLN:CG   | 2:B:791:ALA:H    | 2.24                     | 0.51              |
| 2:D:183:ASN:HB2  | 2:D:185:LEU:HD12 | 1.91                     | 0.51              |
| 2:D:452:ARG:NH1  | 2:D:452:ARG:HG2  | 1.97                     | 0.51              |
| 2:B:613:ASP:C    | 2:B:613:ASP:OD2  | 2.49                     | 0.51              |
| 2:D:137:LEU:HB3  | 2:D:138:PRO:HD2  | 1.92                     | 0.51              |
| 1:A:118:SER:O    | 1:A:119:PHE:C    | 2.49                     | 0.50              |
| 2:B:38:VAL:HG21  | 2:B:240:ARG:CD   | 2.40                     | 0.50              |
| 2:D:605:TRP:CE3  | 2:D:606:ASN:HB2  | 2.45                     | 0.50              |
| 1:A:86:ARG:HG2   | 1:A:90:GLU:CD    | 2.31                     | 0.50              |
| 2:B:232:LEU:O    | 2:B:235:LYS:HB3  | 2.10                     | 0.50              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:744:TYR:OH  | 2:B:747:LYS:N    | 2.44                     | 0.50              |
| 1:C:132:GLU:CD  | 2:D:574:LEU:HD11 | 2.31                     | 0.50              |
| 2:D:731:GLY:HA2 | 2:D:735:VAL:CG1  | 2.41                     | 0.50              |
| 2:B:614:PHE:CZ  | 1:C:94:VAL:HG22  | 2.46                     | 0.50              |
| 2:D:441:LYS:HG2 | 2:D:441:LYS:O    | 2.09                     | 0.50              |
| 2:B:520:VAL:O   | 2:B:523:MET:HB2  | 2.11                     | 0.50              |
| 2:D:672:LYS:O   | 2:D:674:ASP:CG   | 2.49                     | 0.50              |
| 2:D:85:ARG:HB3  | 2:D:88:LEU:HD11  | 1.91                     | 0.50              |
| 1:A:185:ILE:O   | 1:A:186:ARG:HB2  | 2.11                     | 0.50              |
| 1:A:243:PHE:CD2 | 1:A:257:VAL:HG12 | 2.46                     | 0.50              |
| 1:A:300:GLU:CB  | 1:A:312:LEU:HD11 | 2.41                     | 0.50              |
| 2:B:177:ARG:HA  | 2:B:187:LEU:HD13 | 1.93                     | 0.50              |
| 2:D:137:LEU:HB3 | 2:D:138:PRO:CD   | 2.42                     | 0.50              |
| 2:B:138:PRO:O   | 2:B:139:ALA:O    | 2.30                     | 0.50              |
| 1:C:211:GLY:O   | 1:C:294:ALA:HA   | 2.11                     | 0.50              |
| 2:D:41:SER:HA   | 2:D:148:ARG:HH21 | 1.77                     | 0.50              |
| 2:B:525:HIS:HE1 | 2:B:547:SER:OG   | 1.94                     | 0.50              |
| 2:D:54:ALA:O    | 2:D:55:GLN:O     | 2.29                     | 0.50              |
| 2:D:670:GLU:OE2 | 2:D:671:ARG:NH2  | 2.44                     | 0.50              |
| 1:A:97:PRO:HD2  | 2:B:605:TRP:CD1  | 2.47                     | 0.50              |
| 2:B:687:ASN:C   | 2:B:687:ASN:OD1  | 2.49                     | 0.50              |
| 2:D:346:ARG:N   | 2:D:346:ARG:HD2  | 2.27                     | 0.50              |
| 2:D:53:CYS:O    | 2:D:54:ALA:O     | 2.30                     | 0.50              |
| 2:B:698:ARG:H   | 1:C:325:GLN:NE2  | 2.10                     | 0.50              |
| 1:C:149:HIS:O   | 1:C:150:PRO:C    | 2.50                     | 0.50              |
| 1:C:58:ALA:HA   | 1:C:60:ILE:CG2   | 2.39                     | 0.50              |
| 1:A:268:GLU:HB3 | 1:A:301:ARG:HH21 | 1.78                     | 0.49              |
| 2:B:122:PHE:CD1 | 2:B:127:ILE:CD1  | 2.95                     | 0.49              |
| 2:B:37:PRO:HA   | 2:B:156:ASN:HD22 | 1.75                     | 0.49              |
| 2:B:591:MET:HE3 | 2:B:684:LEU:O    | 2.11                     | 0.49              |
| 1:C:251:THR:HB  | 1:C:273:GLY:HA3  | 1.93                     | 0.49              |
| 2:D:515:PHE:CD1 | 2:D:544:MET:HE1  | 2.37                     | 0.49              |
| 2:B:741:PHE:HB3 | 2:D:603:GLU:HG3  | 1.94                     | 0.49              |
| 1:C:50:PRO:O    | 1:C:52:GLU:N     | 2.45                     | 0.49              |
| 2:D:17:ASP:HB3  | 2:D:20:ALA:H     | 1.76                     | 0.49              |
| 2:D:279:ARG:NH1 | 2:D:280:MET:O    | 2.45                     | 0.49              |
| 2:D:547:SER:OG  | 2:D:549:TRP:HB2  | 2.12                     | 0.49              |
| 2:B:123:SER:C   | 2:B:125:LEU:H    | 2.15                     | 0.49              |
| 1:C:265:LYS:NZ  | 2:D:33:ASP:HB2   | 2.27                     | 0.49              |
| 1:C:265:LYS:HD2 | 1:C:266:TRP:N    | 2.27                     | 0.49              |
| 1:C:69:GLN:HE21 | 1:C:69:GLN:CA    | 2.23                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:83:ASN:O     | 2:B:134:ILE:HD11 | 2.12                     | 0.49              |
| 2:B:204:PRO:HD2  | 2:B:275:GLY:HA2  | 1.94                     | 0.49              |
| 2:B:90:VAL:CG1   | 2:B:91:ALA:N     | 2.75                     | 0.49              |
| 1:A:195:ARG:HD2  | 1:A:206:PHE:HE1  | 1.77                     | 0.49              |
| 2:B:208:GLU:O    | 2:B:209:ALA:HB2  | 2.13                     | 0.49              |
| 2:B:271:ARG:HH21 | 2:B:321:HIS:CD2  | 2.29                     | 0.49              |
| 2:B:615:TYR:HB2  | 1:C:99:ARG:NH1   | 2.28                     | 0.49              |
| 1:A:143:LEU:O    | 1:A:250:PHE:HB3  | 2.12                     | 0.49              |
| 2:B:181:VAL:HG11 | 2:B:433:LEU:HD13 | 1.94                     | 0.49              |
| 2:B:653:TYR:O    | 2:B:657:GLU:O    | 2.30                     | 0.49              |
| 1:C:174:GLN:OE1  | 1:C:210:GLU:OE2  | 2.30                     | 0.49              |
| 2:D:54:ALA:HB3   | 2:D:64:VAL:HG13  | 1.94                     | 0.49              |
| 2:D:668:GLU:HG2  | 2:D:672:LYS:HE3  | 1.93                     | 0.49              |
| 1:A:189:ALA:HB3  | 1:A:210:GLU:HB2  | 1.94                     | 0.49              |
| 1:C:105:GLY:HA3  | 2:D:508:GLN:OE1  | 2.12                     | 0.49              |
| 2:B:338:PHE:HB3  | 2:B:343:ILE:HD11 | 1.94                     | 0.49              |
| 2:B:515:PHE:HD1  | 2:B:544:MET:CE   | 2.24                     | 0.49              |
| 2:B:583:PRO:C    | 2:B:584:LEU:O    | 2.51                     | 0.49              |
| 2:B:625:LEU:C    | 2:B:627:LEU:H    | 2.09                     | 0.49              |
| 2:B:794:ARG:HA   | 2:B:795:ASP:C    | 2.34                     | 0.49              |
| 1:C:216:THR:O    | 1:C:217:ASN:O    | 2.30                     | 0.49              |
| 1:C:45:LEU:CB    | 1:C:46:ARG:HA    | 2.42                     | 0.49              |
| 1:C:54:PRO:N     | 1:C:55:ALA:CA    | 2.70                     | 0.49              |
| 1:C:202:HIS:HA   | 4:C:999:AMP:HN61 | 1.76                     | 0.49              |
| 2:D:630:LYS:NZ   | 2:D:691:ASP:O    | 2.35                     | 0.49              |
| 2:D:548:LEU:HD12 | 2:D:548:LEU:N    | 2.28                     | 0.49              |
| 2:B:111:ARG:CG   | 2:B:111:ARG:HH11 | 2.26                     | 0.49              |
| 2:B:280:MET:HG3  | 2:B:299:ALA:O    | 2.13                     | 0.49              |
| 1:C:242:ARG:O    | 1:C:257:VAL:HA   | 2.12                     | 0.49              |
| 2:D:113:GLU:O    | 2:D:114:PRO:O    | 2.30                     | 0.49              |
| 2:D:713:VAL:H    | 2:D:792:SER:HA   | 1.78                     | 0.49              |
| 2:B:710:ILE:HD11 | 2:B:758:ILE:HB   | 1.95                     | 0.48              |
| 2:D:493:LEU:HB2  | 2:D:692:ARG:HD3  | 1.94                     | 0.48              |
| 2:B:309:LYS:NZ   | 2:B:321:HIS:CE1  | 2.81                     | 0.48              |
| 1:C:244:ARG:O    | 1:C:255:ALA:HB1  | 2.14                     | 0.48              |
| 2:D:556:VAL:HG23 | 2:D:560:GLN:OE1  | 2.12                     | 0.48              |
| 2:D:570:PHE:HA   | 2:D:593:ALA:O    | 2.13                     | 0.48              |
| 2:D:634:VAL:HG22 | 2:D:654:LEU:CB   | 2.34                     | 0.48              |
| 1:A:182:GLN:HG3  | 1:A:183:PRO:HD2  | 1.95                     | 0.48              |
| 1:A:230:PHE:HB2  | 2:D:485:MET:HE1  | 1.94                     | 0.48              |
| 2:B:522:GLN:NE2  | 2:B:529:GLU:CD   | 2.66                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:99:ARG:HB3   | 2:B:607:LEU:HD21 | 1.95                     | 0.48              |
| 1:C:59:VAL:H     | 1:C:60:ILE:CB    | 2.23                     | 0.48              |
| 2:D:55:GLN:HG3   | 2:D:56:HIS:HA    | 1.95                     | 0.48              |
| 2:D:631:LEU:O    | 2:D:633:GLU:N    | 2.45                     | 0.48              |
| 1:A:107:HIS:NE2  | 1:A:109:VAL:HG13 | 2.29                     | 0.48              |
| 1:A:170:THR:C    | 1:A:210:GLU:HG3  | 2.24                     | 0.48              |
| 2:B:644:LEU:HA   | 2:B:666:HIS:N    | 2.28                     | 0.48              |
| 1:C:235:PHE:HA   | 1:C:306:ARG:NH1  | 2.29                     | 0.48              |
| 1:C:239:LEU:HD13 | 1:C:241:ILE:HD12 | 1.96                     | 0.48              |
| 1:C:66:GLN:O     | 1:C:67:VAL:HG22  | 2.13                     | 0.48              |
| 2:D:7:TRP:CD2    | 2:D:172:ILE:HD12 | 2.48                     | 0.48              |
| 1:C:277:PRO:HG3  | 2:D:459:GLU:OE1  | 2.13                     | 0.48              |
| 2:B:236:GLU:HG3  | 2:B:240:ARG:HE   | 1.79                     | 0.48              |
| 2:B:252:VAL:HG21 | 2:B:380:LEU:HD13 | 1.95                     | 0.48              |
| 2:B:631:LEU:CD2  | 2:B:632:ASN:N    | 2.77                     | 0.48              |
| 2:D:30:LEU:N     | 2:D:30:LEU:HD23  | 2.29                     | 0.48              |
| 2:D:664:VAL:HB   | 2:D:680:LEU:HD13 | 1.96                     | 0.48              |
| 2:B:131:HIS:O    | 2:B:132:SER:HB2  | 2.14                     | 0.48              |
| 2:B:432:ARG:CG   | 2:B:432:ARG:NH1  | 2.72                     | 0.48              |
| 2:B:517:ASP:OD1  | 2:B:519:LYS:N    | 2.45                     | 0.48              |
| 1:C:164:ARG:HH12 | 2:D:531:LEU:HD11 | 1.78                     | 0.48              |
| 2:D:402:LYS:HB2  | 2:D:403:ARG:NH2  | 2.29                     | 0.48              |
| 2:D:57:PRO:HG3   | 2:D:63:ARG:HH22  | 1.78                     | 0.48              |
| 2:B:230:THR:HG23 | 2:B:234:MET:HE2  | 1.96                     | 0.48              |
| 2:B:600:ARG:HH12 | 2:B:616:ASP:CG   | 2.12                     | 0.48              |
| 2:B:666:HIS:CE1  | 2:B:668:GLU:OE2  | 2.67                     | 0.48              |
| 2:D:234:MET:O    | 2:D:238:LEU:HB2  | 2.14                     | 0.48              |
| 2:D:672:LYS:O    | 2:D:674:ASP:N    | 2.47                     | 0.48              |
| 1:A:248:PHE:HD2  | 1:A:254:SER:HB3  | 1.79                     | 0.48              |
| 1:A:289:VAL:HG12 | 1:A:290:TYR:CD1  | 2.48                     | 0.48              |
| 2:D:11:TRP:CZ3   | 2:D:173:ILE:HG13 | 2.48                     | 0.48              |
| 2:D:634:VAL:HA   | 2:D:654:LEU:HA   | 1.96                     | 0.48              |
| 2:D:762:LEU:CD1  | 2:D:774:ILE:HG23 | 2.43                     | 0.48              |
| 1:A:107:HIS:HD2  | 1:A:109:VAL:H    | 1.59                     | 0.48              |
| 1:A:145:ILE:CG2  | 1:A:146:PRO:CA   | 2.91                     | 0.48              |
| 1:A:174:GLN:HG3  | 1:A:212:LEU:HG   | 1.96                     | 0.48              |
| 2:B:410:ARG:HH22 | 2:B:421:ILE:C    | 2.17                     | 0.48              |
| 1:C:140:PHE:CE2  | 1:C:165:LEU:HD11 | 2.48                     | 0.48              |
| 1:C:279:VAL:O    | 1:C:282:ASN:HB2  | 2.14                     | 0.48              |
| 1:C:32:LEU:HA    | 1:C:35:LYS:HD3   | 1.96                     | 0.48              |
| 2:D:306:ASP:HB3  | 2:D:311:LEU:HD21 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:452:ARG:HH21 | 2:B:464:GLU:CD   | 2.17                     | 0.48              |
| 2:B:703:PHE:O    | 2:B:763:GLN:NE2  | 2.47                     | 0.48              |
| 2:B:778:VAL:C    | 2:B:780:LYS:H    | 2.17                     | 0.48              |
| 2:D:338:PHE:HD2  | 2:D:360:TYR:CD1  | 2.32                     | 0.48              |
| 1:C:205:MET:HE2  | 2:D:513:TYR:HA   | 1.95                     | 0.48              |
| 1:A:146:PRO:HG2  | 1:A:147:GLY:H    | 1.80                     | 0.47              |
| 1:A:195:ARG:HB3  | 1:A:196:ASN:H    | 1.56                     | 0.47              |
| 1:A:313:ARG:NH1  | 1:A:317:GLU:OE1  | 2.47                     | 0.47              |
| 1:A:203:THR:N    | 4:A:992:AMP:HN61 | 2.00                     | 0.47              |
| 1:C:284:GLY:C    | 1:C:285:ILE:HD12 | 2.35                     | 0.47              |
| 1:C:324:LYS:HZ2  | 1:C:325:GLN:HB3  | 1.79                     | 0.47              |
| 1:A:107:HIS:HD2  | 1:A:109:VAL:N    | 2.12                     | 0.47              |
| 1:A:269:VAL:HG13 | 1:A:302:LEU:HD11 | 1.95                     | 0.47              |
| 2:B:599:ASN:HA   | 2:B:611:THR:HA   | 1.95                     | 0.47              |
| 1:C:265:LYS:HD2  | 1:C:266:TRP:H    | 1.80                     | 0.47              |
| 2:D:55:GLN:O     | 2:D:63:ARG:HD3   | 2.14                     | 0.47              |
| 1:A:169:GLN:CA   | 1:A:193:VAL:HG11 | 2.43                     | 0.47              |
| 2:B:425:GLN:NE2  | 2:B:469:TYR:CD1  | 2.82                     | 0.47              |
| 2:D:42:PHE:CE2   | 2:D:125:LEU:HD22 | 2.49                     | 0.47              |
| 2:D:571:GLU:N    | 2:D:593:ALA:O    | 2.44                     | 0.47              |
| 2:D:9:ARG:HA     | 2:D:12:VAL:O     | 2.14                     | 0.47              |
| 1:A:199:ASP:OD1  | 1:A:202:HIS:HD2  | 1.97                     | 0.47              |
| 1:C:238:ASP:CG   | 1:C:238:ASP:O    | 2.53                     | 0.47              |
| 2:D:127:ILE:HD13 | 2:D:127:ILE:O    | 2.13                     | 0.47              |
| 2:B:236:GLU:OE2  | 2:B:236:GLU:HA   | 2.15                     | 0.47              |
| 2:B:306:ASP:OD1  | 2:B:308:ASN:HB3  | 2.14                     | 0.47              |
| 2:D:111:ARG:C    | 2:D:113:GLU:N    | 2.68                     | 0.47              |
| 2:D:184:GLN:HA   | 2:D:432:ARG:NH1  | 2.29                     | 0.47              |
| 2:B:134:ILE:H    | 2:B:134:ILE:HD12 | 1.80                     | 0.47              |
| 2:B:316:ILE:HD11 | 2:B:343:ILE:HG23 | 1.96                     | 0.47              |
| 2:B:498:VAL:HG13 | 2:B:624:VAL:HG13 | 1.96                     | 0.47              |
| 2:B:647:GLY:HA2  | 1:C:91:THR:HB    | 1.97                     | 0.47              |
| 2:D:133:GLY:O    | 2:D:134:ILE:HG22 | 2.14                     | 0.47              |
| 2:D:139:ALA:O    | 2:D:141:ALA:N    | 2.48                     | 0.47              |
| 1:C:192:ARG:NH2  | 2:D:511:ILE:HG23 | 2.29                     | 0.47              |
| 2:B:769:LEU:H    | 2:B:769:LEU:HD22 | 1.79                     | 0.47              |
| 2:D:165:ASN:O    | 2:D:166:ARG:C    | 2.53                     | 0.47              |
| 2:D:605:TRP:CZ3  | 2:D:606:ASN:HB2  | 2.50                     | 0.47              |
| 2:D:705:ALA:HB2  | 2:D:763:GLN:CD   | 2.35                     | 0.47              |
| 2:D:99:LEU:O     | 2:D:102:ASP:HA   | 2.15                     | 0.47              |
| 1:A:185:ILE:HG13 | 1:A:186:ARG:N    | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:270:LEU:HA   | 1:A:297:MET:HA   | 1.96                     | 0.47              |
| 2:B:659:ILE:HD11 | 2:B:688:LYS:HD3  | 1.95                     | 0.47              |
| 1:C:268:GLU:CD   | 4:C:999:AMP:H3'  | 2.34                     | 0.47              |
| 2:D:452:ARG:CG   | 2:D:452:ARG:NH1  | 2.72                     | 0.47              |
| 2:D:621:LEU:O    | 2:D:625:LEU:HB3  | 2.14                     | 0.47              |
| 2:D:671:ARG:HD3  | 2:D:671:ARG:HA   | 1.57                     | 0.47              |
| 1:A:178:MET:CE   | 1:A:280:LEU:CD2  | 2.92                     | 0.47              |
| 2:B:194:PRO:HA   | 2:B:374:GLU:CG   | 2.45                     | 0.47              |
| 2:B:311:LEU:O    | 2:B:319:GLY:CA   | 2.62                     | 0.47              |
| 2:B:427:THR:O    | 2:B:431:ARG:HB2  | 2.15                     | 0.47              |
| 2:B:47:VAL:HG23  | 2:B:137:LEU:HD23 | 1.97                     | 0.47              |
| 2:D:217:LEU:HB2  | 2:D:335:CYS:O    | 2.15                     | 0.47              |
| 2:D:289:LEU:O    | 2:D:291:ASP:N    | 2.48                     | 0.47              |
| 2:D:319:GLY:C    | 2:D:321:HIS:N    | 2.64                     | 0.47              |
| 2:D:54:ALA:O     | 2:D:55:GLN:C     | 2.53                     | 0.47              |
| 2:D:632:ASN:OD1  | 2:D:632:ASN:C    | 2.52                     | 0.47              |
| 1:A:276:HIS:CD2  | 1:A:278:ASN:HB2  | 2.50                     | 0.47              |
| 2:B:140:ASP:O    | 2:B:140:ASP:CG   | 2.53                     | 0.47              |
| 2:B:165:ASN:N    | 2:B:165:ASN:ND2  | 2.60                     | 0.47              |
| 2:B:194:PRO:HA   | 2:B:374:GLU:HG3  | 1.97                     | 0.47              |
| 2:B:429:ILE:O    | 2:B:433:LEU:HD22 | 2.15                     | 0.47              |
| 2:B:502:LEU:HA   | 2:B:502:LEU:HD12 | 1.80                     | 0.47              |
| 2:D:38:VAL:HG13  | 2:D:155:ASP:O    | 2.15                     | 0.47              |
| 1:A:140:PHE:CA   | 1:A:145:ILE:CG1  | 2.88                     | 0.46              |
| 1:A:144:ASN:HB2  | 1:A:279:VAL:HG22 | 1.96                     | 0.46              |
| 2:B:178:ASP:OD1  | 2:B:467:ARG:NH1  | 2.45                     | 0.46              |
| 2:B:231:PRO:O    | 2:B:233:TRP:N    | 2.48                     | 0.46              |
| 1:C:86:ARG:HG2   | 1:C:90:GLU:OE1   | 2.15                     | 0.46              |
| 1:A:107:HIS:CD2  | 1:A:108:PRO:HD2  | 2.50                     | 0.46              |
| 1:A:151:ALA:O    | 1:A:152:ARG:C    | 2.53                     | 0.46              |
| 2:B:749:VAL:HG21 | 2:B:755:SER:HB2  | 1.97                     | 0.46              |
| 2:B:767:ARG:NH1  | 2:B:767:ARG:CB   | 2.79                     | 0.46              |
| 1:C:112:THR:HG1  | 1:C:234:PHE:HZ   | 1.63                     | 0.46              |
| 1:C:196:ASN:OD1  | 2:D:537:ILE:HG23 | 2.16                     | 0.46              |
| 1:C:83:LEU:HD13  | 1:C:83:LEU:O     | 2.16                     | 0.46              |
| 2:D:271:ARG:HD3  | 2:D:321:HIS:CE1  | 2.49                     | 0.46              |
| 2:D:669:LEU:HA   | 2:D:672:LYS:HD2  | 1.97                     | 0.46              |
| 1:A:86:ARG:HG2   | 1:A:90:GLU:OE2   | 2.16                     | 0.46              |
| 2:B:230:THR:HG22 | 2:B:235:LYS:HB2  | 1.96                     | 0.46              |
| 2:D:107:ALA:HA   | 2:D:116:GLU:HB3  | 1.98                     | 0.46              |
| 1:A:261:GLY:O    | 1:A:262:LYS:C    | 2.54                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:48:LEU:O     | 1:C:49:PRO:C     | 2.53                     | 0.46              |
| 1:C:69:GLN:HA    | 1:C:69:GLN:NE2   | 2.26                     | 0.46              |
| 2:D:201:ASP:N    | 2:D:201:ASP:OD1  | 2.48                     | 0.46              |
| 2:D:17:ASP:HB2   | 2:D:20:ALA:HB2   | 1.96                     | 0.46              |
| 2:D:699:GLU:OE1  | 2:D:699:GLU:CA   | 2.62                     | 0.46              |
| 1:C:172:GLY:O    | 1:C:176:ARG:HG3  | 2.15                     | 0.46              |
| 1:C:202:HIS:HE1  | 1:C:301:ARG:HH22 | 1.54                     | 0.46              |
| 2:D:278:VAL:HG13 | 2:D:302:LEU:HD21 | 1.96                     | 0.46              |
| 2:B:501:LEU:O    | 2:B:505:LYS:HG2  | 2.16                     | 0.46              |
| 2:D:109:LYS:HB3  | 2:D:113:GLU:O    | 2.16                     | 0.46              |
| 2:D:127:ILE:O    | 2:D:127:ILE:CD1  | 2.63                     | 0.46              |
| 2:D:546:LEU:H    | 2:D:546:LEU:HD12 | 1.79                     | 0.46              |
| 1:A:244:ARG:HD3  | 1:A:258:ASP:OD1  | 2.16                     | 0.46              |
| 2:B:224:ILE:HG13 | 2:B:329:GLN:O    | 2.16                     | 0.46              |
| 1:C:235:PHE:HA   | 1:C:306:ARG:HH11 | 1.81                     | 0.46              |
| 2:D:203:LEU:HD21 | 2:D:269:LYS:HE3  | 1.97                     | 0.46              |
| 2:D:346:ARG:H    | 2:D:346:ARG:HD2  | 1.80                     | 0.46              |
| 2:D:65:THR:HG23  | 2:D:77:ILE:O     | 2.16                     | 0.46              |
| 1:A:205:MET:O    | 1:A:206:PHE:CB   | 2.62                     | 0.46              |
| 1:A:213:ILE:O    | 1:A:292:GLY:HA2  | 2.15                     | 0.46              |
| 1:C:58:ALA:HB1   | 1:C:60:ILE:CB    | 2.40                     | 0.46              |
| 2:D:666:HIS:ND1  | 2:D:668:GLU:OE1  | 2.49                     | 0.46              |
| 1:A:108:PRO:HB2  | 1:A:303:THR:HG21 | 1.97                     | 0.46              |
| 1:A:98:GLY:HA2   | 2:D:615:TYR:HB3  | 1.98                     | 0.46              |
| 2:B:575:ARG:HG2  | 2:B:591:MET:SD   | 2.55                     | 0.46              |
| 2:B:568:ARG:HB2  | 2:B:596:ILE:HG22 | 1.97                     | 0.46              |
| 1:C:83:LEU:O     | 1:C:87:LEU:HG    | 2.14                     | 0.46              |
| 1:A:279:VAL:CA   | 1:A:282:ASN:HD21 | 2.12                     | 0.46              |
| 2:B:230:THR:HA   | 2:B:231:PRO:HD3  | 1.87                     | 0.46              |
| 2:B:630:LYS:CB   | 2:B:631:LEU:CA   | 2.93                     | 0.46              |
| 2:B:678:ARG:HD2  | 2:B:680:LEU:HD11 | 1.97                     | 0.46              |
| 1:C:107:HIS:C    | 1:C:107:HIS:ND1  | 2.69                     | 0.46              |
| 1:C:147:GLY:HA2  | 1:C:152:ARG:CZ   | 2.46                     | 0.46              |
| 1:C:136:ASP:OD1  | 1:C:152:ARG:NH2  | 2.49                     | 0.46              |
| 1:C:301:ARG:NE   | 4:C:999:AMP:C2   | 2.84                     | 0.46              |
| 2:D:507:TYR:HB3  | 2:D:570:PHE:HD2  | 1.80                     | 0.46              |
| 2:B:47:VAL:HG13  | 2:B:144:GLY:H    | 1.81                     | 0.45              |
| 2:B:409:ARG:O    | 2:B:410:ARG:C    | 2.54                     | 0.45              |
| 1:A:257:VAL:HG22 | 1:A:270:LEU:HG   | 1.98                     | 0.45              |
| 2:B:111:ARG:N    | 2:B:112:GLY:CA   | 2.71                     | 0.45              |
| 2:B:183:ASN:O    | 2:B:184:GLN:HG2  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:127:ILE:HG13 | 2:B:239:ARG:NH2  | 2.32                     | 0.45              |
| 2:B:276:ILE:HG22 | 2:B:276:ILE:O    | 2.16                     | 0.45              |
| 2:B:701:SER:HB2  | 2:B:703:PHE:HB2  | 1.99                     | 0.45              |
| 2:B:73:ARG:HG3   | 2:B:73:ARG:HH11  | 1.81                     | 0.45              |
| 1:C:320:LEU:HD13 | 1:C:320:LEU:HA   | 1.56                     | 0.45              |
| 2:D:264:MET:SD   | 2:D:335:CYS:HB2  | 2.55                     | 0.45              |
| 1:A:119:PHE:N    | 1:A:119:PHE:CD1  | 2.82                     | 0.45              |
| 1:A:251:THR:HA   | 1:A:274:MET:O    | 2.16                     | 0.45              |
| 1:C:241:ILE:CD1  | 1:C:241:ILE:N    | 2.79                     | 0.45              |
| 2:B:521:GLN:HE22 | 2:B:546:LEU:H    | 1.64                     | 0.45              |
| 2:B:522:GLN:HE22 | 2:B:529:GLU:CD   | 2.17                     | 0.45              |
| 2:B:672:LYS:O    | 2:B:673:LEU:CB   | 2.65                     | 0.45              |
| 1:C:111:ARG:O    | 1:C:115:ARG:HB2  | 2.17                     | 0.45              |
| 2:D:257:LEU:HA   | 2:D:262:GLN:O    | 2.16                     | 0.45              |
| 1:A:222:ASN:HA   | 2:B:477:GLU:O    | 2.17                     | 0.45              |
| 1:C:192:ARG:CG   | 1:C:207:HIS:CE1  | 2.99                     | 0.45              |
| 2:D:635:GLU:HG2  | 2:D:653:TYR:HB2  | 1.99                     | 0.45              |
| 2:B:231:PRO:CG   | 2:B:383:ILE:HG12 | 2.47                     | 0.45              |
| 2:D:199:ILE:HG12 | 2:D:388:ALA:O    | 2.17                     | 0.45              |
| 2:B:110:LEU:O    | 2:B:111:ARG:CB   | 2.65                     | 0.45              |
| 2:B:56:HIS:HB2   | 2:B:59:ALA:O     | 2.17                     | 0.45              |
| 1:C:58:ALA:HA    | 1:C:60:ILE:CD1   | 2.45                     | 0.45              |
| 1:C:64:LYS:O     | 1:C:65:GLU:HB3   | 2.17                     | 0.45              |
| 2:D:631:LEU:C    | 2:D:633:GLU:N    | 2.70                     | 0.45              |
| 2:D:644:LEU:HD13 | 2:D:649:SER:CB   | 2.40                     | 0.45              |
| 1:A:176:ARG:NH2  | 1:A:176:ARG:HG3  | 2.32                     | 0.45              |
| 1:A:190:PRO:HA   | 1:A:208:GLN:O    | 2.16                     | 0.45              |
| 1:A:304:MET:HG2  | 1:A:309:VAL:HB   | 1.99                     | 0.45              |
| 2:B:272:ILE:CD1  | 2:B:273:GLU:H    | 2.29                     | 0.45              |
| 2:B:625:LEU:HA   | 2:B:625:LEU:HD23 | 1.47                     | 0.45              |
| 1:C:149:HIS:O    | 1:C:151:ALA:N    | 2.50                     | 0.45              |
| 1:C:311:ASP:OD1  | 1:C:313:ARG:HB3  | 2.16                     | 0.45              |
| 2:B:56:HIS:O     | 2:B:58:ASN:N     | 2.50                     | 0.44              |
| 1:C:124:GLY:HA3  | 1:C:186:ARG:NH1  | 2.30                     | 0.44              |
| 1:C:65:GLU:N     | 1:C:66:GLN:O     | 2.50                     | 0.44              |
| 2:D:113:GLU:O    | 2:D:114:PRO:C    | 2.55                     | 0.44              |
| 2:D:517:ASP:OD1  | 2:D:519:LYS:CG   | 2.64                     | 0.44              |
| 1:A:143:LEU:O    | 1:A:144:ASN:HB3  | 2.17                     | 0.44              |
| 1:A:304:MET:O    | 1:A:308:GLY:N    | 2.49                     | 0.44              |
| 2:B:221:VAL:O    | 2:B:221:VAL:HG13 | 2.17                     | 0.44              |
| 2:B:705:ALA:HB2  | 2:B:763:GLN:NE2  | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:731:GLY:O    | 2:D:732:VAL:HG12 | 2.16                     | 0.44              |
| 2:B:518:PRO:HG3  | 2:B:543:ALA:HB2  | 1.99                     | 0.44              |
| 2:D:561:ASN:C    | 2:D:563:GLN:H    | 2.20                     | 0.44              |
| 2:B:424:GLU:CD   | 2:B:424:GLU:H    | 2.21                     | 0.44              |
| 1:C:143:LEU:HD22 | 1:C:250:PHE:CD2  | 2.53                     | 0.44              |
| 2:D:151:LEU:O    | 2:D:152:LYS:C    | 2.55                     | 0.44              |
| 2:D:183:ASN:C    | 2:D:185:LEU:H    | 2.21                     | 0.44              |
| 2:D:271:ARG:HD3  | 2:D:321:HIS:NE2  | 2.33                     | 0.44              |
| 2:D:271:ARG:NH1  | 2:D:321:HIS:O    | 2.50                     | 0.44              |
| 2:D:532:LEU:O    | 2:D:534:PRO:HD3  | 2.16                     | 0.44              |
| 2:B:460:ASP:O    | 2:B:463:GLU:HG2  | 2.17                     | 0.44              |
| 2:B:581:GLN:HE21 | 2:B:581:GLN:HB3  | 1.60                     | 0.44              |
| 2:B:630:LYS:CB   | 2:B:631:LEU:HA   | 2.47                     | 0.44              |
| 1:C:105:GLY:CA   | 2:D:508:GLN:OE1  | 2.65                     | 0.44              |
| 1:C:218:ILE:C    | 1:C:218:ILE:HD13 | 2.38                     | 0.44              |
| 2:D:621:LEU:HD12 | 2:D:625:LEU:HD22 | 1.98                     | 0.44              |
| 1:A:204:PRO:HD2  | 2:B:513:TYR:CE1  | 2.52                     | 0.44              |
| 2:B:540:GLU:HG3  | 2:B:541:MET:HG3  | 1.99                     | 0.44              |
| 2:B:499:LYS:HG2  | 2:B:570:PHE:CE1  | 2.53                     | 0.44              |
| 1:C:133:ILE:HD12 | 2:D:576:PHE:CD1  | 2.53                     | 0.44              |
| 1:A:205:MET:HG2  | 1:A:206:PHE:N    | 2.32                     | 0.44              |
| 1:A:302:LEU:HA   | 1:A:302:LEU:HD12 | 1.85                     | 0.44              |
| 2:B:52:GLU:OE2   | 2:B:52:GLU:HA    | 2.17                     | 0.44              |
| 2:B:56:HIS:O     | 2:B:57:PRO:C     | 2.56                     | 0.44              |
| 2:D:375:ARG:HA   | 2:D:375:ARG:HD3  | 1.78                     | 0.44              |
| 2:D:337:PHE:CZ   | 2:D:401:PRO:CG   | 3.00                     | 0.44              |
| 2:D:416:LEU:HD23 | 2:D:416:LEU:HA   | 1.87                     | 0.44              |
| 1:A:216:THR:HG22 | 1:A:289:VAL:O    | 2.18                     | 0.44              |
| 2:B:226:VAL:HG11 | 2:B:328:THR:O    | 2.17                     | 0.44              |
| 2:D:108:ALA:O    | 2:D:115:SER:HA   | 2.18                     | 0.44              |
| 1:A:123:LEU:HD21 | 2:D:485:MET:HG2  | 2.00                     | 0.44              |
| 1:A:199:ASP:OD1  | 1:A:202:HIS:CD2  | 2.71                     | 0.44              |
| 1:A:299:MET:HA   | 1:A:299:MET:CE   | 2.48                     | 0.44              |
| 1:C:300:GLU:HB2  | 1:C:315:PHE:CE1  | 2.53                     | 0.44              |
| 2:B:731:GLY:O    | 2:B:733:ASN:N    | 2.51                     | 0.43              |
| 2:D:535:SER:N    | 2:D:536:PRO:HD3  | 2.33                     | 0.43              |
| 2:D:617:LEU:HA   | 2:D:617:LEU:HD12 | 1.87                     | 0.43              |
| 2:D:625:LEU:CD1  | 2:D:659:ILE:HD11 | 2.48                     | 0.43              |
| 1:A:150:PRO:O    | 1:A:154:ASP:HB2  | 2.18                     | 0.43              |
| 2:B:205:ILE:HG13 | 2:B:394:ILE:HD11 | 1.99                     | 0.43              |
| 2:B:570:PHE:CD1  | 2:B:570:PHE:C    | 2.91                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:625:LEU:HD13 | 2:B:634:VAL:CG1  | 2.48                     | 0.43              |
| 2:B:696:GLN:O    | 2:B:697:ALA:C    | 2.56                     | 0.43              |
| 2:B:774:ILE:C    | 2:B:776:ALA:N    | 2.71                     | 0.43              |
| 2:D:26:THR:CG2   | 2:D:32:VAL:HG22  | 2.48                     | 0.43              |
| 1:A:167:ARG:HH11 | 1:A:167:ARG:HD2  | 1.65                     | 0.43              |
| 1:A:218:ILE:HG12 | 1:A:292:GLY:HA2  | 2.00                     | 0.43              |
| 1:C:192:ARG:NH2  | 2:D:571:GLU:OE2  | 2.52                     | 0.43              |
| 2:D:36:GLU:O     | 2:D:156:ASN:HA   | 2.17                     | 0.43              |
| 2:D:257:LEU:HD23 | 2:D:263:PRO:HA   | 2.00                     | 0.43              |
| 2:D:289:LEU:C    | 2:D:291:ASP:H    | 2.22                     | 0.43              |
| 2:D:427:THR:HG21 | 2:D:439:GLU:OE2  | 2.18                     | 0.43              |
| 2:D:5:GLU:OE1    | 2:D:18:SER:OG    | 2.36                     | 0.43              |
| 2:D:729:LYS:H    | 2:D:731:GLY:H    | 1.65                     | 0.43              |
| 1:A:140:PHE:O    | 1:A:145:ILE:CB   | 2.67                     | 0.43              |
| 1:A:269:VAL:HG12 | 1:A:270:LEU:N    | 2.33                     | 0.43              |
| 2:B:515:PHE:CD1  | 2:B:544:MET:HE1  | 2.42                     | 0.43              |
| 2:D:262:GLN:HA   | 2:D:263:PRO:HD3  | 1.76                     | 0.43              |
| 2:D:55:GLN:H     | 2:D:55:GLN:HG2   | 1.50                     | 0.43              |
| 2:D:724:LEU:HD21 | 2:D:740:LEU:HB2  | 2.00                     | 0.43              |
| 1:A:195:ARG:HD2  | 1:A:206:PHE:CE1  | 2.53                     | 0.43              |
| 2:B:234:MET:O    | 2:B:234:MET:HG2  | 2.19                     | 0.43              |
| 2:B:284:GLY:HA2  | 2:B:296:LYS:HE3  | 2.00                     | 0.43              |
| 2:B:545:ARG:HG3  | 2:B:547:SER:O    | 2.18                     | 0.43              |
| 2:B:661:PHE:O    | 2:B:682:PHE:HA   | 2.18                     | 0.43              |
| 1:C:194:TYR:CE1  | 1:C:205:MET:HG3  | 2.54                     | 0.43              |
| 1:C:29:VAL:HG11  | 1:C:75:LYS:HB3   | 1.99                     | 0.43              |
| 1:C:301:ARG:NE   | 4:C:999:AMP:N1   | 2.67                     | 0.43              |
| 2:D:241:CYS:HB3  | 2:D:258:LEU:HD22 | 1.99                     | 0.43              |
| 1:A:156:ASP:HB2  | 1:A:196:ASN:HB3  | 1.99                     | 0.43              |
| 1:A:263:ASN:CB   | 1:A:264:GLY:CA   | 2.92                     | 0.43              |
| 2:B:289:LEU:N    | 2:B:293:THR:O    | 2.34                     | 0.43              |
| 2:B:344:THR:O    | 2:B:345:GLY:C    | 2.57                     | 0.43              |
| 2:B:622:GLU:HB2  | 1:C:100:ARG:HD3  | 1.99                     | 0.43              |
| 2:B:629:GLY:CA   | 2:B:692:ARG:HB2  | 2.47                     | 0.43              |
| 2:B:790:GLN:HG3  | 2:B:791:ALA:N    | 2.34                     | 0.43              |
| 2:D:147:ILE:HD12 | 2:D:148:ARG:N    | 2.34                     | 0.43              |
| 2:D:1:MET:HB2    | 2:D:2:LYS:H      | 1.58                     | 0.43              |
| 2:D:326:ASP:OD1  | 2:D:326:ASP:N    | 2.51                     | 0.43              |
| 2:B:170:LEU:HD12 | 2:B:170:LEU:HA   | 1.86                     | 0.43              |
| 2:B:352:LEU:HD12 | 2:B:352:LEU:HA   | 1.87                     | 0.43              |
| 2:B:522:GLN:CD   | 2:B:529:GLU:HG3  | 2.31                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:536:PRO:HB2  | 2:D:537:ILE:HD12 | 2.01                     | 0.43              |
| 1:A:123:LEU:HB3  | 2:D:483:LEU:HD13 | 1.99                     | 0.43              |
| 2:B:1:MET:O      | 2:B:1:MET:HG3    | 2.16                     | 0.43              |
| 2:B:225:ASN:ND2  | 2:B:227:LYS:HG2  | 2.34                     | 0.43              |
| 2:B:55:GLN:HE22  | 2:B:63:ARG:HH21  | 1.67                     | 0.43              |
| 2:B:629:GLY:O    | 2:B:630:LYS:O    | 2.36                     | 0.43              |
| 2:B:741:PHE:HB2  | 2:D:603:GLU:HG3  | 2.00                     | 0.43              |
| 1:C:101:ILE:O    | 1:C:102:GLU:C    | 2.57                     | 0.43              |
| 2:D:431:ARG:CZ   | 2:D:437:VAL:HG23 | 2.48                     | 0.43              |
| 2:D:565:ASN:O    | 2:D:565:ASN:CG   | 2.57                     | 0.43              |
| 2:D:673:LEU:O    | 2:D:674:ASP:C    | 2.56                     | 0.43              |
| 2:D:678:ARG:HG3  | 2:D:678:ARG:O    | 2.18                     | 0.43              |
| 2:B:596:ILE:CD1  | 2:B:612:VAL:HG21 | 2.36                     | 0.43              |
| 2:B:674:ASP:O    | 2:B:675:LEU:HB2  | 2.17                     | 0.43              |
| 2:D:254:ASN:HA   | 2:D:254:ASN:HD22 | 1.66                     | 0.43              |
| 1:A:167:ARG:CD   | 1:A:193:VAL:HG12 | 2.49                     | 0.43              |
| 2:B:142:PRO:O    | 2:B:144:GLY:N    | 2.52                     | 0.43              |
| 2:B:614:PHE:HA   | 2:B:680:LEU:HD21 | 2.00                     | 0.43              |
| 2:D:703:PHE:HE2  | 2:D:766:SER:O    | 1.98                     | 0.43              |
| 2:D:358:HIS:CD2  | 2:D:362:ARG:NH2  | 2.87                     | 0.42              |
| 2:D:545:ARG:HB2  | 2:D:547:SER:O    | 2.19                     | 0.42              |
| 2:D:590:LEU:HD12 | 2:D:686:TRP:CD1  | 2.54                     | 0.42              |
| 2:D:641:ASN:HB3  | 2:D:644:LEU:HD11 | 2.00                     | 0.42              |
| 2:D:595:VAL:HA   | 2:D:680:LEU:O    | 2.19                     | 0.42              |
| 2:B:224:ILE:N    | 2:B:329:GLN:O    | 2.45                     | 0.42              |
| 2:B:715:ALA:O    | 2:B:717:ASN:N    | 2.49                     | 0.42              |
| 2:B:790:GLN:CG   | 2:B:791:ALA:N    | 2.82                     | 0.42              |
| 2:D:631:LEU:O    | 2:D:632:ASN:OD1  | 2.36                     | 0.42              |
| 1:A:218:ILE:HD12 | 1:A:218:ILE:C    | 2.39                     | 0.42              |
| 1:A:201:THR:O    | 1:A:312:LEU:HD23 | 2.20                     | 0.42              |
| 2:B:113:GLU:HB2  | 2:B:114:PRO:HD3  | 2.00                     | 0.42              |
| 2:B:291:ASP:OD1  | 2:B:293:THR:HG22 | 2.19                     | 0.42              |
| 2:B:309:LYS:HZ1  | 2:B:321:HIS:CE1  | 2.37                     | 0.42              |
| 1:C:301:ARG:O    | 1:C:305:LEU:HD23 | 2.19                     | 0.42              |
| 1:C:324:LYS:NZ   | 1:C:325:GLN:HB3  | 2.33                     | 0.42              |
| 2:D:342:SER:HA   | 2:D:346:ARG:NH2  | 2.34                     | 0.42              |
| 2:D:624:VAL:O    | 2:D:626:ASP:N    | 2.52                     | 0.42              |
| 2:B:111:ARG:CG   | 2:B:111:ARG:NH1  | 2.82                     | 0.42              |
| 2:B:172:ILE:O    | 2:B:173:ILE:C    | 2.57                     | 0.42              |
| 2:B:774:ILE:O    | 2:B:778:VAL:HG12 | 2.19                     | 0.42              |
| 4:C:999:AMP:N3   | 4:C:999:AMP:H2'  | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:215:ARG:HB2  | 2:D:395:THR:HG23 | 2.01                     | 0.42              |
| 2:D:215:ARG:HD3  | 2:D:369:GLN:HB2  | 2.01                     | 0.42              |
| 2:D:553:LEU:HA   | 2:D:556:VAL:HG13 | 2.00                     | 0.42              |
| 2:B:138:PRO:O    | 2:B:139:ALA:C    | 2.58                     | 0.42              |
| 2:B:338:PHE:HB2  | 2:B:343:ILE:HD11 | 2.00                     | 0.42              |
| 1:C:244:ARG:HA   | 1:C:245:PRO:HD3  | 1.89                     | 0.42              |
| 1:C:71:LEU:C     | 1:C:73:ALA:N     | 2.72                     | 0.42              |
| 1:C:75:LYS:CG    | 1:C:75:LYS:O     | 2.51                     | 0.42              |
| 2:D:17:ASP:HB2   | 2:D:20:ALA:CB    | 2.50                     | 0.42              |
| 2:D:411:SER:O    | 2:D:412:LYS:C    | 2.56                     | 0.42              |
| 2:D:741:PHE:HE1  | 2:D:759:SER:HB3  | 1.84                     | 0.42              |
| 1:A:264:GLY:HA3  | 1:A:265:LYS:HA   | 1.77                     | 0.42              |
| 2:B:262:GLN:OE1  | 2:B:369:GLN:NE2  | 2.50                     | 0.42              |
| 2:B:425:GLN:NE2  | 2:B:469:TYR:HD1  | 2.17                     | 0.42              |
| 2:B:566:ARG:HG2  | 2:B:566:ARG:O    | 2.18                     | 0.42              |
| 2:B:567:VAL:HG23 | 2:B:569:ILE:HG23 | 2.00                     | 0.42              |
| 2:D:134:ILE:HG23 | 2:D:134:ILE:O    | 2.20                     | 0.42              |
| 2:D:583:PRO:O    | 2:D:584:LEU:HB2  | 2.20                     | 0.42              |
| 2:B:42:PHE:CE1   | 2:B:147:ILE:HD11 | 2.55                     | 0.42              |
| 2:D:273:GLU:HG2  | 2:D:306:ASP:OD1  | 2.19                     | 0.42              |
| 1:A:188:ILE:HB   | 1:A:189:ALA:H    | 1.76                     | 0.42              |
| 2:B:12:VAL:HG12  | 2:B:185:LEU:HD12 | 2.02                     | 0.42              |
| 1:C:154:ASP:C    | 1:C:156:ASP:H    | 2.23                     | 0.42              |
| 1:C:219:SER:O    | 1:C:222:ASN:HB2  | 2.19                     | 0.42              |
| 2:D:246:ILE:HG22 | 2:D:247:ASP:HB2  | 2.01                     | 0.42              |
| 2:D:537:ILE:H    | 2:D:537:ILE:HD12 | 1.82                     | 0.42              |
| 2:D:165:ASN:HD22 | 2:D:165:ASN:N    | 2.18                     | 0.42              |
| 2:D:667:PRO:O    | 2:D:670:GLU:N    | 2.52                     | 0.42              |
| 1:A:111:ARG:NH1  | 2:D:490:GLU:OE2  | 2.53                     | 0.42              |
| 3:A:980:PHE:N    | 4:A:992:AMP:O3'  | 2.48                     | 0.42              |
| 2:B:714:VAL:HG22 | 2:B:715:ALA:H    | 1.85                     | 0.42              |
| 2:B:734:GLN:HE21 | 2:B:734:GLN:H    | 1.68                     | 0.42              |
| 2:B:747:LYS:O    | 2:B:747:LYS:HG2  | 2.20                     | 0.42              |
| 1:C:301:ARG:NH1  | 4:C:999:AMP:O3P  | 2.51                     | 0.42              |
| 2:D:208:GLU:HB3  | 2:D:279:ARG:HB3  | 2.02                     | 0.42              |
| 2:D:592:LEU:O    | 2:D:683:GLU:HA   | 2.20                     | 0.42              |
| 2:D:79:CYS:SG    | 2:D:80:GLY:N     | 2.93                     | 0.42              |
| 1:A:107:HIS:CD2  | 1:A:109:VAL:HG13 | 2.55                     | 0.41              |
| 1:A:158:PHE:CZ   | 1:A:195:ARG:O    | 2.66                     | 0.41              |
| 2:B:311:LEU:HB2  | 2:B:322:SER:OG   | 2.20                     | 0.41              |
| 1:C:76:ALA:O     | 1:C:80:SER:OG    | 2.32                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:229:PRO:O    | 2:D:230:THR:C    | 2.58                     | 0.41              |
| 2:D:461:LEU:HA   | 2:D:461:LEU:HD23 | 1.91                     | 0.41              |
| 2:D:600:ARG:NH1  | 2:D:616:ASP:OD2  | 2.44                     | 0.41              |
| 1:A:143:LEU:CD1  | 1:A:171:SER:HB3  | 2.49                     | 0.41              |
| 1:A:176:ARG:HH21 | 1:A:176:ARG:HG3  | 1.85                     | 0.41              |
| 1:A:321:ARG:HH21 | 2:B:562:ARG:HD3  | 1.85                     | 0.41              |
| 2:B:90:VAL:HG11  | 2:B:119:LEU:HG   | 2.02                     | 0.41              |
| 2:B:207:VAL:HG23 | 2:B:278:VAL:HB   | 2.02                     | 0.41              |
| 2:B:787:GLU:CG   | 2:B:787:GLU:O    | 2.66                     | 0.41              |
| 1:C:52:GLU:HA    | 1:C:53:ARG:HA    | 1.86                     | 0.41              |
| 2:D:116:GLU:HB2  | 2:D:117:GLY:CA   | 2.50                     | 0.41              |
| 2:D:534:PRO:O    | 2:D:535:SER:CB   | 2.64                     | 0.41              |
| 1:A:133:ILE:HD12 | 2:B:576:PHE:HD1  | 1.80                     | 0.41              |
| 2:B:209:ALA:H    | 2:B:210:PRO:CD   | 2.32                     | 0.41              |
| 2:B:231:PRO:O    | 2:B:232:LEU:C    | 2.59                     | 0.41              |
| 2:B:32:VAL:O     | 2:B:32:VAL:HG23  | 2.20                     | 0.41              |
| 2:B:520:VAL:O    | 2:B:521:GLN:C    | 2.58                     | 0.41              |
| 2:B:528:VAL:O    | 2:B:529:GLU:HG2  | 2.20                     | 0.41              |
| 2:B:788:ARG:HA   | 2:B:788:ARG:HH11 | 1.84                     | 0.41              |
| 1:C:59:VAL:CG2   | 1:C:62:GLU:HG2   | 2.40                     | 0.41              |
| 2:D:77:ILE:HB    | 2:D:117:GLY:H    | 1.85                     | 0.41              |
| 2:D:121:SER:H    | 2:D:124:GLU:HG3  | 1.85                     | 0.41              |
| 2:D:346:ARG:H    | 2:D:346:ARG:CD   | 2.32                     | 0.41              |
| 2:D:536:PRO:HG3  | 2:D:542:SER:HB3  | 2.03                     | 0.41              |
| 2:D:53:CYS:O     | 2:D:54:ALA:C     | 2.58                     | 0.41              |
| 2:D:67:VAL:HB    | 2:D:77:ILE:HD12  | 2.03                     | 0.41              |
| 2:D:790:GLN:NE2  | 2:D:791:ALA:O    | 2.53                     | 0.41              |
| 1:A:322:PHE:O    | 1:A:325:GLN:HG2  | 2.21                     | 0.41              |
| 2:B:4:SER:HB3    | 2:B:7:TRP:CB     | 2.50                     | 0.41              |
| 2:B:790:GLN:HG3  | 2:B:791:ALA:H    | 1.85                     | 0.41              |
| 2:D:345:GLY:H    | 2:D:346:ARG:NH1  | 2.12                     | 0.41              |
| 2:D:455:MET:HB2  | 2:D:455:MET:HE2  | 1.89                     | 0.41              |
| 2:D:53:CYS:C     | 2:D:54:ALA:O     | 2.57                     | 0.41              |
| 2:D:597:CYS:HB2  | 2:D:679:THR:HG22 | 2.03                     | 0.41              |
| 2:D:645:HIS:O    | 2:D:649:SER:HB3  | 2.20                     | 0.41              |
| 1:A:164:ARG:HH11 | 2:B:584:LEU:HB3  | 1.86                     | 0.41              |
| 2:D:166:ARG:HB2  | 2:D:166:ARG:CZ   | 2.50                     | 0.41              |
| 2:D:512:THR:HB   | 2:D:571:GLU:CD   | 2.41                     | 0.41              |
| 2:D:536:PRO:C    | 2:D:538:SER:H    | 2.23                     | 0.41              |
| 1:A:145:ILE:HB   | 1:A:146:PRO:O    | 2.21                     | 0.41              |
| 1:A:160:PHE:HE1  | 1:A:166:LEU:HG   | 1.83                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:163:THR:HA   | 2:B:164:PRO:HD3  | 1.91                     | 0.41              |
| 1:C:139:ASN:ND2  | 1:C:168:THR:H    | 2.17                     | 0.41              |
| 2:D:517:ASP:OD1  | 2:D:519:LYS:HG3  | 2.21                     | 0.41              |
| 2:D:72:ASP:HB3   | 2:D:73:ARG:H     | 1.69                     | 0.41              |
| 2:D:278:VAL:O    | 2:D:278:VAL:HG12 | 2.19                     | 0.41              |
| 1:A:202:HIS:HA   | 4:A:992:AMP:N6   | 2.36                     | 0.41              |
| 2:B:657:GLU:O    | 2:B:659:ILE:HD13 | 2.20                     | 0.41              |
| 1:A:101:ILE:H    | 1:A:101:ILE:HG12 | 1.59                     | 0.41              |
| 2:B:288:VAL:O    | 2:B:320:GLU:N    | 2.54                     | 0.41              |
| 2:B:67:VAL:HG22  | 2:B:77:ILE:HD12  | 2.03                     | 0.41              |
| 2:B:790:GLN:CD   | 2:B:791:ALA:H    | 2.24                     | 0.41              |
| 1:C:299:MET:CA   | 1:C:299:MET:CE   | 2.96                     | 0.41              |
| 1:C:78:LEU:HD23  | 1:C:78:LEU:HA    | 1.90                     | 0.41              |
| 2:D:644:LEU:HD22 | 2:D:663:GLY:HA3  | 2.03                     | 0.41              |
| 2:D:97:ALA:O     | 2:D:104:LYS:NZ   | 2.43                     | 0.41              |
| 2:B:123:SER:C    | 2:B:125:LEU:N    | 2.74                     | 0.41              |
| 2:B:635:GLU:HB2  | 2:B:653:TYR:HB2  | 2.03                     | 0.41              |
| 2:D:17:ASP:CB    | 2:D:20:ALA:H     | 2.33                     | 0.41              |
| 2:D:224:ILE:H    | 2:D:224:ILE:HG13 | 1.70                     | 0.41              |
| 2:D:506:GLY:O    | 2:D:568:ARG:HD3  | 2.21                     | 0.41              |
| 2:D:708:ARG:HD3  | 2:D:708:ARG:HA   | 1.75                     | 0.41              |
| 2:B:306:ASP:OD1  | 2:B:308:ASN:CB   | 2.69                     | 0.40              |
| 2:D:682:PHE:C    | 2:D:682:PHE:CD2  | 2.94                     | 0.40              |
| 2:B:89:ARG:HG2   | 2:B:141:ALA:HB3  | 2.02                     | 0.40              |
| 1:A:99:ARG:NH2   | 2:B:606:ASN:OD1  | 2.55                     | 0.40              |
| 1:C:21:VAL:HG12  | 1:C:24:LEU:HD22  | 2.04                     | 0.40              |
| 1:C:262:LYS:CG   | 1:C:263:ASN:N    | 2.85                     | 0.40              |
| 2:D:673:LEU:C    | 2:D:674:ASP:O    | 2.60                     | 0.40              |
| 2:D:778:VAL:CG2  | 2:D:779:ALA:N    | 2.84                     | 0.40              |
| 1:A:133:ILE:CD1  | 2:B:576:PHE:CE1  | 3.04                     | 0.40              |
| 2:B:89:ARG:CD    | 2:B:141:ALA:HB3  | 2.50                     | 0.40              |
| 2:B:35:VAL:HG12  | 2:B:158:ILE:HB   | 2.04                     | 0.40              |
| 2:B:432:ARG:NH1  | 2:B:432:ARG:HG2  | 2.22                     | 0.40              |
| 2:B:739:ASN:HD22 | 2:B:740:LEU:H    | 1.69                     | 0.40              |
| 2:B:90:VAL:HG13  | 2:B:91:ALA:H     | 1.83                     | 0.40              |
| 2:D:181:VAL:HB   | 2:D:432:ARG:HG3  | 2.03                     | 0.40              |
| 2:D:316:ILE:HG22 | 2:D:317:PHE:HB2  | 2.04                     | 0.40              |
| 2:D:524:ILE:O    | 2:D:643:ALA:HB2  | 2.21                     | 0.40              |
| 2:D:643:ALA:HB1  | 2:D:669:LEU:HD22 | 2.03                     | 0.40              |
| 2:D:739:ASN:O    | 2:D:758:ILE:O    | 2.39                     | 0.40              |
| 2:B:280:MET:O    | 2:B:281:ALA:HB2  | 2.20                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:452:ARG:CG   | 2:B:452:ARG:NH1  | 2.60                     | 0.40              |
| 2:B:662:VAL:HG13 | 2:B:682:PHE:CB   | 2.51                     | 0.40              |
| 2:B:668:GLU:CD   | 2:B:668:GLU:N    | 2.74                     | 0.40              |
| 2:D:173:ILE:HG23 | 2:D:174:GLY:N    | 2.37                     | 0.40              |
| 2:D:767:ARG:HD3  | 2:D:769:LEU:HD23 | 2.02                     | 0.40              |
| 1:A:295:PHE:CD2  | 1:A:295:PHE:C    | 2.94                     | 0.40              |
| 2:B:121:SER:H    | 2:B:124:GLU:CG   | 2.35                     | 0.40              |
| 1:A:221:THR:HG23 | 2:B:417:ILE:O    | 2.22                     | 0.40              |
| 2:B:514:SER:O    | 2:B:545:ARG:HD2  | 2.22                     | 0.40              |
| 1:C:169:GLN:OE1  | 3:C:990:PHE:N    | 2.55                     | 0.40              |
| 1:C:167:ARG:HH21 | 1:C:191:GLY:HA3  | 1.86                     | 0.40              |
| 1:C:216:THR:O    | 1:C:217:ASN:C    | 2.58                     | 0.40              |
| 1:C:60:ILE:O     | 1:C:61:ASN:O     | 2.39                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 240/327 (73%)   | 197 (82%)  | 31 (13%)  | 12 (5%)  | 2           | 12 |
| 1   | C     | 321/327 (98%)   | 231 (72%)  | 57 (18%)  | 33 (10%) | 0           | 2  |
| 2   | B     | 793/795 (100%)  | 631 (80%)  | 120 (15%) | 42 (5%)  | 2           | 11 |
| 2   | D     | 793/795 (100%)  | 628 (79%)  | 106 (13%) | 59 (7%)  | 1           | 5  |
| All | All   | 2147/2244 (96%) | 1687 (79%) | 314 (15%) | 146 (7%) | 1           | 6  |

All (146) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 146 | PRO  |
| 1   | A     | 167 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 184 | PRO  |
| 1   | A     | 189 | ALA  |
| 1   | A     | 217 | ASN  |
| 2   | B     | 52  | GLU  |
| 2   | B     | 111 | ARG  |
| 2   | B     | 132 | SER  |
| 2   | B     | 139 | ALA  |
| 2   | B     | 140 | ASP  |
| 2   | B     | 143 | ILE  |
| 2   | B     | 209 | ALA  |
| 2   | B     | 232 | LEU  |
| 2   | B     | 280 | MET  |
| 2   | B     | 346 | ARG  |
| 2   | B     | 564 | GLN  |
| 2   | B     | 602 | GLU  |
| 2   | B     | 630 | LYS  |
| 2   | B     | 677 | GLY  |
| 2   | B     | 788 | ARG  |
| 1   | C     | 27  | VAL  |
| 1   | C     | 48  | LEU  |
| 1   | C     | 49  | PRO  |
| 1   | C     | 50  | PRO  |
| 1   | C     | 51  | GLU  |
| 1   | C     | 60  | ILE  |
| 1   | C     | 61  | ASN  |
| 1   | C     | 62  | GLU  |
| 1   | C     | 63  | ALA  |
| 1   | C     | 66  | GLN  |
| 1   | C     | 67  | VAL  |
| 1   | C     | 146 | PRO  |
| 1   | C     | 151 | ALA  |
| 1   | C     | 184 | PRO  |
| 1   | C     | 239 | LEU  |
| 2   | D     | 55  | GLN  |
| 2   | D     | 56  | HIS  |
| 2   | D     | 102 | ASP  |
| 2   | D     | 116 | GLU  |
| 2   | D     | 118 | MET  |
| 2   | D     | 140 | ASP  |
| 2   | D     | 200 | ASP  |
| 2   | D     | 290 | LEU  |
| 2   | D     | 566 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 624 | VAL  |
| 2   | D     | 626 | ASP  |
| 2   | D     | 627 | LEU  |
| 2   | D     | 642 | PRO  |
| 2   | D     | 673 | LEU  |
| 2   | D     | 674 | ASP  |
| 2   | D     | 699 | GLU  |
| 2   | D     | 759 | SER  |
| 1   | A     | 186 | ARG  |
| 2   | B     | 18  | SER  |
| 2   | B     | 71  | GLY  |
| 2   | B     | 200 | ASP  |
| 2   | B     | 273 | GLU  |
| 2   | B     | 345 | GLY  |
| 2   | B     | 584 | LEU  |
| 2   | B     | 716 | GLU  |
| 1   | C     | 54  | PRO  |
| 1   | C     | 58  | ALA  |
| 1   | C     | 72  | ASN  |
| 1   | C     | 76  | ALA  |
| 1   | C     | 83  | LEU  |
| 1   | C     | 152 | ARG  |
| 1   | C     | 217 | ASN  |
| 1   | C     | 261 | GLY  |
| 1   | C     | 262 | LYS  |
| 2   | D     | 54  | ALA  |
| 2   | D     | 86  | GLN  |
| 2   | D     | 143 | ILE  |
| 2   | D     | 320 | GLU  |
| 2   | D     | 581 | GLN  |
| 2   | D     | 655 | LYS  |
| 2   | D     | 747 | LYS  |
| 2   | D     | 787 | GLU  |
| 1   | A     | 262 | LYS  |
| 2   | B     | 566 | ARG  |
| 2   | B     | 654 | LEU  |
| 1   | C     | 150 | PRO  |
| 1   | C     | 197 | ASP  |
| 2   | D     | 5   | GLU  |
| 2   | D     | 17  | ASP  |
| 2   | D     | 58  | ASN  |
| 2   | D     | 114 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 129 | ASP  |
| 2   | D     | 134 | ILE  |
| 2   | D     | 196 | GLY  |
| 2   | D     | 603 | GLU  |
| 2   | D     | 625 | LEU  |
| 2   | D     | 630 | LYS  |
| 2   | D     | 729 | LYS  |
| 2   | D     | 732 | VAL  |
| 1   | A     | 206 | PHE  |
| 1   | A     | 252 | GLU  |
| 1   | A     | 263 | ASN  |
| 2   | B     | 124 | GLU  |
| 2   | B     | 226 | VAL  |
| 2   | B     | 285 | GLU  |
| 2   | B     | 308 | ASN  |
| 2   | B     | 344 | THR  |
| 2   | B     | 675 | LEU  |
| 2   | B     | 697 | ALA  |
| 2   | B     | 732 | VAL  |
| 1   | C     | 15  | ILE  |
| 1   | C     | 65  | GLU  |
| 1   | C     | 258 | ASP  |
| 2   | D     | 69  | VAL  |
| 2   | D     | 165 | ASN  |
| 2   | D     | 203 | LEU  |
| 2   | D     | 211 | GLU  |
| 2   | D     | 321 | HIS  |
| 2   | D     | 536 | PRO  |
| 2   | D     | 563 | GLN  |
| 2   | D     | 632 | ASN  |
| 2   | D     | 654 | LEU  |
| 2   | D     | 667 | PRO  |
| 1   | A     | 188 | ILE  |
| 2   | B     | 129 | ASP  |
| 2   | B     | 184 | GLN  |
| 2   | B     | 270 | ASP  |
| 2   | B     | 281 | ALA  |
| 2   | B     | 642 | PRO  |
| 2   | B     | 779 | ALA  |
| 1   | C     | 82  | ALA  |
| 1   | C     | 218 | ILE  |
| 2   | D     | 144 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 248 | ALA  |
| 2   | D     | 257 | LEU  |
| 2   | D     | 441 | LYS  |
| 2   | D     | 701 | SER  |
| 2   | D     | 754 | LYS  |
| 2   | B     | 199 | ILE  |
| 1   | C     | 59  | VAL  |
| 1   | C     | 145 | ILE  |
| 2   | D     | 95  | ILE  |
| 2   | D     | 535 | SER  |
| 2   | D     | 537 | ILE  |
| 1   | A     | 145 | ILE  |
| 2   | B     | 138 | PRO  |
| 2   | D     | 229 | PRO  |
| 2   | D     | 677 | GLY  |
| 2   | B     | 246 | ILE  |
| 2   | D     | 429 | ILE  |
| 2   | B     | 746 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 212/276 (77%)   | 164 (77%)  | 48 (23%)  | 1           | 4  |
| 1   | C     | 240/276 (87%)   | 202 (84%)  | 38 (16%)  | 2           | 12 |
| 2   | B     | 656/663 (99%)   | 496 (76%)  | 160 (24%) | 0           | 3  |
| 2   | D     | 657/663 (99%)   | 504 (77%)  | 153 (23%) | 1           | 3  |
| All | All   | 1765/1878 (94%) | 1366 (77%) | 399 (23%) | 1           | 4  |

All (399) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 86  | ARG  |
| 1   | A     | 96  | LEU  |
| 1   | A     | 99  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 101 | ILE  |
| 1   | A     | 103 | ASN  |
| 1   | A     | 106 | LEU  |
| 1   | A     | 109 | VAL  |
| 1   | A     | 123 | LEU  |
| 1   | A     | 127 | VAL  |
| 1   | A     | 134 | GLU  |
| 1   | A     | 141 | ASP  |
| 1   | A     | 145 | ILE  |
| 1   | A     | 154 | ASP  |
| 1   | A     | 164 | ARG  |
| 1   | A     | 165 | LEU  |
| 1   | A     | 167 | ARG  |
| 1   | A     | 168 | THR  |
| 1   | A     | 169 | GLN  |
| 1   | A     | 171 | SER  |
| 1   | A     | 173 | VAL  |
| 1   | A     | 178 | MET  |
| 1   | A     | 181 | GLN  |
| 1   | A     | 185 | ILE  |
| 1   | A     | 186 | ARG  |
| 1   | A     | 188 | ILE  |
| 1   | A     | 195 | ARG  |
| 1   | A     | 199 | ASP  |
| 1   | A     | 212 | LEU  |
| 1   | A     | 218 | ILE  |
| 1   | A     | 223 | LEU  |
| 1   | A     | 239 | LEU  |
| 1   | A     | 241 | ILE  |
| 1   | A     | 244 | ARG  |
| 1   | A     | 257 | VAL  |
| 1   | A     | 263 | ASN  |
| 1   | A     | 268 | GLU  |
| 1   | A     | 269 | VAL  |
| 1   | A     | 282 | ASN  |
| 1   | A     | 283 | VAL  |
| 1   | A     | 288 | GLU  |
| 1   | A     | 293 | PHE  |
| 1   | A     | 302 | LEU  |
| 1   | A     | 305 | LEU  |
| 1   | A     | 310 | THR  |
| 1   | A     | 313 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 317 | GLU  |
| 1   | A     | 320 | LEU  |
| 1   | A     | 323 | LEU  |
| 2   | B     | 1   | MET  |
| 2   | B     | 6   | LEU  |
| 2   | B     | 12  | VAL  |
| 2   | B     | 16  | ILE  |
| 2   | B     | 23  | ASN  |
| 2   | B     | 26  | THR  |
| 2   | B     | 31  | GLU  |
| 2   | B     | 33  | ASP  |
| 2   | B     | 38  | VAL  |
| 2   | B     | 52  | GLU  |
| 2   | B     | 53  | CYS  |
| 2   | B     | 56  | HIS  |
| 2   | B     | 62  | LEU  |
| 2   | B     | 76  | ASP  |
| 2   | B     | 77  | ILE  |
| 2   | B     | 78  | VAL  |
| 2   | B     | 84  | CYS  |
| 2   | B     | 85  | ARG  |
| 2   | B     | 86  | GLN  |
| 2   | B     | 89  | ARG  |
| 2   | B     | 103 | PHE  |
| 2   | B     | 104 | LYS  |
| 2   | B     | 106 | LYS  |
| 2   | B     | 111 | ARG  |
| 2   | B     | 113 | GLU  |
| 2   | B     | 124 | GLU  |
| 2   | B     | 127 | ILE  |
| 2   | B     | 130 | ASP  |
| 2   | B     | 131 | HIS  |
| 2   | B     | 134 | ILE  |
| 2   | B     | 140 | ASP  |
| 2   | B     | 145 | THR  |
| 2   | B     | 147 | ILE  |
| 2   | B     | 152 | LYS  |
| 2   | B     | 155 | ASP  |
| 2   | B     | 157 | THR  |
| 2   | B     | 158 | ILE  |
| 2   | B     | 159 | GLU  |
| 2   | B     | 165 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 170 | LEU  |
| 2   | B     | 175 | VAL  |
| 2   | B     | 177 | ARG  |
| 2   | B     | 178 | ASP  |
| 2   | B     | 184 | GLN  |
| 2   | B     | 189 | GLN  |
| 2   | B     | 193 | VAL  |
| 2   | B     | 207 | VAL  |
| 2   | B     | 208 | GLU  |
| 2   | B     | 225 | ASN  |
| 2   | B     | 227 | LYS  |
| 2   | B     | 244 | ARG  |
| 2   | B     | 246 | ILE  |
| 2   | B     | 249 | VAL  |
| 2   | B     | 269 | LYS  |
| 2   | B     | 272 | ILE  |
| 2   | B     | 285 | GLU  |
| 2   | B     | 293 | THR  |
| 2   | B     | 294 | GLU  |
| 2   | B     | 303 | VAL  |
| 2   | B     | 311 | LEU  |
| 2   | B     | 317 | PHE  |
| 2   | B     | 327 | GLU  |
| 2   | B     | 342 | SER  |
| 2   | B     | 344 | THR  |
| 2   | B     | 352 | LEU  |
| 2   | B     | 359 | ARG  |
| 2   | B     | 362 | ARG  |
| 2   | B     | 370 | HIS  |
| 2   | B     | 371 | LYS  |
| 2   | B     | 375 | ARG  |
| 2   | B     | 378 | ARG  |
| 2   | B     | 379 | LEU  |
| 2   | B     | 387 | GLU  |
| 2   | B     | 391 | VAL  |
| 2   | B     | 392 | ILE  |
| 2   | B     | 394 | ILE  |
| 2   | B     | 396 | ASN  |
| 2   | B     | 402 | LYS  |
| 2   | B     | 403 | ARG  |
| 2   | B     | 407 | THR  |
| 2   | B     | 408 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 414 | ASP  |
| 2   | B     | 416 | LEU  |
| 2   | B     | 424 | GLU  |
| 2   | B     | 430 | LEU  |
| 2   | B     | 431 | ARG  |
| 2   | B     | 432 | ARG  |
| 2   | B     | 433 | LEU  |
| 2   | B     | 437 | VAL  |
| 2   | B     | 438 | THR  |
| 2   | B     | 445 | GLN  |
| 2   | B     | 452 | ARG  |
| 2   | B     | 457 | ILE  |
| 2   | B     | 472 | ASN  |
| 2   | B     | 473 | ASN  |
| 2   | B     | 476 | ASP  |
| 2   | B     | 477 | GLU  |
| 2   | B     | 479 | VAL  |
| 2   | B     | 487 | THR  |
| 2   | B     | 502 | LEU  |
| 2   | B     | 512 | THR  |
| 2   | B     | 515 | PHE  |
| 2   | B     | 519 | LYS  |
| 2   | B     | 520 | VAL  |
| 2   | B     | 533 | LEU  |
| 2   | B     | 537 | ILE  |
| 2   | B     | 538 | SER  |
| 2   | B     | 539 | VAL  |
| 2   | B     | 540 | GLU  |
| 2   | B     | 545 | ARG  |
| 2   | B     | 546 | LEU  |
| 2   | B     | 548 | LEU  |
| 2   | B     | 552 | LEU  |
| 2   | B     | 556 | VAL  |
| 2   | B     | 563 | GLN  |
| 2   | B     | 567 | VAL  |
| 2   | B     | 574 | LEU  |
| 2   | B     | 575 | ARG  |
| 2   | B     | 577 | VAL  |
| 2   | B     | 584 | LEU  |
| 2   | B     | 586 | ILE  |
| 2   | B     | 590 | LEU  |
| 2   | B     | 595 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 611 | THR  |
| 2   | B     | 612 | VAL  |
| 2   | B     | 613 | ASP  |
| 2   | B     | 617 | LEU  |
| 2   | B     | 618 | LYS  |
| 2   | B     | 628 | THR  |
| 2   | B     | 630 | LYS  |
| 2   | B     | 631 | LEU  |
| 2   | B     | 641 | ASN  |
| 2   | B     | 662 | VAL  |
| 2   | B     | 668 | GLU  |
| 2   | B     | 671 | ARG  |
| 2   | B     | 676 | ASN  |
| 2   | B     | 678 | ARG  |
| 2   | B     | 685 | GLU  |
| 2   | B     | 688 | LYS  |
| 2   | B     | 689 | LEU  |
| 2   | B     | 700 | ILE  |
| 2   | B     | 714 | VAL  |
| 2   | B     | 716 | GLU  |
| 2   | B     | 724 | LEU  |
| 2   | B     | 728 | LYS  |
| 2   | B     | 732 | VAL  |
| 2   | B     | 733 | ASN  |
| 2   | B     | 734 | GLN  |
| 2   | B     | 738 | VAL  |
| 2   | B     | 739 | ASN  |
| 2   | B     | 751 | GLU  |
| 2   | B     | 756 | LEU  |
| 2   | B     | 760 | LEU  |
| 2   | B     | 761 | ILE  |
| 2   | B     | 768 | THR  |
| 2   | B     | 769 | LEU  |
| 2   | B     | 770 | GLU  |
| 2   | B     | 780 | LYS  |
| 2   | B     | 787 | GLU  |
| 2   | B     | 788 | ARG  |
| 1   | C     | 21  | VAL  |
| 1   | C     | 62  | GLU  |
| 1   | C     | 65  | GLU  |
| 1   | C     | 69  | GLN  |
| 1   | C     | 74  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 75  | LYS  |
| 1   | C     | 83  | LEU  |
| 1   | C     | 91  | THR  |
| 1   | C     | 94  | VAL  |
| 1   | C     | 96  | LEU  |
| 1   | C     | 101 | ILE  |
| 1   | C     | 103 | ASN  |
| 1   | C     | 111 | ARG  |
| 1   | C     | 112 | THR  |
| 1   | C     | 115 | ARG  |
| 1   | C     | 123 | LEU  |
| 1   | C     | 126 | THR  |
| 1   | C     | 155 | HIS  |
| 1   | C     | 164 | ARG  |
| 1   | C     | 165 | LEU  |
| 1   | C     | 181 | GLN  |
| 1   | C     | 185 | ILE  |
| 1   | C     | 209 | MET  |
| 1   | C     | 218 | ILE  |
| 1   | C     | 238 | ASP  |
| 1   | C     | 241 | ILE  |
| 1   | C     | 246 | SER  |
| 1   | C     | 259 | VAL  |
| 1   | C     | 262 | LYS  |
| 1   | C     | 265 | LYS  |
| 1   | C     | 270 | LEU  |
| 1   | C     | 291 | SER  |
| 1   | C     | 302 | LEU  |
| 1   | C     | 312 | LEU  |
| 1   | C     | 313 | ARG  |
| 1   | C     | 320 | LEU  |
| 1   | C     | 323 | LEU  |
| 1   | C     | 324 | LYS  |
| 2   | D     | 1   | MET  |
| 2   | D     | 18  | SER  |
| 2   | D     | 19  | ASP  |
| 2   | D     | 21  | LEU  |
| 2   | D     | 30  | LEU  |
| 2   | D     | 36  | GLU  |
| 2   | D     | 47  | VAL  |
| 2   | D     | 50  | VAL  |
| 2   | D     | 52  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 53  | CYS  |
| 2   | D     | 55  | GLN  |
| 2   | D     | 62  | LEU  |
| 2   | D     | 63  | ARG  |
| 2   | D     | 65  | THR  |
| 2   | D     | 66  | LYS  |
| 2   | D     | 67  | VAL  |
| 2   | D     | 68  | ASN  |
| 2   | D     | 72  | ASP  |
| 2   | D     | 74  | LEU  |
| 2   | D     | 77  | ILE  |
| 2   | D     | 95  | ILE  |
| 2   | D     | 102 | ASP  |
| 2   | D     | 104 | LYS  |
| 2   | D     | 110 | LEU  |
| 2   | D     | 111 | ARG  |
| 2   | D     | 121 | SER  |
| 2   | D     | 124 | GLU  |
| 2   | D     | 127 | ILE  |
| 2   | D     | 129 | ASP  |
| 2   | D     | 131 | HIS  |
| 2   | D     | 143 | ILE  |
| 2   | D     | 152 | LYS  |
| 2   | D     | 158 | ILE  |
| 2   | D     | 161 | SER  |
| 2   | D     | 165 | ASN  |
| 2   | D     | 172 | ILE  |
| 2   | D     | 181 | VAL  |
| 2   | D     | 182 | LEU  |
| 2   | D     | 198 | THR  |
| 2   | D     | 199 | ILE  |
| 2   | D     | 201 | ASP  |
| 2   | D     | 202 | THR  |
| 2   | D     | 203 | LEU  |
| 2   | D     | 211 | GLU  |
| 2   | D     | 222 | LYS  |
| 2   | D     | 227 | LYS  |
| 2   | D     | 244 | ARG  |
| 2   | D     | 269 | LYS  |
| 2   | D     | 272 | ILE  |
| 2   | D     | 276 | ILE  |
| 2   | D     | 279 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 280 | MET  |
| 2   | D     | 282 | LYS  |
| 2   | D     | 290 | LEU  |
| 2   | D     | 294 | GLU  |
| 2   | D     | 304 | ILE  |
| 2   | D     | 308 | ASN  |
| 2   | D     | 317 | PHE  |
| 2   | D     | 322 | SER  |
| 2   | D     | 326 | ASP  |
| 2   | D     | 327 | GLU  |
| 2   | D     | 328 | THR  |
| 2   | D     | 330 | ASN  |
| 2   | D     | 341 | LEU  |
| 2   | D     | 348 | ARG  |
| 2   | D     | 362 | ARG  |
| 2   | D     | 375 | ARG  |
| 2   | D     | 379 | LEU  |
| 2   | D     | 381 | ILE  |
| 2   | D     | 392 | ILE  |
| 2   | D     | 394 | ILE  |
| 2   | D     | 395 | THR  |
| 2   | D     | 396 | ASN  |
| 2   | D     | 400 | LEU  |
| 2   | D     | 402 | LYS  |
| 2   | D     | 403 | ARG  |
| 2   | D     | 408 | LEU  |
| 2   | D     | 423 | ASP  |
| 2   | D     | 426 | VAL  |
| 2   | D     | 427 | THR  |
| 2   | D     | 430 | LEU  |
| 2   | D     | 437 | VAL  |
| 2   | D     | 438 | THR  |
| 2   | D     | 441 | LYS  |
| 2   | D     | 443 | GLU  |
| 2   | D     | 445 | GLN  |
| 2   | D     | 452 | ARG  |
| 2   | D     | 462 | VAL  |
| 2   | D     | 473 | ASN  |
| 2   | D     | 479 | VAL  |
| 2   | D     | 480 | GLN  |
| 2   | D     | 487 | THR  |
| 2   | D     | 510 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 512 | THR  |
| 2   | D     | 515 | PHE  |
| 2   | D     | 519 | LYS  |
| 2   | D     | 522 | GLN  |
| 2   | D     | 528 | VAL  |
| 2   | D     | 532 | LEU  |
| 2   | D     | 537 | ILE  |
| 2   | D     | 538 | SER  |
| 2   | D     | 546 | LEU  |
| 2   | D     | 556 | VAL  |
| 2   | D     | 560 | GLN  |
| 2   | D     | 563 | GLN  |
| 2   | D     | 564 | GLN  |
| 2   | D     | 566 | ARG  |
| 2   | D     | 574 | LEU  |
| 2   | D     | 577 | VAL  |
| 2   | D     | 583 | PRO  |
| 2   | D     | 584 | LEU  |
| 2   | D     | 586 | ILE  |
| 2   | D     | 590 | LEU  |
| 2   | D     | 592 | LEU  |
| 2   | D     | 603 | GLU  |
| 2   | D     | 609 | LYS  |
| 2   | D     | 611 | THR  |
| 2   | D     | 621 | LEU  |
| 2   | D     | 623 | SER  |
| 2   | D     | 625 | LEU  |
| 2   | D     | 628 | THR  |
| 2   | D     | 630 | LYS  |
| 2   | D     | 631 | LEU  |
| 2   | D     | 632 | ASN  |
| 2   | D     | 639 | GLU  |
| 2   | D     | 657 | GLU  |
| 2   | D     | 664 | VAL  |
| 2   | D     | 668 | GLU  |
| 2   | D     | 671 | ARG  |
| 2   | D     | 674 | ASP  |
| 2   | D     | 678 | ARG  |
| 2   | D     | 688 | LYS  |
| 2   | D     | 689 | LEU  |
| 2   | D     | 691 | ASP  |
| 2   | D     | 692 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 698 | ARG  |
| 2   | D     | 699 | GLU  |
| 2   | D     | 700 | ILE  |
| 2   | D     | 702 | ARG  |
| 2   | D     | 708 | ARG  |
| 2   | D     | 714 | VAL  |
| 2   | D     | 717 | ASN  |
| 2   | D     | 732 | VAL  |
| 2   | D     | 735 | VAL  |
| 2   | D     | 740 | LEU  |
| 2   | D     | 760 | LEU  |
| 2   | D     | 761 | ILE  |
| 2   | D     | 767 | ARG  |
| 2   | D     | 768 | THR  |
| 2   | D     | 771 | GLU  |
| 2   | D     | 780 | LYS  |
| 2   | D     | 786 | LYS  |
| 2   | D     | 790 | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 107 | HIS  |
| 1   | A     | 138 | HIS  |
| 1   | A     | 155 | HIS  |
| 1   | A     | 169 | GLN  |
| 1   | A     | 181 | GLN  |
| 1   | A     | 202 | HIS  |
| 1   | A     | 207 | HIS  |
| 1   | A     | 228 | HIS  |
| 1   | A     | 276 | HIS  |
| 1   | A     | 282 | ASN  |
| 1   | A     | 318 | ASN  |
| 2   | B     | 24  | GLN  |
| 2   | B     | 86  | GLN  |
| 2   | B     | 156 | ASN  |
| 2   | B     | 165 | ASN  |
| 2   | B     | 183 | ASN  |
| 2   | B     | 184 | GLN  |
| 2   | B     | 225 | ASN  |
| 2   | B     | 254 | ASN  |
| 2   | B     | 265 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 321 | HIS  |
| 2   | B     | 350 | HIS  |
| 2   | B     | 370 | HIS  |
| 2   | B     | 420 | HIS  |
| 2   | B     | 521 | GLN  |
| 2   | B     | 525 | HIS  |
| 2   | B     | 560 | GLN  |
| 2   | B     | 581 | GLN  |
| 2   | B     | 641 | ASN  |
| 2   | B     | 734 | GLN  |
| 2   | B     | 739 | ASN  |
| 2   | B     | 763 | GLN  |
| 1   | C     | 66  | GLN  |
| 1   | C     | 69  | GLN  |
| 1   | C     | 138 | HIS  |
| 1   | C     | 139 | ASN  |
| 1   | C     | 149 | HIS  |
| 1   | C     | 174 | GLN  |
| 1   | C     | 181 | GLN  |
| 1   | C     | 207 | HIS  |
| 1   | C     | 208 | GLN  |
| 1   | C     | 222 | ASN  |
| 1   | C     | 240 | GLN  |
| 1   | C     | 276 | HIS  |
| 1   | C     | 325 | GLN  |
| 2   | D     | 56  | HIS  |
| 2   | D     | 156 | ASN  |
| 2   | D     | 165 | ASN  |
| 2   | D     | 225 | ASN  |
| 2   | D     | 254 | ASN  |
| 2   | D     | 445 | GLN  |
| 2   | D     | 473 | ASN  |
| 2   | D     | 480 | GLN  |
| 2   | D     | 521 | GLN  |
| 2   | D     | 525 | HIS  |
| 2   | D     | 564 | GLN  |
| 2   | D     | 641 | ASN  |
| 2   | D     | 763 | GLN  |
| 2   | D     | 790 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 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$ |
| 3   | PHE  | A     | 980 | -    | 9,12,12      | 0.46 | 0           | 10,15,15    | 0.29 | 0           |
| 3   | PHE  | C     | 990 | -    | 9,12,12      | 0.56 | 0           | 10,15,15    | 0.26 | 0           |
| 4   | AMP  | C     | 999 | -    | 22,25,25     | 1.42 | 2 (9%)      | 25,38,38    | 1.40 | 3 (12%)     |
| 4   | AMP  | A     | 992 | -    | 22,25,25     | 1.43 | 3 (13%)     | 25,38,38    | 2.06 | 6 (24%)     |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | PHE  | A     | 980 | -    | -       | 2/4/8/8   | 0/1/1/1 |
| 3   | PHE  | C     | 990 | -    | -       | 2/4/8/8   | 0/1/1/1 |
| 4   | AMP  | C     | 999 | -    | -       | 5/6/26/26 | 0/3/3/3 |
| 4   | AMP  | A     | 992 | -    | -       | 5/6/26/26 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | A     | 992 | AMP  | P-O1P   | 4.17  | 1.64        | 1.50     |
| 4   | C     | 999 | AMP  | P-O1P   | 4.08  | 1.63        | 1.50     |
| 4   | C     | 999 | AMP  | O4'-C1' | 3.62  | 1.46        | 1.41     |
| 4   | A     | 992 | AMP  | C5-N7   | -2.04 | 1.32        | 1.39     |
| 4   | A     | 992 | AMP  | P-O3P   | 2.03  | 1.62        | 1.54     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | A     | 992 | AMP  | O4'-C1'-C2' | -5.84 | 98.40       | 106.93   |
| 4   | A     | 992 | AMP  | N3-C2-N1    | -4.82 | 121.14      | 128.68   |
| 4   | C     | 999 | AMP  | N3-C2-N1    | -4.64 | 121.42      | 128.68   |
| 4   | A     | 992 | AMP  | P-O5'-C5'   | 3.25  | 127.23      | 118.30   |
| 4   | A     | 992 | AMP  | O2P-P-O5'   | 3.16  | 115.13      | 106.73   |
| 4   | A     | 992 | AMP  | O3P-P-O5'   | -2.53 | 100.01      | 106.73   |
| 4   | C     | 999 | AMP  | C3'-C2'-C1' | 2.47  | 104.69      | 100.98   |
| 4   | A     | 992 | AMP  | C2-N1-C6    | 2.09  | 122.34      | 118.75   |
| 4   | C     | 999 | AMP  | P-O5'-C5'   | 2.06  | 123.98      | 118.30   |

There are no chirality outliers.

All (14) torsion outliers are listed below:

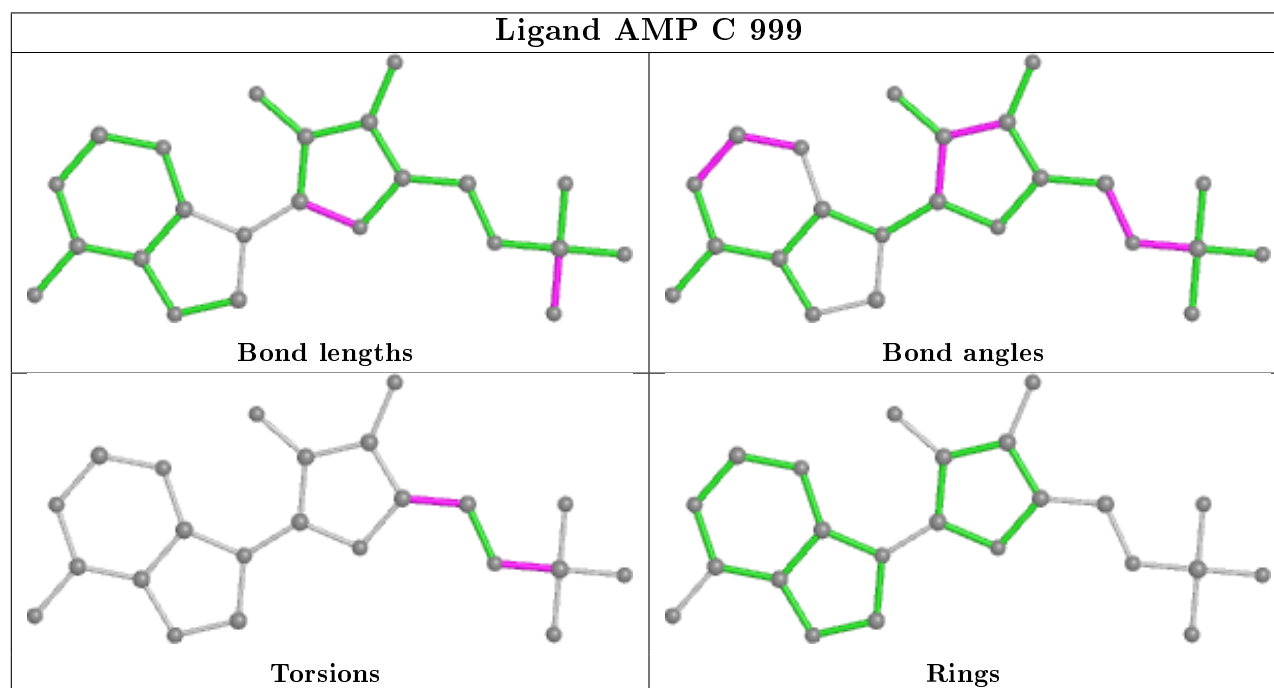
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | C     | 990 | PHE  | N-CA-CB-CG      |
| 3   | C     | 990 | PHE  | C-CA-CB-CG      |
| 4   | C     | 999 | AMP  | C5'-O5'-P-O1P   |
| 4   | C     | 999 | AMP  | C5'-O5'-P-O2P   |
| 4   | C     | 999 | AMP  | C5'-O5'-P-O3P   |
| 4   | C     | 999 | AMP  | O4'-C4'-C5'-O5' |
| 4   | C     | 999 | AMP  | C3'-C4'-C5'-O5' |
| 4   | A     | 992 | AMP  | C5'-O5'-P-O2P   |
| 4   | A     | 992 | AMP  | C5'-O5'-P-O3P   |
| 4   | A     | 992 | AMP  | O4'-C4'-C5'-O5' |
| 4   | A     | 992 | AMP  | C3'-C4'-C5'-O5' |
| 3   | A     | 980 | PHE  | CA-CB-CG-CD2    |
| 3   | A     | 980 | PHE  | CA-CB-CG-CD1    |
| 4   | A     | 992 | AMP  | C4'-C5'-O5'-P   |

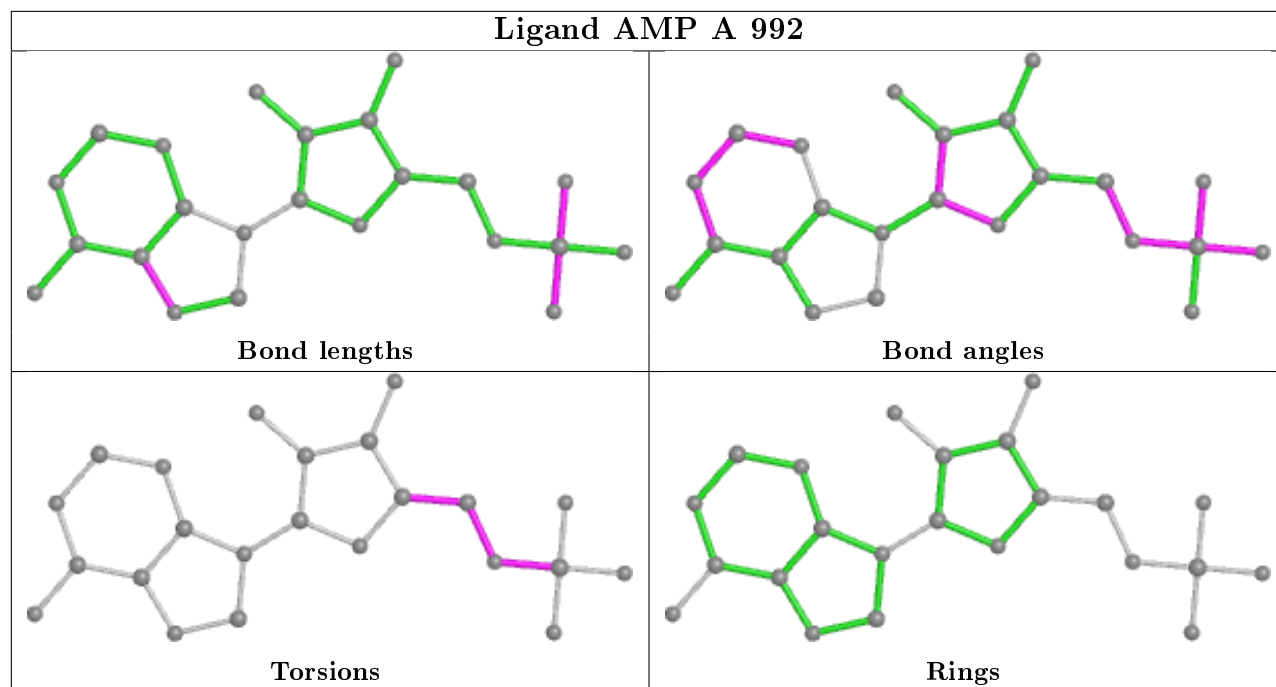
There are no ring outliers.

4 monomers are involved in 19 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 980 | PHE  | 2       | 0            |
| 3   | C     | 990 | PHE  | 1       | 0            |
| 4   | C     | 999 | AMP  | 9       | 0            |
| 4   | A     | 992 | AMP  | 9       | 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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|---------------|-----------------------|--------|
| 1   | A     | 242/327 (74%)   | -0.19  | 3 (1%) 79 53  | 50, 63, 87, 145       | 0      |
| 1   | C     | 323/327 (98%)   | 0.36   | 28 (8%) 10 3  | 36, 89, 164, 169      | 8 (2%) |
| 2   | B     | 795/795 (100%)  | -0.21  | 3 (0%) 92 78  | 51, 89, 128, 148      | 0      |
| 2   | D     | 795/795 (100%)  | -0.03  | 9 (1%) 80 55  | 58, 97, 132, 148      | 0      |
| All | All   | 2155/2244 (96%) | -0.06  | 43 (1%) 65 36 | 36, 90, 138, 169      | 8 (0%) |

All (43) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 19  | SER  | 5.8  |
| 1   | C     | 5   | ALA  | 4.7  |
| 1   | C     | 18  | ALA  | 4.7  |
| 1   | C     | 59  | VAL  | 4.4  |
| 1   | C     | 29  | VAL  | 4.2  |
| 1   | C     | 40  | LEU  | 4.1  |
| 1   | C     | 11  | ALA  | 4.0  |
| 2   | D     | 201 | ASP  | 4.0  |
| 1   | C     | 26  | ASN  | 3.8  |
| 1   | C     | 15  | ILE  | 3.7  |
| 1   | C     | 55  | ALA  | 3.6  |
| 1   | C     | 261 | GLY  | 3.5  |
| 1   | C     | 31  | TYR  | 3.4  |
| 1   | A     | 264 | GLY  | 3.4  |
| 1   | C     | 28  | ARG  | 3.3  |
| 1   | C     | 58  | ALA  | 3.3  |
| 1   | C     | 56  | ALA  | 3.3  |
| 1   | C     | 54  | PRO  | 3.1  |
| 2   | B     | 781 | CYS  | 3.1  |
| 1   | C     | 43  | THR  | 2.9  |
| 1   | A     | 87  | LEU  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 44  | THR  | 2.7  |
| 2   | D     | 211 | GLU  | 2.6  |
| 2   | D     | 114 | PRO  | 2.6  |
| 1   | C     | 41  | GLN  | 2.5  |
| 1   | C     | 57  | GLY  | 2.4  |
| 1   | C     | 243 | PHE  | 2.4  |
| 1   | C     | 45  | LEU  | 2.4  |
| 1   | A     | 88  | ALA  | 2.3  |
| 1   | C     | 163 | THR  | 2.3  |
| 1   | C     | 254 | SER  | 2.3  |
| 2   | D     | 75  | LEU  | 2.2  |
| 2   | D     | 202 | THR  | 2.2  |
| 1   | C     | 60  | ILE  | 2.2  |
| 2   | D     | 71  | GLY  | 2.2  |
| 2   | D     | 109 | LYS  | 2.2  |
| 1   | C     | 39  | THR  | 2.2  |
| 1   | C     | 62  | GLU  | 2.1  |
| 2   | B     | 131 | HIS  | 2.1  |
| 1   | C     | 16  | SER  | 2.1  |
| 2   | B     | 785 | LEU  | 2.1  |
| 2   | D     | 91  | ALA  | 2.1  |
| 2   | D     | 345 | GLY  | 2.1  |

## 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 monosaccharides 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | AMP  | C     | 999 | 23/23 | 0.80 | 0.34 | 137,145,147,147            | 0     |

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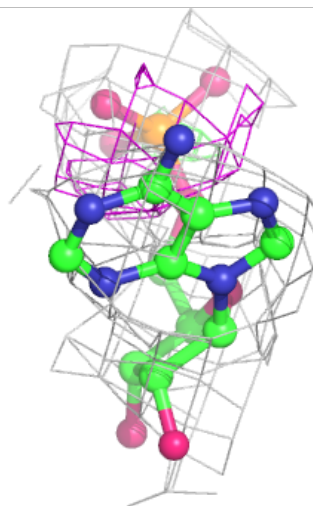
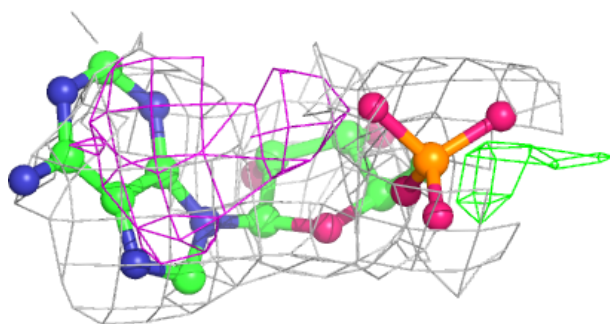
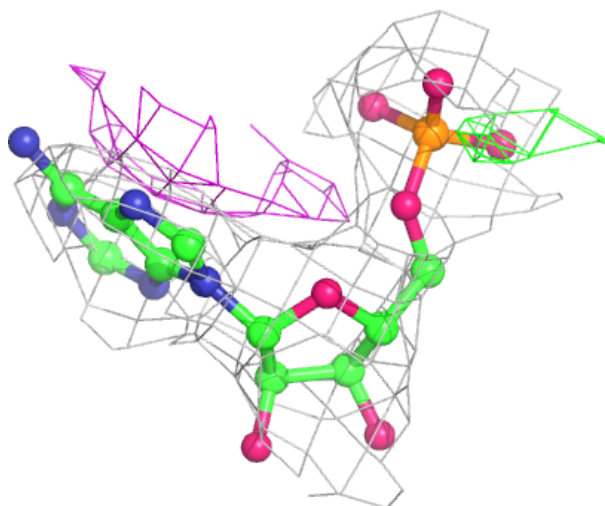
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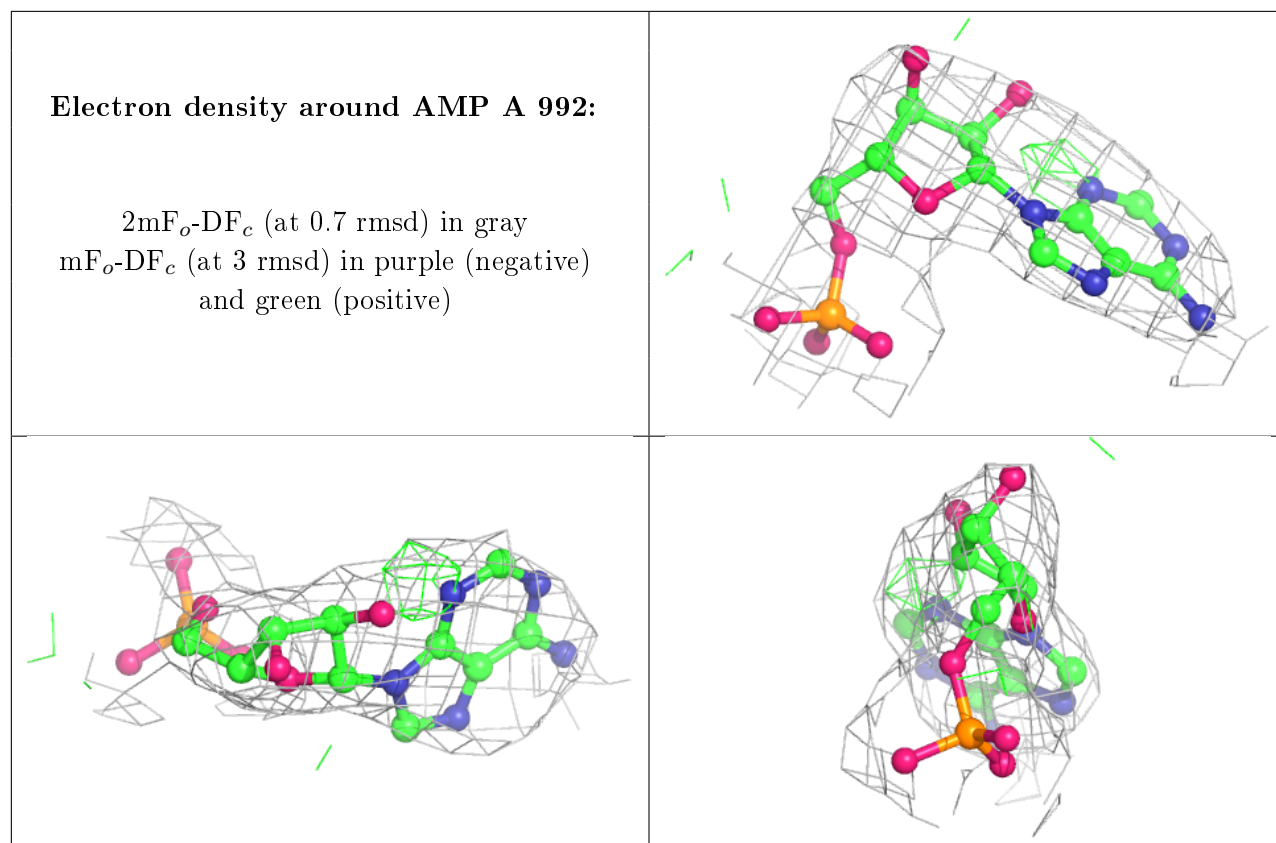
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | PHE  | A     | 980 | 12/12 | 0.89 | 0.38 | 73,80,87,87                 | 0     |
| 4   | AMP  | A     | 992 | 23/23 | 0.91 | 0.37 | 96,99,101,101               | 0     |
| 3   | PHE  | C     | 990 | 12/12 | 0.93 | 0.30 | 95,98,99,99                 | 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 AMP C 999:**

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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.