



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:40 AM UTC

PDB ID : 6LBA / pdb\_00006lba  
EMDB ID : EMD-0868  
Title : Cryo-EM structure of the AtMLKL2 tetramer  
Authors : Lisa, M.; Huang, M.; Zhang, X.; Ryohei, T.N.; Leila, B.K.; Isabel, M.L.S.;  
Florence, J.; Viera, K.; Dmitry, L.; Jane, E.P.; James, M.M.; Kay, H.; Paul,  
S.L.; Chai, J.; Takaki, M.  
Deposited on : 2019-11-13  
Resolution : 4.10 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

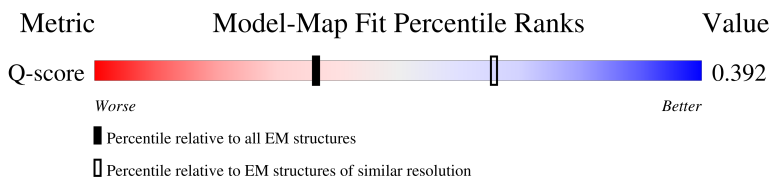
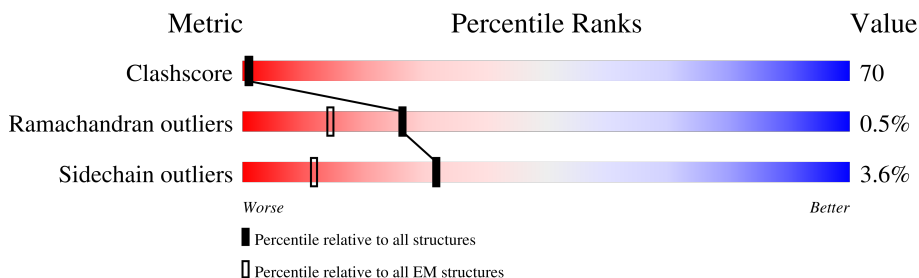
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 6458 ( 3.60 - 4.60 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                      |
|-----|-------|--------|---------------------------------------------------------------------------------------|
| 1   | A     | 572    | <div> <div>11%</div> <div>34%</div> <div>44%</div> <div>•</div> <div>19%</div> </div> |
| 1   | B     | 572    | <div> <div>10%</div> <div>34%</div> <div>43%</div> <div>•</div> <div>19%</div> </div> |
| 1   | C     | 572    | <div> <div>10%</div> <div>35%</div> <div>42%</div> <div>•</div> <div>19%</div> </div> |
| 1   | D     | 572    | <div> <div>10%</div> <div>35%</div> <div>42%</div> <div>•</div> <div>19%</div> </div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14992 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Protein kinase family protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 466      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3748  | 2414 | 656 | 653 | 25 |         |       |
| 1   | C     | 466      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3748  | 2414 | 656 | 653 | 25 |         |       |
| 1   | B     | 466      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3748  | 2414 | 656 | 653 | 25 |         |       |
| 1   | D     | 466      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3748  | 2414 | 656 | 653 | 25 |         |       |

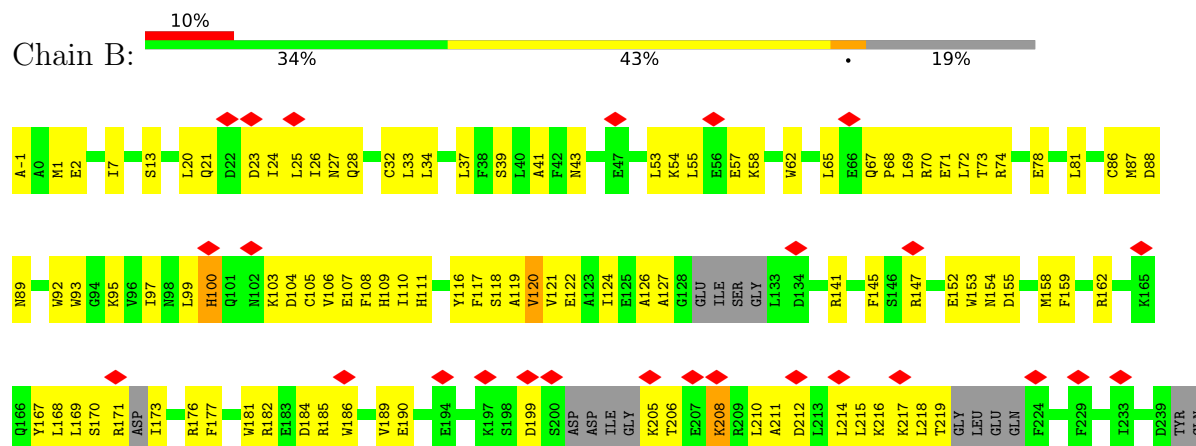
There are 20 discrepancies between the modelled and reference sequences:

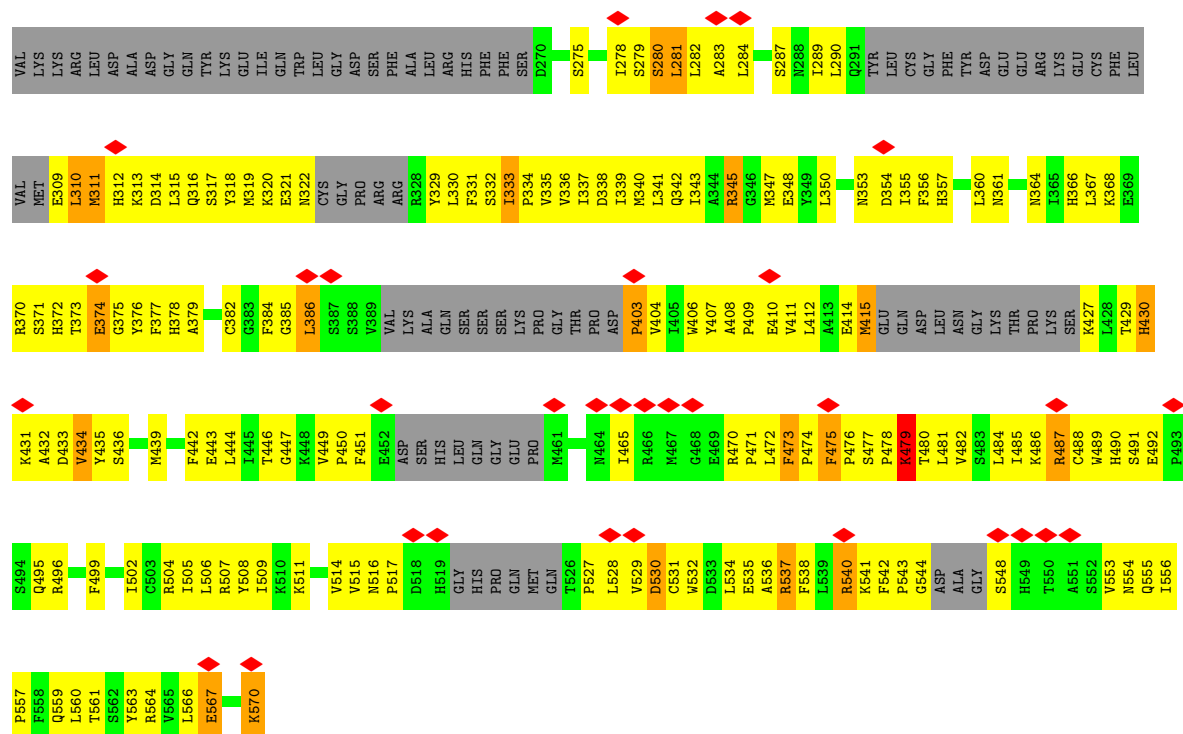
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -1      | ALA      | -      | expression tag | UNP Q9FGG5 |
| A     | 0       | ALA      | -      | expression tag | UNP Q9FGG5 |
| A     | 73      | THR      | TYR    | conflict       | UNP Q9FGG5 |
| A     | 480     | THR      | TYR    | conflict       | UNP Q9FGG5 |
| A     | 561     | THR      | TYR    | conflict       | UNP Q9FGG5 |
| C     | -1      | ALA      | -      | expression tag | UNP Q9FGG5 |
| C     | 0       | ALA      | -      | expression tag | UNP Q9FGG5 |
| C     | 73      | THR      | TYR    | conflict       | UNP Q9FGG5 |
| C     | 480     | THR      | TYR    | conflict       | UNP Q9FGG5 |
| C     | 561     | THR      | TYR    | conflict       | UNP Q9FGG5 |
| B     | -1      | ALA      | -      | expression tag | UNP Q9FGG5 |
| B     | 0       | ALA      | -      | expression tag | UNP Q9FGG5 |
| B     | 73      | THR      | TYR    | conflict       | UNP Q9FGG5 |
| B     | 480     | THR      | TYR    | conflict       | UNP Q9FGG5 |
| B     | 561     | THR      | TYR    | conflict       | UNP Q9FGG5 |
| D     | -1      | ALA      | -      | expression tag | UNP Q9FGG5 |
| D     | 0       | ALA      | -      | expression tag | UNP Q9FGG5 |
| D     | 73      | THR      | TYR    | conflict       | UNP Q9FGG5 |
| D     | 480     | THR      | TYR    | conflict       | UNP Q9FGG5 |
| D     | 561     | THR      | TYR    | conflict       | UNP Q9FGG5 |



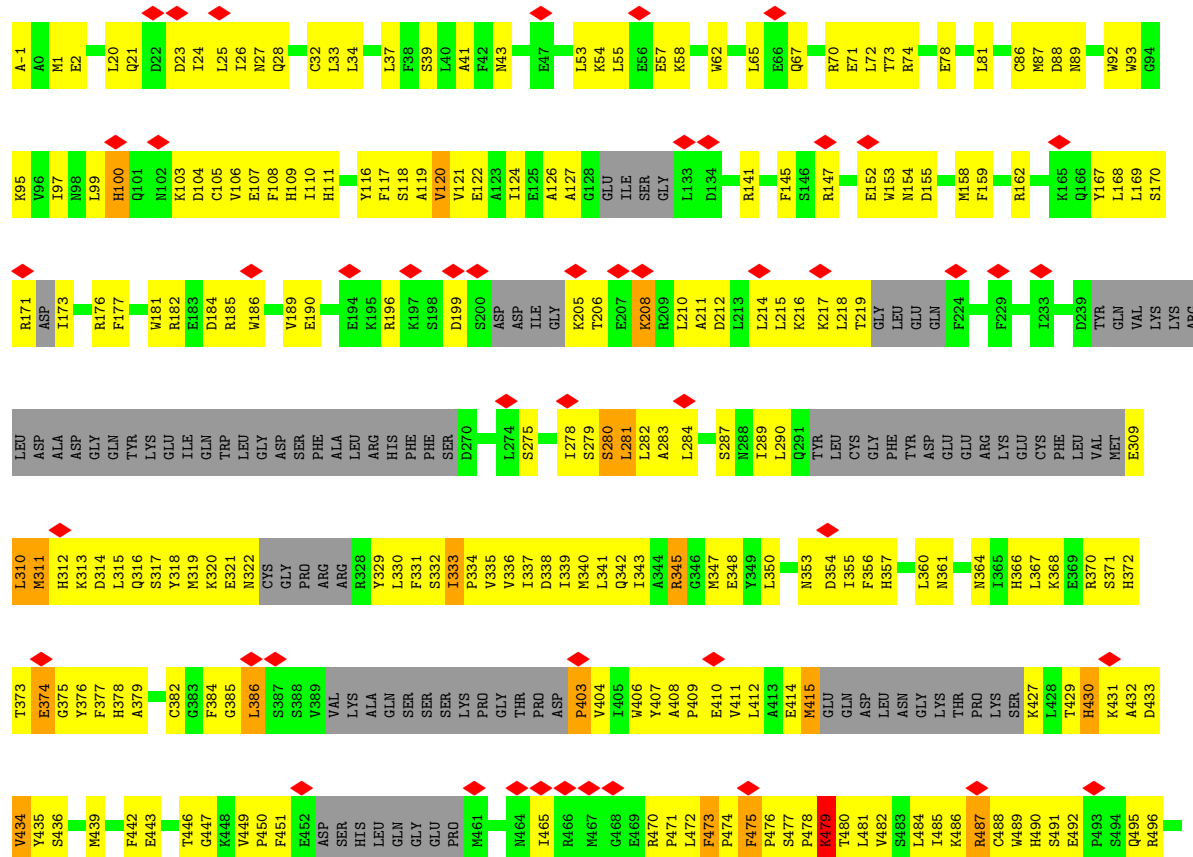


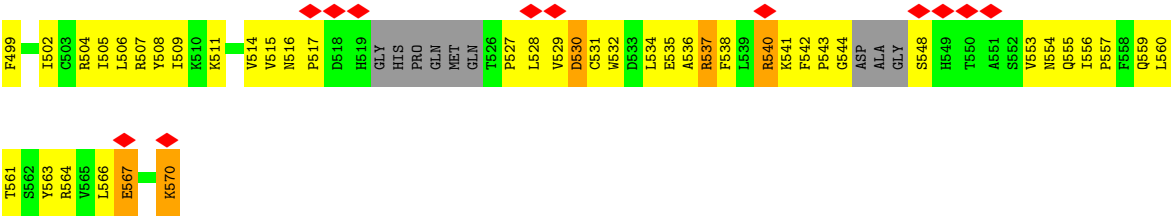
• Molecule 1: Protein kinase family protein





• Molecule 1: Protein kinase family protein





## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, Not provided       |           |
| Number of particles used             | 1527009                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF         | Depositor |
| CTF correction method                | NONE                      | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.5625                    | Depositor |
| Minimum defocus (nm)                 | Not provided              |           |
| Maximum defocus (nm)                 | Not provided              |           |
| Magnification                        | Not provided              |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value                    | 0.105                     | Depositor |
| Minimum map value                    | -0.065                    | Depositor |
| Average map value                    | 0.000                     | Depositor |
| Map value standard deviation         | 0.004                     | Depositor |
| Recommended contour level            | 0.026                     | Depositor |
| Map size ( $\text{\AA}$ )            | 261.308, 261.308, 261.308 | wwPDB     |
| Map dimensions                       | 200, 200, 200             | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.30654, 1.30654, 1.30654 | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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     | 0.32         | 0/3830      | 0.75        | 14/5160 (0.3%)  |
| 1   | B     | 0.32         | 0/3830      | 0.75        | 14/5160 (0.3%)  |
| 1   | C     | 0.32         | 0/3830      | 0.75        | 14/5160 (0.3%)  |
| 1   | D     | 0.32         | 0/3830      | 0.75        | 14/5160 (0.3%)  |
| All | All   | 0.32         | 0/15320     | 0.75        | 56/20640 (0.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

There are no bond length outliers.

All (56) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 403 | PRO  | CA-N-CD | -9.31 | 98.96       | 112.00   |
| 1   | C     | 403 | PRO  | CA-N-CD | -9.31 | 98.97       | 112.00   |
| 1   | A     | 403 | PRO  | CA-N-CD | -9.30 | 98.98       | 112.00   |
| 1   | B     | 540 | ARG  | N-CA-C  | 9.29  | 121.01      | 111.07   |
| 1   | D     | 403 | PRO  | CA-N-CD | -9.28 | 99.00       | 112.00   |
| 1   | A     | 540 | ARG  | N-CA-C  | 9.25  | 120.97      | 111.07   |
| 1   | D     | 540 | ARG  | N-CA-C  | 9.23  | 120.94      | 111.07   |
| 1   | C     | 540 | ARG  | N-CA-C  | 8.93  | 121.01      | 111.28   |
| 1   | B     | 333 | ILE  | CA-C-N  | -8.01 | 111.90      | 120.47   |
| 1   | B     | 333 | ILE  | C-N-CA  | -8.01 | 111.90      | 120.47   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 333 | ILE  | CA-C-N  | -8.01 | 111.90      | 120.47   |
| 1   | A     | 333 | ILE  | C-N-CA  | -8.01 | 111.90      | 120.47   |
| 1   | C     | 333 | ILE  | CA-C-N  | -8.01 | 111.90      | 120.47   |
| 1   | C     | 333 | ILE  | C-N-CA  | -8.01 | 111.90      | 120.47   |
| 1   | D     | 333 | ILE  | CA-C-N  | -7.98 | 111.93      | 120.47   |
| 1   | D     | 333 | ILE  | C-N-CA  | -7.98 | 111.93      | 120.47   |
| 1   | B     | 280 | SER  | N-CA-C  | -6.98 | 103.67      | 111.28   |
| 1   | D     | 280 | SER  | N-CA-C  | -6.96 | 103.69      | 111.28   |
| 1   | A     | 280 | SER  | N-CA-C  | -6.93 | 103.72      | 111.28   |
| 1   | C     | 280 | SER  | N-CA-C  | -6.92 | 103.73      | 111.28   |
| 1   | B     | 473 | PHE  | CA-C-N  | 6.83  | 126.80      | 120.03   |
| 1   | B     | 473 | PHE  | C-N-CA  | 6.83  | 126.80      | 120.03   |
| 1   | D     | 473 | PHE  | CA-C-N  | 6.82  | 126.78      | 120.03   |
| 1   | D     | 473 | PHE  | C-N-CA  | 6.82  | 126.78      | 120.03   |
| 1   | A     | 473 | PHE  | CA-C-N  | 6.80  | 126.76      | 120.03   |
| 1   | A     | 473 | PHE  | C-N-CA  | 6.80  | 126.76      | 120.03   |
| 1   | C     | 473 | PHE  | CA-C-N  | 6.76  | 126.72      | 120.03   |
| 1   | C     | 473 | PHE  | C-N-CA  | 6.76  | 126.72      | 120.03   |
| 1   | C     | 530 | ASP  | N-CA-C  | -6.43 | 100.51      | 110.10   |
| 1   | D     | 530 | ASP  | N-CA-C  | -6.42 | 100.53      | 110.10   |
| 1   | A     | 530 | ASP  | N-CA-C  | -6.42 | 100.54      | 110.10   |
| 1   | B     | 530 | ASP  | N-CA-C  | -6.41 | 100.55      | 110.10   |
| 1   | D     | 491 | SER  | N-CA-C  | 6.32  | 118.17      | 111.28   |
| 1   | B     | 491 | SER  | N-CA-C  | 6.31  | 118.16      | 111.28   |
| 1   | A     | 491 | SER  | N-CA-C  | 6.29  | 118.13      | 111.28   |
| 1   | C     | 491 | SER  | N-CA-C  | 6.28  | 118.13      | 111.28   |
| 1   | B     | 477 | SER  | CA-C-N  | 5.71  | 125.68      | 120.03   |
| 1   | B     | 477 | SER  | C-N-CA  | 5.71  | 125.68      | 120.03   |
| 1   | D     | 477 | SER  | CA-C-N  | 5.71  | 125.68      | 120.03   |
| 1   | D     | 477 | SER  | C-N-CA  | 5.71  | 125.68      | 120.03   |
| 1   | A     | 477 | SER  | CA-C-N  | 5.70  | 125.67      | 120.03   |
| 1   | A     | 477 | SER  | C-N-CA  | 5.70  | 125.67      | 120.03   |
| 1   | C     | 477 | SER  | CA-C-N  | 5.70  | 125.67      | 120.03   |
| 1   | C     | 477 | SER  | C-N-CA  | 5.70  | 125.67      | 120.03   |
| 1   | B     | 371 | SER  | CB-CA-C | -5.47 | 109.78      | 117.23   |
| 1   | D     | 371 | SER  | CB-CA-C | -5.46 | 109.80      | 117.23   |
| 1   | A     | 371 | SER  | CB-CA-C | -5.46 | 109.80      | 117.23   |
| 1   | C     | 371 | SER  | CB-CA-C | -5.45 | 109.81      | 117.23   |
| 1   | D     | 120 | VAL  | N-CA-C  | -5.40 | 105.12      | 113.16   |
| 1   | A     | 120 | VAL  | N-CA-C  | -5.39 | 105.13      | 113.16   |
| 1   | C     | 120 | VAL  | N-CA-C  | -5.38 | 105.15      | 113.16   |
| 1   | B     | 120 | VAL  | N-CA-C  | -5.37 | 105.15      | 113.16   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | D     | 479 | LYS  | N-CA-C | 5.12 | 116.86      | 111.28   |
| 1   | C     | 479 | LYS  | N-CA-C | 5.10 | 116.84      | 111.28   |
| 1   | A     | 479 | LYS  | N-CA-C | 5.08 | 116.82      | 111.28   |
| 1   | B     | 479 | LYS  | N-CA-C | 5.08 | 116.81      | 111.28   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 100 | HIS  | Peptide |
| 1   | B     | 100 | HIS  | Peptide |
| 1   | C     | 100 | HIS  | Peptide |
| 1   | D     | 100 | HIS  | 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     | 3748  | 0        | 3653     | 532     | 0            |
| 1   | B     | 3748  | 0        | 3653     | 529     | 0            |
| 1   | C     | 3748  | 0        | 3653     | 518     | 0            |
| 1   | D     | 3748  | 0        | 3653     | 522     | 0            |
| All | All   | 14992 | 0        | 14612    | 2081    | 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 70.

All (2081) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:470:ARG:HB2  | 1:B:489:TRP:CZ2 | 1.47                     | 1.48              |
| 1:A:470:ARG:HB2  | 1:A:489:TRP:CZ2 | 1.47                     | 1.48              |
| 1:C:470:ARG:HB2  | 1:C:489:TRP:CZ2 | 1.47                     | 1.46              |
| 1:D:470:ARG:HB2  | 1:D:489:TRP:CZ2 | 1.47                     | 1.46              |
| 1:D:411:VAL:HG12 | 1:D:427:LYS:CB  | 1.53                     | 1.38              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:411:VAL:HG12 | 1:C:427:LYS:CB   | 1.53                     | 1.38              |
| 1:C:170:SER:HB3  | 1:C:173:ILE:N    | 1.39                     | 1.38              |
| 1:D:170:SER:HB3  | 1:D:173:ILE:N    | 1.39                     | 1.38              |
| 1:B:411:VAL:HG12 | 1:B:427:LYS:CB   | 1.53                     | 1.37              |
| 1:A:411:VAL:HG12 | 1:A:427:LYS:CB   | 1.53                     | 1.36              |
| 1:C:118:SER:CB   | 1:C:560:LEU:HD23 | 1.58                     | 1.34              |
| 1:D:118:SER:CB   | 1:D:560:LEU:HD23 | 1.58                     | 1.34              |
| 1:A:118:SER:CB   | 1:A:560:LEU:HD23 | 1.58                     | 1.33              |
| 1:B:118:SER:CB   | 1:B:560:LEU:HD23 | 1.58                     | 1.33              |
| 1:C:470:ARG:HB2  | 1:C:489:TRP:CE2  | 1.65                     | 1.32              |
| 1:D:470:ARG:HB2  | 1:D:489:TRP:CE2  | 1.65                     | 1.32              |
| 1:A:170:SER:HB3  | 1:A:173:ILE:N    | 1.39                     | 1.31              |
| 1:B:170:SER:HB3  | 1:B:173:ILE:N    | 1.39                     | 1.31              |
| 1:B:470:ARG:HB2  | 1:B:489:TRP:CE2  | 1.65                     | 1.31              |
| 1:A:470:ARG:HB2  | 1:A:489:TRP:CE2  | 1.65                     | 1.30              |
| 1:C:275:SER:O    | 1:C:278:ILE:HG22 | 1.11                     | 1.28              |
| 1:D:275:SER:O    | 1:D:278:ILE:HG22 | 1.11                     | 1.28              |
| 1:C:118:SER:CB   | 1:C:560:LEU:CD2  | 2.13                     | 1.26              |
| 1:D:118:SER:CB   | 1:D:560:LEU:CD2  | 2.13                     | 1.26              |
| 1:A:118:SER:CB   | 1:A:560:LEU:CD2  | 2.13                     | 1.25              |
| 1:C:470:ARG:HD2  | 1:C:489:TRP:CD2  | 1.71                     | 1.25              |
| 1:B:118:SER:CB   | 1:B:560:LEU:CD2  | 2.13                     | 1.25              |
| 1:D:470:ARG:HD2  | 1:D:489:TRP:CD2  | 1.71                     | 1.25              |
| 1:A:470:ARG:HD2  | 1:A:489:TRP:CD2  | 1.71                     | 1.25              |
| 1:B:470:ARG:HD2  | 1:B:489:TRP:CD2  | 1.71                     | 1.24              |
| 1:B:275:SER:O    | 1:B:278:ILE:HG22 | 1.11                     | 1.23              |
| 1:D:290:LEU:HD11 | 1:D:309:GLU:O    | 1.38                     | 1.23              |
| 1:C:290:LEU:HD11 | 1:C:309:GLU:O    | 1.38                     | 1.23              |
| 1:A:275:SER:O    | 1:A:278:ILE:HG22 | 1.11                     | 1.22              |
| 1:A:290:LEU:HD11 | 1:A:309:GLU:C    | 1.63                     | 1.22              |
| 1:B:290:LEU:HD11 | 1:B:309:GLU:C    | 1.63                     | 1.22              |
| 1:C:290:LEU:HD11 | 1:C:309:GLU:C    | 1.63                     | 1.22              |
| 1:D:290:LEU:HD11 | 1:D:309:GLU:C    | 1.63                     | 1.22              |
| 1:C:290:LEU:HD23 | 1:C:382:CYS:SG   | 1.80                     | 1.21              |
| 1:D:290:LEU:HD23 | 1:D:382:CYS:SG   | 1.80                     | 1.21              |
| 1:A:290:LEU:HD23 | 1:A:382:CYS:SG   | 1.80                     | 1.21              |
| 1:B:290:LEU:HD23 | 1:B:382:CYS:SG   | 1.80                     | 1.21              |
| 1:C:538:PHE:O    | 1:C:543:PRO:HD3  | 1.40                     | 1.20              |
| 1:D:538:PHE:O    | 1:D:543:PRO:HD3  | 1.40                     | 1.20              |
| 1:B:118:SER:HB2  | 1:B:560:LEU:CD2  | 1.72                     | 1.19              |
| 1:A:118:SER:HB2  | 1:A:560:LEU:CD2  | 1.72                     | 1.19              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:538:PHE:O    | 1:A:543:PRO:HD3  | 1.40                     | 1.19              |
| 1:B:538:PHE:O    | 1:B:543:PRO:HD3  | 1.40                     | 1.19              |
| 1:A:290:LEU:HD11 | 1:A:309:GLU:O    | 1.38                     | 1.18              |
| 1:B:290:LEU:HD11 | 1:B:309:GLU:O    | 1.38                     | 1.18              |
| 1:A:356:PHE:HE1  | 1:A:430:HIS:CB   | 1.56                     | 1.18              |
| 1:B:356:PHE:HE1  | 1:B:430:HIS:CB   | 1.56                     | 1.18              |
| 1:D:356:PHE:HE1  | 1:D:430:HIS:CB   | 1.56                     | 1.18              |
| 1:C:356:PHE:HE1  | 1:C:430:HIS:CB   | 1.56                     | 1.18              |
| 1:C:310:LEU:HD22 | 1:C:311:MET:N    | 1.59                     | 1.17              |
| 1:D:310:LEU:HD22 | 1:D:311:MET:N    | 1.59                     | 1.17              |
| 1:A:471:PRO:HD2  | 1:A:489:TRP:CZ2  | 1.80                     | 1.17              |
| 1:B:471:PRO:HD2  | 1:B:489:TRP:CZ2  | 1.80                     | 1.16              |
| 1:A:310:LEU:HD22 | 1:A:311:MET:N    | 1.59                     | 1.16              |
| 1:C:53:LEU:HD23  | 1:C:126:ALA:HB1  | 1.24                     | 1.16              |
| 1:B:431:LYS:O    | 1:B:434:VAL:HG12 | 1.45                     | 1.16              |
| 1:A:431:LYS:O    | 1:A:434:VAL:HG12 | 1.45                     | 1.16              |
| 1:B:310:LEU:HD22 | 1:B:311:MET:N    | 1.59                     | 1.16              |
| 1:A:408:ALA:HA   | 1:A:435:TYR:CD2  | 1.81                     | 1.15              |
| 1:C:312:HIS:HD2  | 1:C:368:LYS:CG   | 1.59                     | 1.15              |
| 1:B:408:ALA:HA   | 1:B:435:TYR:CD2  | 1.81                     | 1.15              |
| 1:D:312:HIS:HD2  | 1:D:368:LYS:CG   | 1.59                     | 1.15              |
| 1:C:408:ALA:HA   | 1:C:435:TYR:CD2  | 1.81                     | 1.15              |
| 1:D:53:LEU:HD23  | 1:D:126:ALA:HB1  | 1.24                     | 1.15              |
| 1:C:356:PHE:HE1  | 1:C:430:HIS:HB2  | 1.01                     | 1.15              |
| 1:C:118:SER:HB2  | 1:C:560:LEU:CD2  | 1.72                     | 1.15              |
| 1:D:471:PRO:HD2  | 1:D:489:TRP:CZ2  | 1.79                     | 1.15              |
| 1:D:118:SER:HB2  | 1:D:560:LEU:CD2  | 1.72                     | 1.14              |
| 1:D:408:ALA:HA   | 1:D:435:TYR:CD2  | 1.81                     | 1.14              |
| 1:C:431:LYS:O    | 1:C:434:VAL:HG12 | 1.45                     | 1.14              |
| 1:C:471:PRO:HD2  | 1:C:489:TRP:CZ2  | 1.80                     | 1.14              |
| 1:B:284:LEU:HD22 | 1:B:353:ASN:HD22 | 1.08                     | 1.14              |
| 1:D:431:LYS:O    | 1:D:434:VAL:HG12 | 1.45                     | 1.14              |
| 1:C:284:LEU:HD22 | 1:C:353:ASN:HD22 | 1.09                     | 1.14              |
| 1:D:356:PHE:HE1  | 1:D:430:HIS:HB2  | 1.01                     | 1.14              |
| 1:A:284:LEU:HD22 | 1:A:353:ASN:HD22 | 1.09                     | 1.14              |
| 1:D:284:LEU:HD22 | 1:D:353:ASN:HD22 | 1.09                     | 1.14              |
| 1:B:312:HIS:HD2  | 1:B:368:LYS:CG   | 1.59                     | 1.13              |
| 1:A:312:HIS:HD2  | 1:A:368:LYS:CG   | 1.59                     | 1.13              |
| 1:C:290:LEU:HD22 | 1:C:311:MET:HG3  | 1.18                     | 1.13              |
| 1:D:290:LEU:HD22 | 1:D:311:MET:HG3  | 1.18                     | 1.13              |
| 1:A:442:PHE:HE1  | 1:A:485:ILE:HB   | 1.07                     | 1.13              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:442:PHE:HE1  | 1:B:485:ILE:HB   | 1.07                     | 1.12              |
| 1:A:471:PRO:HD2  | 1:A:489:TRP:HZ2  | 0.96                     | 1.12              |
| 1:B:471:PRO:HD2  | 1:B:489:TRP:HZ2  | 0.96                     | 1.12              |
| 1:C:312:HIS:HD2  | 1:C:368:LYS:HG3  | 1.06                     | 1.12              |
| 1:B:312:HIS:HD2  | 1:B:368:LYS:HG3  | 1.06                     | 1.12              |
| 1:A:170:SER:CB   | 1:A:173:ILE:N    | 2.12                     | 1.11              |
| 1:C:170:SER:CB   | 1:C:173:ILE:N    | 2.12                     | 1.11              |
| 1:C:284:LEU:CD2  | 1:C:353:ASN:HD22 | 1.62                     | 1.11              |
| 1:A:312:HIS:HD2  | 1:A:368:LYS:HG3  | 1.06                     | 1.11              |
| 1:B:170:SER:CB   | 1:B:173:ILE:N    | 2.12                     | 1.11              |
| 1:D:170:SER:CB   | 1:D:173:ILE:N    | 2.12                     | 1.11              |
| 1:D:442:PHE:HE1  | 1:D:485:ILE:HB   | 1.07                     | 1.11              |
| 1:C:442:PHE:HE1  | 1:C:485:ILE:HB   | 1.07                     | 1.11              |
| 1:B:284:LEU:CD2  | 1:B:353:ASN:HD22 | 1.62                     | 1.11              |
| 1:D:284:LEU:CD2  | 1:D:353:ASN:HD22 | 1.62                     | 1.11              |
| 1:D:312:HIS:HD2  | 1:D:368:LYS:HG3  | 1.06                     | 1.11              |
| 1:A:284:LEU:CD2  | 1:A:353:ASN:HD22 | 1.62                     | 1.11              |
| 1:A:356:PHE:HE1  | 1:A:430:HIS:HB2  | 1.01                     | 1.10              |
| 1:B:332:SER:OG   | 1:B:334:PRO:HG2  | 1.51                     | 1.10              |
| 1:B:356:PHE:HE1  | 1:B:430:HIS:HB2  | 1.01                     | 1.10              |
| 1:A:332:SER:OG   | 1:A:334:PRO:HG2  | 1.51                     | 1.10              |
| 1:A:53:LEU:HD23  | 1:A:126:ALA:HB1  | 1.24                     | 1.10              |
| 1:A:53:LEU:CD2   | 1:A:126:ALA:HB1  | 1.82                     | 1.10              |
| 1:C:332:SER:OG   | 1:C:334:PRO:HG2  | 1.51                     | 1.10              |
| 1:B:53:LEU:CD2   | 1:B:126:ALA:HB1  | 1.82                     | 1.10              |
| 1:C:311:MET:HB3  | 1:C:366:HIS:HB3  | 1.34                     | 1.09              |
| 1:D:332:SER:OG   | 1:D:334:PRO:HG2  | 1.51                     | 1.09              |
| 1:B:53:LEU:HD23  | 1:B:126:ALA:HB1  | 1.24                     | 1.09              |
| 1:B:290:LEU:HD22 | 1:B:311:MET:HG3  | 1.18                     | 1.09              |
| 1:D:311:MET:HB3  | 1:D:366:HIS:HB3  | 1.34                     | 1.09              |
| 1:D:53:LEU:CD2   | 1:D:126:ALA:HB1  | 1.82                     | 1.09              |
| 1:A:290:LEU:HD22 | 1:A:311:MET:HG3  | 1.18                     | 1.09              |
| 1:A:470:ARG:CB   | 1:A:489:TRP:CE2  | 2.34                     | 1.09              |
| 1:C:53:LEU:CD2   | 1:C:126:ALA:HB1  | 1.82                     | 1.09              |
| 1:B:470:ARG:CB   | 1:B:489:TRP:CE2  | 2.34                     | 1.09              |
| 1:D:470:ARG:CB   | 1:D:489:TRP:CE2  | 2.34                     | 1.08              |
| 1:A:356:PHE:CE1  | 1:A:430:HIS:CB   | 2.37                     | 1.08              |
| 1:C:470:ARG:CB   | 1:C:489:TRP:CE2  | 2.34                     | 1.08              |
| 1:B:356:PHE:CE1  | 1:B:430:HIS:CB   | 2.37                     | 1.08              |
| 1:A:411:VAL:CG1  | 1:A:427:LYS:CB   | 2.32                     | 1.07              |
| 1:C:367:LEU:HD23 | 1:C:379:ALA:HB2  | 1.14                     | 1.07              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:411:VAL:CG1  | 1:C:427:LYS:CB  | 2.32                     | 1.07              |
| 1:B:411:VAL:CG1  | 1:B:427:LYS:CB  | 2.32                     | 1.07              |
| 1:D:367:LEU:HD23 | 1:D:379:ALA:HB2 | 1.14                     | 1.07              |
| 1:D:411:VAL:CG1  | 1:D:427:LYS:CB  | 2.32                     | 1.07              |
| 1:A:312:HIS:CD2  | 1:A:368:LYS:HG3 | 1.89                     | 1.07              |
| 1:B:312:HIS:CD2  | 1:B:368:LYS:HG3 | 1.89                     | 1.07              |
| 1:A:275:SER:O    | 1:A:278:ILE:CG2 | 2.03                     | 1.07              |
| 1:A:367:LEU:HD23 | 1:A:379:ALA:HB2 | 1.14                     | 1.07              |
| 1:B:275:SER:O    | 1:B:278:ILE:CG2 | 2.03                     | 1.07              |
| 1:C:356:PHE:CE1  | 1:C:430:HIS:CB  | 2.37                     | 1.06              |
| 1:C:275:SER:O    | 1:C:278:ILE:CG2 | 2.03                     | 1.06              |
| 1:C:471:PRO:HD2  | 1:C:489:TRP:HZ2 | 0.96                     | 1.06              |
| 1:B:367:LEU:HD23 | 1:B:379:ALA:HB2 | 1.14                     | 1.06              |
| 1:D:275:SER:O    | 1:D:278:ILE:CG2 | 2.03                     | 1.06              |
| 1:D:356:PHE:CE1  | 1:D:430:HIS:CB  | 2.36                     | 1.06              |
| 1:D:471:PRO:HD2  | 1:D:489:TRP:HZ2 | 0.96                     | 1.06              |
| 1:C:470:ARG:HB3  | 1:C:489:TRP:NE1 | 1.71                     | 1.05              |
| 1:C:312:HIS:CD2  | 1:C:368:LYS:HG3 | 1.89                     | 1.05              |
| 1:D:470:ARG:HB3  | 1:D:489:TRP:NE1 | 1.71                     | 1.05              |
| 1:D:312:HIS:CD2  | 1:D:368:LYS:HG3 | 1.89                     | 1.05              |
| 1:A:470:ARG:HB3  | 1:A:489:TRP:NE1 | 1.71                     | 1.04              |
| 1:A:81:LEU:HD11  | 1:A:372:HIS:CE1 | 1.93                     | 1.04              |
| 1:B:81:LEU:HD11  | 1:B:372:HIS:CE1 | 1.93                     | 1.04              |
| 1:A:311:MET:HB3  | 1:A:366:HIS:HB3 | 1.34                     | 1.03              |
| 1:A:356:PHE:CE1  | 1:A:430:HIS:HB2 | 1.93                     | 1.03              |
| 1:B:356:PHE:CE1  | 1:B:430:HIS:HB2 | 1.93                     | 1.03              |
| 1:B:470:ARG:HB3  | 1:B:489:TRP:NE1 | 1.71                     | 1.03              |
| 1:C:81:LEU:HD11  | 1:C:372:HIS:CE1 | 1.93                     | 1.03              |
| 1:C:470:ARG:CB   | 1:C:489:TRP:NE1 | 2.21                     | 1.03              |
| 1:D:470:ARG:CB   | 1:D:489:TRP:NE1 | 2.21                     | 1.03              |
| 1:B:311:MET:HB3  | 1:B:366:HIS:HB3 | 1.34                     | 1.03              |
| 1:D:81:LEU:HD11  | 1:D:372:HIS:CE1 | 1.93                     | 1.03              |
| 1:A:490:HIS:O    | 1:A:496:ARG:HD2 | 1.59                     | 1.03              |
| 1:A:470:ARG:CB   | 1:A:489:TRP:NE1 | 2.21                     | 1.02              |
| 1:C:81:LEU:HD11  | 1:C:372:HIS:ND1 | 1.74                     | 1.02              |
| 1:B:470:ARG:CB   | 1:B:489:TRP:NE1 | 2.21                     | 1.02              |
| 1:B:490:HIS:O    | 1:B:496:ARG:HD2 | 1.59                     | 1.02              |
| 1:D:81:LEU:HD11  | 1:D:372:HIS:ND1 | 1.74                     | 1.02              |
| 1:C:312:HIS:CD2  | 1:C:368:LYS:CG  | 2.43                     | 1.02              |
| 1:B:470:ARG:HD2  | 1:B:489:TRP:CE2 | 1.94                     | 1.02              |
| 1:D:312:HIS:CD2  | 1:D:368:LYS:CG  | 2.43                     | 1.02              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:312:HIS:CD2  | 1:D:368:LYS:HE2  | 1.94                     | 1.02              |
| 1:A:470:ARG:HD2  | 1:A:489:TRP:CE2  | 1.94                     | 1.02              |
| 1:C:312:HIS:CD2  | 1:C:368:LYS:HE2  | 1.95                     | 1.02              |
| 1:D:470:ARG:HD2  | 1:D:489:TRP:CE2  | 1.94                     | 1.02              |
| 1:A:312:HIS:CD2  | 1:A:368:LYS:HE2  | 1.94                     | 1.01              |
| 1:C:470:ARG:HD2  | 1:C:489:TRP:CE2  | 1.94                     | 1.01              |
| 1:B:312:HIS:CD2  | 1:B:368:LYS:CG   | 2.43                     | 1.01              |
| 1:B:312:HIS:CD2  | 1:B:368:LYS:HE2  | 1.95                     | 1.01              |
| 1:A:81:LEU:HD11  | 1:A:372:HIS:ND1  | 1.74                     | 1.01              |
| 1:C:356:PHE:CE1  | 1:C:430:HIS:HB2  | 1.93                     | 1.01              |
| 1:B:81:LEU:HD11  | 1:B:372:HIS:ND1  | 1.74                     | 1.01              |
| 1:D:356:PHE:CE1  | 1:D:430:HIS:HB2  | 1.93                     | 1.01              |
| 1:D:490:HIS:O    | 1:D:496:ARG:HD2  | 1.59                     | 1.01              |
| 1:A:412:LEU:HD11 | 1:A:465:ILE:CG2  | 1.91                     | 1.01              |
| 1:C:470:ARG:CB   | 1:C:489:TRP:CZ2  | 2.44                     | 1.01              |
| 1:C:490:HIS:O    | 1:C:496:ARG:HD2  | 1.59                     | 1.01              |
| 1:B:412:LEU:HD11 | 1:B:465:ILE:CG2  | 1.91                     | 1.01              |
| 1:D:470:ARG:CB   | 1:D:489:TRP:CZ2  | 2.44                     | 1.01              |
| 1:C:367:LEU:HD23 | 1:C:379:ALA:CB   | 1.92                     | 1.00              |
| 1:D:367:LEU:HD23 | 1:D:379:ALA:CB   | 1.92                     | 1.00              |
| 1:D:412:LEU:HD11 | 1:D:465:ILE:CG2  | 1.91                     | 1.00              |
| 1:C:412:LEU:HD11 | 1:C:465:ILE:CG2  | 1.91                     | 1.00              |
| 1:A:370:ARG:HG3  | 1:A:376:TYR:C    | 1.87                     | 1.00              |
| 1:B:370:ARG:HG3  | 1:B:376:TYR:C    | 1.87                     | 1.00              |
| 1:D:370:ARG:HG3  | 1:D:376:TYR:C    | 1.87                     | 1.00              |
| 1:C:370:ARG:HG3  | 1:C:376:TYR:C    | 1.87                     | 1.00              |
| 1:A:311:MET:HG2  | 1:A:366:HIS:CD2  | 1.98                     | 0.99              |
| 1:B:121:VAL:HG11 | 1:B:564:ARG:HH12 | 1.27                     | 0.99              |
| 1:D:121:VAL:HG11 | 1:D:564:ARG:HH12 | 1.27                     | 0.99              |
| 1:A:121:VAL:HG11 | 1:A:564:ARG:HH12 | 1.27                     | 0.99              |
| 1:B:311:MET:HG2  | 1:B:366:HIS:CD2  | 1.98                     | 0.99              |
| 1:A:67:GLN:HG3   | 1:A:517:PRO:HB3  | 1.43                     | 0.99              |
| 1:C:312:HIS:CD2  | 1:C:368:LYS:CD   | 2.45                     | 0.99              |
| 1:D:312:HIS:CD2  | 1:D:368:LYS:CD   | 2.45                     | 0.99              |
| 1:A:470:ARG:CB   | 1:A:489:TRP:CZ2  | 2.44                     | 0.99              |
| 1:C:67:GLN:HG3   | 1:C:517:PRO:HB3  | 1.43                     | 0.99              |
| 1:D:67:GLN:HG3   | 1:D:517:PRO:HB3  | 1.43                     | 0.99              |
| 1:A:367:LEU:HD23 | 1:A:379:ALA:CB   | 1.92                     | 0.99              |
| 1:C:121:VAL:HG11 | 1:C:564:ARG:HH12 | 1.27                     | 0.99              |
| 1:B:67:GLN:HG3   | 1:B:517:PRO:HB3  | 1.43                     | 0.99              |
| 1:B:367:LEU:HD23 | 1:B:379:ALA:CB   | 1.92                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:470:ARG:CB   | 1:B:489:TRP:CZ2  | 2.44                     | 0.99              |
| 1:D:111:HIS:CE1  | 1:D:345:ARG:CD   | 2.46                     | 0.99              |
| 1:C:111:HIS:CE1  | 1:C:345:ARG:CD   | 2.46                     | 0.98              |
| 1:A:312:HIS:CD2  | 1:A:368:LYS:CG   | 2.43                     | 0.98              |
| 1:B:313:LYS:HD2  | 1:B:318:TYR:CE2  | 1.99                     | 0.98              |
| 1:A:312:HIS:CD2  | 1:A:368:LYS:CD   | 2.45                     | 0.98              |
| 1:A:313:LYS:HD2  | 1:A:318:TYR:CE2  | 1.99                     | 0.98              |
| 1:B:312:HIS:CD2  | 1:B:368:LYS:CD   | 2.45                     | 0.98              |
| 1:A:470:ARG:HD3  | 1:A:489:TRP:CD1  | 1.98                     | 0.98              |
| 1:B:470:ARG:HD3  | 1:B:489:TRP:CD1  | 1.98                     | 0.98              |
| 1:C:118:SER:OG   | 1:C:560:LEU:HD23 | 1.62                     | 0.98              |
| 1:C:311:MET:HG2  | 1:C:366:HIS:CD2  | 1.98                     | 0.98              |
| 1:B:111:HIS:CE1  | 1:B:345:ARG:CD   | 2.46                     | 0.98              |
| 1:B:470:ARG:HB3  | 1:B:489:TRP:HE1  | 1.28                     | 0.98              |
| 1:A:111:HIS:CE1  | 1:A:345:ARG:CD   | 2.46                     | 0.98              |
| 1:A:470:ARG:HB3  | 1:A:489:TRP:HE1  | 1.28                     | 0.98              |
| 1:D:311:MET:HG2  | 1:D:366:HIS:CD2  | 1.98                     | 0.98              |
| 1:B:412:LEU:HD11 | 1:B:465:ILE:HG22 | 1.46                     | 0.98              |
| 1:D:118:SER:OG   | 1:D:560:LEU:HD23 | 1.62                     | 0.98              |
| 1:A:412:LEU:HD11 | 1:A:465:ILE:HG22 | 1.46                     | 0.98              |
| 1:C:313:LYS:HD2  | 1:C:318:TYR:CE2  | 1.99                     | 0.97              |
| 1:B:367:LEU:CD2  | 1:B:379:ALA:HB2  | 1.94                     | 0.97              |
| 1:D:313:LYS:HD2  | 1:D:318:TYR:CE2  | 1.99                     | 0.97              |
| 1:D:470:ARG:HD3  | 1:D:489:TRP:CD1  | 1.98                     | 0.97              |
| 1:A:118:SER:OG   | 1:A:560:LEU:HD23 | 1.62                     | 0.97              |
| 1:A:367:LEU:CD2  | 1:A:379:ALA:HB2  | 1.94                     | 0.97              |
| 1:C:442:PHE:CE1  | 1:C:485:ILE:HB   | 2.00                     | 0.97              |
| 1:B:118:SER:OG   | 1:B:560:LEU:HD23 | 1.62                     | 0.97              |
| 1:C:470:ARG:HD3  | 1:C:489:TRP:CD1  | 1.98                     | 0.97              |
| 1:D:442:PHE:CE1  | 1:D:485:ILE:HB   | 2.00                     | 0.97              |
| 1:D:367:LEU:CD2  | 1:D:379:ALA:HB2  | 1.94                     | 0.97              |
| 1:D:118:SER:CB   | 1:D:560:LEU:HD21 | 1.95                     | 0.96              |
| 1:C:118:SER:CB   | 1:C:560:LEU:HD21 | 1.95                     | 0.96              |
| 1:C:367:LEU:CD2  | 1:C:379:ALA:HB2  | 1.94                     | 0.96              |
| 1:A:53:LEU:CD2   | 1:A:126:ALA:CB   | 2.44                     | 0.96              |
| 1:A:442:PHE:CE1  | 1:A:485:ILE:HB   | 2.00                     | 0.96              |
| 1:B:442:PHE:CE1  | 1:B:485:ILE:HB   | 2.00                     | 0.96              |
| 1:B:53:LEU:CD2   | 1:B:126:ALA:CB   | 2.44                     | 0.96              |
| 1:A:111:HIS:CE1  | 1:A:345:ARG:HD2  | 2.01                     | 0.96              |
| 1:B:111:HIS:CE1  | 1:B:345:ARG:HD2  | 2.01                     | 0.96              |
| 1:A:118:SER:CB   | 1:A:560:LEU:HD21 | 1.95                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:118:SER:CB   | 1:B:560:LEU:HD21 | 1.95                     | 0.95              |
| 1:C:370:ARG:HG2  | 1:C:377:PHE:HA   | 1.47                     | 0.95              |
| 1:C:53:LEU:CD2   | 1:C:126:ALA:CB   | 2.44                     | 0.95              |
| 1:D:53:LEU:CD2   | 1:D:126:ALA:CB   | 2.44                     | 0.95              |
| 1:D:370:ARG:HG2  | 1:D:377:PHE:HA   | 1.47                     | 0.95              |
| 1:D:484:LEU:HD21 | 1:D:502:ILE:HD11 | 1.48                     | 0.95              |
| 1:C:484:LEU:HD21 | 1:C:502:ILE:HD11 | 1.48                     | 0.94              |
| 1:A:407:TYR:O    | 1:A:435:TYR:HE2  | 1.50                     | 0.94              |
| 1:C:412:LEU:HD11 | 1:C:465:ILE:HG22 | 1.46                     | 0.94              |
| 1:B:407:TYR:O    | 1:B:435:TYR:HE2  | 1.50                     | 0.94              |
| 1:B:484:LEU:HD21 | 1:B:502:ILE:HD11 | 1.48                     | 0.94              |
| 1:A:370:ARG:HG2  | 1:A:377:PHE:HA   | 1.47                     | 0.94              |
| 1:B:332:SER:OG   | 1:B:334:PRO:CG   | 2.16                     | 0.94              |
| 1:D:412:LEU:HD11 | 1:D:465:ILE:HG22 | 1.46                     | 0.94              |
| 1:A:332:SER:OG   | 1:A:334:PRO:CG   | 2.16                     | 0.94              |
| 1:A:484:LEU:HD21 | 1:A:502:ILE:HD11 | 1.48                     | 0.94              |
| 1:A:313:LYS:HD2  | 1:A:318:TYR:HE2  | 1.32                     | 0.94              |
| 1:B:313:LYS:HD2  | 1:B:318:TYR:HE2  | 1.32                     | 0.94              |
| 1:B:370:ARG:HG2  | 1:B:377:PHE:HA   | 1.47                     | 0.94              |
| 1:D:111:HIS:CE1  | 1:D:345:ARG:HD2  | 2.01                     | 0.94              |
| 1:C:111:HIS:CE1  | 1:C:345:ARG:HD2  | 2.01                     | 0.94              |
| 1:D:470:ARG:HB3  | 1:D:489:TRP:HE1  | 1.28                     | 0.94              |
| 1:C:290:LEU:HD22 | 1:C:311:MET:CG   | 1.99                     | 0.94              |
| 1:D:290:LEU:HD22 | 1:D:311:MET:CG   | 1.99                     | 0.94              |
| 1:D:407:TYR:O    | 1:D:435:TYR:HE2  | 1.50                     | 0.94              |
| 1:A:290:LEU:HD22 | 1:A:311:MET:CG   | 1.98                     | 0.93              |
| 1:A:360:LEU:O    | 1:A:361:ASN:OD1  | 1.86                     | 0.93              |
| 1:B:360:LEU:O    | 1:B:361:ASN:OD1  | 1.86                     | 0.93              |
| 1:C:407:TYR:O    | 1:C:435:TYR:HE2  | 1.50                     | 0.93              |
| 1:B:290:LEU:HD22 | 1:B:311:MET:CG   | 1.99                     | 0.93              |
| 1:D:290:LEU:CD2  | 1:D:382:CYS:SG   | 2.56                     | 0.93              |
| 1:C:290:LEU:CD2  | 1:C:382:CYS:SG   | 2.56                     | 0.93              |
| 1:C:470:ARG:HB3  | 1:C:489:TRP:HE1  | 1.28                     | 0.93              |
| 1:A:385:GLY:O    | 1:A:386:LEU:HB2  | 1.69                     | 0.93              |
| 1:D:332:SER:OG   | 1:D:334:PRO:CG   | 2.16                     | 0.93              |
| 1:B:385:GLY:O    | 1:B:386:LEU:HB2  | 1.69                     | 0.93              |
| 1:C:332:SER:OG   | 1:C:334:PRO:CG   | 2.16                     | 0.92              |
| 1:D:312:HIS:CD2  | 1:D:368:LYS:CE   | 2.52                     | 0.92              |
| 1:C:312:HIS:CD2  | 1:C:368:LYS:CE   | 2.52                     | 0.92              |
| 1:A:280:SER:O    | 1:A:282:LEU:N    | 2.02                     | 0.92              |
| 1:B:280:SER:O    | 1:B:282:LEU:N    | 2.02                     | 0.92              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:312:HIS:CD2 | 1:A:368:LYS:CE  | 2.52                     | 0.92              |
| 1:C:360:LEU:O   | 1:C:361:ASN:OD1 | 1.86                     | 0.92              |
| 1:B:312:HIS:CD2 | 1:B:368:LYS:CE  | 2.52                     | 0.92              |
| 1:A:290:LEU:CD2 | 1:A:382:CYS:SG  | 2.56                     | 0.92              |
| 1:B:290:LEU:CD2 | 1:B:382:CYS:SG  | 2.57                     | 0.92              |
| 1:D:360:LEU:O   | 1:D:361:ASN:OD1 | 1.86                     | 0.92              |
| 1:D:488:CYS:O   | 1:D:496:ARG:HG2 | 1.70                     | 0.92              |
| 1:A:199:ASP:CB  | 1:A:208:LYS:HD3 | 2.00                     | 0.92              |
| 1:A:311:MET:HB3 | 1:A:366:HIS:CB  | 2.00                     | 0.92              |
| 1:C:488:CYS:O   | 1:C:496:ARG:HG2 | 1.70                     | 0.92              |
| 1:B:199:ASP:CB  | 1:B:208:LYS:HD3 | 2.00                     | 0.92              |
| 1:B:311:MET:HB3 | 1:B:366:HIS:CB  | 2.00                     | 0.92              |
| 1:D:280:SER:O   | 1:D:282:LEU:N   | 2.02                     | 0.92              |
| 1:C:280:SER:O   | 1:C:282:LEU:N   | 2.02                     | 0.91              |
| 1:A:488:CYS:O   | 1:A:496:ARG:HG2 | 1.70                     | 0.91              |
| 1:C:370:ARG:HB2 | 1:C:376:TYR:O   | 1.70                     | 0.91              |
| 1:B:370:ARG:HB2 | 1:B:376:TYR:O   | 1.70                     | 0.91              |
| 1:B:488:CYS:O   | 1:B:496:ARG:HG2 | 1.70                     | 0.91              |
| 1:D:370:ARG:HB2 | 1:D:376:TYR:O   | 1.71                     | 0.91              |
| 1:D:385:GLY:O   | 1:D:386:LEU:HB2 | 1.69                     | 0.91              |
| 1:A:370:ARG:HB2 | 1:A:376:TYR:O   | 1.70                     | 0.91              |
| 1:C:385:GLY:O   | 1:C:386:LEU:HB2 | 1.69                     | 0.91              |
| 1:C:311:MET:HB3 | 1:C:366:HIS:CB  | 2.00                     | 0.91              |
| 1:C:318:TYR:O   | 1:C:322:ASN:CG  | 2.14                     | 0.91              |
| 1:D:311:MET:HB3 | 1:D:366:HIS:CB  | 2.00                     | 0.91              |
| 1:D:318:TYR:O   | 1:D:322:ASN:CG  | 2.14                     | 0.91              |
| 1:D:412:LEU:O   | 1:D:415:MET:SD  | 2.29                     | 0.91              |
| 1:C:313:LYS:HD2 | 1:C:318:TYR:HE2 | 1.32                     | 0.91              |
| 1:C:412:LEU:O   | 1:C:415:MET:SD  | 2.29                     | 0.91              |
| 1:D:199:ASP:CB  | 1:D:208:LYS:HD3 | 2.00                     | 0.91              |
| 1:C:199:ASP:CB  | 1:C:208:LYS:HD3 | 2.00                     | 0.91              |
| 1:A:318:TYR:O   | 1:A:322:ASN:CG  | 2.14                     | 0.90              |
| 1:A:412:LEU:O   | 1:A:415:MET:SD  | 2.29                     | 0.90              |
| 1:B:412:LEU:O   | 1:B:415:MET:SD  | 2.29                     | 0.90              |
| 1:D:313:LYS:HD2 | 1:D:318:TYR:HE2 | 1.32                     | 0.90              |
| 1:A:290:LEU:CD2 | 1:A:311:MET:HG3 | 2.02                     | 0.90              |
| 1:A:370:ARG:CG  | 1:A:376:TYR:O   | 2.20                     | 0.90              |
| 1:B:290:LEU:CD2 | 1:B:311:MET:HG3 | 2.02                     | 0.90              |
| 1:B:318:TYR:O   | 1:B:322:ASN:CG  | 2.14                     | 0.90              |
| 1:B:370:ARG:CG  | 1:B:376:TYR:O   | 2.20                     | 0.90              |
| 1:B:475:PHE:CD2 | 1:B:476:PRO:HD3 | 2.06                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:370:ARG:CG   | 1:C:376:TYR:O    | 2.20                     | 0.90              |
| 1:D:370:ARG:CG   | 1:D:376:TYR:O    | 2.20                     | 0.90              |
| 1:A:475:PHE:CD2  | 1:A:476:PRO:HD3  | 2.07                     | 0.90              |
| 1:A:442:PHE:CZ   | 1:A:489:TRP:CE3  | 2.60                     | 0.90              |
| 1:B:442:PHE:CZ   | 1:B:489:TRP:CE3  | 2.60                     | 0.90              |
| 1:C:442:PHE:CZ   | 1:C:489:TRP:CE3  | 2.60                     | 0.89              |
| 1:D:370:ARG:CG   | 1:D:376:TYR:C    | 2.45                     | 0.89              |
| 1:D:442:PHE:CZ   | 1:D:489:TRP:CE3  | 2.60                     | 0.89              |
| 1:C:370:ARG:CG   | 1:C:376:TYR:C    | 2.45                     | 0.89              |
| 1:B:370:ARG:CG   | 1:B:376:TYR:C    | 2.45                     | 0.89              |
| 1:C:407:TYR:O    | 1:C:435:TYR:CE2  | 2.26                     | 0.89              |
| 1:A:370:ARG:CG   | 1:A:376:TYR:C    | 2.45                     | 0.89              |
| 1:B:311:MET:H    | 1:B:311:MET:HE2  | 1.37                     | 0.89              |
| 1:D:407:TYR:O    | 1:D:435:TYR:CE2  | 2.26                     | 0.89              |
| 1:A:311:MET:HE2  | 1:A:311:MET:H    | 1.37                     | 0.88              |
| 1:C:475:PHE:CD2  | 1:C:476:PRO:HD3  | 2.06                     | 0.88              |
| 1:C:290:LEU:HB3  | 1:C:382:CYS:SG   | 2.14                     | 0.88              |
| 1:B:290:LEU:HB3  | 1:B:382:CYS:SG   | 2.14                     | 0.88              |
| 1:D:290:LEU:CD2  | 1:D:311:MET:HG3  | 2.02                     | 0.88              |
| 1:A:290:LEU:HB3  | 1:A:382:CYS:SG   | 2.14                     | 0.88              |
| 1:D:290:LEU:HB3  | 1:D:382:CYS:SG   | 2.14                     | 0.88              |
| 1:C:290:LEU:CD1  | 1:C:309:GLU:C    | 2.47                     | 0.88              |
| 1:D:118:SER:HB3  | 1:D:560:LEU:CD2  | 2.03                     | 0.88              |
| 1:D:290:LEU:CD1  | 1:D:309:GLU:C    | 2.47                     | 0.88              |
| 1:D:475:PHE:CD2  | 1:D:476:PRO:HD3  | 2.07                     | 0.88              |
| 1:C:290:LEU:CD2  | 1:C:311:MET:HG3  | 2.02                     | 0.88              |
| 1:D:311:MET:HE2  | 1:D:311:MET:H    | 1.37                     | 0.88              |
| 1:C:118:SER:HB3  | 1:C:560:LEU:CD2  | 2.03                     | 0.88              |
| 1:C:311:MET:H    | 1:C:311:MET:HE2  | 1.37                     | 0.88              |
| 1:D:508:TYR:OH   | 1:D:528:LEU:HD12 | 1.74                     | 0.87              |
| 1:A:370:ARG:CB   | 1:A:376:TYR:O    | 2.23                     | 0.87              |
| 1:C:508:TYR:OH   | 1:C:528:LEU:HD12 | 1.74                     | 0.87              |
| 1:B:407:TYR:O    | 1:B:435:TYR:CE2  | 2.26                     | 0.87              |
| 1:A:407:TYR:O    | 1:A:435:TYR:CE2  | 2.26                     | 0.87              |
| 1:B:336:VAL:HG12 | 1:B:340:MET:HE2  | 1.56                     | 0.87              |
| 1:B:370:ARG:CB   | 1:B:376:TYR:O    | 2.23                     | 0.87              |
| 1:A:336:VAL:HG12 | 1:A:340:MET:HE2  | 1.56                     | 0.87              |
| 1:B:118:SER:HB3  | 1:B:560:LEU:CD2  | 2.03                     | 0.87              |
| 1:B:508:TYR:OH   | 1:B:528:LEU:HD12 | 1.74                     | 0.87              |
| 1:A:118:SER:HB3  | 1:A:560:LEU:CD2  | 2.03                     | 0.87              |
| 1:B:332:SER:CB   | 1:B:334:PRO:HD2  | 2.05                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:332:SER:CB   | 1:A:334:PRO:HD2  | 2.05                     | 0.87              |
| 1:A:479:LYS:NZ   | 1:A:479:LYS:HB3  | 1.90                     | 0.87              |
| 1:A:508:TYR:OH   | 1:A:528:LEU:HD12 | 1.74                     | 0.87              |
| 1:C:374:GLU:N    | 1:C:374:GLU:OE2  | 2.08                     | 0.87              |
| 1:D:374:GLU:N    | 1:D:374:GLU:OE2  | 2.08                     | 0.87              |
| 1:D:470:ARG:HD2  | 1:D:489:TRP:CG   | 2.09                     | 0.87              |
| 1:B:479:LYS:NZ   | 1:B:479:LYS:HB3  | 1.90                     | 0.86              |
| 1:C:284:LEU:CD2  | 1:C:353:ASN:ND2  | 2.37                     | 0.86              |
| 1:C:321:GLU:OE1  | 1:C:321:GLU:N    | 2.08                     | 0.86              |
| 1:C:370:ARG:CB   | 1:C:376:TYR:O    | 2.23                     | 0.86              |
| 1:B:470:ARG:HD2  | 1:B:489:TRP:CG   | 2.09                     | 0.86              |
| 1:D:284:LEU:CD2  | 1:D:353:ASN:ND2  | 2.37                     | 0.86              |
| 1:A:284:LEU:CD2  | 1:A:353:ASN:ND2  | 2.37                     | 0.86              |
| 1:C:470:ARG:HD2  | 1:C:489:TRP:CG   | 2.09                     | 0.86              |
| 1:B:284:LEU:CD2  | 1:B:353:ASN:ND2  | 2.37                     | 0.86              |
| 1:A:470:ARG:HD2  | 1:A:489:TRP:CG   | 2.09                     | 0.86              |
| 1:C:479:LYS:NZ   | 1:C:479:LYS:HB3  | 1.90                     | 0.86              |
| 1:D:321:GLU:OE1  | 1:D:321:GLU:N    | 2.08                     | 0.86              |
| 1:D:370:ARG:CB   | 1:D:376:TYR:O    | 2.23                     | 0.86              |
| 1:C:446:THR:HG21 | 1:C:473:PHE:HD2  | 1.40                     | 0.86              |
| 1:B:290:LEU:CD1  | 1:B:309:GLU:C    | 2.47                     | 0.86              |
| 1:D:446:THR:HG21 | 1:D:473:PHE:HD2  | 1.40                     | 0.86              |
| 1:A:290:LEU:CD1  | 1:A:309:GLU:C    | 2.47                     | 0.86              |
| 1:A:321:GLU:OE1  | 1:A:321:GLU:N    | 2.08                     | 0.86              |
| 1:B:446:THR:HG21 | 1:B:473:PHE:HD2  | 1.40                     | 0.86              |
| 1:D:479:LYS:NZ   | 1:D:479:LYS:HB3  | 1.90                     | 0.86              |
| 1:B:321:GLU:OE1  | 1:B:321:GLU:N    | 2.08                     | 0.86              |
| 1:A:446:THR:HG21 | 1:A:473:PHE:HD2  | 1.40                     | 0.86              |
| 1:D:332:SER:CB   | 1:D:334:PRO:HD2  | 2.05                     | 0.86              |
| 1:C:332:SER:CB   | 1:C:334:PRO:HD2  | 2.05                     | 0.86              |
| 1:A:199:ASP:HB2  | 1:A:208:LYS:HD3  | 1.58                     | 0.85              |
| 1:B:199:ASP:HB2  | 1:B:208:LYS:HD3  | 1.58                     | 0.85              |
| 1:C:312:HIS:HD2  | 1:C:368:LYS:CD   | 1.83                     | 0.85              |
| 1:C:415:MET:SD   | 1:C:415:MET:N    | 2.48                     | 0.85              |
| 1:A:374:GLU:N    | 1:A:374:GLU:OE2  | 2.08                     | 0.85              |
| 1:B:374:GLU:N    | 1:B:374:GLU:OE2  | 2.08                     | 0.85              |
| 1:D:415:MET:SD   | 1:D:415:MET:N    | 2.48                     | 0.85              |
| 1:D:312:HIS:HD2  | 1:D:368:LYS:CD   | 1.83                     | 0.85              |
| 1:B:515:VAL:C    | 1:B:516:ASN:HD22 | 1.84                     | 0.85              |
| 1:A:515:VAL:C    | 1:A:516:ASN:HD22 | 1.84                     | 0.85              |
| 1:C:470:ARG:HB2  | 1:C:489:TRP:HZ2  | 1.38                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:515:VAL:C    | 1:C:516:ASN:HD22 | 1.84                     | 0.85              |
| 1:D:515:VAL:C    | 1:D:516:ASN:HD22 | 1.84                     | 0.85              |
| 1:A:118:SER:HB2  | 1:A:560:LEU:HD21 | 1.57                     | 0.84              |
| 1:D:431:LYS:O    | 1:D:434:VAL:CG1  | 2.25                     | 0.84              |
| 1:C:431:LYS:O    | 1:C:434:VAL:CG1  | 2.25                     | 0.84              |
| 1:B:310:LEU:HD22 | 1:B:311:MET:H    | 1.41                     | 0.84              |
| 1:D:470:ARG:HB2  | 1:D:489:TRP:HZ2  | 1.38                     | 0.84              |
| 1:C:336:VAL:HG12 | 1:C:340:MET:HE2  | 1.56                     | 0.84              |
| 1:B:118:SER:HB2  | 1:B:560:LEU:HD21 | 1.57                     | 0.84              |
| 1:A:310:LEU:HD22 | 1:A:311:MET:H    | 1.41                     | 0.84              |
| 1:A:488:CYS:O    | 1:A:496:ARG:CG   | 2.26                     | 0.84              |
| 1:B:284:LEU:HD22 | 1:B:353:ASN:ND2  | 1.91                     | 0.84              |
| 1:B:470:ARG:CD   | 1:B:489:TRP:CE2  | 2.60                     | 0.84              |
| 1:D:118:SER:HB2  | 1:D:560:LEU:HD23 | 1.35                     | 0.84              |
| 1:A:431:LYS:O    | 1:A:434:VAL:CG1  | 2.25                     | 0.84              |
| 1:A:470:ARG:CD   | 1:A:489:TRP:CE2  | 2.60                     | 0.84              |
| 1:B:488:CYS:O    | 1:B:496:ARG:CG   | 2.26                     | 0.84              |
| 1:D:336:VAL:HG12 | 1:D:340:MET:HE2  | 1.56                     | 0.84              |
| 1:A:284:LEU:HD22 | 1:A:353:ASN:ND2  | 1.92                     | 0.84              |
| 1:B:431:LYS:O    | 1:B:434:VAL:CG1  | 2.25                     | 0.84              |
| 1:D:488:CYS:O    | 1:D:496:ARG:CG   | 2.26                     | 0.84              |
| 1:C:284:LEU:HD22 | 1:C:353:ASN:ND2  | 1.92                     | 0.84              |
| 1:C:442:PHE:CD1  | 1:C:473:PHE:HZ   | 1.96                     | 0.84              |
| 1:D:284:LEU:HD22 | 1:D:353:ASN:ND2  | 1.92                     | 0.84              |
| 1:D:442:PHE:CD1  | 1:D:473:PHE:HZ   | 1.96                     | 0.84              |
| 1:D:470:ARG:CD   | 1:D:489:TRP:CE2  | 2.60                     | 0.84              |
| 1:C:470:ARG:CD   | 1:C:489:TRP:CE2  | 2.60                     | 0.83              |
| 1:C:488:CYS:O    | 1:C:496:ARG:CG   | 2.26                     | 0.83              |
| 1:C:118:SER:HB2  | 1:C:560:LEU:HD23 | 1.36                     | 0.83              |
| 1:C:332:SER:OG   | 1:C:334:PRO:CD   | 2.27                     | 0.83              |
| 1:A:332:SER:OG   | 1:A:334:PRO:CD   | 2.27                     | 0.83              |
| 1:B:332:SER:OG   | 1:B:334:PRO:CD   | 2.27                     | 0.83              |
| 1:D:332:SER:OG   | 1:D:334:PRO:CD   | 2.27                     | 0.83              |
| 1:D:470:ARG:CD   | 1:D:489:TRP:CD1  | 2.61                     | 0.83              |
| 1:C:470:ARG:CD   | 1:C:489:TRP:CD1  | 2.61                     | 0.83              |
| 1:C:199:ASP:HB2  | 1:C:208:LYS:HD3  | 1.58                     | 0.83              |
| 1:D:199:ASP:HB2  | 1:D:208:LYS:HD3  | 1.58                     | 0.83              |
| 1:B:370:ARG:HG2  | 1:B:377:PHE:CA   | 2.09                     | 0.83              |
| 1:B:415:MET:SD   | 1:B:415:MET:N    | 2.48                     | 0.83              |
| 1:A:312:HIS:HD2  | 1:A:368:LYS:CD   | 1.83                     | 0.82              |
| 1:A:370:ARG:HG2  | 1:A:377:PHE:CA   | 2.09                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:415:MET:SD   | 1:A:415:MET:N    | 2.48                     | 0.82              |
| 1:B:442:PHE:CD1  | 1:B:473:PHE:HZ   | 1.96                     | 0.82              |
| 1:A:470:ARG:CD   | 1:A:489:TRP:CD1  | 2.61                     | 0.82              |
| 1:B:312:HIS:HD2  | 1:B:368:LYS:CD   | 1.83                     | 0.82              |
| 1:A:442:PHE:CD1  | 1:A:473:PHE:HZ   | 1.96                     | 0.82              |
| 1:B:470:ARG:CD   | 1:B:489:TRP:CD1  | 2.61                     | 0.82              |
| 1:B:111:HIS:CE1  | 1:B:345:ARG:HD3  | 2.14                     | 0.82              |
| 1:A:111:HIS:CE1  | 1:A:345:ARG:HD3  | 2.14                     | 0.82              |
| 1:D:370:ARG:HG2  | 1:D:377:PHE:CA   | 2.09                     | 0.82              |
| 1:C:111:HIS:CE1  | 1:C:345:ARG:HD3  | 2.14                     | 0.82              |
| 1:D:111:HIS:CE1  | 1:D:345:ARG:HD3  | 2.14                     | 0.82              |
| 1:D:311:MET:CG   | 1:D:366:HIS:CD2  | 2.63                     | 0.82              |
| 1:C:311:MET:CG   | 1:C:366:HIS:CD2  | 2.63                     | 0.82              |
| 1:C:370:ARG:HG2  | 1:C:377:PHE:CA   | 2.09                     | 0.81              |
| 1:D:310:LEU:HD22 | 1:D:311:MET:H    | 1.41                     | 0.81              |
| 1:C:470:ARG:CD   | 1:C:489:TRP:CD2  | 2.62                     | 0.81              |
| 1:A:311:MET:CG   | 1:A:366:HIS:CD2  | 2.63                     | 0.81              |
| 1:C:118:SER:HB3  | 1:C:560:LEU:HD21 | 1.61                     | 0.81              |
| 1:D:470:ARG:CD   | 1:D:489:TRP:CD2  | 2.62                     | 0.81              |
| 1:C:310:LEU:HD22 | 1:C:311:MET:H    | 1.41                     | 0.81              |
| 1:A:446:THR:CG2  | 1:A:473:PHE:HD2  | 1.94                     | 0.81              |
| 1:B:311:MET:CG   | 1:B:366:HIS:CD2  | 2.63                     | 0.81              |
| 1:B:446:THR:CG2  | 1:B:473:PHE:HD2  | 1.94                     | 0.81              |
| 1:B:538:PHE:O    | 1:B:543:PRO:CD   | 2.26                     | 0.81              |
| 1:D:118:SER:HB3  | 1:D:560:LEU:HD21 | 1.61                     | 0.81              |
| 1:A:538:PHE:O    | 1:A:543:PRO:CD   | 2.26                     | 0.80              |
| 1:C:471:PRO:HG2  | 1:C:489:TRP:HH2  | 1.45                     | 0.80              |
| 1:A:471:PRO:HG2  | 1:A:489:TRP:HH2  | 1.45                     | 0.80              |
| 1:C:557:PRO:O    | 1:C:561:THR:HG23 | 1.81                     | 0.80              |
| 1:B:471:PRO:HG2  | 1:B:489:TRP:HH2  | 1.45                     | 0.80              |
| 1:A:159:PHE:CZ   | 1:A:561:THR:HG21 | 2.16                     | 0.80              |
| 1:D:470:ARG:CD   | 1:D:489:TRP:CG   | 2.64                     | 0.80              |
| 1:D:471:PRO:HG2  | 1:D:489:TRP:HH2  | 1.45                     | 0.80              |
| 1:D:557:PRO:O    | 1:D:561:THR:HG23 | 1.81                     | 0.80              |
| 1:C:470:ARG:CD   | 1:C:489:TRP:CG   | 2.65                     | 0.80              |
| 1:B:159:PHE:CZ   | 1:B:561:THR:HG21 | 2.16                     | 0.80              |
| 1:C:472:LEU:HD12 | 1:C:472:LEU:O    | 1.82                     | 0.80              |
| 1:D:116:TYR:CE1  | 1:D:514:VAL:HG21 | 2.17                     | 0.80              |
| 1:D:446:THR:CG2  | 1:D:473:PHE:HD2  | 1.94                     | 0.80              |
| 1:D:472:LEU:HD12 | 1:D:472:LEU:O    | 1.82                     | 0.80              |
| 1:C:116:TYR:CE1  | 1:C:514:VAL:HG21 | 2.17                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:446:THR:CG2  | 1:C:473:PHE:HD2  | 1.94                     | 0.80              |
| 1:D:538:PHE:O    | 1:D:543:PRO:CD   | 2.26                     | 0.80              |
| 1:C:311:MET:HG2  | 1:C:366:HIS:CG   | 2.17                     | 0.79              |
| 1:C:538:PHE:O    | 1:C:543:PRO:CD   | 2.26                     | 0.79              |
| 1:B:557:PRO:O    | 1:B:561:THR:HG23 | 1.81                     | 0.79              |
| 1:A:470:ARG:HB2  | 1:A:489:TRP:HZ2  | 1.38                     | 0.79              |
| 1:A:557:PRO:O    | 1:A:561:THR:HG23 | 1.81                     | 0.79              |
| 1:D:311:MET:HG2  | 1:D:366:HIS:CG   | 2.17                     | 0.79              |
| 1:D:505:ILE:HD11 | 1:D:531:CYS:HB3  | 1.64                     | 0.79              |
| 1:A:116:TYR:CE1  | 1:A:514:VAL:HG21 | 2.17                     | 0.79              |
| 1:A:470:ARG:CD   | 1:A:489:TRP:CG   | 2.64                     | 0.79              |
| 1:B:311:MET:HG2  | 1:B:366:HIS:CG   | 2.17                     | 0.79              |
| 1:A:570:LYS:NZ   | 1:A:570:LYS:HB2  | 1.98                     | 0.79              |
| 1:C:159:PHE:CZ   | 1:C:561:THR:HG21 | 2.16                     | 0.79              |
| 1:C:505:ILE:HD11 | 1:C:531:CYS:HB3  | 1.64                     | 0.79              |
| 1:B:116:TYR:CE1  | 1:B:514:VAL:HG21 | 2.17                     | 0.79              |
| 1:B:470:ARG:HB2  | 1:B:489:TRP:HZ2  | 1.38                     | 0.79              |
| 1:B:470:ARG:CD   | 1:B:489:TRP:CG   | 2.65                     | 0.79              |
| 1:B:570:LYS:HB2  | 1:B:570:LYS:NZ   | 1.98                     | 0.79              |
| 1:D:159:PHE:CZ   | 1:D:561:THR:HG21 | 2.16                     | 0.79              |
| 1:A:311:MET:HG2  | 1:A:366:HIS:CG   | 2.17                     | 0.79              |
| 1:A:118:SER:HB3  | 1:A:560:LEU:HD21 | 1.61                     | 0.79              |
| 1:D:336:VAL:HG12 | 1:D:340:MET:CE   | 2.13                     | 0.79              |
| 1:C:336:VAL:HG12 | 1:C:340:MET:CE   | 2.13                     | 0.79              |
| 1:B:118:SER:HB3  | 1:B:560:LEU:HD21 | 1.61                     | 0.79              |
| 1:C:208:LYS:HB2  | 1:C:208:LYS:NZ   | 1.98                     | 0.79              |
| 1:B:505:ILE:HD11 | 1:B:531:CYS:CB   | 2.13                     | 0.79              |
| 1:A:505:ILE:HD11 | 1:A:531:CYS:CB   | 2.13                     | 0.78              |
| 1:D:208:LYS:HB2  | 1:D:208:LYS:NZ   | 1.98                     | 0.78              |
| 1:A:385:GLY:O    | 1:A:386:LEU:CB   | 2.31                     | 0.78              |
| 1:B:385:GLY:O    | 1:B:386:LEU:CB   | 2.31                     | 0.78              |
| 1:C:81:LEU:CD1   | 1:C:372:HIS:ND1  | 2.46                     | 0.78              |
| 1:A:472:LEU:HD12 | 1:A:472:LEU:O    | 1.82                     | 0.78              |
| 1:C:408:ALA:HB3  | 1:C:411:VAL:HG22 | 1.66                     | 0.78              |
| 1:B:81:LEU:CD1   | 1:B:372:HIS:ND1  | 2.46                     | 0.78              |
| 1:B:472:LEU:HD12 | 1:B:472:LEU:O    | 1.82                     | 0.78              |
| 1:D:81:LEU:CD1   | 1:D:372:HIS:ND1  | 2.46                     | 0.78              |
| 1:A:81:LEU:CD1   | 1:A:372:HIS:ND1  | 2.46                     | 0.78              |
| 1:D:408:ALA:HB3  | 1:D:411:VAL:HG22 | 1.66                     | 0.78              |
| 1:A:336:VAL:HG12 | 1:A:340:MET:CE   | 2.13                     | 0.78              |
| 1:B:336:VAL:HG12 | 1:B:340:MET:CE   | 2.13                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:470:ARG:CD   | 1:A:489:TRP:CD2  | 2.62                     | 0.78              |
| 1:C:414:GLU:OE1  | 1:C:414:GLU:N    | 2.16                     | 0.78              |
| 1:D:414:GLU:OE1  | 1:D:414:GLU:N    | 2.16                     | 0.78              |
| 1:A:505:ILE:HD11 | 1:A:531:CYS:HB3  | 1.64                     | 0.77              |
| 1:C:74:ARG:CZ    | 1:C:376:TYR:CE1  | 2.67                     | 0.77              |
| 1:C:385:GLY:O    | 1:C:386:LEU:CB   | 2.31                     | 0.77              |
| 1:D:74:ARG:CZ    | 1:D:376:TYR:CE1  | 2.67                     | 0.77              |
| 1:A:408:ALA:HB3  | 1:A:411:VAL:HG22 | 1.66                     | 0.77              |
| 1:B:408:ALA:HB3  | 1:B:411:VAL:HG22 | 1.66                     | 0.77              |
| 1:B:505:ILE:HD11 | 1:B:531:CYS:HB3  | 1.64                     | 0.77              |
| 1:D:385:GLY:O    | 1:D:386:LEU:CB   | 2.31                     | 0.77              |
| 1:A:356:PHE:CE1  | 1:A:430:HIS:HB3  | 2.18                     | 0.77              |
| 1:C:505:ILE:HD11 | 1:C:531:CYS:CB   | 2.13                     | 0.77              |
| 1:B:537:ARG:HB2  | 1:B:566:LEU:HD13 | 1.67                     | 0.77              |
| 1:A:537:ARG:HB2  | 1:A:566:LEU:HD13 | 1.67                     | 0.77              |
| 1:B:356:PHE:CE1  | 1:B:430:HIS:HB3  | 2.18                     | 0.77              |
| 1:D:505:ILE:HD11 | 1:D:531:CYS:CB   | 2.13                     | 0.77              |
| 1:A:74:ARG:CZ    | 1:A:376:TYR:CE1  | 2.67                     | 0.77              |
| 1:A:414:GLU:N    | 1:A:414:GLU:OE1  | 2.16                     | 0.77              |
| 1:A:555:GLN:O    | 1:A:559:GLN:HG3  | 1.84                     | 0.77              |
| 1:B:74:ARG:CZ    | 1:B:376:TYR:CE1  | 2.67                     | 0.77              |
| 1:B:470:ARG:CD   | 1:B:489:TRP:CD2  | 2.62                     | 0.77              |
| 1:D:311:MET:SD   | 1:D:366:HIS:CD2  | 2.77                     | 0.77              |
| 1:C:555:GLN:O    | 1:C:559:GLN:HG3  | 1.84                     | 0.77              |
| 1:C:570:LYS:HB2  | 1:C:570:LYS:NZ   | 1.98                     | 0.77              |
| 1:C:311:MET:SD   | 1:C:366:HIS:CD2  | 2.77                     | 0.77              |
| 1:B:555:GLN:O    | 1:B:559:GLN:HG3  | 1.84                     | 0.77              |
| 1:D:356:PHE:CE1  | 1:D:430:HIS:HB3  | 2.18                     | 0.77              |
| 1:C:406:TRP:CZ3  | 1:C:439:MET:HB3  | 2.20                     | 0.77              |
| 1:B:414:GLU:OE1  | 1:B:414:GLU:N    | 2.16                     | 0.77              |
| 1:B:53:LEU:HD21  | 1:B:126:ALA:CB   | 2.14                     | 0.77              |
| 1:B:208:LYS:NZ   | 1:B:208:LYS:HB2  | 1.98                     | 0.77              |
| 1:B:406:TRP:CZ3  | 1:B:439:MET:HB3  | 2.20                     | 0.77              |
| 1:D:313:LYS:CD   | 1:D:318:TYR:HE2  | 1.98                     | 0.77              |
| 1:D:406:TRP:CZ3  | 1:D:439:MET:HB3  | 2.20                     | 0.77              |
| 1:D:555:GLN:O    | 1:D:559:GLN:HG3  | 1.84                     | 0.77              |
| 1:D:570:LYS:HB2  | 1:D:570:LYS:NZ   | 1.98                     | 0.77              |
| 1:A:53:LEU:HD21  | 1:A:126:ALA:CB   | 2.14                     | 0.76              |
| 1:A:208:LYS:HB2  | 1:A:208:LYS:NZ   | 1.98                     | 0.76              |
| 1:C:313:LYS:CD   | 1:C:318:TYR:HE2  | 1.98                     | 0.76              |
| 1:C:412:LEU:CD1  | 1:C:465:ILE:HG22 | 2.15                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:33:LEU:HD21  | 1:B:177:PHE:HD1  | 1.50                     | 0.76              |
| 1:D:412:LEU:CD1  | 1:D:465:ILE:HG22 | 2.15                     | 0.76              |
| 1:A:33:LEU:HD21  | 1:A:177:PHE:HD1  | 1.50                     | 0.76              |
| 1:A:406:TRP:CZ3  | 1:A:439:MET:HB3  | 2.20                     | 0.76              |
| 1:C:356:PHE:CE1  | 1:C:430:HIS:HB3  | 2.18                     | 0.76              |
| 1:C:280:SER:O    | 1:C:281:LEU:C    | 2.28                     | 0.76              |
| 1:C:537:ARG:HB2  | 1:C:566:LEU:HD13 | 1.67                     | 0.76              |
| 1:B:311:MET:SD   | 1:B:366:HIS:CD2  | 2.78                     | 0.76              |
| 1:D:537:ARG:HB2  | 1:D:566:LEU:HD13 | 1.67                     | 0.76              |
| 1:A:311:MET:SD   | 1:A:366:HIS:CD2  | 2.77                     | 0.76              |
| 1:C:53:LEU:HD21  | 1:C:126:ALA:CB   | 2.14                     | 0.76              |
| 1:D:53:LEU:HD21  | 1:D:126:ALA:CB   | 2.14                     | 0.76              |
| 1:D:280:SER:O    | 1:D:281:LEU:C    | 2.28                     | 0.76              |
| 1:B:311:MET:CG   | 1:B:366:HIS:CG   | 2.68                     | 0.76              |
| 1:C:214:LEU:O    | 1:C:218:LEU:HD12 | 1.86                     | 0.76              |
| 1:D:471:PRO:CD   | 1:D:489:TRP:HZ2  | 1.90                     | 0.76              |
| 1:A:311:MET:CG   | 1:A:366:HIS:CG   | 2.69                     | 0.75              |
| 1:D:214:LEU:O    | 1:D:218:LEU:HD12 | 1.86                     | 0.75              |
| 1:B:121:VAL:CG1  | 1:B:564:ARG:HH12 | 1.99                     | 0.75              |
| 1:A:37:LEU:HD11  | 1:A:177:PHE:HE1  | 1.51                     | 0.75              |
| 1:A:214:LEU:O    | 1:A:218:LEU:HD12 | 1.86                     | 0.75              |
| 1:B:37:LEU:HD11  | 1:B:177:PHE:HE1  | 1.51                     | 0.75              |
| 1:B:214:LEU:O    | 1:B:218:LEU:HD12 | 1.86                     | 0.75              |
| 1:A:121:VAL:CG1  | 1:A:564:ARG:HH12 | 1.99                     | 0.75              |
| 1:A:290:LEU:CB   | 1:A:382:CYS:SG   | 2.74                     | 0.75              |
| 1:C:471:PRO:CD   | 1:C:489:TRP:HZ2  | 1.90                     | 0.75              |
| 1:B:290:LEU:CB   | 1:B:382:CYS:SG   | 2.74                     | 0.75              |
| 1:C:21:GLN:NE2   | 1:C:32:CYS:SG    | 2.60                     | 0.75              |
| 1:D:33:LEU:HD21  | 1:D:177:PHE:HD1  | 1.50                     | 0.75              |
| 1:A:21:GLN:NE2   | 1:A:32:CYS:SG    | 2.60                     | 0.75              |
| 1:C:33:LEU:HD21  | 1:C:177:PHE:HD1  | 1.50                     | 0.75              |
| 1:C:311:MET:CG   | 1:C:366:HIS:CG   | 2.69                     | 0.75              |
| 1:B:311:MET:H    | 1:B:311:MET:CE   | 2.00                     | 0.75              |
| 1:D:21:GLN:NE2   | 1:D:32:CYS:SG    | 2.60                     | 0.75              |
| 1:C:290:LEU:CB   | 1:C:382:CYS:SG   | 2.74                     | 0.75              |
| 1:B:21:GLN:NE2   | 1:B:32:CYS:SG    | 2.60                     | 0.75              |
| 1:D:311:MET:CG   | 1:D:366:HIS:CG   | 2.69                     | 0.75              |
| 1:A:311:MET:H    | 1:A:311:MET:CE   | 2.00                     | 0.75              |
| 1:B:118:SER:HB2  | 1:B:560:LEU:HD23 | 1.36                     | 0.75              |
| 1:A:313:LYS:CD   | 1:A:318:TYR:HE2  | 1.98                     | 0.74              |
| 1:C:515:VAL:HG12 | 1:C:516:ASN:ND2  | 2.02                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:412:LEU:CD1  | 1:B:465:ILE:HG22 | 2.15                     | 0.74              |
| 1:B:542:PHE:N    | 1:B:543:PRO:HD2  | 2.02                     | 0.74              |
| 1:D:515:VAL:HG12 | 1:D:516:ASN:ND2  | 2.02                     | 0.74              |
| 1:A:542:PHE:N    | 1:A:543:PRO:HD2  | 2.02                     | 0.74              |
| 1:C:490:HIS:O    | 1:C:496:ARG:CD   | 2.36                     | 0.74              |
| 1:B:313:LYS:CD   | 1:B:318:TYR:HE2  | 1.98                     | 0.74              |
| 1:B:408:ALA:HA   | 1:B:435:TYR:HD2  | 1.51                     | 0.74              |
| 1:D:290:LEU:CB   | 1:D:382:CYS:SG   | 2.74                     | 0.74              |
| 1:A:217:LYS:HB2  | 1:A:217:LYS:NZ   | 2.00                     | 0.74              |
| 1:A:412:LEU:CD1  | 1:A:465:ILE:HG22 | 2.15                     | 0.74              |
| 1:C:217:LYS:HB2  | 1:C:217:LYS:NZ   | 2.00                     | 0.74              |
| 1:B:368:LYS:O    | 1:B:377:PHE:HB3  | 1.87                     | 0.74              |
| 1:D:368:LYS:O    | 1:D:377:PHE:HB3  | 1.87                     | 0.74              |
| 1:A:118:SER:HB2  | 1:A:560:LEU:HD23 | 1.36                     | 0.74              |
| 1:A:368:LYS:O    | 1:A:377:PHE:HB3  | 1.87                     | 0.74              |
| 1:A:408:ALA:HA   | 1:A:435:TYR:HD2  | 1.51                     | 0.74              |
| 1:C:368:LYS:O    | 1:C:377:PHE:HB3  | 1.87                     | 0.74              |
| 1:C:529:VAL:HG13 | 1:C:530:ASP:O    | 1.88                     | 0.74              |
| 1:B:217:LYS:HB2  | 1:B:217:LYS:NZ   | 2.00                     | 0.74              |
| 1:A:490:HIS:O    | 1:A:496:ARG:CD   | 2.36                     | 0.74              |
| 1:B:490:HIS:O    | 1:B:496:ARG:CD   | 2.36                     | 0.74              |
| 1:D:529:VAL:HG13 | 1:D:530:ASP:O    | 1.88                     | 0.74              |
| 1:C:311:MET:H    | 1:C:311:MET:CE   | 2.00                     | 0.74              |
| 1:D:217:LYS:HB2  | 1:D:217:LYS:NZ   | 2.00                     | 0.74              |
| 1:D:311:MET:H    | 1:D:311:MET:CE   | 2.00                     | 0.74              |
| 1:D:37:LEU:HD11  | 1:D:177:PHE:HE1  | 1.51                     | 0.74              |
| 1:C:37:LEU:HD11  | 1:C:177:PHE:HE1  | 1.51                     | 0.74              |
| 1:C:332:SER:O    | 1:C:336:VAL:HG23 | 1.88                     | 0.74              |
| 1:B:280:SER:O    | 1:B:281:LEU:C    | 2.28                     | 0.74              |
| 1:B:515:VAL:HG12 | 1:B:516:ASN:ND2  | 2.02                     | 0.74              |
| 1:D:332:SER:O    | 1:D:336:VAL:HG23 | 1.88                     | 0.74              |
| 1:A:515:VAL:HG12 | 1:A:516:ASN:ND2  | 2.02                     | 0.74              |
| 1:D:205:LYS:HG3  | 1:D:206:THR:HG23 | 1.70                     | 0.74              |
| 1:A:280:SER:O    | 1:A:281:LEU:C    | 2.28                     | 0.73              |
| 1:C:205:LYS:HG3  | 1:C:206:THR:HG23 | 1.70                     | 0.73              |
| 1:A:332:SER:O    | 1:A:336:VAL:HG23 | 1.88                     | 0.73              |
| 1:C:118:SER:HB2  | 1:C:560:LEU:HD21 | 1.57                     | 0.73              |
| 1:A:529:VAL:HG13 | 1:A:530:ASP:O    | 1.88                     | 0.73              |
| 1:C:542:PHE:N    | 1:C:543:PRO:HD2  | 2.02                     | 0.73              |
| 1:B:332:SER:O    | 1:B:336:VAL:HG23 | 1.88                     | 0.73              |
| 1:D:118:SER:HB2  | 1:D:560:LEU:HD21 | 1.57                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:449:VAL:HG13 | 1:D:450:PRO:HD2  | 1.69                     | 0.73              |
| 1:C:332:SER:HB2  | 1:C:334:PRO:HD2  | 1.70                     | 0.73              |
| 1:B:529:VAL:HG13 | 1:B:530:ASP:O    | 1.88                     | 0.73              |
| 1:D:542:PHE:N    | 1:D:543:PRO:HD2  | 2.02                     | 0.73              |
| 1:C:449:VAL:HG13 | 1:C:450:PRO:HD2  | 1.69                     | 0.73              |
| 1:D:332:SER:HB2  | 1:D:334:PRO:HD2  | 1.70                     | 0.73              |
| 1:C:116:TYR:HE1  | 1:C:514:VAL:HG21 | 1.53                     | 0.73              |
| 1:D:93:TRP:HZ3   | 1:D:214:LEU:HD12 | 1.52                     | 0.73              |
| 1:D:116:TYR:HE1  | 1:D:514:VAL:HG21 | 1.53                     | 0.73              |
| 1:D:439:MET:SD   | 1:D:442:PHE:CD2  | 2.82                     | 0.73              |
| 1:A:439:MET:SD   | 1:A:442:PHE:CD2  | 2.82                     | 0.73              |
| 1:A:449:VAL:HG13 | 1:A:450:PRO:HD2  | 1.69                     | 0.73              |
| 1:C:439:MET:SD   | 1:C:442:PHE:CD2  | 2.82                     | 0.73              |
| 1:C:439:MET:SD   | 1:C:442:PHE:HD2  | 2.12                     | 0.73              |
| 1:B:439:MET:SD   | 1:B:442:PHE:CD2  | 2.82                     | 0.73              |
| 1:B:449:VAL:HG13 | 1:B:450:PRO:HD2  | 1.69                     | 0.73              |
| 1:D:439:MET:SD   | 1:D:442:PHE:HD2  | 2.12                     | 0.73              |
| 1:A:93:TRP:HZ3   | 1:A:214:LEU:HD12 | 1.52                     | 0.73              |
| 1:C:93:TRP:HZ3   | 1:C:214:LEU:HD12 | 1.52                     | 0.73              |
| 1:B:93:TRP:HZ3   | 1:B:214:LEU:HD12 | 1.52                     | 0.73              |
| 1:A:439:MET:SD   | 1:A:442:PHE:HD2  | 2.12                     | 0.72              |
| 1:A:570:LYS:HB2  | 1:A:570:LYS:HZ2  | 1.54                     | 0.72              |
| 1:A:205:LYS:HG3  | 1:A:206:THR:HG23 | 1.70                     | 0.72              |
| 1:C:121:VAL:CG1  | 1:C:564:ARG:HH12 | 1.99                     | 0.72              |
| 1:B:333:ILE:N    | 1:B:334:PRO:CD   | 2.52                     | 0.72              |
| 1:B:439:MET:SD   | 1:B:442:PHE:HD2  | 2.12                     | 0.72              |
| 1:D:121:VAL:CG1  | 1:D:564:ARG:HH12 | 1.99                     | 0.72              |
| 1:A:333:ILE:N    | 1:A:334:PRO:CD   | 2.52                     | 0.72              |
| 1:B:205:LYS:HG3  | 1:B:206:THR:HG23 | 1.71                     | 0.72              |
| 1:D:311:MET:SD   | 1:D:366:HIS:NE2  | 2.63                     | 0.72              |
| 1:A:332:SER:HB2  | 1:A:334:PRO:HD2  | 1.70                     | 0.72              |
| 1:C:311:MET:SD   | 1:C:366:HIS:NE2  | 2.63                     | 0.72              |
| 1:B:332:SER:HB2  | 1:B:334:PRO:HD2  | 1.70                     | 0.72              |
| 1:B:409:PRO:HG2  | 1:B:410:GLU:OE1  | 1.90                     | 0.71              |
| 1:A:409:PRO:HG2  | 1:A:410:GLU:OE1  | 1.91                     | 0.71              |
| 1:C:333:ILE:N    | 1:C:334:PRO:HD2  | 2.05                     | 0.71              |
| 1:B:111:HIS:HE1  | 1:B:345:ARG:HD2  | 1.54                     | 0.71              |
| 1:D:333:ILE:N    | 1:D:334:PRO:HD2  | 2.05                     | 0.71              |
| 1:D:408:ALA:HA   | 1:D:435:TYR:HD2  | 1.51                     | 0.71              |
| 1:D:470:ARG:HH21 | 1:D:486:LYS:CE   | 2.02                     | 0.71              |
| 1:A:116:TYR:HE1  | 1:A:514:VAL:HG21 | 1.53                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:111:HIS:HE1  | 1:A:345:ARG:HD2  | 1.54                     | 0.71              |
| 1:A:470:ARG:HH21 | 1:A:486:LYS:CE   | 2.02                     | 0.71              |
| 1:C:470:ARG:HH21 | 1:C:486:LYS:CE   | 2.02                     | 0.71              |
| 1:B:470:ARG:HH21 | 1:B:486:LYS:CE   | 2.02                     | 0.71              |
| 1:C:408:ALA:HA   | 1:C:435:TYR:HD2  | 1.51                     | 0.71              |
| 1:B:116:TYR:HE1  | 1:B:514:VAL:HG21 | 1.53                     | 0.71              |
| 1:A:484:LEU:C    | 1:A:484:LEU:HD23 | 2.15                     | 0.71              |
| 1:B:484:LEU:HD23 | 1:B:484:LEU:C    | 2.16                     | 0.71              |
| 1:A:511:LYS:O    | 1:A:515:VAL:HG23 | 1.91                     | 0.71              |
| 1:B:511:LYS:O    | 1:B:515:VAL:HG23 | 1.91                     | 0.71              |
| 1:C:290:LEU:CD1  | 1:C:309:GLU:O    | 2.31                     | 0.71              |
| 1:B:311:MET:SD   | 1:B:366:HIS:NE2  | 2.63                     | 0.71              |
| 1:D:484:LEU:C    | 1:D:484:LEU:HD23 | 2.15                     | 0.71              |
| 1:C:409:PRO:HG2  | 1:C:410:GLU:OE1  | 1.91                     | 0.71              |
| 1:B:471:PRO:CD   | 1:B:489:TRP:CZ2  | 2.67                     | 0.71              |
| 1:A:471:PRO:CD   | 1:A:489:TRP:CZ2  | 2.67                     | 0.70              |
| 1:C:484:LEU:HD23 | 1:C:484:LEU:C    | 2.16                     | 0.70              |
| 1:D:333:ILE:N    | 1:D:334:PRO:CD   | 2.52                     | 0.70              |
| 1:D:409:PRO:HG2  | 1:D:410:GLU:OE1  | 1.91                     | 0.70              |
| 1:A:311:MET:SD   | 1:A:366:HIS:NE2  | 2.63                     | 0.70              |
| 1:A:333:ILE:N    | 1:A:334:PRO:HD2  | 2.05                     | 0.70              |
| 1:C:333:ILE:N    | 1:C:334:PRO:CD   | 2.52                     | 0.70              |
| 1:B:333:ILE:N    | 1:B:334:PRO:HD2  | 2.05                     | 0.70              |
| 1:D:490:HIS:O    | 1:D:496:ARG:CD   | 2.36                     | 0.70              |
| 1:D:471:PRO:CD   | 1:D:489:TRP:CZ2  | 2.67                     | 0.70              |
| 1:C:169:LEU:HD11 | 1:C:557:PRO:HG3  | 1.74                     | 0.70              |
| 1:D:169:LEU:HD11 | 1:D:557:PRO:HG3  | 1.74                     | 0.70              |
| 1:D:311:MET:CB   | 1:D:366:HIS:HB3  | 2.18                     | 0.70              |
| 1:A:451:PHE:HZ   | 1:A:465:ILE:HD11 | 1.56                     | 0.70              |
| 1:C:111:HIS:HE1  | 1:C:345:ARG:HD2  | 1.54                     | 0.70              |
| 1:B:451:PHE:HZ   | 1:B:465:ILE:HD11 | 1.56                     | 0.70              |
| 1:C:471:PRO:CD   | 1:C:489:TRP:CZ2  | 2.67                     | 0.69              |
| 1:A:169:LEU:HD11 | 1:A:557:PRO:HG3  | 1.74                     | 0.69              |
| 1:A:313:LYS:CD   | 1:A:318:TYR:CE2  | 2.75                     | 0.69              |
| 1:A:439:MET:HA   | 1:A:442:PHE:CD2  | 2.27                     | 0.69              |
| 1:C:311:MET:CB   | 1:C:366:HIS:HB3  | 2.18                     | 0.69              |
| 1:B:313:LYS:CD   | 1:B:318:TYR:CE2  | 2.75                     | 0.69              |
| 1:D:111:HIS:HE1  | 1:D:345:ARG:HD2  | 1.55                     | 0.69              |
| 1:B:169:LEU:HD11 | 1:B:557:PRO:HG3  | 1.74                     | 0.69              |
| 1:B:439:MET:HA   | 1:B:442:PHE:CD2  | 2.27                     | 0.69              |
| 1:C:511:LYS:O    | 1:C:515:VAL:HG23 | 1.91                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:535:GLU:OE1  | 1:D:563:TYR:OH   | 2.10                     | 0.69              |
| 1:C:451:PHE:HZ   | 1:C:465:ILE:HD11 | 1.56                     | 0.69              |
| 1:D:508:TYR:OH   | 1:D:528:LEU:CD1  | 2.40                     | 0.69              |
| 1:D:511:LYS:O    | 1:D:515:VAL:HG23 | 1.91                     | 0.69              |
| 1:C:312:HIS:CD2  | 1:C:368:LYS:HD3  | 2.28                     | 0.69              |
| 1:C:508:TYR:OH   | 1:C:528:LEU:CD1  | 2.40                     | 0.69              |
| 1:C:310:LEU:C    | 1:C:310:LEU:HD13 | 2.18                     | 0.69              |
| 1:C:535:GLU:OE1  | 1:C:563:TYR:OH   | 2.10                     | 0.69              |
| 1:D:310:LEU:HD13 | 1:D:310:LEU:C    | 2.18                     | 0.69              |
| 1:D:312:HIS:CD2  | 1:D:368:LYS:HD3  | 2.28                     | 0.69              |
| 1:A:312:HIS:CD2  | 1:A:368:LYS:HD3  | 2.28                     | 0.69              |
| 1:B:312:HIS:CD2  | 1:B:368:LYS:HD3  | 2.28                     | 0.69              |
| 1:D:451:PHE:HZ   | 1:D:465:ILE:HD11 | 1.56                     | 0.69              |
| 1:D:470:ARG:HH21 | 1:D:486:LYS:HE3  | 1.58                     | 0.69              |
| 1:C:74:ARG:NH2   | 1:C:376:TYR:CE1  | 2.61                     | 0.69              |
| 1:C:470:ARG:HH21 | 1:C:486:LYS:HE3  | 1.58                     | 0.69              |
| 1:D:74:ARG:NH2   | 1:D:376:TYR:CE1  | 2.61                     | 0.69              |
| 1:A:475:PHE:N    | 1:A:476:PRO:HD2  | 2.08                     | 0.68              |
| 1:A:508:TYR:OH   | 1:A:528:LEU:CD1  | 2.40                     | 0.68              |
| 1:D:570:LYS:HB2  | 1:D:570:LYS:HZ2  | 1.58                     | 0.68              |
| 1:A:332:SER:HG   | 1:A:334:PRO:HG2  | 1.56                     | 0.68              |
| 1:A:535:GLU:OE1  | 1:A:563:TYR:OH   | 2.10                     | 0.68              |
| 1:C:570:LYS:HB2  | 1:C:570:LYS:HZ2  | 1.59                     | 0.68              |
| 1:B:332:SER:HG   | 1:B:334:PRO:HG2  | 1.56                     | 0.68              |
| 1:B:475:PHE:N    | 1:B:476:PRO:HD2  | 2.08                     | 0.68              |
| 1:D:479:LYS:HB3  | 1:D:479:LYS:HZ3  | 1.56                     | 0.68              |
| 1:C:33:LEU:HD21  | 1:C:177:PHE:CD1  | 2.28                     | 0.68              |
| 1:B:508:TYR:OH   | 1:B:528:LEU:CD1  | 2.40                     | 0.68              |
| 1:B:535:GLU:OE1  | 1:B:563:TYR:OH   | 2.10                     | 0.68              |
| 1:A:310:LEU:HD22 | 1:A:310:LEU:C    | 2.18                     | 0.68              |
| 1:C:37:LEU:HD11  | 1:C:177:PHE:CE1  | 2.28                     | 0.68              |
| 1:B:310:LEU:HD13 | 1:B:310:LEU:C    | 2.18                     | 0.68              |
| 1:D:33:LEU:HD21  | 1:D:177:PHE:CD1  | 2.28                     | 0.68              |
| 1:D:37:LEU:HD11  | 1:D:177:PHE:CE1  | 2.28                     | 0.68              |
| 1:A:310:LEU:C    | 1:A:310:LEU:HD13 | 2.18                     | 0.68              |
| 1:B:310:LEU:HD22 | 1:B:310:LEU:C    | 2.18                     | 0.68              |
| 1:A:33:LEU:HD21  | 1:A:177:PHE:CD1  | 2.28                     | 0.68              |
| 1:A:319:MET:HA   | 1:A:322:ASN:CG   | 2.19                     | 0.68              |
| 1:A:37:LEU:HD11  | 1:A:177:PHE:CE1  | 2.28                     | 0.68              |
| 1:A:74:ARG:NH2   | 1:A:376:TYR:CE1  | 2.61                     | 0.68              |
| 1:C:439:MET:HA   | 1:C:442:PHE:CD2  | 2.27                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:446:THR:CG2  | 1:C:473:PHE:CD2  | 2.77                     | 0.68              |
| 1:B:33:LEU:HD21  | 1:B:177:PHE:CD1  | 2.28                     | 0.68              |
| 1:B:74:ARG:NH2   | 1:B:376:TYR:CE1  | 2.61                     | 0.68              |
| 1:B:319:MET:HA   | 1:B:322:ASN:CG   | 2.19                     | 0.68              |
| 1:D:439:MET:HA   | 1:D:442:PHE:CD2  | 2.27                     | 0.68              |
| 1:B:37:LEU:HD11  | 1:B:177:PHE:CE1  | 2.28                     | 0.68              |
| 1:D:446:THR:CG2  | 1:D:473:PHE:CD2  | 2.77                     | 0.68              |
| 1:C:475:PHE:N    | 1:C:476:PRO:HD2  | 2.08                     | 0.68              |
| 1:B:311:MET:CB   | 1:B:366:HIS:HB3  | 2.18                     | 0.68              |
| 1:A:311:MET:CB   | 1:A:366:HIS:HB3  | 2.18                     | 0.68              |
| 1:C:375:GLY:O    | 1:C:377:PHE:CE2  | 2.47                     | 0.68              |
| 1:C:471:PRO:HG2  | 1:C:489:TRP:CH2  | 2.30                     | 0.67              |
| 1:D:375:GLY:O    | 1:D:377:PHE:CE2  | 2.47                     | 0.67              |
| 1:C:479:LYS:HB3  | 1:C:479:LYS:HZ3  | 1.58                     | 0.67              |
| 1:D:475:PHE:N    | 1:D:476:PRO:HD2  | 2.08                     | 0.67              |
| 1:B:471:PRO:HG2  | 1:B:489:TRP:CH2  | 2.30                     | 0.67              |
| 1:D:217:LYS:HB2  | 1:D:217:LYS:HZ3  | 1.58                     | 0.67              |
| 1:B:78:GLU:HG3   | 1:B:109:HIS:CE1  | 2.30                     | 0.67              |
| 1:B:470:ARG:HH21 | 1:B:486:LYS:HE3  | 1.58                     | 0.67              |
| 1:A:78:GLU:HG3   | 1:A:109:HIS:CE1  | 2.30                     | 0.67              |
| 1:A:470:ARG:HH21 | 1:A:486:LYS:HE3  | 1.58                     | 0.67              |
| 1:A:471:PRO:HG2  | 1:A:489:TRP:CH2  | 2.30                     | 0.67              |
| 1:A:499:PHE:HA   | 1:A:502:ILE:HG22 | 1.76                     | 0.67              |
| 1:C:217:LYS:HB2  | 1:C:217:LYS:HZ3  | 1.58                     | 0.67              |
| 1:B:499:PHE:HA   | 1:B:502:ILE:HG22 | 1.76                     | 0.67              |
| 1:C:319:MET:HA   | 1:C:322:ASN:CG   | 2.19                     | 0.67              |
| 1:D:319:MET:HA   | 1:D:322:ASN:CG   | 2.19                     | 0.67              |
| 1:D:499:PHE:HA   | 1:D:502:ILE:HG22 | 1.76                     | 0.67              |
| 1:A:446:THR:CG2  | 1:A:473:PHE:CD2  | 2.77                     | 0.67              |
| 1:C:74:ARG:HG3   | 1:C:373:THR:HG22 | 1.77                     | 0.67              |
| 1:C:280:SER:C    | 1:C:282:LEU:N    | 2.53                     | 0.67              |
| 1:B:74:ARG:HG3   | 1:B:373:THR:HG22 | 1.77                     | 0.67              |
| 1:D:74:ARG:HG3   | 1:D:373:THR:HG22 | 1.77                     | 0.67              |
| 1:D:280:SER:C    | 1:D:282:LEU:N    | 2.53                     | 0.67              |
| 1:A:375:GLY:O    | 1:A:377:PHE:CE2  | 2.47                     | 0.67              |
| 1:B:375:GLY:O    | 1:B:377:PHE:CE2  | 2.47                     | 0.67              |
| 1:B:446:THR:CG2  | 1:B:473:PHE:CD2  | 2.77                     | 0.67              |
| 1:A:74:ARG:HG3   | 1:A:373:THR:HG22 | 1.77                     | 0.67              |
| 1:A:159:PHE:HZ   | 1:A:561:THR:HG21 | 1.60                     | 0.67              |
| 1:C:499:PHE:HA   | 1:C:502:ILE:HG22 | 1.76                     | 0.67              |
| 1:C:216:LYS:HA   | 1:C:219:THR:CG2  | 2.25                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:159:PHE:HZ   | 1:B:561:THR:HG21 | 1.60                     | 0.66              |
| 1:B:311:MET:CB   | 1:B:366:HIS:CG   | 2.79                     | 0.66              |
| 1:D:215:LEU:O    | 1:D:219:THR:HG23 | 1.95                     | 0.66              |
| 1:D:216:LYS:HA   | 1:D:219:THR:CG2  | 2.25                     | 0.66              |
| 1:A:216:LYS:HA   | 1:A:219:THR:CG2  | 2.25                     | 0.66              |
| 1:A:311:MET:CB   | 1:A:366:HIS:CG   | 2.79                     | 0.66              |
| 1:B:216:LYS:HA   | 1:B:219:THR:CG2  | 2.25                     | 0.66              |
| 1:C:215:LEU:O    | 1:C:219:THR:HG23 | 1.96                     | 0.66              |
| 1:D:78:GLU:HG3   | 1:D:109:HIS:CE1  | 2.30                     | 0.66              |
| 1:C:78:GLU:HG3   | 1:C:109:HIS:CE1  | 2.30                     | 0.66              |
| 1:B:290:LEU:CD1  | 1:B:309:GLU:O    | 2.31                     | 0.66              |
| 1:A:280:SER:C    | 1:A:282:LEU:N    | 2.53                     | 0.66              |
| 1:A:290:LEU:CD1  | 1:A:309:GLU:O    | 2.31                     | 0.66              |
| 1:B:406:TRP:HZ3  | 1:B:439:MET:HB3  | 1.61                     | 0.66              |
| 1:D:492:GLU:O    | 1:D:496:ARG:NE   | 2.29                     | 0.66              |
| 1:A:311:MET:CB   | 1:A:366:HIS:CB   | 2.74                     | 0.66              |
| 1:C:492:GLU:O    | 1:C:496:ARG:NE   | 2.29                     | 0.66              |
| 1:B:280:SER:C    | 1:B:282:LEU:N    | 2.53                     | 0.66              |
| 1:B:311:MET:CB   | 1:B:366:HIS:CB   | 2.74                     | 0.66              |
| 1:A:406:TRP:HZ3  | 1:A:439:MET:HB3  | 1.61                     | 0.66              |
| 1:A:471:PRO:CD   | 1:A:489:TRP:HZ2  | 1.90                     | 0.66              |
| 1:C:127:ALA:HB2  | 1:C:141:ARG:HD2  | 1.78                     | 0.66              |
| 1:D:127:ALA:HB2  | 1:D:141:ARG:HD2  | 1.78                     | 0.66              |
| 1:A:215:LEU:O    | 1:A:219:THR:HG23 | 1.96                     | 0.65              |
| 1:C:182:ARG:NH1  | 1:B:190:GLU:OE1  | 2.29                     | 0.65              |
| 1:C:310:LEU:HD22 | 1:C:310:LEU:C    | 2.18                     | 0.65              |
| 1:A:208:LYS:HB2  | 1:A:208:LYS:HZ3  | 1.59                     | 0.65              |
| 1:A:442:PHE:CD1  | 1:A:473:PHE:CZ   | 2.84                     | 0.65              |
| 1:B:215:LEU:O    | 1:B:219:THR:HG23 | 1.96                     | 0.65              |
| 1:B:471:PRO:CD   | 1:B:489:TRP:HZ2  | 1.90                     | 0.65              |
| 1:D:182:ARG:HB3  | 1:D:186:TRP:CZ3  | 2.31                     | 0.65              |
| 1:D:310:LEU:HD22 | 1:D:310:LEU:C    | 2.18                     | 0.65              |
| 1:C:190:GLU:OE1  | 1:B:182:ARG:NH1  | 2.30                     | 0.65              |
| 1:C:182:ARG:HB3  | 1:C:186:TRP:CZ3  | 2.31                     | 0.65              |
| 1:B:182:ARG:HB3  | 1:B:186:TRP:CZ3  | 2.31                     | 0.65              |
| 1:A:182:ARG:HB3  | 1:A:186:TRP:CZ3  | 2.31                     | 0.65              |
| 1:A:492:GLU:O    | 1:A:496:ARG:NE   | 2.29                     | 0.65              |
| 1:D:311:MET:CB   | 1:D:366:HIS:CG   | 2.79                     | 0.65              |
| 1:A:541:LYS:C    | 1:A:543:PRO:HD2  | 2.22                     | 0.65              |
| 1:B:492:GLU:O    | 1:B:496:ARG:NE   | 2.29                     | 0.65              |
| 1:B:541:LYS:C    | 1:B:543:PRO:HD2  | 2.22                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:311:MET:CB   | 1:C:366:HIS:CG   | 2.79                     | 0.65              |
| 1:C:541:LYS:C    | 1:C:543:PRO:HD2  | 2.22                     | 0.65              |
| 1:B:442:PHE:CE2  | 1:B:489:TRP:CZ3  | 2.85                     | 0.65              |
| 1:D:541:LYS:C    | 1:D:543:PRO:HD2  | 2.22                     | 0.65              |
| 1:A:442:PHE:CE2  | 1:A:489:TRP:CZ3  | 2.85                     | 0.65              |
| 1:B:216:LYS:HA   | 1:B:219:THR:HG23 | 1.79                     | 0.65              |
| 1:B:470:ARG:CD   | 1:B:489:TRP:NE1  | 2.60                     | 0.65              |
| 1:D:478:PRO:O    | 1:D:482:VAL:HG23 | 1.97                     | 0.65              |
| 1:A:67:GLN:CG    | 1:A:517:PRO:HB3  | 2.24                     | 0.65              |
| 1:A:216:LYS:HA   | 1:A:219:THR:HG23 | 1.79                     | 0.65              |
| 1:A:310:LEU:HD13 | 1:A:310:LEU:O    | 1.97                     | 0.65              |
| 1:A:470:ARG:CD   | 1:A:489:TRP:NE1  | 2.60                     | 0.65              |
| 1:A:504:ARG:NH1  | 1:A:535:GLU:OE2  | 2.30                     | 0.65              |
| 1:C:478:PRO:O    | 1:C:482:VAL:HG23 | 1.97                     | 0.65              |
| 1:D:470:ARG:CD   | 1:D:489:TRP:NE1  | 2.60                     | 0.65              |
| 1:A:217:LYS:HB2  | 1:A:217:LYS:HZ3  | 1.62                     | 0.64              |
| 1:B:217:LYS:HB2  | 1:B:217:LYS:HZ3  | 1.62                     | 0.64              |
| 1:D:310:LEU:HD13 | 1:D:310:LEU:O    | 1.97                     | 0.64              |
| 1:C:310:LEU:HD13 | 1:C:310:LEU:O    | 1.97                     | 0.64              |
| 1:C:470:ARG:CD   | 1:C:489:TRP:NE1  | 2.60                     | 0.64              |
| 1:C:472:LEU:HD12 | 1:C:472:LEU:C    | 2.22                     | 0.64              |
| 1:B:310:LEU:HD13 | 1:B:310:LEU:O    | 1.97                     | 0.64              |
| 1:B:504:ARG:NH1  | 1:B:535:GLU:OE2  | 2.30                     | 0.64              |
| 1:D:472:LEU:HD12 | 1:D:472:LEU:C    | 2.22                     | 0.64              |
| 1:A:127:ALA:HB2  | 1:A:141:ARG:HD2  | 1.78                     | 0.64              |
| 1:C:442:PHE:CE2  | 1:C:489:TRP:CE3  | 2.85                     | 0.64              |
| 1:B:67:GLN:CG    | 1:B:517:PRO:HB3  | 2.24                     | 0.64              |
| 1:B:127:ALA:HB2  | 1:B:141:ARG:HD2  | 1.78                     | 0.64              |
| 1:D:442:PHE:CE2  | 1:D:489:TRP:CE3  | 2.85                     | 0.64              |
| 1:A:24:ILE:HD11  | 1:A:87:MET:HG2   | 1.79                     | 0.64              |
| 1:C:67:GLN:CG    | 1:C:517:PRO:HB3  | 2.24                     | 0.64              |
| 1:C:504:ARG:NH1  | 1:C:535:GLU:OE2  | 2.30                     | 0.64              |
| 1:B:24:ILE:HD11  | 1:B:87:MET:HG2   | 1.79                     | 0.64              |
| 1:D:313:LYS:CD   | 1:D:318:TYR:CE2  | 2.75                     | 0.64              |
| 1:C:279:SER:O    | 1:C:282:LEU:HD23 | 1.97                     | 0.64              |
| 1:B:25:LEU:HB2   | 1:B:92:TRP:HE1   | 1.63                     | 0.64              |
| 1:D:504:ARG:NH1  | 1:D:535:GLU:OE2  | 2.30                     | 0.64              |
| 1:A:25:LEU:HB2   | 1:A:92:TRP:HE1   | 1.63                     | 0.64              |
| 1:B:490:HIS:HB3  | 1:B:495:GLN:NE2  | 2.13                     | 0.64              |
| 1:D:279:SER:O    | 1:D:282:LEU:HD23 | 1.97                     | 0.64              |
| 1:A:490:HIS:HB3  | 1:A:495:GLN:NE2  | 2.13                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:313:LYS:CD   | 1:C:318:TYR:CE2  | 2.75                     | 0.64              |
| 1:B:472:LEU:HD12 | 1:B:472:LEU:C    | 2.22                     | 0.64              |
| 1:D:67:GLN:CG    | 1:D:517:PRO:HB3  | 2.24                     | 0.64              |
| 1:C:442:PHE:CE2  | 1:C:489:TRP:CZ3  | 2.85                     | 0.64              |
| 1:B:442:PHE:CD1  | 1:B:473:PHE:CZ   | 2.84                     | 0.64              |
| 1:D:442:PHE:CE2  | 1:D:489:TRP:CZ3  | 2.85                     | 0.64              |
| 1:A:472:LEU:HD12 | 1:A:472:LEU:C    | 2.22                     | 0.64              |
| 1:C:373:THR:C    | 1:C:374:GLU:OE2  | 2.41                     | 0.64              |
| 1:D:24:ILE:HD11  | 1:D:87:MET:HG2   | 1.79                     | 0.64              |
| 1:D:373:THR:C    | 1:D:374:GLU:OE2  | 2.41                     | 0.64              |
| 1:C:24:ILE:HD11  | 1:C:87:MET:HG2   | 1.79                     | 0.63              |
| 1:D:25:LEU:HB2   | 1:D:92:TRP:HE1   | 1.63                     | 0.63              |
| 1:D:412:LEU:HD11 | 1:D:465:ILE:HG21 | 1.79                     | 0.63              |
| 1:A:478:PRO:O    | 1:A:482:VAL:HG23 | 1.97                     | 0.63              |
| 1:C:25:LEU:HB2   | 1:C:92:TRP:HE1   | 1.63                     | 0.63              |
| 1:C:159:PHE:HZ   | 1:C:561:THR:HG21 | 1.60                     | 0.63              |
| 1:C:311:MET:CB   | 1:C:366:HIS:CB   | 2.74                     | 0.63              |
| 1:D:311:MET:CB   | 1:D:366:HIS:CB   | 2.74                     | 0.63              |
| 1:A:279:SER:O    | 1:A:282:LEU:HD23 | 1.98                     | 0.63              |
| 1:B:279:SER:O    | 1:B:282:LEU:HD23 | 1.97                     | 0.63              |
| 1:B:439:MET:CE   | 1:B:450:PRO:HG2  | 2.29                     | 0.63              |
| 1:A:373:THR:C    | 1:A:374:GLU:OE2  | 2.41                     | 0.63              |
| 1:A:439:MET:CE   | 1:A:450:PRO:HG2  | 2.29                     | 0.63              |
| 1:A:442:PHE:CE2  | 1:A:489:TRP:CE3  | 2.85                     | 0.63              |
| 1:A:515:VAL:HG12 | 1:A:516:ASN:HD21 | 1.64                     | 0.63              |
| 1:C:412:LEU:HD11 | 1:C:465:ILE:HG21 | 1.79                     | 0.63              |
| 1:C:555:GLN:HB3  | 1:C:559:GLN:HE21 | 1.64                     | 0.63              |
| 1:B:373:THR:C    | 1:B:374:GLU:OE2  | 2.41                     | 0.63              |
| 1:C:216:LYS:HA   | 1:C:219:THR:HG23 | 1.79                     | 0.63              |
| 1:B:442:PHE:CE2  | 1:B:489:TRP:CE3  | 2.85                     | 0.63              |
| 1:B:478:PRO:O    | 1:B:482:VAL:HG23 | 1.97                     | 0.63              |
| 1:B:515:VAL:HG12 | 1:B:516:ASN:HD21 | 1.64                     | 0.63              |
| 1:D:216:LYS:HA   | 1:D:219:THR:HG23 | 1.79                     | 0.63              |
| 1:D:555:GLN:HB3  | 1:D:559:GLN:HE21 | 1.64                     | 0.63              |
| 1:A:475:PHE:CG   | 1:A:476:PRO:CD   | 2.82                     | 0.63              |
| 1:D:159:PHE:HZ   | 1:D:561:THR:HG21 | 1.60                     | 0.63              |
| 1:D:442:PHE:CD1  | 1:D:473:PHE:CZ   | 2.84                     | 0.63              |
| 1:D:515:VAL:C    | 1:D:516:ASN:ND2  | 2.56                     | 0.63              |
| 1:A:479:LYS:HB3  | 1:A:479:LYS:HZ2  | 1.63                     | 0.63              |
| 1:C:169:LEU:HD21 | 1:C:557:PRO:HG3  | 1.80                     | 0.63              |
| 1:C:442:PHE:CD1  | 1:C:473:PHE:CZ   | 2.84                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:515:VAL:C    | 1:C:516:ASN:ND2  | 2.56                     | 0.63              |
| 1:B:475:PHE:CG   | 1:B:476:PRO:CD   | 2.82                     | 0.63              |
| 1:A:280:SER:O    | 1:A:283:ALA:N    | 2.32                     | 0.63              |
| 1:B:280:SER:O    | 1:B:283:ALA:N    | 2.32                     | 0.63              |
| 1:D:490:HIS:HB3  | 1:D:495:GLN:NE2  | 2.13                     | 0.63              |
| 1:D:536:ALA:O    | 1:D:540:ARG:N    | 2.31                     | 0.63              |
| 1:C:439:MET:CE   | 1:C:450:PRO:HG2  | 2.29                     | 0.62              |
| 1:B:479:LYS:HB3  | 1:B:479:LYS:HZ2  | 1.63                     | 0.62              |
| 1:D:439:MET:CE   | 1:D:450:PRO:HG2  | 2.29                     | 0.62              |
| 1:D:475:PHE:CG   | 1:D:476:PRO:CD   | 2.82                     | 0.62              |
| 1:C:319:MET:O    | 1:C:322:ASN:CG   | 2.42                     | 0.62              |
| 1:C:515:VAL:HG12 | 1:C:516:ASN:HD21 | 1.64                     | 0.62              |
| 1:D:169:LEU:HD21 | 1:D:557:PRO:HG3  | 1.80                     | 0.62              |
| 1:C:475:PHE:CG   | 1:C:476:PRO:CD   | 2.82                     | 0.62              |
| 1:C:490:HIS:HB3  | 1:C:495:GLN:NE2  | 2.13                     | 0.62              |
| 1:D:319:MET:O    | 1:D:322:ASN:CG   | 2.42                     | 0.62              |
| 1:A:555:GLN:HB3  | 1:A:559:GLN:HE21 | 1.64                     | 0.62              |
| 1:C:536:ALA:O    | 1:C:540:ARG:N    | 2.31                     | 0.62              |
| 1:B:312:HIS:HD2  | 1:B:368:LYS:CE   | 2.04                     | 0.62              |
| 1:D:515:VAL:HG12 | 1:D:516:ASN:HD21 | 1.64                     | 0.62              |
| 1:A:312:HIS:HD2  | 1:A:368:LYS:CE   | 2.04                     | 0.62              |
| 1:A:487:ARG:NH2  | 1:A:532:TRP:HD1  | 1.98                     | 0.62              |
| 1:C:171:ARG:O    | 1:C:173:ILE:HA   | 1.99                     | 0.62              |
| 1:B:536:ALA:O    | 1:B:540:ARG:N    | 2.31                     | 0.62              |
| 1:D:154:ASN:HB3  | 1:D:542:PHE:CE1  | 2.35                     | 0.62              |
| 1:C:108:PHE:HZ   | 1:C:370:ARG:HH12 | 1.48                     | 0.62              |
| 1:C:154:ASN:HB3  | 1:C:542:PHE:CE1  | 2.35                     | 0.62              |
| 1:B:487:ARG:NH2  | 1:B:532:TRP:HD1  | 1.98                     | 0.62              |
| 1:A:536:ALA:O    | 1:A:540:ARG:N    | 2.31                     | 0.62              |
| 1:B:409:PRO:HA   | 1:B:412:LEU:HG   | 1.82                     | 0.62              |
| 1:D:108:PHE:HZ   | 1:D:370:ARG:HH12 | 1.48                     | 0.62              |
| 1:D:171:ARG:O    | 1:D:173:ILE:HA   | 2.00                     | 0.62              |
| 1:A:409:PRO:HA   | 1:A:412:LEU:HG   | 1.82                     | 0.62              |
| 1:A:515:VAL:C    | 1:A:516:ASN:ND2  | 2.56                     | 0.62              |
| 1:A:541:LYS:NZ   | 1:A:541:LYS:HB3  | 2.15                     | 0.62              |
| 1:C:360:LEU:HB3  | 1:C:436:SER:HB2  | 1.81                     | 0.62              |
| 1:B:541:LYS:NZ   | 1:B:541:LYS:HB3  | 2.15                     | 0.62              |
| 1:B:555:GLN:HB3  | 1:B:559:GLN:HE21 | 1.64                     | 0.62              |
| 1:D:360:LEU:HB3  | 1:D:436:SER:HB2  | 1.81                     | 0.62              |
| 1:D:471:PRO:HG2  | 1:D:489:TRP:CH2  | 2.30                     | 0.62              |
| 1:B:411:VAL:HA   | 1:B:414:GLU:OE2  | 2.00                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:171:ARG:O    | 1:A:173:ILE:HA   | 1.99                     | 0.62              |
| 1:A:411:VAL:HA   | 1:A:414:GLU:OE2  | 2.00                     | 0.62              |
| 1:C:104:ASP:O    | 1:C:107:GLU:HG3  | 2.00                     | 0.62              |
| 1:D:104:ASP:O    | 1:D:107:GLU:HG3  | 2.00                     | 0.62              |
| 1:A:278:ILE:O    | 1:A:278:ILE:HG12 | 1.99                     | 0.61              |
| 1:A:319:MET:O    | 1:A:322:ASN:CG   | 2.42                     | 0.61              |
| 1:C:403:PRO:O    | 1:C:403:PRO:HD2  | 2.00                     | 0.61              |
| 1:B:515:VAL:C    | 1:B:516:ASN:ND2  | 2.56                     | 0.61              |
| 1:D:375:GLY:O    | 1:D:377:PHE:CZ   | 2.52                     | 0.61              |
| 1:A:169:LEU:HD21 | 1:A:557:PRO:HG3  | 1.80                     | 0.61              |
| 1:C:541:LYS:NZ   | 1:C:541:LYS:HB3  | 2.15                     | 0.61              |
| 1:B:171:ARG:O    | 1:B:173:ILE:HA   | 2.00                     | 0.61              |
| 1:B:278:ILE:HG12 | 1:B:278:ILE:O    | 1.99                     | 0.61              |
| 1:B:319:MET:O    | 1:B:322:ASN:CG   | 2.42                     | 0.61              |
| 1:C:312:HIS:HD2  | 1:C:368:LYS:CE   | 2.04                     | 0.61              |
| 1:C:375:GLY:O    | 1:C:377:PHE:CZ   | 2.53                     | 0.61              |
| 1:C:411:VAL:HA   | 1:C:414:GLU:OE2  | 2.00                     | 0.61              |
| 1:D:403:PRO:HD2  | 1:D:403:PRO:O    | 2.00                     | 0.61              |
| 1:A:104:ASP:O    | 1:A:107:GLU:HG3  | 2.00                     | 0.61              |
| 1:A:108:PHE:HZ   | 1:A:370:ARG:HH12 | 1.48                     | 0.61              |
| 1:C:487:ARG:NH2  | 1:C:532:TRP:HD1  | 1.98                     | 0.61              |
| 1:B:375:GLY:O    | 1:B:377:PHE:CZ   | 2.52                     | 0.61              |
| 1:D:312:HIS:HD2  | 1:D:368:LYS:CE   | 2.04                     | 0.61              |
| 1:D:541:LYS:NZ   | 1:D:541:LYS:HB3  | 2.15                     | 0.61              |
| 1:A:375:GLY:O    | 1:A:377:PHE:CZ   | 2.53                     | 0.61              |
| 1:C:560:LEU:HD12 | 1:C:560:LEU:O    | 2.00                     | 0.61              |
| 1:B:104:ASP:O    | 1:B:107:GLU:HG3  | 2.00                     | 0.61              |
| 1:B:108:PHE:HZ   | 1:B:370:ARG:HH12 | 1.48                     | 0.61              |
| 1:B:154:ASN:HB3  | 1:B:542:PHE:CE1  | 2.35                     | 0.61              |
| 1:B:169:LEU:HD21 | 1:B:557:PRO:HG3  | 1.80                     | 0.61              |
| 1:D:360:LEU:C    | 1:D:361:ASN:OD1  | 2.44                     | 0.61              |
| 1:D:411:VAL:HA   | 1:D:414:GLU:OE2  | 2.00                     | 0.61              |
| 1:D:487:ARG:NH2  | 1:D:532:TRP:HD1  | 1.98                     | 0.61              |
| 1:A:154:ASN:HB3  | 1:A:542:PHE:CE1  | 2.35                     | 0.61              |
| 1:C:360:LEU:C    | 1:C:361:ASN:OD1  | 2.44                     | 0.61              |
| 1:D:560:LEU:HD12 | 1:D:560:LEU:O    | 2.01                     | 0.61              |
| 1:A:404:VAL:O    | 1:A:404:VAL:HG12 | 2.00                     | 0.61              |
| 1:A:479:LYS:HB3  | 1:A:479:LYS:HZ3  | 1.62                     | 0.61              |
| 1:B:404:VAL:O    | 1:B:404:VAL:HG12 | 2.00                     | 0.61              |
| 1:A:360:LEU:HB3  | 1:A:436:SER:HB2  | 1.81                     | 0.61              |
| 1:B:360:LEU:HB3  | 1:B:436:SER:HB2  | 1.81                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:479:LYS:HB3  | 1:B:479:LYS:HZ3  | 1.62                     | 0.60              |
| 1:D:278:ILE:O    | 1:D:278:ILE:HG12 | 1.99                     | 0.60              |
| 1:D:290:LEU:CD1  | 1:D:309:GLU:O    | 2.31                     | 0.60              |
| 1:A:560:LEU:HD12 | 1:A:560:LEU:O    | 2.00                     | 0.60              |
| 1:C:409:PRO:HA   | 1:C:412:LEU:HG   | 1.82                     | 0.60              |
| 1:B:412:LEU:HD11 | 1:B:465:ILE:HG21 | 1.79                     | 0.60              |
| 1:B:475:PHE:CG   | 1:B:476:PRO:HD3  | 2.36                     | 0.60              |
| 1:D:409:PRO:HA   | 1:D:412:LEU:HG   | 1.82                     | 0.60              |
| 1:A:475:PHE:CG   | 1:A:476:PRO:HD3  | 2.36                     | 0.60              |
| 1:C:278:ILE:O    | 1:C:278:ILE:HG12 | 1.99                     | 0.60              |
| 1:D:406:TRP:HZ3  | 1:D:439:MET:HB3  | 1.61                     | 0.60              |
| 1:B:560:LEU:O    | 1:B:560:LEU:HD12 | 2.01                     | 0.60              |
| 1:A:412:LEU:HD11 | 1:A:465:ILE:HG21 | 1.79                     | 0.60              |
| 1:C:479:LYS:HG3  | 1:C:527:PRO:HG3  | 1.83                     | 0.60              |
| 1:C:208:LYS:HB2  | 1:C:208:LYS:HZ2  | 1.67                     | 0.60              |
| 1:D:404:VAL:O    | 1:D:404:VAL:HG12 | 2.00                     | 0.60              |
| 1:C:404:VAL:O    | 1:C:404:VAL:HG12 | 2.00                     | 0.60              |
| 1:C:406:TRP:HZ3  | 1:C:439:MET:HB3  | 1.61                     | 0.60              |
| 1:B:403:PRO:HD2  | 1:B:403:PRO:O    | 2.00                     | 0.60              |
| 1:D:479:LYS:HG3  | 1:D:527:PRO:HG3  | 1.84                     | 0.60              |
| 1:A:360:LEU:C    | 1:A:361:ASN:OD1  | 2.44                     | 0.60              |
| 1:C:78:GLU:OE1   | 1:C:78:GLU:HA    | 2.01                     | 0.60              |
| 1:D:78:GLU:OE1   | 1:D:78:GLU:HA    | 2.01                     | 0.60              |
| 1:A:403:PRO:O    | 1:A:403:PRO:HD2  | 2.00                     | 0.60              |
| 1:B:170:SER:C    | 1:B:173:ILE:N    | 2.60                     | 0.60              |
| 1:B:356:PHE:CE1  | 1:B:430:HIS:CA   | 2.84                     | 0.60              |
| 1:B:360:LEU:C    | 1:B:361:ASN:OD1  | 2.44                     | 0.60              |
| 1:A:78:GLU:OE1   | 1:A:78:GLU:HA    | 2.01                     | 0.59              |
| 1:A:170:SER:C    | 1:A:173:ILE:N    | 2.60                     | 0.59              |
| 1:A:356:PHE:CE1  | 1:A:430:HIS:CA   | 2.84                     | 0.59              |
| 1:C:475:PHE:CG   | 1:C:476:PRO:HD3  | 2.36                     | 0.59              |
| 1:D:475:PHE:CG   | 1:D:476:PRO:HD3  | 2.36                     | 0.59              |
| 1:B:78:GLU:OE1   | 1:B:78:GLU:HA    | 2.01                     | 0.59              |
| 1:D:53:LEU:CD2   | 1:D:126:ALA:HB2  | 2.31                     | 0.59              |
| 1:D:356:PHE:CE1  | 1:D:430:HIS:CA   | 2.84                     | 0.59              |
| 1:C:53:LEU:CD2   | 1:C:126:ALA:HB2  | 2.31                     | 0.59              |
| 1:C:108:PHE:HZ   | 1:C:370:ARG:NH1  | 2.01                     | 0.59              |
| 1:C:411:VAL:O    | 1:C:414:GLU:CD   | 2.46                     | 0.59              |
| 1:D:108:PHE:HZ   | 1:D:370:ARG:NH1  | 2.00                     | 0.59              |
| 1:A:108:PHE:HZ   | 1:A:370:ARG:NH1  | 2.00                     | 0.59              |
| 1:A:479:LYS:HG3  | 1:A:527:PRO:HG3  | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:534:LEU:O    | 1:A:537:ARG:HG2  | 2.02                     | 0.59              |
| 1:C:356:PHE:CE1  | 1:C:430:HIS:CA   | 2.84                     | 0.59              |
| 1:B:108:PHE:HZ   | 1:B:370:ARG:NH1  | 2.00                     | 0.59              |
| 1:B:479:LYS:HG3  | 1:B:527:PRO:HG3  | 1.84                     | 0.59              |
| 1:B:534:LEU:O    | 1:B:537:ARG:HG2  | 2.02                     | 0.59              |
| 1:D:411:VAL:O    | 1:D:414:GLU:CD   | 2.46                     | 0.59              |
| 1:C:53:LEU:HD13  | 1:C:62:TRP:CE2   | 2.37                     | 0.59              |
| 1:D:553:VAL:O    | 1:D:556:ILE:HG13 | 2.02                     | 0.59              |
| 1:A:356:PHE:CD1  | 1:A:430:HIS:HA   | 2.38                     | 0.59              |
| 1:A:411:VAL:CA   | 1:A:414:GLU:OE2  | 2.51                     | 0.59              |
| 1:C:280:SER:O    | 1:C:283:ALA:N    | 2.32                     | 0.59              |
| 1:C:411:VAL:CA   | 1:C:414:GLU:OE2  | 2.51                     | 0.59              |
| 1:C:553:VAL:O    | 1:C:556:ILE:HG13 | 2.03                     | 0.59              |
| 1:B:310:LEU:HD22 | 1:B:311:MET:HE2  | 1.84                     | 0.59              |
| 1:B:356:PHE:CD1  | 1:B:430:HIS:HA   | 2.38                     | 0.59              |
| 1:B:411:VAL:CA   | 1:B:414:GLU:OE2  | 2.51                     | 0.59              |
| 1:D:53:LEU:HD13  | 1:D:62:TRP:CE2   | 2.37                     | 0.59              |
| 1:D:310:LEU:HD22 | 1:D:311:MET:HE2  | 1.83                     | 0.59              |
| 1:D:411:VAL:CA   | 1:D:414:GLU:OE2  | 2.51                     | 0.59              |
| 1:D:534:LEU:O    | 1:D:537:ARG:HG2  | 2.02                     | 0.59              |
| 1:C:170:SER:C    | 1:C:173:ILE:N    | 2.60                     | 0.59              |
| 1:C:534:LEU:O    | 1:C:537:ARG:HG2  | 2.02                     | 0.59              |
| 1:A:116:TYR:HE1  | 1:A:514:VAL:CG2  | 2.15                     | 0.59              |
| 1:A:310:LEU:HD22 | 1:A:311:MET:HE2  | 1.84                     | 0.59              |
| 1:A:408:ALA:CA   | 1:A:435:TYR:CD2  | 2.74                     | 0.59              |
| 1:A:411:VAL:O    | 1:A:414:GLU:CD   | 2.46                     | 0.59              |
| 1:C:313:LYS:HD2  | 1:C:318:TYR:CZ   | 2.37                     | 0.59              |
| 1:B:411:VAL:O    | 1:B:414:GLU:CD   | 2.46                     | 0.59              |
| 1:D:154:ASN:HB3  | 1:D:542:PHE:CZ   | 2.38                     | 0.59              |
| 1:D:170:SER:C    | 1:D:173:ILE:N    | 2.60                     | 0.59              |
| 1:D:280:SER:O    | 1:D:283:ALA:N    | 2.32                     | 0.59              |
| 1:A:214:LEU:O    | 1:A:218:LEU:CD1  | 2.51                     | 0.59              |
| 1:C:154:ASN:HB3  | 1:C:542:PHE:CZ   | 2.38                     | 0.59              |
| 1:C:214:LEU:O    | 1:C:218:LEU:CD1  | 2.51                     | 0.59              |
| 1:B:116:TYR:HE1  | 1:B:514:VAL:CG2  | 2.15                     | 0.59              |
| 1:B:214:LEU:O    | 1:B:218:LEU:CD1  | 2.50                     | 0.59              |
| 1:B:408:ALA:CA   | 1:B:435:TYR:CD2  | 2.74                     | 0.59              |
| 1:B:570:LYS:HB2  | 1:B:570:LYS:HZ2  | 1.66                     | 0.59              |
| 1:D:116:TYR:HE1  | 1:D:514:VAL:CG2  | 2.15                     | 0.59              |
| 1:D:214:LEU:O    | 1:D:218:LEU:CD1  | 2.51                     | 0.59              |
| 1:C:310:LEU:HD22 | 1:C:311:MET:HE2  | 1.84                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:313:LYS:HD2  | 1:B:318:TYR:CZ   | 2.37                     | 0.59              |
| 1:D:208:LYS:HB2  | 1:D:208:LYS:HZ2  | 1.68                     | 0.59              |
| 1:D:313:LYS:HD2  | 1:D:318:TYR:CZ   | 2.37                     | 0.59              |
| 1:A:53:LEU:HD13  | 1:A:62:TRP:CE2   | 2.37                     | 0.58              |
| 1:A:313:LYS:HD2  | 1:A:318:TYR:CZ   | 2.37                     | 0.58              |
| 1:C:116:TYR:HE1  | 1:C:514:VAL:CG2  | 2.15                     | 0.58              |
| 1:A:406:TRP:CE3  | 1:A:439:MET:HB3  | 2.38                     | 0.58              |
| 1:B:53:LEU:HD13  | 1:B:62:TRP:CE2   | 2.37                     | 0.58              |
| 1:B:147:ARG:NH2  | 1:D:152:GLU:OE2  | 2.36                     | 0.58              |
| 1:B:406:TRP:CE3  | 1:B:439:MET:HB3  | 2.38                     | 0.58              |
| 1:B:208:LYS:HB2  | 1:B:208:LYS:HZ2  | 1.66                     | 0.58              |
| 1:A:553:VAL:O    | 1:A:556:ILE:HG13 | 2.02                     | 0.58              |
| 1:A:199:ASP:OD2  | 1:A:208:LYS:CD   | 2.51                     | 0.58              |
| 1:B:124:ILE:HG22 | 1:B:124:ILE:O    | 2.03                     | 0.58              |
| 1:B:199:ASP:OD2  | 1:B:208:LYS:CD   | 2.51                     | 0.58              |
| 1:B:332:SER:H    | 1:B:335:VAL:HG22 | 1.68                     | 0.58              |
| 1:B:553:VAL:O    | 1:B:556:ILE:HG13 | 2.02                     | 0.58              |
| 1:D:356:PHE:CD1  | 1:D:430:HIS:HA   | 2.38                     | 0.58              |
| 1:D:370:ARG:HG3  | 1:D:377:PHE:N    | 2.18                     | 0.58              |
| 1:A:124:ILE:O    | 1:A:124:ILE:HG22 | 2.03                     | 0.58              |
| 1:C:321:GLU:CD   | 1:C:321:GLU:H    | 2.12                     | 0.58              |
| 1:D:350:LEU:HB3  | 1:D:355:ILE:HG23 | 1.84                     | 0.58              |
| 1:A:332:SER:H    | 1:A:335:VAL:HG22 | 1.68                     | 0.58              |
| 1:C:70:ARG:O     | 1:C:73:THR:HG22  | 2.04                     | 0.58              |
| 1:C:350:LEU:HB3  | 1:C:355:ILE:HG23 | 1.84                     | 0.58              |
| 1:C:356:PHE:CD1  | 1:C:430:HIS:HA   | 2.38                     | 0.58              |
| 1:B:186:TRP:HA   | 1:B:189:VAL:HG22 | 1.86                     | 0.58              |
| 1:D:70:ARG:O     | 1:D:73:THR:HG22  | 2.04                     | 0.58              |
| 1:A:186:TRP:HA   | 1:A:189:VAL:HG22 | 1.86                     | 0.58              |
| 1:C:370:ARG:HG3  | 1:C:377:PHE:N    | 2.19                     | 0.58              |
| 1:D:321:GLU:H    | 1:D:321:GLU:CD   | 2.12                     | 0.58              |
| 1:D:332:SER:CB   | 1:D:334:PRO:CD   | 2.81                     | 0.58              |
| 1:A:350:LEU:HB3  | 1:A:355:ILE:HG23 | 1.84                     | 0.58              |
| 1:B:81:LEU:CD1   | 1:B:372:HIS:CE1  | 2.80                     | 0.58              |
| 1:B:350:LEU:HB3  | 1:B:355:ILE:HG23 | 1.84                     | 0.58              |
| 1:B:314:ASP:CG   | 1:B:366:HIS:CE1  | 2.82                     | 0.58              |
| 1:A:81:LEU:CD1   | 1:A:372:HIS:CE1  | 2.80                     | 0.57              |
| 1:A:314:ASP:CG   | 1:A:366:HIS:CE1  | 2.82                     | 0.57              |
| 1:B:70:ARG:O     | 1:B:73:THR:HG22  | 2.04                     | 0.57              |
| 1:D:199:ASP:OD2  | 1:D:208:LYS:CD   | 2.51                     | 0.57              |
| 1:D:542:PHE:N    | 1:D:543:PRO:CD   | 2.67                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:70:ARG:O     | 1:A:73:THR:HG22  | 2.04                     | 0.57              |
| 1:C:199:ASP:OD2  | 1:C:208:LYS:CD   | 2.51                     | 0.57              |
| 1:C:542:PHE:N    | 1:C:543:PRO:CD   | 2.67                     | 0.57              |
| 1:B:439:MET:HE2  | 1:B:450:PRO:HG2  | 1.86                     | 0.57              |
| 1:C:314:ASP:CG   | 1:C:366:HIS:CE1  | 2.82                     | 0.57              |
| 1:D:314:ASP:CG   | 1:D:366:HIS:CE1  | 2.82                     | 0.57              |
| 1:A:154:ASN:HB3  | 1:A:542:PHE:CZ   | 2.38                     | 0.57              |
| 1:A:439:MET:HE2  | 1:A:450:PRO:HG2  | 1.86                     | 0.57              |
| 1:B:312:HIS:NE2  | 1:B:368:LYS:HD3  | 2.19                     | 0.57              |
| 1:B:542:PHE:N    | 1:B:543:PRO:CD   | 2.67                     | 0.57              |
| 1:A:312:HIS:NE2  | 1:A:368:LYS:HD3  | 2.19                     | 0.57              |
| 1:A:542:PHE:N    | 1:A:543:PRO:CD   | 2.67                     | 0.57              |
| 1:C:290:LEU:CD2  | 1:C:311:MET:CG   | 2.72                     | 0.57              |
| 1:C:406:TRP:CE3  | 1:C:439:MET:HB3  | 2.38                     | 0.57              |
| 1:B:154:ASN:HB3  | 1:B:542:PHE:CZ   | 2.38                     | 0.57              |
| 1:A:290:LEU:CD2  | 1:A:311:MET:CG   | 2.72                     | 0.57              |
| 1:A:370:ARG:HG3  | 1:A:377:PHE:N    | 2.19                     | 0.57              |
| 1:C:312:HIS:NE2  | 1:C:368:LYS:HD3  | 2.19                     | 0.57              |
| 1:D:332:SER:H    | 1:D:335:VAL:HG22 | 1.68                     | 0.57              |
| 1:D:406:TRP:CE3  | 1:D:439:MET:HB3  | 2.38                     | 0.57              |
| 1:A:484:LEU:HD23 | 1:A:484:LEU:O    | 2.05                     | 0.57              |
| 1:C:332:SER:H    | 1:C:335:VAL:HG22 | 1.68                     | 0.57              |
| 1:D:312:HIS:NE2  | 1:D:368:LYS:HD3  | 2.19                     | 0.57              |
| 1:D:330:LEU:HD12 | 1:D:330:LEU:O    | 2.05                     | 0.57              |
| 1:B:370:ARG:HG3  | 1:B:377:PHE:N    | 2.19                     | 0.57              |
| 1:D:124:ILE:O    | 1:D:124:ILE:HG22 | 2.03                     | 0.57              |
| 1:A:321:GLU:H    | 1:A:321:GLU:CD   | 2.12                     | 0.57              |
| 1:C:27:ASN:ND2   | 1:C:86:CYS:SG    | 2.78                     | 0.57              |
| 1:C:484:LEU:HD23 | 1:C:484:LEU:O    | 2.05                     | 0.57              |
| 1:B:317:SER:O    | 1:B:321:GLU:OE2  | 2.23                     | 0.57              |
| 1:D:484:LEU:HD23 | 1:D:484:LEU:O    | 2.05                     | 0.57              |
| 1:A:317:SER:O    | 1:A:321:GLU:OE2  | 2.23                     | 0.57              |
| 1:C:124:ILE:O    | 1:C:124:ILE:HG22 | 2.03                     | 0.57              |
| 1:C:479:LYS:HB3  | 1:C:479:LYS:HZ2  | 1.67                     | 0.57              |
| 1:B:290:LEU:CD2  | 1:B:311:MET:CG   | 2.72                     | 0.57              |
| 1:B:321:GLU:H    | 1:B:321:GLU:CD   | 2.12                     | 0.57              |
| 1:B:484:LEU:HD23 | 1:B:484:LEU:O    | 2.05                     | 0.57              |
| 1:D:27:ASN:ND2   | 1:D:86:CYS:SG    | 2.78                     | 0.57              |
| 1:D:290:LEU:CD2  | 1:D:311:MET:CG   | 2.72                     | 0.57              |
| 1:C:155:ASP:HB3  | 1:C:158:MET:HB3  | 1.87                     | 0.56              |
| 1:C:330:LEU:HD12 | 1:C:330:LEU:O    | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:439:MET:HE2  | 1:C:450:PRO:HG2  | 1.86                     | 0.56              |
| 1:D:155:ASP:HB3  | 1:D:158:MET:HB3  | 1.87                     | 0.56              |
| 1:C:199:ASP:OD2  | 1:C:208:LYS:HD2  | 2.05                     | 0.56              |
| 1:B:27:ASN:ND2   | 1:B:86:CYS:SG    | 2.78                     | 0.56              |
| 1:D:186:TRP:HA   | 1:D:189:VAL:HG22 | 1.86                     | 0.56              |
| 1:D:208:LYS:HB2  | 1:D:208:LYS:HZ3  | 1.69                     | 0.56              |
| 1:D:310:LEU:CD2  | 1:D:311:MET:HE2  | 2.35                     | 0.56              |
| 1:D:439:MET:HE2  | 1:D:450:PRO:HG2  | 1.86                     | 0.56              |
| 1:A:27:ASN:ND2   | 1:A:86:CYS:SG    | 2.78                     | 0.56              |
| 1:A:314:ASP:HA   | 1:A:366:HIS:HA   | 1.88                     | 0.56              |
| 1:A:330:LEU:HD12 | 1:A:330:LEU:O    | 2.05                     | 0.56              |
| 1:A:541:LYS:HB3  | 1:A:541:LYS:HZ3  | 1.69                     | 0.56              |
| 1:C:186:TRP:HA   | 1:C:189:VAL:HG22 | 1.86                     | 0.56              |
| 1:C:216:LYS:HD2  | 1:C:219:THR:OG1  | 2.06                     | 0.56              |
| 1:C:310:LEU:CD2  | 1:C:311:MET:HE2  | 2.35                     | 0.56              |
| 1:C:314:ASP:HA   | 1:C:366:HIS:HA   | 1.88                     | 0.56              |
| 1:B:199:ASP:OD2  | 1:B:208:LYS:HD2  | 2.05                     | 0.56              |
| 1:B:314:ASP:HA   | 1:B:366:HIS:HA   | 1.88                     | 0.56              |
| 1:B:330:LEU:HD12 | 1:B:330:LEU:O    | 2.05                     | 0.56              |
| 1:B:443:GLU:O    | 1:B:447:GLY:N    | 2.29                     | 0.56              |
| 1:D:216:LYS:HD2  | 1:D:219:THR:OG1  | 2.06                     | 0.56              |
| 1:A:336:VAL:CG1  | 1:A:340:MET:HE2  | 2.33                     | 0.56              |
| 1:B:336:VAL:CG1  | 1:B:340:MET:HE2  | 2.33                     | 0.56              |
| 1:B:541:LYS:HB3  | 1:B:541:LYS:HZ3  | 1.69                     | 0.56              |
| 1:D:199:ASP:OD2  | 1:D:208:LYS:HD2  | 2.05                     | 0.56              |
| 1:D:314:ASP:HA   | 1:D:366:HIS:HA   | 1.88                     | 0.56              |
| 1:A:310:LEU:CD2  | 1:A:311:MET:HE2  | 2.35                     | 0.56              |
| 1:A:443:GLU:O    | 1:A:447:GLY:N    | 2.29                     | 0.56              |
| 1:B:310:LEU:CD2  | 1:B:311:MET:HE2  | 2.36                     | 0.56              |
| 1:D:343:ILE:O    | 1:D:347:MET:N    | 2.38                     | 0.56              |
| 1:A:199:ASP:OD2  | 1:A:208:LYS:HD2  | 2.05                     | 0.56              |
| 1:C:1:MET:HE1    | 1:D:20:LEU:HD12  | 1.87                     | 0.56              |
| 1:C:343:ILE:O    | 1:C:347:MET:N    | 2.38                     | 0.56              |
| 1:B:53:LEU:CD2   | 1:B:126:ALA:HB2  | 2.31                     | 0.56              |
| 1:B:155:ASP:HB3  | 1:B:158:MET:HB3  | 1.87                     | 0.56              |
| 1:A:155:ASP:HB3  | 1:A:158:MET:HB3  | 1.87                     | 0.56              |
| 1:A:370:ARG:HG2  | 1:A:376:TYR:O    | 2.04                     | 0.56              |
| 1:B:370:ARG:HG2  | 1:B:376:TYR:O    | 2.04                     | 0.56              |
| 1:C:317:SER:O    | 1:C:321:GLU:OE2  | 2.23                     | 0.56              |
| 1:A:53:LEU:CD2   | 1:A:126:ALA:HB2  | 2.31                     | 0.56              |
| 1:A:343:ILE:O    | 1:A:347:MET:N    | 2.38                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:370:ARG:CG   | 1:D:377:PHE:CA   | 2.84                     | 0.56              |
| 1:C:370:ARG:CG   | 1:C:377:PHE:CA   | 2.84                     | 0.55              |
| 1:B:216:LYS:O    | 1:B:219:THR:OG1  | 2.12                     | 0.55              |
| 1:B:343:ILE:O    | 1:B:347:MET:N    | 2.38                     | 0.55              |
| 1:D:317:SER:O    | 1:D:321:GLU:OE2  | 2.23                     | 0.55              |
| 1:A:470:ARG:CG   | 1:A:489:TRP:CE2  | 2.90                     | 0.55              |
| 1:C:208:LYS:HB2  | 1:C:208:LYS:HZ3  | 1.71                     | 0.55              |
| 1:B:470:ARG:CG   | 1:B:489:TRP:CE2  | 2.90                     | 0.55              |
| 1:D:370:ARG:HG2  | 1:D:376:TYR:O    | 2.04                     | 0.55              |
| 1:D:449:VAL:CG1  | 1:D:450:PRO:HD2  | 2.37                     | 0.55              |
| 1:A:216:LYS:O    | 1:A:219:THR:OG1  | 2.12                     | 0.55              |
| 1:A:316:GLN:O    | 1:A:320:LYS:NZ   | 2.40                     | 0.55              |
| 1:C:449:VAL:CG1  | 1:C:450:PRO:HD2  | 2.37                     | 0.55              |
| 1:A:216:LYS:HD2  | 1:A:219:THR:OG1  | 2.06                     | 0.55              |
| 1:C:345:ARG:HE   | 1:C:345:ARG:CA   | 2.20                     | 0.55              |
| 1:C:370:ARG:HG2  | 1:C:376:TYR:O    | 2.04                     | 0.55              |
| 1:B:216:LYS:HD2  | 1:B:219:THR:OG1  | 2.06                     | 0.55              |
| 1:B:316:GLN:O    | 1:B:320:LYS:NZ   | 2.40                     | 0.55              |
| 1:D:345:ARG:HE   | 1:D:345:ARG:CA   | 2.20                     | 0.55              |
| 1:D:479:LYS:HB3  | 1:D:479:LYS:HZ2  | 1.69                     | 0.55              |
| 1:D:490:HIS:O    | 1:D:496:ARG:NH1  | 2.40                     | 0.55              |
| 1:C:490:HIS:O    | 1:C:496:ARG:NH1  | 2.40                     | 0.55              |
| 1:C:314:ASP:CG   | 1:C:366:HIS:ND1  | 2.65                     | 0.55              |
| 1:B:345:ARG:HE   | 1:B:345:ARG:CA   | 2.20                     | 0.55              |
| 1:C:216:LYS:O    | 1:C:219:THR:OG1  | 2.12                     | 0.54              |
| 1:D:216:LYS:O    | 1:D:219:THR:OG1  | 2.12                     | 0.54              |
| 1:A:345:ARG:CA   | 1:A:345:ARG:HE   | 2.20                     | 0.54              |
| 1:B:331:PHE:HB3  | 1:B:336:VAL:HG22 | 1.89                     | 0.54              |
| 1:D:314:ASP:CG   | 1:D:366:HIS:ND1  | 2.65                     | 0.54              |
| 1:A:331:PHE:HB3  | 1:A:336:VAL:HG22 | 1.89                     | 0.54              |
| 1:A:505:ILE:HD11 | 1:A:531:CYS:C    | 2.32                     | 0.54              |
| 1:C:505:ILE:HD11 | 1:C:531:CYS:C    | 2.32                     | 0.54              |
| 1:B:366:HIS:CD2  | 1:B:382:CYS:HB2  | 2.43                     | 0.54              |
| 1:B:505:ILE:HD11 | 1:B:531:CYS:C    | 2.32                     | 0.54              |
| 1:D:315:LEU:HD13 | 1:D:367:LEU:CD1  | 2.37                     | 0.54              |
| 1:D:470:ARG:CG   | 1:D:489:TRP:CE2  | 2.90                     | 0.54              |
| 1:D:505:ILE:HD11 | 1:D:531:CYS:C    | 2.32                     | 0.54              |
| 1:A:1:MET:HE1    | 1:B:20:LEU:HD12  | 1.89                     | 0.54              |
| 1:A:315:LEU:HD13 | 1:A:367:LEU:CD1  | 2.37                     | 0.54              |
| 1:A:366:HIS:CD2  | 1:A:382:CYS:HB2  | 2.43                     | 0.54              |
| 1:C:55:LEU:HB2   | 1:D:23:ASP:HB3   | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:208:LYS:HB2  | 1:B:208:LYS:HZ3  | 1.71                     | 0.54              |
| 1:C:65:LEU:HA    | 1:C:122:GLU:HG2  | 1.90                     | 0.54              |
| 1:C:315:LEU:HD13 | 1:C:367:LEU:CD1  | 2.37                     | 0.54              |
| 1:C:316:GLN:O    | 1:C:320:LYS:NZ   | 2.40                     | 0.54              |
| 1:C:470:ARG:CG   | 1:C:489:TRP:CE2  | 2.90                     | 0.54              |
| 1:B:314:ASP:CG   | 1:B:366:HIS:ND1  | 2.65                     | 0.54              |
| 1:B:315:LEU:HD13 | 1:B:367:LEU:CD1  | 2.37                     | 0.54              |
| 1:D:316:GLN:O    | 1:D:320:LYS:NZ   | 2.40                     | 0.54              |
| 1:A:116:TYR:CD1  | 1:A:514:VAL:HG21 | 2.43                     | 0.54              |
| 1:A:310:LEU:CD2  | 1:A:311:MET:CE   | 2.86                     | 0.54              |
| 1:A:314:ASP:CG   | 1:A:366:HIS:ND1  | 2.65                     | 0.54              |
| 1:A:470:ARG:HH21 | 1:A:486:LYS:HE2  | 1.73                     | 0.54              |
| 1:C:331:PHE:HB3  | 1:C:336:VAL:HG22 | 1.89                     | 0.54              |
| 1:B:116:TYR:CD1  | 1:B:514:VAL:HG21 | 2.43                     | 0.54              |
| 1:B:470:ARG:HH21 | 1:B:486:LYS:HE2  | 1.73                     | 0.54              |
| 1:A:65:LEU:HA    | 1:A:122:GLU:HG2  | 1.90                     | 0.54              |
| 1:C:199:ASP:OD1  | 1:C:199:ASP:N    | 2.41                     | 0.54              |
| 1:C:366:HIS:CD2  | 1:C:382:CYS:HB2  | 2.43                     | 0.54              |
| 1:B:310:LEU:CD2  | 1:B:311:MET:CE   | 2.86                     | 0.54              |
| 1:B:490:HIS:O    | 1:B:496:ARG:NH1  | 2.40                     | 0.54              |
| 1:D:65:LEU:HA    | 1:D:122:GLU:HG2  | 1.90                     | 0.54              |
| 1:D:366:HIS:CD2  | 1:D:382:CYS:HB2  | 2.43                     | 0.54              |
| 1:A:490:HIS:O    | 1:A:496:ARG:NH1  | 2.40                     | 0.54              |
| 1:D:199:ASP:N    | 1:D:199:ASP:OD1  | 2.41                     | 0.54              |
| 1:D:331:PHE:HB3  | 1:D:336:VAL:HG22 | 1.89                     | 0.54              |
| 1:A:429:THR:OG1  | 1:A:432:ALA:CB   | 2.56                     | 0.54              |
| 1:C:116:TYR:CD1  | 1:C:514:VAL:HG21 | 2.43                     | 0.54              |
| 1:B:65:LEU:HA    | 1:B:122:GLU:HG2  | 1.90                     | 0.54              |
| 1:B:199:ASP:OD1  | 1:B:199:ASP:N    | 2.41                     | 0.54              |
| 1:B:429:THR:OG1  | 1:B:432:ALA:CB   | 2.56                     | 0.54              |
| 1:D:116:TYR:CD1  | 1:D:514:VAL:HG21 | 2.43                     | 0.54              |
| 1:A:199:ASP:N    | 1:A:199:ASP:OD1  | 2.41                     | 0.53              |
| 1:A:504:ARG:HA   | 1:A:507:ARG:HE   | 1.72                     | 0.53              |
| 1:B:473:PHE:HB3  | 1:B:474:PRO:HD2  | 1.91                     | 0.53              |
| 1:B:504:ARG:HA   | 1:B:507:ARG:HE   | 1.72                     | 0.53              |
| 1:D:473:PHE:HB3  | 1:D:474:PRO:HD2  | 1.91                     | 0.53              |
| 1:A:311:MET:SD   | 1:A:366:HIS:CE1  | 3.01                     | 0.53              |
| 1:A:473:PHE:HB3  | 1:A:474:PRO:HD2  | 1.91                     | 0.53              |
| 1:C:473:PHE:HB3  | 1:C:474:PRO:HD2  | 1.91                     | 0.53              |
| 1:B:311:MET:SD   | 1:B:366:HIS:CE1  | 3.01                     | 0.53              |
| 1:D:368:LYS:O    | 1:D:377:PHE:CD1  | 2.62                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:429:THR:OG1  | 1:A:432:ALA:HB2  | 2.09                     | 0.53              |
| 1:C:107:GLU:HA   | 1:C:110:ILE:HG12 | 1.89                     | 0.53              |
| 1:C:310:LEU:CD2  | 1:C:311:MET:CE   | 2.86                     | 0.53              |
| 1:C:368:LYS:O    | 1:C:377:PHE:CD1  | 2.62                     | 0.53              |
| 1:C:429:THR:OG1  | 1:C:432:ALA:HB2  | 2.09                     | 0.53              |
| 1:B:429:THR:OG1  | 1:B:432:ALA:HB2  | 2.09                     | 0.53              |
| 1:D:310:LEU:CD2  | 1:D:311:MET:CE   | 2.86                     | 0.53              |
| 1:D:429:THR:OG1  | 1:D:432:ALA:HB2  | 2.09                     | 0.53              |
| 1:A:107:GLU:HA   | 1:A:110:ILE:HG12 | 1.89                     | 0.53              |
| 1:C:336:VAL:CG1  | 1:C:340:MET:HE2  | 2.33                     | 0.53              |
| 1:B:107:GLU:HA   | 1:B:110:ILE:HG12 | 1.89                     | 0.53              |
| 1:B:570:LYS:HB2  | 1:B:570:LYS:HZ3  | 1.70                     | 0.53              |
| 1:D:107:GLU:HA   | 1:D:110:ILE:HG12 | 1.89                     | 0.53              |
| 1:C:311:MET:SD   | 1:C:366:HIS:CE1  | 3.01                     | 0.53              |
| 1:C:429:THR:OG1  | 1:C:432:ALA:CB   | 2.56                     | 0.53              |
| 1:D:311:MET:SD   | 1:D:366:HIS:CE1  | 3.01                     | 0.53              |
| 1:A:337:ILE:HA   | 1:A:340:MET:HE3  | 1.91                     | 0.53              |
| 1:C:505:ILE:CD1  | 1:C:531:CYS:HB3  | 2.36                     | 0.53              |
| 1:B:337:ILE:HA   | 1:B:340:MET:HE3  | 1.91                     | 0.53              |
| 1:D:505:ILE:CD1  | 1:D:531:CYS:HB3  | 2.36                     | 0.53              |
| 1:C:439:MET:CE   | 1:C:450:PRO:CG   | 2.86                     | 0.53              |
| 1:C:504:ARG:HA   | 1:C:507:ARG:HE   | 1.72                     | 0.53              |
| 1:D:429:THR:OG1  | 1:D:432:ALA:CB   | 2.56                     | 0.53              |
| 1:A:281:LEU:HD11 | 1:A:385:GLY:HA3  | 1.91                     | 0.53              |
| 1:B:281:LEU:HD11 | 1:B:385:GLY:HA3  | 1.91                     | 0.53              |
| 1:D:336:VAL:CG1  | 1:D:340:MET:HE2  | 2.33                     | 0.53              |
| 1:D:439:MET:CE   | 1:D:450:PRO:CG   | 2.87                     | 0.53              |
| 1:D:504:ARG:HA   | 1:D:507:ARG:HE   | 1.72                     | 0.53              |
| 1:B:439:MET:CE   | 1:B:450:PRO:CG   | 2.86                     | 0.53              |
| 1:A:439:MET:CE   | 1:A:450:PRO:CG   | 2.87                     | 0.52              |
| 1:A:442:PHE:CZ   | 1:A:489:TRP:HE3  | 2.25                     | 0.52              |
| 1:B:368:LYS:O    | 1:B:377:PHE:CD1  | 2.62                     | 0.52              |
| 1:B:442:PHE:CZ   | 1:B:489:TRP:HE3  | 2.25                     | 0.52              |
| 1:A:124:ILE:HG23 | 1:A:145:PHE:CE2  | 2.45                     | 0.52              |
| 1:A:169:LEU:HD11 | 1:A:557:PRO:CG   | 2.38                     | 0.52              |
| 1:A:370:ARG:CG   | 1:A:377:PHE:CA   | 2.84                     | 0.52              |
| 1:C:23:ASP:HB3   | 1:D:55:LEU:HB2   | 1.92                     | 0.52              |
| 1:C:443:GLU:O    | 1:C:447:GLY:N    | 2.29                     | 0.52              |
| 1:B:124:ILE:HG23 | 1:B:145:PHE:CE2  | 2.45                     | 0.52              |
| 1:B:370:ARG:CG   | 1:B:377:PHE:CA   | 2.84                     | 0.52              |
| 1:D:443:GLU:O    | 1:D:447:GLY:N    | 2.29                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:287:SER:O    | 1:A:378:HIS:CE1  | 2.62                     | 0.52              |
| 1:A:368:LYS:O    | 1:A:377:PHE:CD1  | 2.62                     | 0.52              |
| 1:C:310:LEU:HD22 | 1:C:311:MET:CE   | 2.40                     | 0.52              |
| 1:B:169:LEU:HD11 | 1:B:557:PRO:CG   | 2.38                     | 0.52              |
| 1:D:169:LEU:HD11 | 1:D:557:PRO:CG   | 2.38                     | 0.52              |
| 1:D:310:LEU:HD22 | 1:D:311:MET:CE   | 2.39                     | 0.52              |
| 1:A:310:LEU:HD22 | 1:A:311:MET:CE   | 2.39                     | 0.52              |
| 1:C:169:LEU:HD11 | 1:C:557:PRO:CG   | 2.38                     | 0.52              |
| 1:B:287:SER:O    | 1:B:378:HIS:CE1  | 2.62                     | 0.52              |
| 1:B:310:LEU:HD22 | 1:B:311:MET:CE   | 2.39                     | 0.52              |
| 1:A:505:ILE:CD1  | 1:A:531:CYS:HB3  | 2.36                     | 0.52              |
| 1:C:281:LEU:HD11 | 1:C:385:GLY:HA3  | 1.91                     | 0.52              |
| 1:D:281:LEU:HD11 | 1:D:385:GLY:HA3  | 1.91                     | 0.52              |
| 1:D:337:ILE:HA   | 1:D:340:MET:HE3  | 1.91                     | 0.52              |
| 1:C:337:ILE:HA   | 1:C:340:MET:HE3  | 1.91                     | 0.52              |
| 1:B:345:ARG:HE   | 1:B:345:ARG:HA   | 1.75                     | 0.52              |
| 1:B:429:THR:OG1  | 1:B:432:ALA:N    | 2.41                     | 0.52              |
| 1:A:310:LEU:CD2  | 1:A:311:MET:N    | 2.53                     | 0.52              |
| 1:A:345:ARG:HE   | 1:A:345:ARG:HA   | 1.75                     | 0.52              |
| 1:C:335:VAL:HG12 | 1:C:376:TYR:CD2  | 2.44                     | 0.52              |
| 1:B:310:LEU:CD2  | 1:B:311:MET:N    | 2.53                     | 0.52              |
| 1:B:315:LEU:HD13 | 1:B:367:LEU:HD11 | 1.92                     | 0.52              |
| 1:B:505:ILE:CD1  | 1:B:531:CYS:HB3  | 2.36                     | 0.52              |
| 1:D:370:ARG:CG   | 1:D:377:PHE:N    | 2.73                     | 0.52              |
| 1:A:315:LEU:HD13 | 1:A:367:LEU:HD11 | 1.92                     | 0.52              |
| 1:A:370:ARG:CG   | 1:A:377:PHE:N    | 2.73                     | 0.52              |
| 1:C:287:SER:O    | 1:C:378:HIS:CE1  | 2.62                     | 0.52              |
| 1:B:370:ARG:CG   | 1:B:377:PHE:N    | 2.73                     | 0.52              |
| 1:C:370:ARG:CG   | 1:C:377:PHE:N    | 2.73                     | 0.51              |
| 1:D:335:VAL:HG12 | 1:D:376:TYR:CD2  | 2.44                     | 0.51              |
| 1:D:170:SER:CA   | 1:D:173:ILE:N    | 2.73                     | 0.51              |
| 1:D:408:ALA:CA   | 1:D:435:TYR:CD2  | 2.74                     | 0.51              |
| 1:A:335:VAL:HG12 | 1:A:376:TYR:CD2  | 2.44                     | 0.51              |
| 1:C:170:SER:CA   | 1:C:173:ILE:N    | 2.72                     | 0.51              |
| 1:C:345:ARG:HE   | 1:C:345:ARG:HA   | 1.75                     | 0.51              |
| 1:B:335:VAL:HG12 | 1:B:376:TYR:CD2  | 2.44                     | 0.51              |
| 1:D:287:SER:O    | 1:D:378:HIS:CE1  | 2.62                     | 0.51              |
| 1:D:315:LEU:HD13 | 1:D:367:LEU:HD11 | 1.92                     | 0.51              |
| 1:D:345:ARG:HE   | 1:D:345:ARG:HA   | 1.75                     | 0.51              |
| 1:B:570:LYS:NZ   | 1:B:570:LYS:CB   | 2.73                     | 0.51              |
| 1:D:124:ILE:HG23 | 1:D:145:PHE:CE2  | 2.45                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:315:LEU:HD13 | 1:C:367:LEU:HD11 | 1.92                     | 0.51              |
| 1:A:570:LYS:NZ   | 1:A:570:LYS:CB   | 2.73                     | 0.51              |
| 1:C:53:LEU:HG    | 1:C:126:ALA:HB2  | 1.91                     | 0.51              |
| 1:C:124:ILE:HG23 | 1:C:145:PHE:CE2  | 2.45                     | 0.51              |
| 1:C:442:PHE:CG   | 1:C:473:PHE:HZ   | 2.29                     | 0.51              |
| 1:B:411:VAL:C    | 1:B:414:GLU:OE2  | 2.54                     | 0.51              |
| 1:D:442:PHE:CG   | 1:D:473:PHE:HZ   | 2.29                     | 0.51              |
| 1:A:104:ASP:OD1  | 1:A:181:TRP:NE1  | 2.40                     | 0.51              |
| 1:A:411:VAL:C    | 1:A:414:GLU:OE2  | 2.54                     | 0.51              |
| 1:C:408:ALA:CA   | 1:C:435:TYR:CD2  | 2.74                     | 0.51              |
| 1:C:411:VAL:C    | 1:C:414:GLU:OE2  | 2.54                     | 0.51              |
| 1:B:104:ASP:OD1  | 1:B:181:TRP:NE1  | 2.40                     | 0.51              |
| 1:B:449:VAL:CG1  | 1:B:450:PRO:HD2  | 2.37                     | 0.51              |
| 1:A:449:VAL:CG1  | 1:A:450:PRO:HD2  | 2.37                     | 0.51              |
| 1:C:104:ASP:OD1  | 1:C:181:TRP:NE1  | 2.40                     | 0.51              |
| 1:C:341:LEU:HD21 | 1:C:345:ARG:HG3  | 1.93                     | 0.51              |
| 1:D:53:LEU:HG    | 1:D:126:ALA:HB2  | 1.91                     | 0.51              |
| 1:D:411:VAL:C    | 1:D:414:GLU:OE2  | 2.54                     | 0.51              |
| 1:B:53:LEU:HD21  | 1:B:126:ALA:HB2  | 1.93                     | 0.51              |
| 1:B:53:LEU:HG    | 1:B:126:ALA:HB2  | 1.91                     | 0.51              |
| 1:A:53:LEU:HD21  | 1:A:126:ALA:HB2  | 1.93                     | 0.51              |
| 1:A:53:LEU:HG    | 1:A:126:ALA:HB2  | 1.91                     | 0.51              |
| 1:A:71:GLU:OE2   | 1:A:74:ARG:NH1   | 2.44                     | 0.51              |
| 1:B:71:GLU:OE2   | 1:B:74:ARG:NH1   | 2.44                     | 0.51              |
| 1:D:341:LEU:HD21 | 1:D:345:ARG:HG3  | 1.93                     | 0.51              |
| 1:C:280:SER:C    | 1:C:282:LEU:H    | 2.19                     | 0.50              |
| 1:D:104:ASP:OD1  | 1:D:181:TRP:NE1  | 2.40                     | 0.50              |
| 1:A:430:HIS:O    | 1:A:433:ASP:OD1  | 2.30                     | 0.50              |
| 1:C:412:LEU:C    | 1:C:414:GLU:OE1  | 2.55                     | 0.50              |
| 1:C:429:THR:OG1  | 1:C:432:ALA:N    | 2.41                     | 0.50              |
| 1:B:368:LYS:O    | 1:B:377:PHE:HD1  | 1.95                     | 0.50              |
| 1:B:430:HIS:O    | 1:B:433:ASP:OD1  | 2.30                     | 0.50              |
| 1:D:412:LEU:C    | 1:D:414:GLU:OE1  | 2.55                     | 0.50              |
| 1:A:170:SER:CA   | 1:A:173:ILE:N    | 2.73                     | 0.50              |
| 1:A:368:LYS:O    | 1:A:377:PHE:HD1  | 1.95                     | 0.50              |
| 1:D:430:HIS:O    | 1:D:433:ASP:OD1  | 2.29                     | 0.50              |
| 1:A:408:ALA:CB   | 1:A:411:VAL:HG22 | 2.39                     | 0.50              |
| 1:A:412:LEU:C    | 1:A:414:GLU:OE1  | 2.55                     | 0.50              |
| 1:C:430:HIS:O    | 1:C:433:ASP:OD1  | 2.30                     | 0.50              |
| 1:B:170:SER:CA   | 1:B:173:ILE:N    | 2.73                     | 0.50              |
| 1:D:280:SER:C    | 1:D:282:LEU:H    | 2.19                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:71:GLU:OE2   | 1:C:74:ARG:NH1   | 2.44                     | 0.50              |
| 1:B:408:ALA:CB   | 1:B:411:VAL:HG22 | 2.39                     | 0.50              |
| 1:B:412:LEU:C    | 1:B:414:GLU:OE1  | 2.55                     | 0.50              |
| 1:D:71:GLU:OE2   | 1:D:74:ARG:NH1   | 2.44                     | 0.50              |
| 1:D:74:ARG:NH2   | 1:D:376:TYR:HE1  | 2.09                     | 0.50              |
| 1:C:368:LYS:O    | 1:C:377:PHE:HD1  | 1.95                     | 0.50              |
| 1:D:368:LYS:O    | 1:D:377:PHE:HD1  | 1.95                     | 0.50              |
| 1:D:429:THR:OG1  | 1:D:432:ALA:N    | 2.41                     | 0.50              |
| 1:D:470:ARG:HH21 | 1:D:486:LYS:HE2  | 1.73                     | 0.50              |
| 1:C:74:ARG:NH2   | 1:C:376:TYR:HE1  | 2.09                     | 0.50              |
| 1:A:516:ASN:HD22 | 1:A:516:ASN:N    | 2.08                     | 0.50              |
| 1:C:408:ALA:CB   | 1:C:411:VAL:HG22 | 2.39                     | 0.50              |
| 1:C:470:ARG:HH21 | 1:C:486:LYS:HE2  | 1.73                     | 0.50              |
| 1:B:516:ASN:HD22 | 1:B:516:ASN:N    | 2.08                     | 0.50              |
| 1:D:442:PHE:CZ   | 1:D:489:TRP:HE3  | 2.25                     | 0.50              |
| 1:A:199:ASP:HB3  | 1:A:208:LYS:HG2  | 1.94                     | 0.50              |
| 1:B:199:ASP:HB3  | 1:B:208:LYS:HG2  | 1.94                     | 0.50              |
| 1:A:442:PHE:CG   | 1:A:473:PHE:HZ   | 2.29                     | 0.49              |
| 1:C:199:ASP:CB   | 1:C:208:LYS:CD   | 2.83                     | 0.49              |
| 1:B:442:PHE:CG   | 1:B:473:PHE:HZ   | 2.29                     | 0.49              |
| 1:D:41:ALA:HB1   | 1:D:117:PHE:HE2  | 1.77                     | 0.49              |
| 1:C:41:ALA:HB1   | 1:C:117:PHE:HE2  | 1.77                     | 0.49              |
| 1:C:199:ASP:HB3  | 1:C:208:LYS:HG2  | 1.94                     | 0.49              |
| 1:C:541:LYS:HB3  | 1:C:541:LYS:HZ3  | 1.76                     | 0.49              |
| 1:B:57:GLU:OE1   | 1:B:57:GLU:N     | 2.43                     | 0.49              |
| 1:D:199:ASP:CB   | 1:D:208:LYS:CD   | 2.83                     | 0.49              |
| 1:D:199:ASP:HB3  | 1:D:208:LYS:HG2  | 1.94                     | 0.49              |
| 1:D:408:ALA:CB   | 1:D:411:VAL:HG22 | 2.39                     | 0.49              |
| 1:A:57:GLU:OE1   | 1:A:57:GLU:N     | 2.43                     | 0.49              |
| 1:A:341:LEU:HD21 | 1:A:345:ARG:HG3  | 1.93                     | 0.49              |
| 1:C:20:LEU:HD12  | 1:D:1:MET:HE1    | 1.94                     | 0.49              |
| 1:B:341:LEU:HD21 | 1:B:345:ARG:HG3  | 1.93                     | 0.49              |
| 1:D:541:LYS:HB3  | 1:D:541:LYS:HZ3  | 1.76                     | 0.49              |
| 1:C:284:LEU:HD23 | 1:C:353:ASN:ND2  | 2.26                     | 0.49              |
| 1:C:442:PHE:CZ   | 1:C:489:TRP:HE3  | 2.25                     | 0.49              |
| 1:C:516:ASN:ND2  | 1:C:516:ASN:N    | 2.60                     | 0.49              |
| 1:B:41:ALA:HB1   | 1:B:117:PHE:HE2  | 1.76                     | 0.49              |
| 1:A:23:ASP:HB3   | 1:B:55:LEU:HB2   | 1.93                     | 0.49              |
| 1:C:333:ILE:O    | 1:C:337:ILE:CG1  | 2.61                     | 0.49              |
| 1:D:284:LEU:HD23 | 1:D:353:ASN:ND2  | 2.26                     | 0.49              |
| 1:D:333:ILE:O    | 1:D:337:ILE:CG1  | 2.61                     | 0.49              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:516:ASN:ND2  | 1:D:516:ASN:N   | 2.60                     | 0.49              |
| 1:A:41:ALA:HB1   | 1:A:117:PHE:HE2 | 1.77                     | 0.49              |
| 1:A:411:VAL:O    | 1:A:414:GLU:OE1 | 2.31                     | 0.49              |
| 1:A:554:ASN:O    | 1:A:557:PRO:HD2 | 2.13                     | 0.49              |
| 1:B:411:VAL:O    | 1:B:414:GLU:OE1 | 2.31                     | 0.49              |
| 1:A:184:ASP:N    | 1:A:184:ASP:OD1 | 2.46                     | 0.49              |
| 1:B:199:ASP:OD2  | 1:B:208:LYS:HD3 | 2.13                     | 0.49              |
| 1:B:280:SER:C    | 1:B:282:LEU:H   | 2.19                     | 0.49              |
| 1:A:333:ILE:O    | 1:A:337:ILE:CG1 | 2.61                     | 0.49              |
| 1:A:338:ASP:OD1  | 1:A:342:GLN:NE2 | 2.46                     | 0.49              |
| 1:A:484:LEU:C    | 1:A:484:LEU:CD2 | 2.85                     | 0.49              |
| 1:B:333:ILE:O    | 1:B:337:ILE:CG1 | 2.61                     | 0.49              |
| 1:B:338:ASP:OD1  | 1:B:342:GLN:NE2 | 2.46                     | 0.49              |
| 1:B:484:LEU:C    | 1:B:484:LEU:CD2 | 2.85                     | 0.49              |
| 1:B:554:ASN:O    | 1:B:557:PRO:HD2 | 2.13                     | 0.49              |
| 1:A:199:ASP:OD2  | 1:A:208:LYS:HD3 | 2.13                     | 0.49              |
| 1:B:284:LEU:HD23 | 1:B:353:ASN:ND2 | 2.26                     | 0.49              |
| 1:A:280:SER:C    | 1:A:282:LEU:H   | 2.19                     | 0.48              |
| 1:C:57:GLU:OE1   | 1:C:57:GLU:N    | 2.43                     | 0.48              |
| 1:A:284:LEU:HD23 | 1:A:353:ASN:ND2 | 2.26                     | 0.48              |
| 1:C:338:ASP:OD1  | 1:C:342:GLN:NE2 | 2.46                     | 0.48              |
| 1:C:492:GLU:HB2  | 1:C:495:GLN:NE2 | 2.29                     | 0.48              |
| 1:C:570:LYS:HB2  | 1:C:570:LYS:HZ3 | 1.77                     | 0.48              |
| 1:D:57:GLU:OE1   | 1:D:57:GLU:N    | 2.43                     | 0.48              |
| 1:D:121:VAL:HG11 | 1:D:564:ARG:NH1 | 2.11                     | 0.48              |
| 1:D:338:ASP:OD1  | 1:D:342:GLN:NE2 | 2.46                     | 0.48              |
| 1:D:492:GLU:HB2  | 1:D:495:GLN:NE2 | 2.29                     | 0.48              |
| 1:B:411:VAL:HG11 | 1:B:427:LYS:CB  | 2.38                     | 0.48              |
| 1:C:173:ILE:HB   | 1:C:176:ARG:CB  | 2.44                     | 0.48              |
| 1:B:360:LEU:HB3  | 1:B:436:SER:CB  | 2.43                     | 0.48              |
| 1:D:173:ILE:HB   | 1:D:176:ARG:CB  | 2.44                     | 0.48              |
| 1:A:332:SER:C    | 1:A:334:PRO:N   | 2.69                     | 0.48              |
| 1:C:556:ILE:N    | 1:C:557:PRO:HD2 | 2.29                     | 0.48              |
| 1:D:556:ILE:N    | 1:D:557:PRO:HD2 | 2.29                     | 0.48              |
| 1:D:570:LYS:HB2  | 1:D:570:LYS:HZ3 | 1.77                     | 0.48              |
| 1:A:411:VAL:HG11 | 1:A:427:LYS:CB  | 2.37                     | 0.48              |
| 1:C:332:SER:C    | 1:C:334:PRO:N   | 2.69                     | 0.48              |
| 1:B:312:HIS:NE2  | 1:B:368:LYS:CE  | 2.76                     | 0.48              |
| 1:B:332:SER:C    | 1:B:334:PRO:N   | 2.69                     | 0.48              |
| 1:B:470:ARG:HD3  | 1:B:489:TRP:CG  | 2.36                     | 0.48              |
| 1:D:310:LEU:HD21 | 1:D:311:MET:O   | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:312:HIS:NE2  | 1:A:368:LYS:CE   | 2.76                     | 0.48              |
| 1:B:556:ILE:N    | 1:B:557:PRO:HD2  | 2.29                     | 0.48              |
| 1:D:411:VAL:O    | 1:D:414:GLU:OE1  | 2.31                     | 0.48              |
| 1:A:95:LYS:O     | 1:A:99:LEU:HB2   | 2.13                     | 0.48              |
| 1:A:556:ILE:N    | 1:A:557:PRO:HD2  | 2.29                     | 0.48              |
| 1:C:310:LEU:HD21 | 1:C:311:MET:O    | 2.14                     | 0.48              |
| 1:C:411:VAL:O    | 1:C:414:GLU:OE1  | 2.31                     | 0.48              |
| 1:B:95:LYS:O     | 1:B:99:LEU:HB2   | 2.14                     | 0.48              |
| 1:D:199:ASP:CG   | 1:D:208:LYS:HD3  | 2.39                     | 0.48              |
| 1:D:312:HIS:NE2  | 1:D:368:LYS:CE   | 2.76                     | 0.48              |
| 1:A:429:THR:OG1  | 1:A:432:ALA:N    | 2.41                     | 0.48              |
| 1:A:470:ARG:HD3  | 1:A:489:TRP:CG   | 2.36                     | 0.48              |
| 1:C:184:ASP:OD1  | 1:C:185:ARG:N    | 2.47                     | 0.48              |
| 1:C:199:ASP:OD2  | 1:C:208:LYS:HD3  | 2.13                     | 0.48              |
| 1:C:199:ASP:CG   | 1:C:208:LYS:HD3  | 2.39                     | 0.48              |
| 1:C:312:HIS:NE2  | 1:C:368:LYS:CE   | 2.76                     | 0.48              |
| 1:B:199:ASP:CG   | 1:B:208:LYS:HD3  | 2.39                     | 0.48              |
| 1:A:199:ASP:CG   | 1:A:208:LYS:HD3  | 2.39                     | 0.48              |
| 1:A:411:VAL:O    | 1:A:414:GLU:OE2  | 2.31                     | 0.48              |
| 1:C:121:VAL:HG11 | 1:C:564:ARG:NH1  | 2.11                     | 0.48              |
| 1:B:37:LEU:CD1   | 1:B:177:PHE:HE1  | 2.25                     | 0.48              |
| 1:B:411:VAL:O    | 1:B:414:GLU:OE2  | 2.31                     | 0.48              |
| 1:B:492:GLU:HB2  | 1:B:495:GLN:NE2  | 2.29                     | 0.48              |
| 1:D:184:ASP:OD1  | 1:D:185:ARG:N    | 2.47                     | 0.48              |
| 1:D:199:ASP:OD2  | 1:D:208:LYS:HD3  | 2.13                     | 0.48              |
| 1:A:492:GLU:HB2  | 1:A:495:GLN:NE2  | 2.29                     | 0.47              |
| 1:C:95:LYS:O     | 1:C:99:LEU:HB2   | 2.14                     | 0.47              |
| 1:D:95:LYS:O     | 1:D:99:LEU:HB2   | 2.13                     | 0.47              |
| 1:D:216:LYS:CA   | 1:D:219:THR:HG23 | 2.43                     | 0.47              |
| 1:A:37:LEU:CD1   | 1:A:177:PHE:HE1  | 2.25                     | 0.47              |
| 1:C:312:HIS:NE2  | 1:C:368:LYS:CD   | 2.76                     | 0.47              |
| 1:C:554:ASN:O    | 1:C:557:PRO:HD2  | 2.13                     | 0.47              |
| 1:D:332:SER:C    | 1:D:334:PRO:N    | 2.69                     | 0.47              |
| 1:A:216:LYS:CA   | 1:A:219:THR:HG23 | 2.43                     | 0.47              |
| 1:C:216:LYS:CA   | 1:C:219:THR:HG23 | 2.43                     | 0.47              |
| 1:C:404:VAL:O    | 1:C:404:VAL:CG1  | 2.62                     | 0.47              |
| 1:D:411:VAL:O    | 1:D:414:GLU:OE2  | 2.31                     | 0.47              |
| 1:D:554:ASN:O    | 1:D:557:PRO:HD2  | 2.13                     | 0.47              |
| 1:A:516:ASN:ND2  | 1:A:516:ASN:N    | 2.60                     | 0.47              |
| 1:C:360:LEU:HB3  | 1:C:436:SER:CB   | 2.43                     | 0.47              |
| 1:C:411:VAL:O    | 1:C:414:GLU:OE2  | 2.31                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:74:ARG:NH2   | 1:B:376:TYR:HE1  | 2.09                     | 0.47              |
| 1:B:216:LYS:CA   | 1:B:219:THR:HG23 | 2.43                     | 0.47              |
| 1:B:516:ASN:ND2  | 1:B:516:ASN:N    | 2.60                     | 0.47              |
| 1:D:53:LEU:HD23  | 1:D:53:LEU:HA    | 1.78                     | 0.47              |
| 1:D:312:HIS:NE2  | 1:D:368:LYS:CD   | 2.76                     | 0.47              |
| 1:A:74:ARG:NH2   | 1:A:376:TYR:HE1  | 2.09                     | 0.47              |
| 1:A:361:ASN:O    | 1:A:364:ASN:N    | 2.45                     | 0.47              |
| 1:A:374:GLU:N    | 1:A:374:GLU:CD   | 2.73                     | 0.47              |
| 1:C:439:MET:SD   | 1:C:442:PHE:CE2  | 3.08                     | 0.47              |
| 1:B:361:ASN:O    | 1:B:364:ASN:N    | 2.45                     | 0.47              |
| 1:D:404:VAL:O    | 1:D:404:VAL:CG1  | 2.62                     | 0.47              |
| 1:C:439:MET:CE   | 1:C:442:PHE:HD2  | 2.27                     | 0.47              |
| 1:B:310:LEU:HD21 | 1:B:311:MET:O    | 2.14                     | 0.47              |
| 1:B:374:GLU:N    | 1:B:374:GLU:CD   | 2.73                     | 0.47              |
| 1:B:487:ARG:HG2  | 1:B:532:TRP:CD1  | 2.50                     | 0.47              |
| 1:D:81:LEU:CD1   | 1:D:372:HIS:CE1  | 2.80                     | 0.47              |
| 1:D:360:LEU:HB3  | 1:D:436:SER:CB   | 2.43                     | 0.47              |
| 1:D:439:MET:SD   | 1:D:442:PHE:CE2  | 3.08                     | 0.47              |
| 1:A:33:LEU:CD2   | 1:A:177:PHE:HD1  | 2.24                     | 0.47              |
| 1:A:169:LEU:HD21 | 1:A:557:PRO:CG   | 2.44                     | 0.47              |
| 1:A:199:ASP:CB   | 1:A:208:LYS:CD   | 2.83                     | 0.47              |
| 1:A:310:LEU:HD21 | 1:A:311:MET:O    | 2.14                     | 0.47              |
| 1:A:409:PRO:O    | 1:A:412:LEU:HB2  | 2.14                     | 0.47              |
| 1:A:439:MET:SD   | 1:A:442:PHE:CE2  | 3.08                     | 0.47              |
| 1:A:487:ARG:HG2  | 1:A:532:TRP:CD1  | 2.50                     | 0.47              |
| 1:C:55:LEU:HD22  | 1:D:20:LEU:HB3   | 1.94                     | 0.47              |
| 1:C:313:LYS:HD2  | 1:C:318:TYR:OH   | 2.15                     | 0.47              |
| 1:C:341:LEU:CD2  | 1:C:345:ARG:HG3  | 2.45                     | 0.47              |
| 1:C:409:PRO:O    | 1:C:412:LEU:HB2  | 2.14                     | 0.47              |
| 1:C:487:ARG:HG2  | 1:C:532:TRP:CD1  | 2.50                     | 0.47              |
| 1:B:33:LEU:CD2   | 1:B:177:PHE:HD1  | 2.24                     | 0.47              |
| 1:B:439:MET:SD   | 1:B:442:PHE:CE2  | 3.08                     | 0.47              |
| 1:B:492:GLU:HB2  | 1:B:495:GLN:CD   | 2.40                     | 0.47              |
| 1:D:313:LYS:HD2  | 1:D:318:TYR:OH   | 2.15                     | 0.47              |
| 1:D:341:LEU:CD2  | 1:D:345:ARG:HG3  | 2.45                     | 0.47              |
| 1:D:409:PRO:O    | 1:D:412:LEU:HB2  | 2.14                     | 0.47              |
| 1:D:487:ARG:HG2  | 1:D:532:TRP:CD1  | 2.50                     | 0.47              |
| 1:A:173:ILE:HB   | 1:A:176:ARG:CB   | 2.44                     | 0.47              |
| 1:A:414:GLU:N    | 1:A:414:GLU:CD   | 2.73                     | 0.47              |
| 1:A:492:GLU:HB2  | 1:A:495:GLN:CD   | 2.40                     | 0.47              |
| 1:C:88:ASP:O     | 1:C:95:LYS:HE3   | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:169:LEU:HD21 | 1:B:557:PRO:CG   | 2.44                     | 0.47              |
| 1:D:439:MET:CE   | 1:D:442:PHE:HD2  | 2.27                     | 0.47              |
| 1:B:53:LEU:CG    | 1:B:126:ALA:HB2  | 2.45                     | 0.47              |
| 1:B:199:ASP:CB   | 1:B:208:LYS:CD   | 2.83                     | 0.47              |
| 1:B:409:PRO:O    | 1:B:412:LEU:HB2  | 2.14                     | 0.47              |
| 1:B:414:GLU:N    | 1:B:414:GLU:CD   | 2.73                     | 0.47              |
| 1:D:88:ASP:O     | 1:D:95:LYS:HE3   | 2.15                     | 0.47              |
| 1:A:53:LEU:CG    | 1:A:126:ALA:HB2  | 2.45                     | 0.47              |
| 1:A:529:VAL:HG22 | 1:A:530:ASP:H    | 1.80                     | 0.47              |
| 1:B:173:ILE:HB   | 1:B:176:ARG:CB   | 2.44                     | 0.47              |
| 1:B:529:VAL:HG22 | 1:B:530:ASP:H    | 1.80                     | 0.47              |
| 1:A:439:MET:CE   | 1:A:442:PHE:HD2  | 2.27                     | 0.46              |
| 1:C:81:LEU:CD1   | 1:C:372:HIS:CE1  | 2.80                     | 0.46              |
| 1:C:529:VAL:HG22 | 1:C:530:ASP:H    | 1.80                     | 0.46              |
| 1:A:20:LEU:HD12  | 1:B:1:MET:HE1    | 1.97                     | 0.46              |
| 1:A:354:ASP:O    | 1:A:356:PHE:CE2  | 2.69                     | 0.46              |
| 1:B:53:LEU:HD23  | 1:B:53:LEU:HA    | 1.79                     | 0.46              |
| 1:B:354:ASP:O    | 1:B:356:PHE:CE2  | 2.69                     | 0.46              |
| 1:B:439:MET:CE   | 1:B:442:PHE:HD2  | 2.27                     | 0.46              |
| 1:A:341:LEU:CD2  | 1:A:345:ARG:HG3  | 2.45                     | 0.46              |
| 1:B:341:LEU:CD2  | 1:B:345:ARG:HG3  | 2.45                     | 0.46              |
| 1:D:489:TRP:O    | 1:D:489:TRP:HD1  | 1.99                     | 0.46              |
| 1:A:53:LEU:HD23  | 1:A:53:LEU:HA    | 1.78                     | 0.46              |
| 1:C:489:TRP:HD1  | 1:C:489:TRP:O    | 1.99                     | 0.46              |
| 1:B:54:LYS:HB2   | 1:B:57:GLU:OE2   | 2.15                     | 0.46              |
| 1:A:54:LYS:HB2   | 1:A:57:GLU:OE2   | 2.15                     | 0.46              |
| 1:A:360:LEU:HB3  | 1:A:436:SER:CB   | 2.43                     | 0.46              |
| 1:C:335:VAL:O    | 1:C:339:ILE:HG13 | 2.16                     | 0.46              |
| 1:D:529:VAL:HG22 | 1:D:530:ASP:H    | 1.80                     | 0.46              |
| 1:A:57:GLU:H     | 1:A:57:GLU:CD    | 2.24                     | 0.46              |
| 1:A:122:GLU:C    | 1:A:124:ILE:N    | 2.73                     | 0.46              |
| 1:A:182:ARG:NH1  | 1:D:190:GLU:OE1  | 2.49                     | 0.46              |
| 1:A:208:LYS:HB2  | 1:A:208:LYS:HZ2  | 1.78                     | 0.46              |
| 1:A:216:LYS:HA   | 1:A:219:THR:HG21 | 1.96                     | 0.46              |
| 1:A:404:VAL:O    | 1:A:404:VAL:CG1  | 2.62                     | 0.46              |
| 1:C:169:LEU:HD21 | 1:C:557:PRO:CG   | 2.44                     | 0.46              |
| 1:C:414:GLU:N    | 1:C:414:GLU:CD   | 2.73                     | 0.46              |
| 1:B:57:GLU:H     | 1:B:57:GLU:CD    | 2.24                     | 0.46              |
| 1:D:54:LYS:HB2   | 1:D:57:GLU:OE2   | 2.15                     | 0.46              |
| 1:D:215:LEU:C    | 1:D:215:LEU:HD12 | 2.41                     | 0.46              |
| 1:D:335:VAL:O    | 1:D:339:ILE:HG13 | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:374:GLU:N    | 1:D:374:GLU:CD   | 2.73                     | 0.46              |
| 1:C:215:LEU:C    | 1:C:215:LEU:HD12 | 2.41                     | 0.46              |
| 1:C:335:VAL:HG12 | 1:C:376:TYR:CE2  | 2.51                     | 0.46              |
| 1:C:354:ASP:O    | 1:C:356:PHE:CE2  | 2.69                     | 0.46              |
| 1:C:374:GLU:N    | 1:C:374:GLU:CD   | 2.73                     | 0.46              |
| 1:C:449:VAL:HG13 | 1:C:450:PRO:CD   | 2.43                     | 0.46              |
| 1:B:122:GLU:C    | 1:B:124:ILE:N    | 2.73                     | 0.46              |
| 1:B:404:VAL:O    | 1:B:404:VAL:CG1  | 2.62                     | 0.46              |
| 1:D:169:LEU:HD21 | 1:D:557:PRO:CG   | 2.44                     | 0.46              |
| 1:D:354:ASP:O    | 1:D:356:PHE:CE2  | 2.69                     | 0.46              |
| 1:D:414:GLU:N    | 1:D:414:GLU:CD   | 2.73                     | 0.46              |
| 1:D:449:VAL:HG13 | 1:D:450:PRO:CD   | 2.43                     | 0.46              |
| 1:A:313:LYS:HD2  | 1:A:318:TYR:OH   | 2.15                     | 0.46              |
| 1:A:470:ARG:HD2  | 1:A:489:TRP:CD1  | 2.41                     | 0.46              |
| 1:C:54:LYS:HB2   | 1:C:57:GLU:OE2   | 2.15                     | 0.46              |
| 1:B:216:LYS:HA   | 1:B:219:THR:HG21 | 1.96                     | 0.46              |
| 1:B:470:ARG:HD2  | 1:B:489:TRP:CD1  | 2.41                     | 0.46              |
| 1:D:356:PHE:CE1  | 1:D:430:HIS:HA   | 2.51                     | 0.46              |
| 1:D:570:LYS:NZ   | 1:D:570:LYS:CB   | 2.73                     | 0.46              |
| 1:A:335:VAL:O    | 1:A:339:ILE:HG13 | 2.16                     | 0.46              |
| 1:C:20:LEU:HB3   | 1:D:55:LEU:HD22  | 1.97                     | 0.46              |
| 1:C:370:ARG:HB2  | 1:C:373:THR:OG1  | 2.16                     | 0.46              |
| 1:B:313:LYS:HD2  | 1:B:318:TYR:OH   | 2.15                     | 0.46              |
| 1:B:335:VAL:O    | 1:B:339:ILE:HG13 | 2.16                     | 0.46              |
| 1:B:490:HIS:O    | 1:B:496:ARG:CZ   | 2.64                     | 0.46              |
| 1:D:335:VAL:HG12 | 1:D:376:TYR:CE2  | 2.51                     | 0.46              |
| 1:D:370:ARG:HB2  | 1:D:373:THR:OG1  | 2.16                     | 0.46              |
| 1:D:446:THR:HG23 | 1:D:473:PHE:CD2  | 2.51                     | 0.46              |
| 1:D:490:HIS:O    | 1:D:496:ARG:CZ   | 2.64                     | 0.46              |
| 1:A:490:HIS:O    | 1:A:496:ARG:CZ   | 2.64                     | 0.46              |
| 1:C:88:ASP:OD1   | 1:C:89:ASN:N     | 2.49                     | 0.46              |
| 1:C:184:ASP:OD1  | 1:C:184:ASP:N    | 2.46                     | 0.46              |
| 1:C:356:PHE:CE1  | 1:C:430:HIS:HA   | 2.51                     | 0.46              |
| 1:C:446:THR:HG23 | 1:C:473:PHE:CD2  | 2.51                     | 0.46              |
| 1:C:470:ARG:CB   | 1:C:489:TRP:HE1  | 2.02                     | 0.46              |
| 1:C:490:HIS:O    | 1:C:496:ARG:CZ   | 2.64                     | 0.46              |
| 1:B:356:PHE:CE1  | 1:B:430:HIS:HA   | 2.51                     | 0.46              |
| 1:D:492:GLU:HB2  | 1:D:495:GLN:CD   | 2.40                     | 0.46              |
| 1:A:88:ASP:OD1   | 1:A:89:ASN:N     | 2.49                     | 0.45              |
| 1:A:171:ARG:O    | 1:A:173:ILE:CA   | 2.64                     | 0.45              |
| 1:A:356:PHE:CE1  | 1:A:430:HIS:HA   | 2.51                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:492:GLU:HB2  | 1:C:495:GLN:CD   | 2.40                     | 0.45              |
| 1:B:88:ASP:OD1   | 1:B:89:ASN:N     | 2.49                     | 0.45              |
| 1:D:21:GLN:HE21  | 1:D:28:GLN:HB2   | 1.81                     | 0.45              |
| 1:D:88:ASP:OD1   | 1:D:89:ASN:N     | 2.49                     | 0.45              |
| 1:D:171:ARG:O    | 1:D:173:ILE:CA   | 2.64                     | 0.45              |
| 1:D:184:ASP:OD1  | 1:D:184:ASP:N    | 2.46                     | 0.45              |
| 1:A:184:ASP:OD1  | 1:A:185:ARG:N    | 2.47                     | 0.45              |
| 1:C:21:GLN:HE21  | 1:C:28:GLN:HB2   | 1.81                     | 0.45              |
| 1:C:53:LEU:CG    | 1:C:126:ALA:HB2  | 2.45                     | 0.45              |
| 1:C:171:ARG:O    | 1:C:173:ILE:CA   | 2.64                     | 0.45              |
| 1:C:570:LYS:NZ   | 1:C:570:LYS:CB   | 2.73                     | 0.45              |
| 1:B:152:GLU:OE2  | 1:D:147:ARG:NH2  | 2.49                     | 0.45              |
| 1:B:312:HIS:NE2  | 1:B:368:LYS:CD   | 2.76                     | 0.45              |
| 1:B:475:PHE:N    | 1:B:476:PRO:CD   | 2.78                     | 0.45              |
| 1:D:53:LEU:CG    | 1:D:126:ALA:HB2  | 2.45                     | 0.45              |
| 1:D:484:LEU:C    | 1:D:484:LEU:CD2  | 2.85                     | 0.45              |
| 1:A:88:ASP:O     | 1:A:95:LYS:HE3   | 2.15                     | 0.45              |
| 1:A:310:LEU:C    | 1:A:310:LEU:CD1  | 2.85                     | 0.45              |
| 1:A:312:HIS:NE2  | 1:A:368:LYS:CD   | 2.76                     | 0.45              |
| 1:C:484:LEU:C    | 1:C:484:LEU:CD2  | 2.85                     | 0.45              |
| 1:B:88:ASP:O     | 1:B:95:LYS:HE3   | 2.15                     | 0.45              |
| 1:B:171:ARG:O    | 1:B:173:ILE:CA   | 2.64                     | 0.45              |
| 1:B:366:HIS:HD2  | 1:B:382:CYS:SG   | 2.40                     | 0.45              |
| 1:A:366:HIS:HD2  | 1:A:382:CYS:SG   | 2.40                     | 0.45              |
| 1:A:489:TRP:O    | 1:A:489:TRP:HD1  | 1.99                     | 0.45              |
| 1:B:184:ASP:OD1  | 1:B:185:ARG:N    | 2.47                     | 0.45              |
| 1:B:331:PHE:HB3  | 1:B:336:VAL:CG2  | 2.46                     | 0.45              |
| 1:B:332:SER:C    | 1:B:334:PRO:HD2  | 2.42                     | 0.45              |
| 1:B:335:VAL:HG12 | 1:B:376:TYR:CE2  | 2.51                     | 0.45              |
| 1:D:348:GLU:HB3  | 1:D:499:PHE:HB2  | 1.99                     | 0.45              |
| 1:A:74:ARG:NH1   | 1:A:376:TYR:CZ   | 2.84                     | 0.45              |
| 1:A:215:LEU:C    | 1:A:215:LEU:HD12 | 2.41                     | 0.45              |
| 1:A:331:PHE:HB3  | 1:A:336:VAL:CG2  | 2.46                     | 0.45              |
| 1:A:332:SER:C    | 1:A:334:PRO:HD2  | 2.42                     | 0.45              |
| 1:A:335:VAL:HG12 | 1:A:376:TYR:CE2  | 2.51                     | 0.45              |
| 1:C:74:ARG:NH1   | 1:C:376:TYR:CZ   | 2.84                     | 0.45              |
| 1:B:215:LEU:C    | 1:B:215:LEU:HD12 | 2.41                     | 0.45              |
| 1:B:310:LEU:C    | 1:B:310:LEU:CD1  | 2.85                     | 0.45              |
| 1:D:366:HIS:HD2  | 1:D:382:CYS:SG   | 2.40                     | 0.45              |
| 1:A:408:ALA:N    | 1:A:411:VAL:CG2  | 2.79                     | 0.45              |
| 1:C:78:GLU:HG3   | 1:C:109:HIS:HE1  | 1.80                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:122:GLU:C   | 1:C:124:ILE:N    | 2.73                     | 0.45              |
| 1:C:366:HIS:HD2 | 1:C:382:CYS:SG   | 2.40                     | 0.45              |
| 1:C:408:ALA:N   | 1:C:411:VAL:CG2  | 2.79                     | 0.45              |
| 1:B:74:ARG:NH1  | 1:B:376:TYR:CZ   | 2.84                     | 0.45              |
| 1:B:489:TRP:O   | 1:B:489:TRP:HD1  | 1.99                     | 0.45              |
| 1:D:74:ARG:NH1  | 1:D:376:TYR:CZ   | 2.84                     | 0.45              |
| 1:D:78:GLU:HG3  | 1:D:109:HIS:HE1  | 1.80                     | 0.45              |
| 1:D:152:GLU:HB2 | 1:D:153:TRP:CZ3  | 2.52                     | 0.45              |
| 1:D:216:LYS:HA  | 1:D:219:THR:HG21 | 1.96                     | 0.45              |
| 1:D:470:ARG:CB  | 1:D:489:TRP:HE1  | 2.02                     | 0.45              |
| 1:D:475:PHE:N   | 1:D:476:PRO:CD   | 2.78                     | 0.45              |
| 1:A:348:GLU:HB3 | 1:A:499:PHE:HB2  | 1.99                     | 0.45              |
| 1:C:152:GLU:HB2 | 1:C:153:TRP:CZ3  | 2.52                     | 0.45              |
| 1:C:348:GLU:HB3 | 1:C:499:PHE:HB2  | 1.99                     | 0.45              |
| 1:C:350:LEU:O   | 1:C:355:ILE:HG22 | 2.17                     | 0.45              |
| 1:C:475:PHE:N   | 1:C:476:PRO:CD   | 2.78                     | 0.45              |
| 1:B:170:SER:OG  | 1:B:171:ARG:N    | 2.50                     | 0.45              |
| 1:D:408:ALA:N   | 1:D:411:VAL:CG2  | 2.79                     | 0.45              |
| 1:D:489:TRP:CD1 | 1:D:489:TRP:O    | 2.70                     | 0.45              |
| 1:A:21:GLN:HE21 | 1:A:28:GLN:HB2   | 1.81                     | 0.45              |
| 1:A:170:SER:OG  | 1:A:171:ARG:N    | 2.50                     | 0.45              |
| 1:C:37:LEU:CD1  | 1:C:177:PHE:HE1  | 2.25                     | 0.45              |
| 1:C:173:ILE:HB  | 1:C:176:ARG:HB2  | 1.99                     | 0.45              |
| 1:C:489:TRP:CD1 | 1:C:489:TRP:O    | 2.70                     | 0.45              |
| 1:B:21:GLN:HE21 | 1:B:28:GLN:HB2   | 1.81                     | 0.45              |
| 1:B:408:ALA:N   | 1:B:411:VAL:CG2  | 2.80                     | 0.45              |
| 1:D:37:LEU:CD1  | 1:D:177:PHE:HE1  | 2.25                     | 0.45              |
| 1:D:122:GLU:C   | 1:D:124:ILE:N    | 2.73                     | 0.45              |
| 1:D:350:LEU:O   | 1:D:355:ILE:HG22 | 2.17                     | 0.45              |
| 1:A:489:TRP:CD1 | 1:A:489:TRP:O    | 2.70                     | 0.45              |
| 1:C:216:LYS:HA  | 1:C:219:THR:HG21 | 1.96                     | 0.45              |
| 1:B:348:GLU:HB3 | 1:B:499:PHE:HB2  | 1.99                     | 0.45              |
| 1:D:173:ILE:HB  | 1:D:176:ARG:HB2  | 1.99                     | 0.45              |
| 1:A:332:SER:CB  | 1:A:334:PRO:CD   | 2.81                     | 0.45              |
| 1:A:350:LEU:O   | 1:A:355:ILE:HG22 | 2.17                     | 0.45              |
| 1:C:361:ASN:O   | 1:C:364:ASN:N    | 2.45                     | 0.45              |
| 1:D:542:PHE:H   | 1:D:542:PHE:HD2  | 1.65                     | 0.45              |
| 1:C:33:LEU:CD2  | 1:C:177:PHE:HD1  | 2.24                     | 0.44              |
| 1:C:310:LEU:CD2 | 1:C:311:MET:O    | 2.65                     | 0.44              |
| 1:C:329:TYR:O   | 1:C:329:TYR:CD1  | 2.70                     | 0.44              |
| 1:C:542:PHE:H   | 1:C:542:PHE:HD2  | 1.65                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:332:SER:CB   | 1:B:334:PRO:CD   | 2.81                     | 0.44              |
| 1:B:350:LEU:O    | 1:B:355:ILE:HG22 | 2.17                     | 0.44              |
| 1:B:489:TRP:CD1  | 1:B:489:TRP:O    | 2.70                     | 0.44              |
| 1:D:310:LEU:CD2  | 1:D:311:MET:O    | 2.65                     | 0.44              |
| 1:D:329:TYR:CD1  | 1:D:329:TYR:O    | 2.70                     | 0.44              |
| 1:D:537:ARG:HB3  | 1:D:537:ARG:HH21 | 1.82                     | 0.44              |
| 1:C:537:ARG:HH21 | 1:C:537:ARG:HB3  | 1.82                     | 0.44              |
| 1:B:34:LEU:HD23  | 1:B:34:LEU:HA    | 1.77                     | 0.44              |
| 1:B:184:ASP:OD1  | 1:B:184:ASP:N    | 2.46                     | 0.44              |
| 1:A:152:GLU:HB2  | 1:A:153:TRP:CZ3  | 2.52                     | 0.44              |
| 1:A:152:GLU:OE2  | 1:C:147:ARG:NH2  | 2.51                     | 0.44              |
| 1:A:370:ARG:HB2  | 1:A:373:THR:OG1  | 2.16                     | 0.44              |
| 1:A:480:THR:CG2  | 1:A:527:PRO:HB3  | 2.48                     | 0.44              |
| 1:C:475:PHE:CG   | 1:C:476:PRO:HD2  | 2.53                     | 0.44              |
| 1:B:34:LEU:HG    | 1:B:106:VAL:HG23 | 2.00                     | 0.44              |
| 1:B:103:LYS:NZ   | 1:B:105:CYS:HB2  | 2.33                     | 0.44              |
| 1:B:370:ARG:HB2  | 1:B:373:THR:OG1  | 2.16                     | 0.44              |
| 1:B:403:PRO:O    | 1:B:403:PRO:CD   | 2.66                     | 0.44              |
| 1:D:34:LEU:HA    | 1:D:34:LEU:HD23  | 1.77                     | 0.44              |
| 1:D:331:PHE:HB3  | 1:D:336:VAL:CG2  | 2.46                     | 0.44              |
| 1:D:361:ASN:O    | 1:D:364:ASN:N    | 2.45                     | 0.44              |
| 1:A:34:LEU:HG    | 1:A:106:VAL:HG23 | 2.00                     | 0.44              |
| 1:A:55:LEU:HB2   | 1:B:23:ASP:HB3   | 1.98                     | 0.44              |
| 1:A:103:LYS:NZ   | 1:A:105:CYS:HB2  | 2.33                     | 0.44              |
| 1:A:173:ILE:HB   | 1:A:176:ARG:HB2  | 1.99                     | 0.44              |
| 1:A:190:GLU:OE1  | 1:D:182:ARG:NH1  | 2.49                     | 0.44              |
| 1:A:329:TYR:O    | 1:A:329:TYR:CD1  | 2.70                     | 0.44              |
| 1:A:567:GLU:CD   | 1:A:567:GLU:C    | 2.85                     | 0.44              |
| 1:C:72:LEU:HD12  | 1:C:72:LEU:HA    | 1.78                     | 0.44              |
| 1:B:103:LYS:HZ2  | 1:B:105:CYS:HB2  | 1.83                     | 0.44              |
| 1:B:310:LEU:CD2  | 1:B:311:MET:O    | 2.65                     | 0.44              |
| 1:B:329:TYR:CD1  | 1:B:329:TYR:O    | 2.70                     | 0.44              |
| 1:B:480:THR:CG2  | 1:B:527:PRO:HB3  | 2.48                     | 0.44              |
| 1:B:567:GLU:C    | 1:B:567:GLU:CD   | 2.85                     | 0.44              |
| 1:D:442:PHE:CZ   | 1:D:489:TRP:CZ3  | 3.02                     | 0.44              |
| 1:D:475:PHE:CG   | 1:D:476:PRO:HD2  | 2.53                     | 0.44              |
| 1:A:103:LYS:HZ2  | 1:A:105:CYS:HB2  | 1.83                     | 0.44              |
| 1:A:310:LEU:CD2  | 1:A:311:MET:O    | 2.65                     | 0.44              |
| 1:A:482:VAL:O    | 1:A:486:LYS:HG3  | 2.18                     | 0.44              |
| 1:C:331:PHE:HB3  | 1:C:336:VAL:CG2  | 2.46                     | 0.44              |
| 1:B:152:GLU:HB2  | 1:B:153:TRP:CZ3  | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:537:ARG:HB3  | 1:B:537:ARG:HH21 | 1.82                     | 0.44              |
| 1:A:537:ARG:HB3  | 1:A:537:ARG:HH21 | 1.82                     | 0.44              |
| 1:B:173:ILE:HB   | 1:B:176:ARG:HB2  | 1.99                     | 0.44              |
| 1:D:33:LEU:CD2   | 1:D:177:PHE:HD1  | 2.24                     | 0.44              |
| 1:A:34:LEU:HD23  | 1:A:34:LEU:HA    | 1.77                     | 0.44              |
| 1:A:488:CYS:HA   | 1:A:496:ARG:HG3  | 2.00                     | 0.44              |
| 1:C:332:SER:H    | 1:C:335:VAL:CG2  | 2.31                     | 0.44              |
| 1:B:39:SER:O     | 1:B:43:ASN:ND2   | 2.50                     | 0.44              |
| 1:B:482:VAL:O    | 1:B:486:LYS:HG3  | 2.18                     | 0.44              |
| 1:D:39:SER:O     | 1:D:43:ASN:ND2   | 2.50                     | 0.44              |
| 1:D:488:CYS:O    | 1:D:496:ARG:HG3  | 2.17                     | 0.44              |
| 1:A:39:SER:O     | 1:A:43:ASN:ND2   | 2.50                     | 0.44              |
| 1:C:39:SER:O     | 1:C:43:ASN:ND2   | 2.51                     | 0.44              |
| 1:C:69:LEU:HA    | 1:C:69:LEU:HD23  | 1.79                     | 0.44              |
| 1:C:120:VAL:HG11 | 1:C:167:TYR:CE1  | 2.53                     | 0.44              |
| 1:C:170:SER:OG   | 1:C:171:ARG:N    | 2.50                     | 0.44              |
| 1:C:442:PHE:CZ   | 1:C:489:TRP:CZ3  | 3.02                     | 0.44              |
| 1:B:53:LEU:CG    | 1:B:126:ALA:CB   | 2.96                     | 0.44              |
| 1:D:93:TRP:O     | 1:D:97:ILE:HG13  | 2.18                     | 0.44              |
| 1:D:319:MET:CA   | 1:D:322:ASN:CG   | 2.88                     | 0.44              |
| 1:D:332:SER:H    | 1:D:335:VAL:CG2  | 2.31                     | 0.44              |
| 1:A:53:LEU:CG    | 1:A:126:ALA:CB   | 2.96                     | 0.44              |
| 1:C:117:PHE:C    | 1:C:119:ALA:N    | 2.76                     | 0.44              |
| 1:B:488:CYS:HA   | 1:B:496:ARG:HG3  | 2.00                     | 0.44              |
| 1:D:117:PHE:C    | 1:D:119:ALA:N    | 2.76                     | 0.44              |
| 1:D:120:VAL:HG11 | 1:D:167:TYR:CE1  | 2.53                     | 0.44              |
| 1:C:93:TRP:O     | 1:C:97:ILE:HG13  | 2.18                     | 0.43              |
| 1:C:479:LYS:NZ   | 1:C:479:LYS:CB   | 2.73                     | 0.43              |
| 1:C:488:CYS:HA   | 1:C:496:ARG:HG3  | 2.00                     | 0.43              |
| 1:B:1:MET:HG2    | 1:B:58:LYS:HD2   | 2.00                     | 0.43              |
| 1:D:170:SER:OG   | 1:D:171:ARG:N    | 2.50                     | 0.43              |
| 1:A:1:MET:HG2    | 1:A:58:LYS:HD2   | 2.01                     | 0.43              |
| 1:C:415:MET:N    | 1:C:415:MET:CE   | 2.81                     | 0.43              |
| 1:D:488:CYS:HA   | 1:D:496:ARG:HG3  | 2.00                     | 0.43              |
| 1:A:69:LEU:HD23  | 1:A:69:LEU:HA    | 1.78                     | 0.43              |
| 1:A:120:VAL:HG11 | 1:A:167:TYR:CE1  | 2.53                     | 0.43              |
| 1:A:370:ARG:HG3  | 1:A:376:TYR:HB3  | 2.01                     | 0.43              |
| 1:A:433:ASP:O    | 1:A:436:SER:OG   | 2.29                     | 0.43              |
| 1:A:475:PHE:N    | 1:A:476:PRO:CD   | 2.78                     | 0.43              |
| 1:C:319:MET:CA   | 1:C:322:ASN:CG   | 2.88                     | 0.43              |
| 1:C:480:THR:CG2  | 1:C:527:PRO:HB3  | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:567:GLU:C    | 1:C:567:GLU:CD   | 2.85                     | 0.43              |
| 1:B:370:ARG:HG3  | 1:B:376:TYR:HB3  | 2.01                     | 0.43              |
| 1:B:433:ASP:O    | 1:B:436:SER:OG   | 2.29                     | 0.43              |
| 1:D:480:THR:CG2  | 1:D:527:PRO:HB3  | 2.48                     | 0.43              |
| 1:D:567:GLU:CD   | 1:D:567:GLU:C    | 2.85                     | 0.43              |
| 1:A:289:ILE:CG2  | 1:A:384:PHE:CZ   | 3.01                     | 0.43              |
| 1:C:26:ILE:HG21  | 1:C:99:LEU:HB3   | 2.01                     | 0.43              |
| 1:C:57:GLU:H     | 1:C:57:GLU:CD    | 2.24                     | 0.43              |
| 1:B:120:VAL:HG11 | 1:B:167:TYR:CE1  | 2.53                     | 0.43              |
| 1:B:289:ILE:CG2  | 1:B:384:PHE:CZ   | 3.02                     | 0.43              |
| 1:B:313:LYS:HB2  | 1:B:318:TYR:HE2  | 1.84                     | 0.43              |
| 1:D:26:ILE:HG21  | 1:D:99:LEU:HB3   | 2.01                     | 0.43              |
| 1:D:72:LEU:HA    | 1:D:72:LEU:HD12  | 1.79                     | 0.43              |
| 1:D:415:MET:N    | 1:D:415:MET:CE   | 2.81                     | 0.43              |
| 1:A:117:PHE:C    | 1:A:119:ALA:N    | 2.76                     | 0.43              |
| 1:A:313:LYS:HB2  | 1:A:318:TYR:HE2  | 1.84                     | 0.43              |
| 1:A:415:MET:N    | 1:A:415:MET:CE   | 2.81                     | 0.43              |
| 1:A:506:LEU:HA   | 1:A:509:ILE:HD12 | 2.00                     | 0.43              |
| 1:B:117:PHE:C    | 1:B:119:ALA:N    | 2.76                     | 0.43              |
| 1:B:506:LEU:HA   | 1:B:509:ILE:HD12 | 2.00                     | 0.43              |
| 1:D:57:GLU:H     | 1:D:57:GLU:CD    | 2.24                     | 0.43              |
| 1:C:34:LEU:HG    | 1:C:106:VAL:HG23 | 2.00                     | 0.43              |
| 1:C:289:ILE:CG2  | 1:C:384:PHE:CZ   | 3.01                     | 0.43              |
| 1:C:332:SER:C    | 1:C:334:PRO:HD2  | 2.42                     | 0.43              |
| 1:B:415:MET:N    | 1:B:415:MET:CE   | 2.81                     | 0.43              |
| 1:A:319:MET:CA   | 1:A:322:ASN:CG   | 2.88                     | 0.43              |
| 1:D:34:LEU:HG    | 1:D:106:VAL:HG23 | 2.00                     | 0.43              |
| 1:D:289:ILE:CG2  | 1:D:384:PHE:CZ   | 3.01                     | 0.43              |
| 1:D:446:THR:HG21 | 1:D:473:PHE:CD2  | 2.32                     | 0.43              |
| 1:A:93:TRP:O     | 1:A:97:ILE:HG13  | 2.18                     | 0.43              |
| 1:A:147:ARG:NH2  | 1:C:152:GLU:OE2  | 2.52                     | 0.43              |
| 1:A:357:HIS:CD2  | 1:A:360:LEU:HD13 | 2.54                     | 0.43              |
| 1:A:446:THR:HG23 | 1:A:473:PHE:CD2  | 2.51                     | 0.43              |
| 1:A:542:PHE:H    | 1:A:542:PHE:HD2  | 1.65                     | 0.43              |
| 1:B:357:HIS:CD2  | 1:B:360:LEU:HD13 | 2.54                     | 0.43              |
| 1:B:446:THR:HG23 | 1:B:473:PHE:CD2  | 2.51                     | 0.43              |
| 1:A:84:LYS:HE2   | 1:A:84:LYS:HB3   | 1.89                     | 0.43              |
| 1:A:153:TRP:HE1  | 1:A:162:ARG:CZ   | 2.32                     | 0.43              |
| 1:C:482:VAL:O    | 1:C:486:LYS:HG3  | 2.18                     | 0.43              |
| 1:B:319:MET:CA   | 1:B:322:ASN:CG   | 2.88                     | 0.43              |
| 1:A:26:ILE:HG21  | 1:A:99:LEU:HB3   | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:69:LEU:HD23  | 1:B:69:LEU:HA    | 1.78                     | 0.43              |
| 1:B:93:TRP:O     | 1:B:97:ILE:HG13  | 2.18                     | 0.43              |
| 1:B:153:TRP:HE1  | 1:B:162:ARG:CZ   | 2.32                     | 0.43              |
| 1:B:542:PHE:HD2  | 1:B:542:PHE:H    | 1.65                     | 0.43              |
| 1:D:153:TRP:HE1  | 1:D:162:ARG:CZ   | 2.32                     | 0.43              |
| 1:D:332:SER:C    | 1:D:334:PRO:HD2  | 2.42                     | 0.43              |
| 1:D:506:LEU:HA   | 1:D:509:ILE:HD12 | 2.00                     | 0.43              |
| 1:A:20:LEU:HB3   | 1:B:55:LEU:HD22  | 2.01                     | 0.42              |
| 1:A:78:GLU:HG3   | 1:A:109:HIS:HE1  | 1.79                     | 0.42              |
| 1:C:153:TRP:HE1  | 1:C:162:ARG:CZ   | 2.32                     | 0.42              |
| 1:C:403:PRO:O    | 1:C:403:PRO:CD   | 2.66                     | 0.42              |
| 1:C:506:LEU:HA   | 1:C:509:ILE:HD12 | 2.00                     | 0.42              |
| 1:B:26:ILE:HG21  | 1:B:99:LEU:HB3   | 2.01                     | 0.42              |
| 1:D:-1:ALA:HB3   | 1:D:2:GLU:HB3    | 2.01                     | 0.42              |
| 1:D:118:SER:HG   | 1:D:560:LEU:HD23 | 1.75                     | 0.42              |
| 1:D:287:SER:O    | 1:D:378:HIS:NE2  | 2.52                     | 0.42              |
| 1:D:482:VAL:O    | 1:D:486:LYS:HG3  | 2.18                     | 0.42              |
| 1:A:154:ASN:O    | 1:A:542:PHE:HE1  | 2.03                     | 0.42              |
| 1:C:-1:ALA:HB3   | 1:C:2:GLU:HB3    | 2.00                     | 0.42              |
| 1:C:287:SER:O    | 1:C:378:HIS:NE2  | 2.53                     | 0.42              |
| 1:B:154:ASN:O    | 1:B:542:PHE:HE1  | 2.02                     | 0.42              |
| 1:C:103:LYS:NZ   | 1:C:105:CYS:HB2  | 2.33                     | 0.42              |
| 1:C:446:THR:HG21 | 1:C:473:PHE:CD2  | 2.32                     | 0.42              |
| 1:D:103:LYS:NZ   | 1:D:105:CYS:HB2  | 2.33                     | 0.42              |
| 1:A:407:TYR:HB3  | 1:A:411:VAL:HG23 | 2.01                     | 0.42              |
| 1:A:570:LYS:HB2  | 1:A:570:LYS:HZ3  | 1.82                     | 0.42              |
| 1:C:407:TYR:HB3  | 1:C:411:VAL:HG23 | 2.01                     | 0.42              |
| 1:B:78:GLU:HG3   | 1:B:109:HIS:HE1  | 1.80                     | 0.42              |
| 1:D:310:LEU:C    | 1:D:310:LEU:CD1  | 2.85                     | 0.42              |
| 1:D:403:PRO:O    | 1:D:403:PRO:CD   | 2.66                     | 0.42              |
| 1:A:481:LEU:HD23 | 1:A:481:LEU:HA   | 1.89                     | 0.42              |
| 1:A:559:GLN:O    | 1:A:563:TYR:HD2  | 2.02                     | 0.42              |
| 1:B:332:SER:H    | 1:B:335:VAL:CG2  | 2.31                     | 0.42              |
| 1:B:407:TYR:HB3  | 1:B:411:VAL:HG23 | 2.01                     | 0.42              |
| 1:B:559:GLN:O    | 1:B:563:TYR:HD2  | 2.02                     | 0.42              |
| 1:A:332:SER:H    | 1:A:335:VAL:CG2  | 2.31                     | 0.42              |
| 1:A:347:MET:HB3  | 1:A:499:PHE:CE2  | 2.55                     | 0.42              |
| 1:C:118:SER:HG   | 1:C:560:LEU:HD23 | 1.75                     | 0.42              |
| 1:C:337:ILE:HG22 | 1:C:481:LEU:HD21 | 2.02                     | 0.42              |
| 1:C:559:GLN:O    | 1:C:563:TYR:HD2  | 2.02                     | 0.42              |
| 1:D:1:MET:HG2    | 1:D:58:LYS:HD2   | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:-1:ALA:HB3   | 1:A:2:GLU:HB3    | 2.01                     | 0.42              |
| 1:A:449:VAL:CG1  | 1:A:450:PRO:CD   | 2.97                     | 0.42              |
| 1:B:449:VAL:CG1  | 1:B:450:PRO:CD   | 2.97                     | 0.42              |
| 1:B:544:GLY:O    | 1:B:548:SER:N    | 2.53                     | 0.42              |
| 1:A:408:ALA:H    | 1:A:411:VAL:CG2  | 2.33                     | 0.42              |
| 1:A:449:VAL:HG13 | 1:A:450:PRO:CD   | 2.43                     | 0.42              |
| 1:A:475:PHE:N    | 1:A:475:PHE:CD1  | 2.73                     | 0.42              |
| 1:A:544:GLY:O    | 1:A:548:SER:N    | 2.53                     | 0.42              |
| 1:C:1:MET:HG2    | 1:C:58:LYS:HD2   | 2.01                     | 0.42              |
| 1:B:-1:ALA:HB3   | 1:B:2:GLU:HB3    | 2.01                     | 0.42              |
| 1:B:347:MET:HB3  | 1:B:499:PHE:CE2  | 2.55                     | 0.42              |
| 1:D:337:ILE:HG22 | 1:D:481:LEU:HD21 | 2.02                     | 0.42              |
| 1:D:407:TYR:HB3  | 1:D:411:VAL:HG23 | 2.01                     | 0.42              |
| 1:D:411:VAL:HG11 | 1:D:427:LYS:CB   | 2.38                     | 0.42              |
| 1:D:559:GLN:O    | 1:D:563:TYR:HD2  | 2.02                     | 0.42              |
| 1:A:475:PHE:CG   | 1:A:476:PRO:HD2  | 2.53                     | 0.42              |
| 1:C:53:LEU:CG    | 1:C:126:ALA:CB   | 2.96                     | 0.42              |
| 1:C:370:ARG:HG3  | 1:C:376:TYR:HB3  | 2.01                     | 0.42              |
| 1:B:408:ALA:H    | 1:B:411:VAL:CG2  | 2.33                     | 0.42              |
| 1:B:444:LEU:HD23 | 1:B:444:LEU:HA   | 1.87                     | 0.42              |
| 1:D:449:VAL:CG1  | 1:D:450:PRO:CD   | 2.97                     | 0.42              |
| 1:D:563:TYR:O    | 1:D:567:GLU:HB3  | 2.20                     | 0.42              |
| 1:A:72:LEU:HD12  | 1:A:72:LEU:HA    | 1.79                     | 0.42              |
| 1:C:357:HIS:CD2  | 1:C:360:LEU:HD13 | 2.54                     | 0.42              |
| 1:C:563:TYR:O    | 1:C:567:GLU:HB3  | 2.20                     | 0.42              |
| 1:B:337:ILE:HG22 | 1:B:481:LEU:HD21 | 2.02                     | 0.42              |
| 1:B:449:VAL:HG13 | 1:B:450:PRO:CD   | 2.43                     | 0.42              |
| 1:B:475:PHE:CG   | 1:B:476:PRO:HD2  | 2.53                     | 0.42              |
| 1:D:53:LEU:CG    | 1:D:126:ALA:CB   | 2.96                     | 0.42              |
| 1:D:212:ASP:HA   | 1:D:215:LEU:CD2  | 2.50                     | 0.42              |
| 1:D:370:ARG:HG3  | 1:D:376:TYR:HB3  | 2.01                     | 0.42              |
| 1:A:210:LEU:O    | 1:A:211:ALA:C    | 2.63                     | 0.41              |
| 1:A:337:ILE:HG22 | 1:A:481:LEU:HD21 | 2.02                     | 0.41              |
| 1:A:563:TYR:O    | 1:A:567:GLU:HB3  | 2.20                     | 0.41              |
| 1:C:212:ASP:HA   | 1:C:215:LEU:CD2  | 2.50                     | 0.41              |
| 1:C:347:MET:HB3  | 1:C:499:PHE:CE2  | 2.55                     | 0.41              |
| 1:C:449:VAL:CG1  | 1:C:450:PRO:CD   | 2.97                     | 0.41              |
| 1:B:210:LEU:O    | 1:B:211:ALA:C    | 2.63                     | 0.41              |
| 1:D:357:HIS:CD2  | 1:D:360:LEU:HD13 | 2.54                     | 0.41              |
| 1:D:544:GLY:O    | 1:D:548:SER:N    | 2.53                     | 0.41              |
| 1:A:343:ILE:O    | 1:A:347:MET:HG2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:444:LEU:HD23 | 1:A:444:LEU:HA   | 1.87                     | 0.41              |
| 1:C:122:GLU:C    | 1:C:124:ILE:H    | 2.28                     | 0.41              |
| 1:B:99:LEU:HD23  | 1:B:99:LEU:HA    | 1.79                     | 0.41              |
| 1:B:343:ILE:O    | 1:B:347:MET:HG2  | 2.20                     | 0.41              |
| 1:D:122:GLU:C    | 1:D:124:ILE:H    | 2.28                     | 0.41              |
| 1:D:310:LEU:CD2  | 1:D:311:MET:N    | 2.53                     | 0.41              |
| 1:D:347:MET:HB3  | 1:D:499:PHE:CE2  | 2.55                     | 0.41              |
| 1:A:287:SER:O    | 1:A:378:HIS:NE2  | 2.52                     | 0.41              |
| 1:C:99:LEU:HA    | 1:C:99:LEU:HD23  | 1.79                     | 0.41              |
| 1:C:544:GLY:O    | 1:C:548:SER:N    | 2.53                     | 0.41              |
| 1:B:212:ASP:HA   | 1:B:215:LEU:CD2  | 2.50                     | 0.41              |
| 1:B:481:LEU:HD23 | 1:B:481:LEU:HA   | 1.89                     | 0.41              |
| 1:B:563:TYR:O    | 1:B:567:GLU:HB3  | 2.20                     | 0.41              |
| 1:D:332:SER:HG   | 1:D:334:PRO:HG2  | 1.71                     | 0.41              |
| 1:A:212:ASP:HA   | 1:A:215:LEU:CD2  | 2.50                     | 0.41              |
| 1:C:313:LYS:HB2  | 1:C:318:TYR:HE2  | 1.84                     | 0.41              |
| 1:B:127:ALA:CB   | 1:B:141:ARG:HD2  | 2.48                     | 0.41              |
| 1:B:287:SER:O    | 1:B:378:HIS:NE2  | 2.52                     | 0.41              |
| 1:B:442:PHE:CZ   | 1:B:489:TRP:CZ3  | 3.02                     | 0.41              |
| 1:B:475:PHE:N    | 1:B:475:PHE:CD1  | 2.73                     | 0.41              |
| 1:B:505:ILE:CG1  | 1:B:531:CYS:HB3  | 2.51                     | 0.41              |
| 1:A:108:PHE:O    | 1:A:111:HIS:HB3  | 2.21                     | 0.41              |
| 1:A:127:ALA:CB   | 1:A:141:ARG:HD2  | 2.48                     | 0.41              |
| 1:A:185:ARG:NE   | 1:A:218:LEU:HD23 | 2.36                     | 0.41              |
| 1:A:505:ILE:CG1  | 1:A:531:CYS:HB3  | 2.51                     | 0.41              |
| 1:B:108:PHE:O    | 1:B:111:HIS:HB3  | 2.21                     | 0.41              |
| 1:B:185:ARG:NE   | 1:B:218:LEU:HD23 | 2.36                     | 0.41              |
| 1:A:5:ARG:NH2    | 1:B:13:SER:OG    | 2.44                     | 0.41              |
| 1:C:108:PHE:O    | 1:C:111:HIS:HB3  | 2.21                     | 0.41              |
| 1:C:332:SER:HG   | 1:C:334:PRO:HG2  | 1.71                     | 0.41              |
| 1:C:408:ALA:H    | 1:C:411:VAL:CG2  | 2.33                     | 0.41              |
| 1:C:411:VAL:HG11 | 1:C:427:LYS:CB   | 2.38                     | 0.41              |
| 1:D:408:ALA:H    | 1:D:411:VAL:CG2  | 2.33                     | 0.41              |
| 1:A:99:LEU:HD23  | 1:A:99:LEU:HA    | 1.79                     | 0.41              |
| 1:A:100:HIS:HA   | 1:A:103:LYS:HB2  | 2.03                     | 0.41              |
| 1:A:122:GLU:C    | 1:A:124:ILE:H    | 2.28                     | 0.41              |
| 1:C:127:ALA:CB   | 1:C:141:ARG:HD2  | 2.48                     | 0.41              |
| 1:C:153:TRP:HA   | 1:C:158:MET:SD   | 2.61                     | 0.41              |
| 1:C:310:LEU:CD2  | 1:C:311:MET:N    | 2.53                     | 0.41              |
| 1:C:505:ILE:CG1  | 1:C:531:CYS:HB3  | 2.51                     | 0.41              |
| 1:B:72:LEU:HD12  | 1:B:72:LEU:HA    | 1.79                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:100:HIS:HA   | 1:B:103:LYS:HB2  | 2.03                     | 0.41              |
| 1:B:407:TYR:O    | 1:B:435:TYR:CD2  | 2.72                     | 0.41              |
| 1:D:53:LEU:HD21  | 1:D:126:ALA:HB2  | 1.93                     | 0.41              |
| 1:D:108:PHE:O    | 1:D:111:HIS:HB3  | 2.21                     | 0.41              |
| 1:D:127:ALA:CB   | 1:D:141:ARG:HD2  | 2.48                     | 0.41              |
| 1:D:153:TRP:HA   | 1:D:158:MET:SD   | 2.61                     | 0.41              |
| 1:D:313:LYS:HB2  | 1:D:318:TYR:HE2  | 1.84                     | 0.41              |
| 1:D:505:ILE:CG1  | 1:D:531:CYS:HB3  | 2.51                     | 0.41              |
| 1:A:407:TYR:O    | 1:A:435:TYR:CD2  | 2.72                     | 0.41              |
| 1:A:442:PHE:CZ   | 1:A:489:TRP:CZ3  | 3.02                     | 0.41              |
| 1:C:117:PHE:CE2  | 1:C:168:LEU:HD11 | 2.56                     | 0.41              |
| 1:C:343:ILE:O    | 1:C:347:MET:HG2  | 2.20                     | 0.41              |
| 1:B:122:GLU:C    | 1:B:124:ILE:H    | 2.28                     | 0.41              |
| 1:B:470:ARG:HD3  | 1:B:489:TRP:NE1  | 2.27                     | 0.41              |
| 1:A:153:TRP:HA   | 1:A:158:MET:SD   | 2.61                     | 0.41              |
| 1:A:403:PRO:O    | 1:A:403:PRO:CD   | 2.66                     | 0.41              |
| 1:A:470:ARG:HD3  | 1:A:489:TRP:NE1  | 2.27                     | 0.41              |
| 1:A:488:CYS:O    | 1:A:496:ARG:HG3  | 2.16                     | 0.41              |
| 1:C:210:LEU:O    | 1:C:211:ALA:C    | 2.63                     | 0.41              |
| 1:C:475:PHE:N    | 1:C:475:PHE:CD1  | 2.73                     | 0.41              |
| 1:C:475:PHE:H    | 1:C:475:PHE:HD1  | 1.59                     | 0.41              |
| 1:B:118:SER:C    | 1:B:120:VAL:H    | 2.29                     | 0.41              |
| 1:B:121:VAL:HG11 | 1:B:564:ARG:NH1  | 2.11                     | 0.41              |
| 1:B:488:CYS:O    | 1:B:496:ARG:HG3  | 2.17                     | 0.41              |
| 1:D:103:LYS:HZ2  | 1:D:105:CYS:HB2  | 1.86                     | 0.41              |
| 1:D:117:PHE:CE2  | 1:D:168:LEU:HD11 | 2.56                     | 0.41              |
| 1:D:210:LEU:O    | 1:D:211:ALA:C    | 2.63                     | 0.41              |
| 1:A:118:SER:C    | 1:A:120:VAL:H    | 2.29                     | 0.41              |
| 1:D:99:LEU:HA    | 1:D:99:LEU:HD23  | 1.79                     | 0.41              |
| 1:D:343:ILE:O    | 1:D:347:MET:HG2  | 2.20                     | 0.41              |
| 1:A:536:ALA:O    | 1:A:540:ARG:CB   | 2.69                     | 0.40              |
| 1:C:154:ASN:O    | 1:C:542:PHE:HE1  | 2.03                     | 0.40              |
| 1:B:74:ARG:CZ    | 1:B:376:TYR:CZ   | 3.04                     | 0.40              |
| 1:B:153:TRP:HA   | 1:B:158:MET:SD   | 2.61                     | 0.40              |
| 1:D:154:ASN:O    | 1:D:542:PHE:HE1  | 2.02                     | 0.40              |
| 1:D:185:ARG:NE   | 1:D:218:LEU:HD23 | 2.36                     | 0.40              |
| 1:A:74:ARG:CZ    | 1:A:376:TYR:CZ   | 3.05                     | 0.40              |
| 1:A:408:ALA:CA   | 1:A:435:TYR:HD2  | 2.28                     | 0.40              |
| 1:C:53:LEU:HD21  | 1:C:126:ALA:HB2  | 1.93                     | 0.40              |
| 1:C:185:ARG:NE   | 1:C:218:LEU:HD23 | 2.36                     | 0.40              |
| 1:B:67:GLN:N     | 1:B:68:PRO:HD2   | 2.36                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:536:ALA:O    | 1:B:540:ARG:CB   | 2.69                     | 0.40              |
| 1:D:415:MET:N    | 1:D:415:MET:HE3  | 2.36                     | 0.40              |
| 1:A:67:GLN:N     | 1:A:68:PRO:HD2   | 2.36                     | 0.40              |
| 1:A:117:PHE:CE2  | 1:A:168:LEU:HD11 | 2.56                     | 0.40              |
| 1:A:556:ILE:HG13 | 1:A:556:ILE:H    | 1.69                     | 0.40              |
| 1:C:415:MET:N    | 1:C:415:MET:HE3  | 2.36                     | 0.40              |
| 1:B:117:PHE:CE2  | 1:B:168:LEU:HD11 | 2.56                     | 0.40              |
| 1:D:100:HIS:HA   | 1:D:103:LYS:HB2  | 2.03                     | 0.40              |
| 1:D:475:PHE:N    | 1:D:475:PHE:CD1  | 2.73                     | 0.40              |
| 1:A:124:ILE:HG23 | 1:A:145:PHE:CZ   | 2.57                     | 0.40              |
| 1:C:100:HIS:HA   | 1:C:103:LYS:HB2  | 2.03                     | 0.40              |
| 1:C:290:LEU:CG   | 1:C:382:CYS:SG   | 3.10                     | 0.40              |
| 1:C:329:TYR:CD1  | 1:C:329:TYR:C    | 3.00                     | 0.40              |
| 1:C:414:GLU:HB2  | 1:C:415:MET:HE1  | 2.03                     | 0.40              |
| 1:B:124:ILE:HG23 | 1:B:145:PHE:CZ   | 2.57                     | 0.40              |
| 1:B:556:ILE:HG13 | 1:B:556:ILE:H    | 1.69                     | 0.40              |
| 1:D:196:ARG:HD2  | 1:D:212:ASP:OD1  | 2.22                     | 0.40              |
| 1:D:290:LEU:CG   | 1:D:382:CYS:SG   | 3.10                     | 0.40              |
| 1:D:472:LEU:C    | 1:D:472:LEU:CD1  | 2.93                     | 0.40              |
| 1:A:148:LYS:O    | 1:A:148:LYS:HG2  | 2.22                     | 0.40              |
| 1:A:196:ARG:HD2  | 1:A:212:ASP:OD1  | 2.22                     | 0.40              |
| 1:A:500:SER:HA   | 1:A:503:CYS:SG   | 2.62                     | 0.40              |
| 1:C:196:ARG:HD2  | 1:C:212:ASP:OD1  | 2.22                     | 0.40              |
| 1:B:7:ILE:H      | 1:B:7:ILE:HG12   | 1.70                     | 0.40              |
| 1:D:329:TYR:CD1  | 1:D:329:TYR:C    | 3.00                     | 0.40              |
| 1:D:475:PHE:H    | 1:D:475:PHE:HD1  | 1.59                     | 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 PDB entries followed by that with respect to all EM entries.

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     | 440/572 (77%)   | 390 (89%)  | 48 (11%)  | 2 (0%)   | 24          | 61 |
| 1   | B     | 440/572 (77%)   | 390 (89%)  | 48 (11%)  | 2 (0%)   | 24          | 61 |
| 1   | C     | 440/572 (77%)   | 390 (89%)  | 48 (11%)  | 2 (0%)   | 24          | 61 |
| 1   | D     | 440/572 (77%)   | 390 (89%)  | 48 (11%)  | 2 (0%)   | 24          | 61 |
| All | All   | 1760/2288 (77%) | 1560 (89%) | 192 (11%) | 8 (0%)   | 26          | 61 |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 281 | LEU  |
| 1   | A     | 386 | LEU  |
| 1   | C     | 281 | LEU  |
| 1   | C     | 386 | LEU  |
| 1   | B     | 281 | LEU  |
| 1   | B     | 386 | LEU  |
| 1   | D     | 281 | LEU  |
| 1   | D     | 386 | LEU  |

### 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 PDB entries followed by that with respect to all EM entries.

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     | 393/518 (76%)   | 379 (96%)  | 14 (4%)  | 31          | 53 |
| 1   | B     | 393/518 (76%)   | 379 (96%)  | 14 (4%)  | 31          | 53 |
| 1   | C     | 393/518 (76%)   | 379 (96%)  | 14 (4%)  | 31          | 53 |
| 1   | D     | 393/518 (76%)   | 379 (96%)  | 14 (4%)  | 31          | 53 |
| All | All   | 1572/2072 (76%) | 1516 (96%) | 56 (4%)  | 32          | 53 |

All (56) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 208 | LYS  |
| 1   | A     | 310 | LEU  |
| 1   | A     | 311 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 345 | ARG  |
| 1   | A     | 374 | GLU  |
| 1   | A     | 415 | MET  |
| 1   | A     | 430 | HIS  |
| 1   | A     | 434 | VAL  |
| 1   | A     | 475 | PHE  |
| 1   | A     | 479 | LYS  |
| 1   | A     | 487 | ARG  |
| 1   | A     | 537 | ARG  |
| 1   | A     | 567 | GLU  |
| 1   | A     | 570 | LYS  |
| 1   | C     | 208 | LYS  |
| 1   | C     | 310 | LEU  |
| 1   | C     | 311 | MET  |
| 1   | C     | 345 | ARG  |
| 1   | C     | 374 | GLU  |
| 1   | C     | 415 | MET  |
| 1   | C     | 430 | HIS  |
| 1   | C     | 434 | VAL  |
| 1   | C     | 475 | PHE  |
| 1   | C     | 479 | LYS  |
| 1   | C     | 487 | ARG  |
| 1   | C     | 537 | ARG  |
| 1   | C     | 567 | GLU  |
| 1   | C     | 570 | LYS  |
| 1   | B     | 208 | LYS  |
| 1   | B     | 310 | LEU  |
| 1   | B     | 311 | MET  |
| 1   | B     | 345 | ARG  |
| 1   | B     | 374 | GLU  |
| 1   | B     | 415 | MET  |
| 1   | B     | 430 | HIS  |
| 1   | B     | 434 | VAL  |
| 1   | B     | 475 | PHE  |
| 1   | B     | 479 | LYS  |
| 1   | B     | 487 | ARG  |
| 1   | B     | 537 | ARG  |
| 1   | B     | 567 | GLU  |
| 1   | B     | 570 | LYS  |
| 1   | D     | 208 | LYS  |
| 1   | D     | 310 | LEU  |
| 1   | D     | 311 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 345 | ARG  |
| 1   | D     | 374 | GLU  |
| 1   | D     | 415 | MET  |
| 1   | D     | 430 | HIS  |
| 1   | D     | 434 | VAL  |
| 1   | D     | 475 | PHE  |
| 1   | D     | 479 | LYS  |
| 1   | D     | 487 | ARG  |
| 1   | D     | 537 | ARG  |
| 1   | D     | 567 | GLU  |
| 1   | D     | 570 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | GLN  |
| 1   | A     | 21  | GLN  |
| 1   | A     | 27  | ASN  |
| 1   | A     | 43  | ASN  |
| 1   | A     | 51  | GLN  |
| 1   | A     | 67  | GLN  |
| 1   | A     | 109 | HIS  |
| 1   | A     | 111 | HIS  |
| 1   | A     | 312 | HIS  |
| 1   | A     | 353 | ASN  |
| 1   | A     | 364 | ASN  |
| 1   | A     | 366 | HIS  |
| 1   | A     | 495 | GLN  |
| 1   | A     | 516 | ASN  |
| 1   | A     | 519 | HIS  |
| 1   | A     | 559 | GLN  |
| 1   | C     | 3   | GLN  |
| 1   | C     | 21  | GLN  |
| 1   | C     | 27  | ASN  |
| 1   | C     | 43  | ASN  |
| 1   | C     | 51  | GLN  |
| 1   | C     | 67  | GLN  |
| 1   | C     | 109 | HIS  |
| 1   | C     | 111 | HIS  |
| 1   | C     | 312 | HIS  |
| 1   | C     | 353 | ASN  |
| 1   | C     | 364 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 366 | HIS  |
| 1   | C     | 495 | GLN  |
| 1   | C     | 516 | ASN  |
| 1   | C     | 519 | HIS  |
| 1   | C     | 559 | GLN  |
| 1   | B     | 3   | GLN  |
| 1   | B     | 21  | GLN  |
| 1   | B     | 27  | ASN  |
| 1   | B     | 43  | ASN  |
| 1   | B     | 51  | GLN  |
| 1   | B     | 67  | GLN  |
| 1   | B     | 109 | HIS  |
| 1   | B     | 111 | HIS  |
| 1   | B     | 312 | HIS  |
| 1   | B     | 353 | ASN  |
| 1   | B     | 364 | ASN  |
| 1   | B     | 366 | HIS  |
| 1   | B     | 495 | GLN  |
| 1   | B     | 516 | ASN  |
| 1   | B     | 519 | HIS  |
| 1   | B     | 559 | GLN  |
| 1   | D     | 3   | GLN  |
| 1   | D     | 21  | GLN  |
| 1   | D     | 27  | ASN  |
| 1   | D     | 43  | ASN  |
| 1   | D     | 51  | GLN  |
| 1   | D     | 67  | GLN  |
| 1   | D     | 109 | HIS  |
| 1   | D     | 111 | HIS  |
| 1   | D     | 312 | HIS  |
| 1   | D     | 353 | ASN  |
| 1   | D     | 364 | ASN  |
| 1   | D     | 366 | HIS  |
| 1   | D     | 495 | GLN  |
| 1   | D     | 516 | ASN  |
| 1   | D     | 519 | HIS  |
| 1   | D     | 559 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

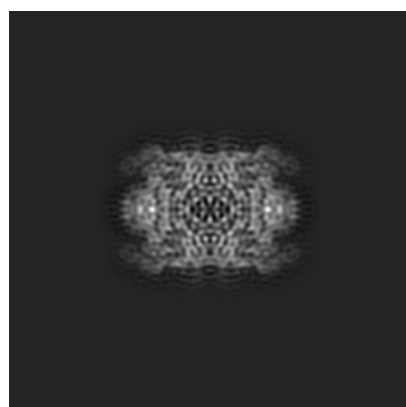
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0868. These allow visual inspection of the internal detail of the map and identification of artifacts.

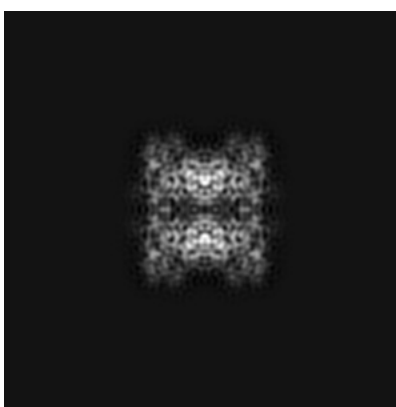
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

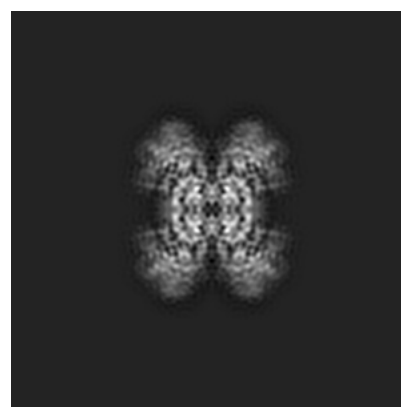
#### 6.1.1 Primary map



X



Y



Z

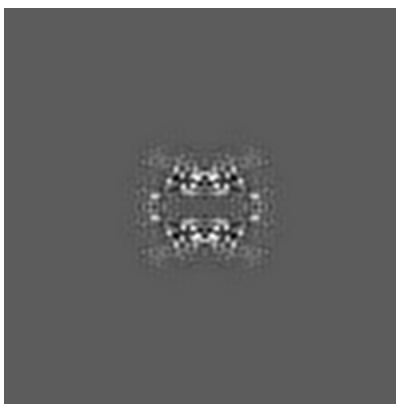
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

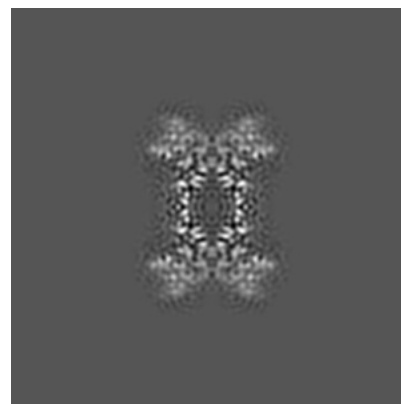
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

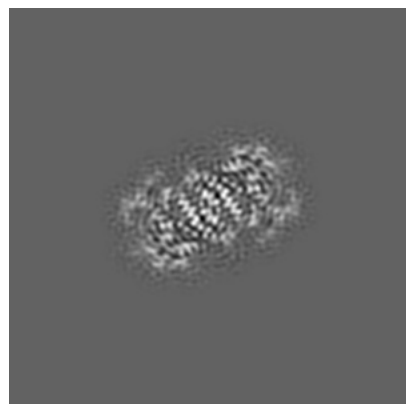


Z Index: 100

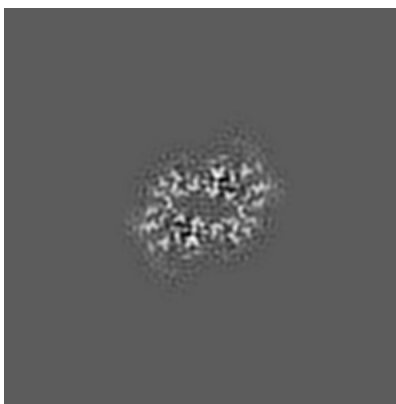
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

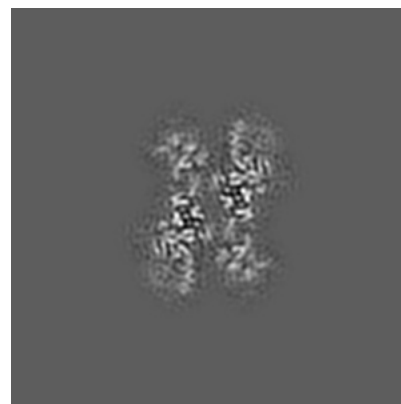
### 6.3.1 Primary map



X Index: 84



Y Index: 93

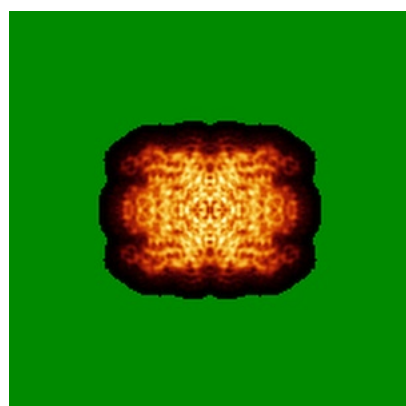


Z Index: 92

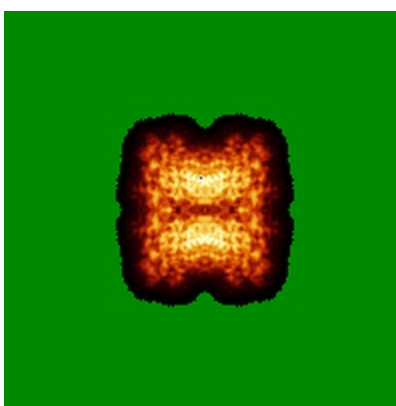
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

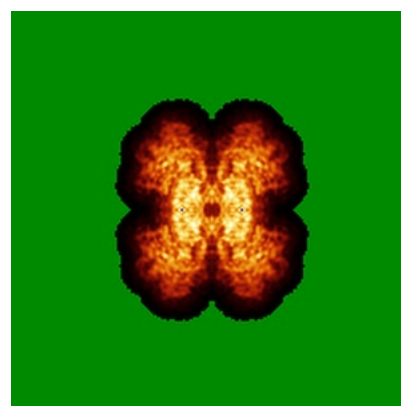
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views

This section was not generated.

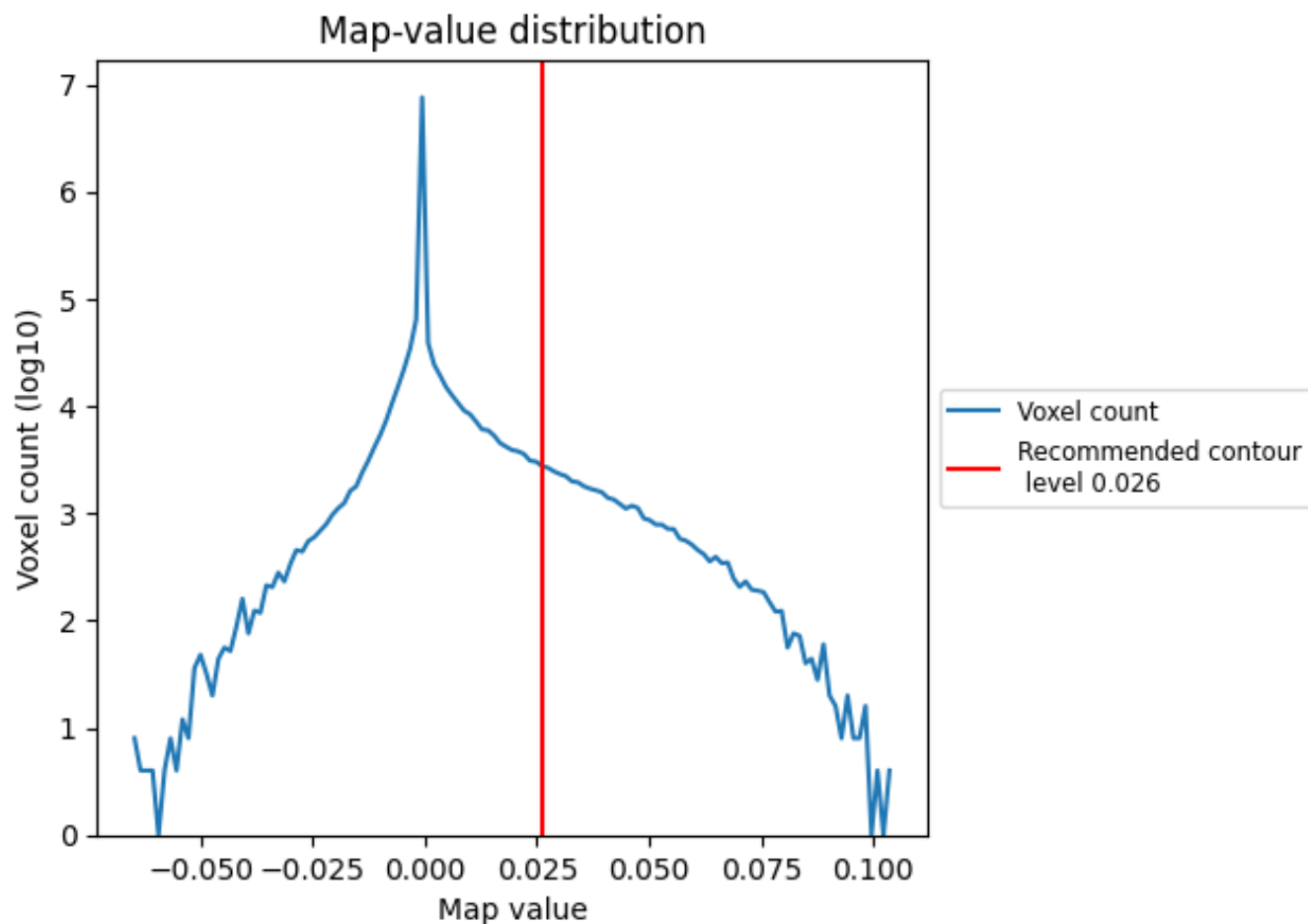
## 6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

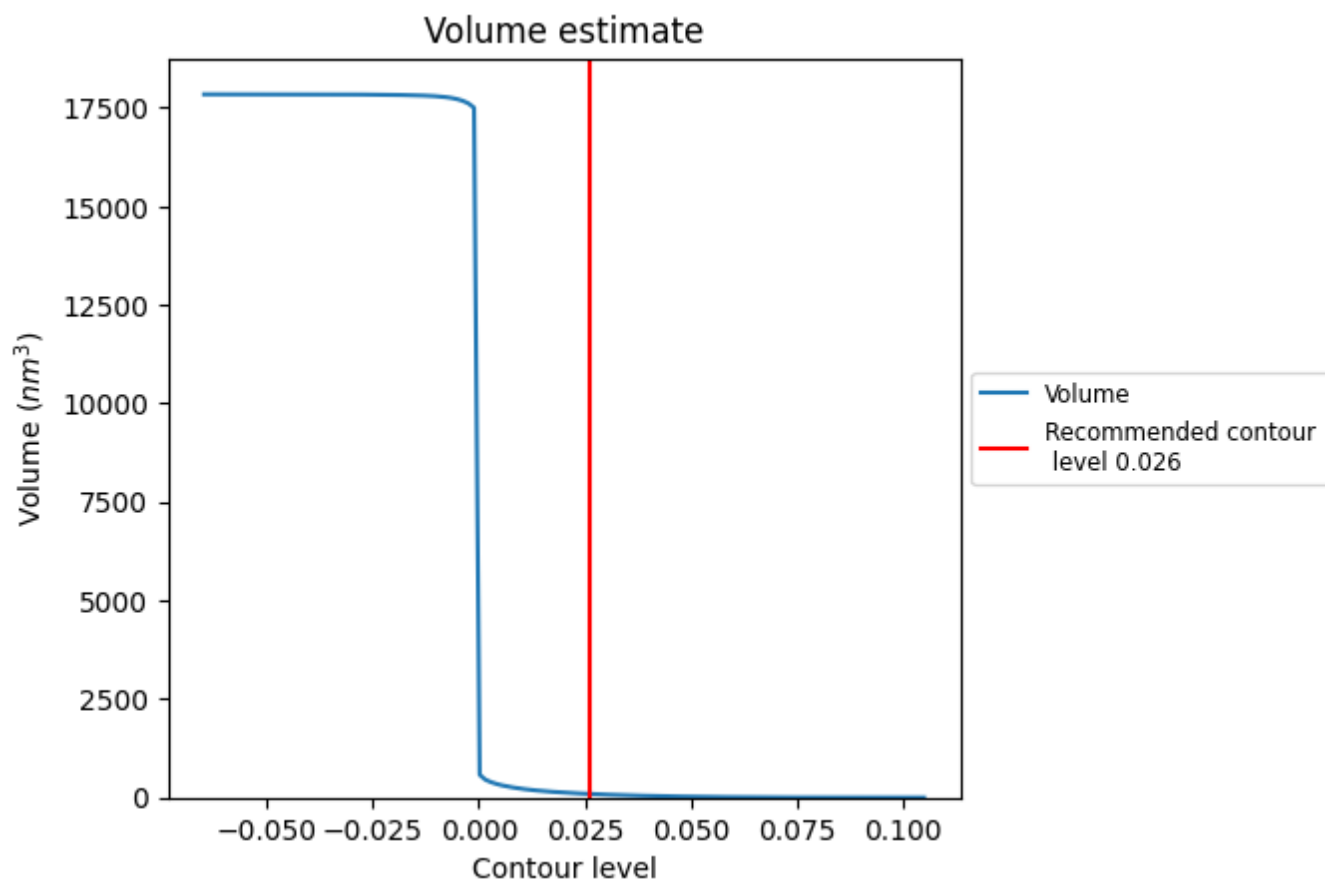
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

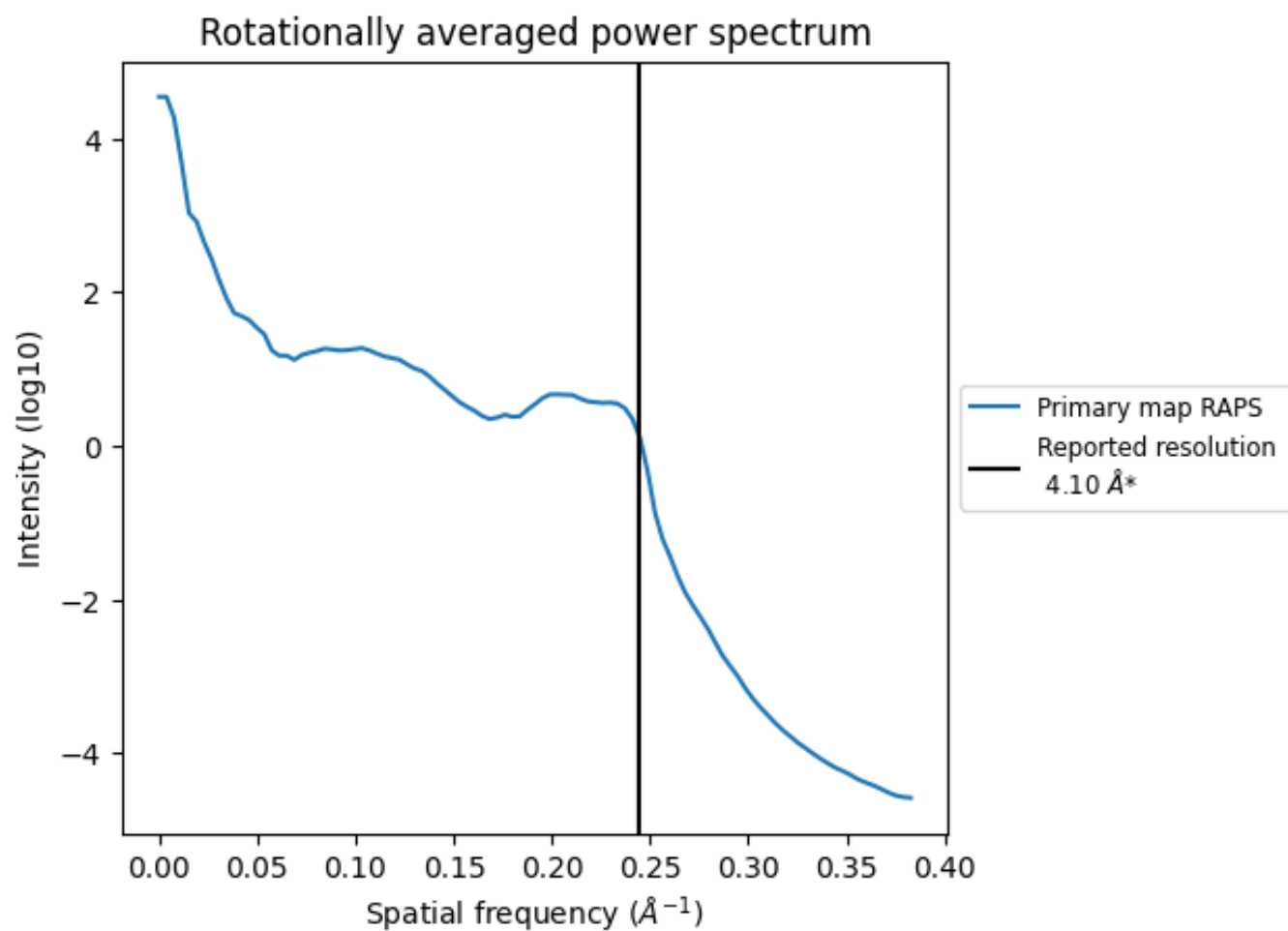
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm<sup>3</sup>; this corresponds to an approximate mass of 84 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

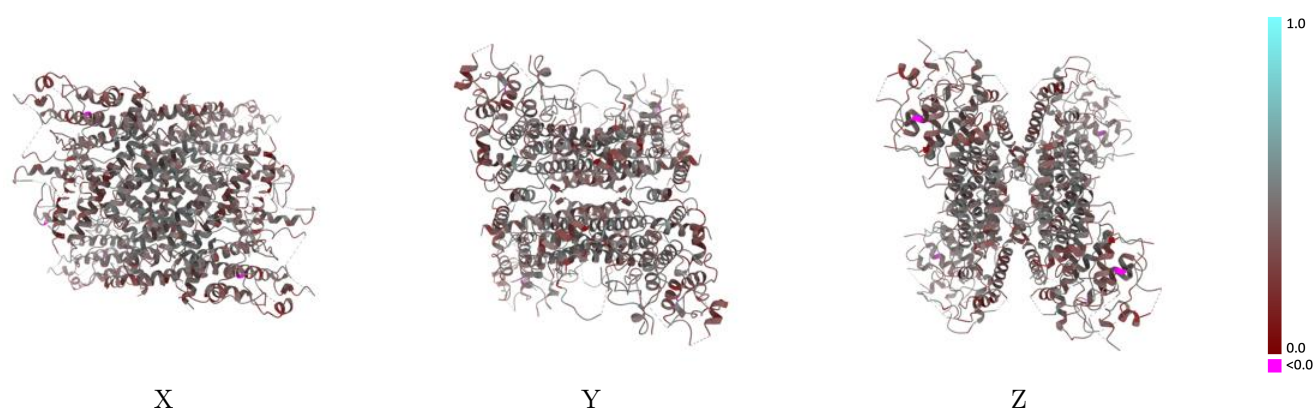
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0868 and PDB model 6LBA. Per-residue inclusion information can be found in section 3 on page 4.

### 9.1 Map-model overlay [i](#)

This section was not generated.

### 9.2 Q-score mapped to coordinate model [i](#)

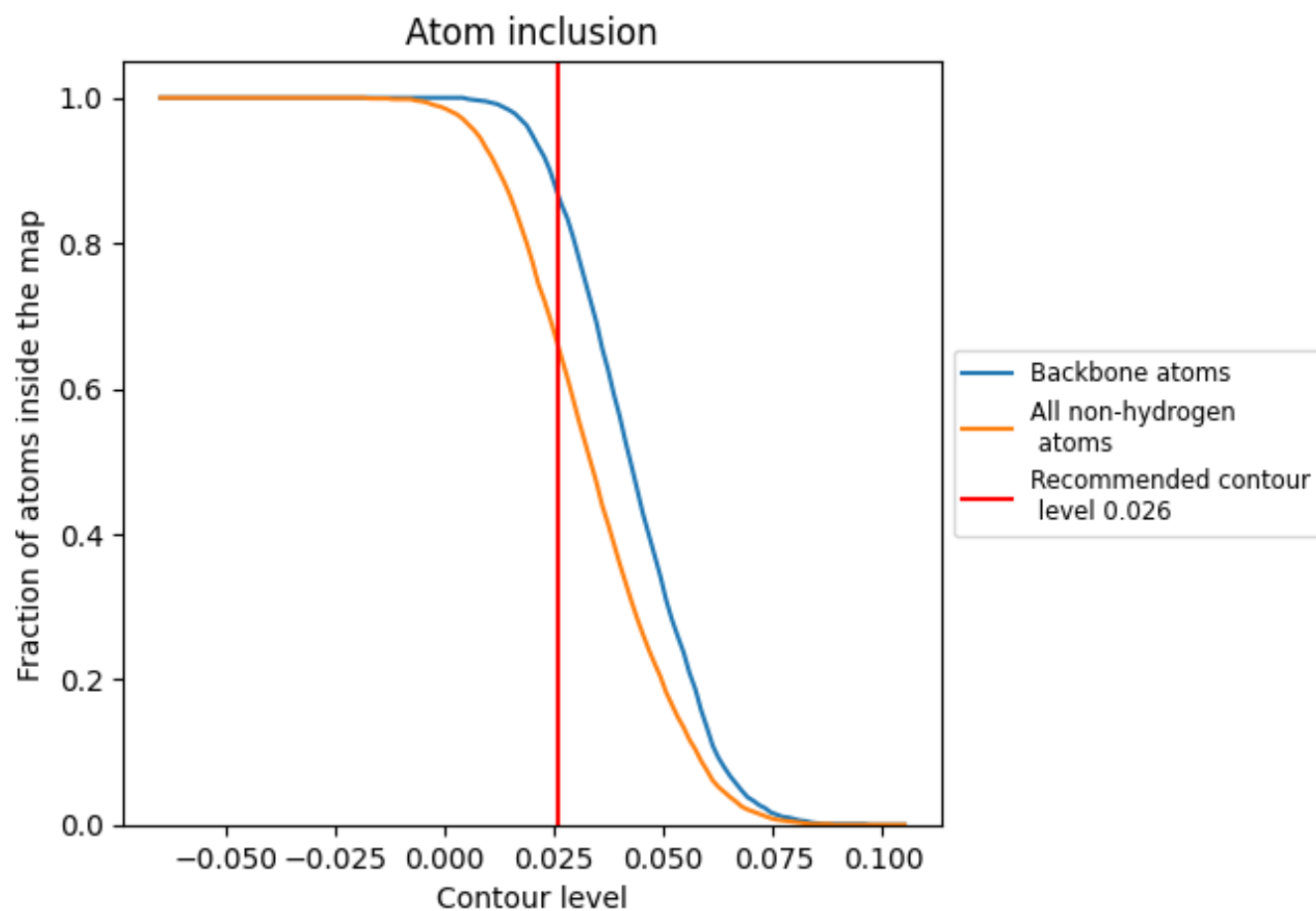


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.026) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6570 | <div></div> 0.3920 |
| A     | <div></div> 0.6570 | <div></div> 0.3930 |
| B     | <div></div> 0.6550 | <div></div> 0.3930 |
| C     | <div></div> 0.6580 | <div></div> 0.3930 |
| D     | <div></div> 0.6590 | <div></div> 0.3920 |

