



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:24 PM UTC

PDB ID : 2DIK / pdb\_00002dik  
Title : R337A MUTANT OF PYRUVATE PHOSPHATE DIKINASE  
Authors : Huang, K.; Herzberg, O.  
Deposited on : 1998-09-03  
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

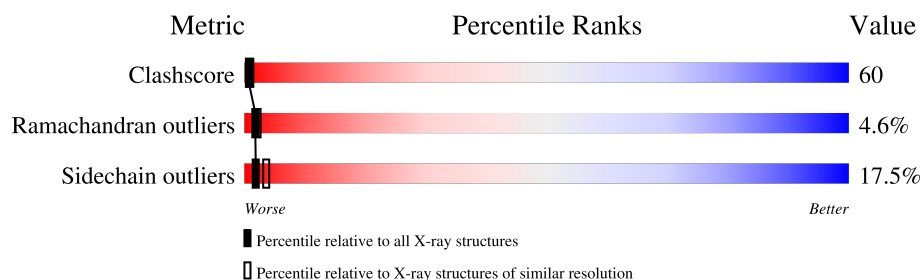
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

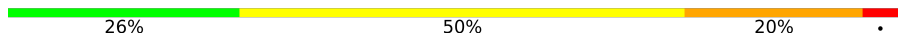
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 873    |  |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6778 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

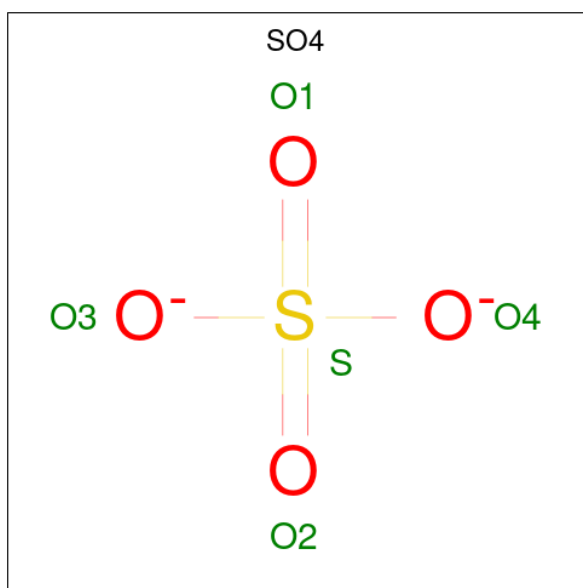
- Molecule 1 is a protein called PROTEIN (PYRUVATE PHOSPHATE DIKINASE).

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
|     |       |          | Total | C    | N    | O    | S  |         |         |       |
| 1   | A     | 869      | 6724  | 4233 | 1137 | 1303 | 51 | 0       | 0       | 0     |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 337     | ALA      | ARG    | engineered mutation | UNP P22983 |

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
|     |       |          | Total | O | S |         |         |
| 2   | A     | 1        | 5     | 4 | 1 | 0       | 0       |
| 2   | A     | 1        | 5     | 4 | 1 | 0       | 0       |

- Molecule 3 is water.

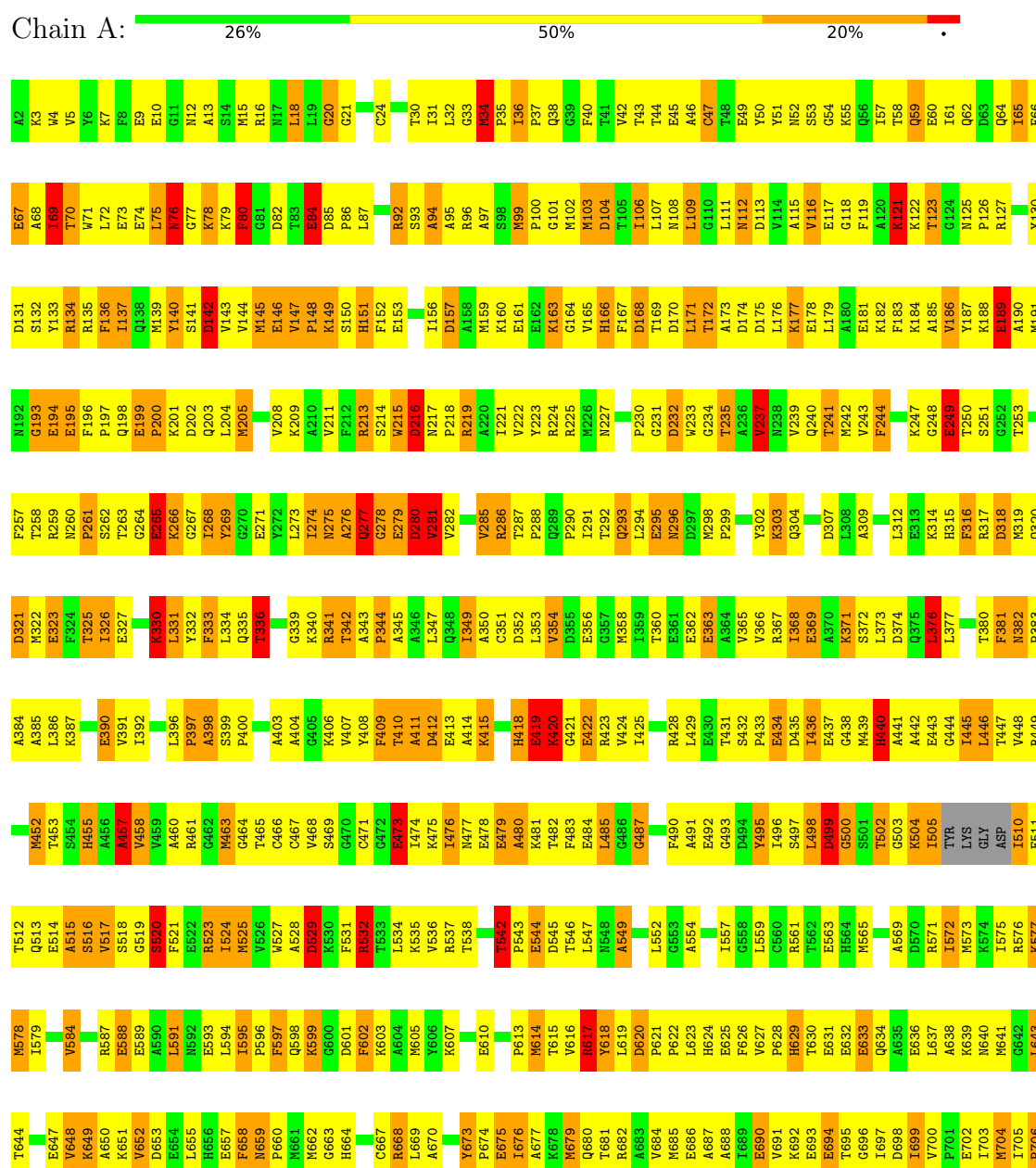
| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | A     | 44       | Total<br>44 | O<br>44 | 0       | 0       |

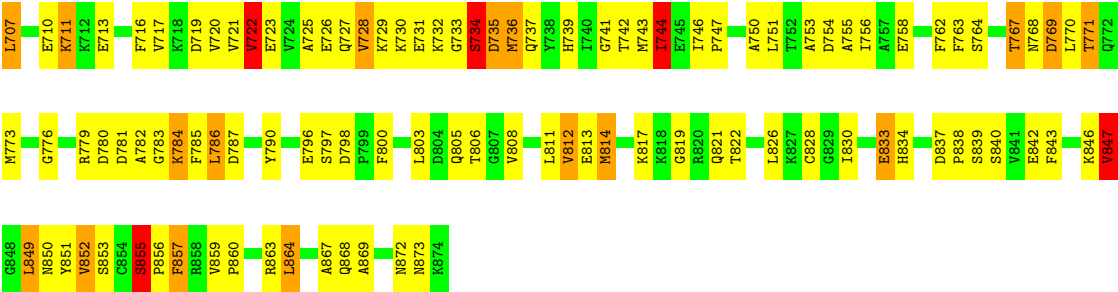
### 3 Residue-property plots

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

Note EDS was not executed.

#### • Molecule 1: PROTEIN (PYRUVATE PHOSPHATE DIKINASE)





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                                    | Source    |
|----------------------------------------------------------|----------------------------------------------------------|-----------|
| Space group                                              | P 1 2 1                                                  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 89.80 Å   58.80 Å   102.00 Å<br>90.00°   94.80°   90.00° | Depositor |
| Resolution (Å)                                           | 8.00 – 2.50                                              | Depositor |
| % Data completeness<br>(in resolution range)             | 75.0 (8.00-2.50)                                         | Depositor |
| $R_{merge}$                                              | (Not available)                                          | Depositor |
| $R_{sym}$                                                | 9.90                                                     | Depositor |
| Refinement program                                       | TNT                                                      | Depositor |
| R, $R_{free}$                                            | 0.185 , (Not available)                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                                   | Xtriage   |
| Total number of atoms                                    | 6778                                                     | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 29.0                                                     | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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     | 1.59         | 38/6846 (0.6%) | 1.94        | 163/9227 (1.8%) |

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                   | 2                   |

All (38) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 341 | ARG  | CA-C   | -7.91 | 1.43        | 1.52     |
| 1   | A     | 699 | ILE  | CA-CB  | -7.69 | 1.45        | 1.54     |
| 1   | A     | 458 | VAL  | C-N    | -6.61 | 1.25        | 1.33     |
| 1   | A     | 704 | MET  | CA-C   | -6.52 | 1.44        | 1.52     |
| 1   | A     | 331 | LEU  | CA-C   | -6.50 | 1.44        | 1.52     |
| 1   | A     | 369 | GLU  | CA-C   | -6.45 | 1.44        | 1.53     |
| 1   | A     | 722 | VAL  | N-CA   | -6.14 | 1.39        | 1.46     |
| 1   | A     | 872 | ASN  | CA-C   | -6.14 | 1.45        | 1.52     |
| 1   | A     | 265 | GLU  | CD-OE1 | 5.99  | 1.36        | 1.25     |
| 1   | A     | 731 | GLU  | CA-CB  | -5.98 | 1.44        | 1.53     |
| 1   | A     | 834 | HIS  | N-CA   | -5.98 | 1.38        | 1.46     |
| 1   | A     | 813 | GLU  | N-CA   | -5.93 | 1.39        | 1.46     |
| 1   | A     | 625 | GLU  | CD-OE1 | 5.88  | 1.36        | 1.25     |
| 1   | A     | 549 | ALA  | CA-C   | -5.87 | 1.45        | 1.52     |
| 1   | A     | 851 | TYR  | N-CA   | -5.80 | 1.39        | 1.46     |
| 1   | A     | 852 | VAL  | CA-C   | -5.73 | 1.46        | 1.53     |
| 1   | A     | 542 | THR  | CA-C   | -5.72 | 1.47        | 1.52     |
| 1   | A     | 720 | VAL  | CA-CB  | -5.72 | 1.46        | 1.54     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 249 | GLU  | CD-OE1 | 5.67  | 1.36        | 1.25     |
| 1   | A     | 769 | ASP  | C-N    | -5.66 | 1.26        | 1.33     |
| 1   | A     | 499 | ASP  | CG-OD2 | 5.64  | 1.36        | 1.25     |
| 1   | A     | 610 | GLU  | CD-OE2 | 5.52  | 1.35        | 1.25     |
| 1   | A     | 344 | PRO  | N-CA   | -5.51 | 1.40        | 1.47     |
| 1   | A     | 323 | GLU  | CD-OE2 | 5.46  | 1.35        | 1.25     |
| 1   | A     | 798 | ASP  | CG-OD2 | 5.46  | 1.35        | 1.25     |
| 1   | A     | 833 | GLU  | CD-OE1 | 5.42  | 1.35        | 1.25     |
| 1   | A     | 652 | VAL  | CA-CB  | -5.40 | 1.48        | 1.54     |
| 1   | A     | 595 | ILE  | CA-C   | -5.31 | 1.47        | 1.52     |
| 1   | A     | 542 | THR  | CA-CB  | -5.30 | 1.47        | 1.53     |
| 1   | A     | 859 | VAL  | CA-C   | -5.27 | 1.47        | 1.52     |
| 1   | A     | 321 | ASP  | CA-C   | 5.22  | 1.59        | 1.52     |
| 1   | A     | 764 | SER  | N-CA   | -5.21 | 1.40        | 1.46     |
| 1   | A     | 591 | LEU  | N-CA   | -5.17 | 1.40        | 1.46     |
| 1   | A     | 411 | ALA  | CA-C   | -5.11 | 1.46        | 1.52     |
| 1   | A     | 853 | SER  | N-CA   | -5.10 | 1.40        | 1.46     |
| 1   | A     | 299 | PRO  | N-CA   | -5.09 | 1.40        | 1.47     |
| 1   | A     | 780 | ASP  | CG-OD1 | 5.09  | 1.35        | 1.25     |
| 1   | A     | 142 | ASP  | CG-OD1 | 5.02  | 1.34        | 1.25     |

All (163) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | A     | 735 | ASP  | N-CA-C   | -11.04 | 97.13       | 111.92   |
| 1   | A     | 736 | MET  | N-CA-C   | -10.01 | 95.46       | 110.28   |
| 1   | A     | 99  | MET  | CA-C-N   | 9.30   | 131.47      | 119.84   |
| 1   | A     | 99  | MET  | C-N-CA   | 9.30   | 131.47      | 119.84   |
| 1   | A     | 166 | HIS  | N-CA-C   | 9.14   | 124.68      | 113.17   |
| 1   | A     | 146 | GLU  | N-CA-C   | -9.10  | 101.07      | 112.72   |
| 1   | A     | 800 | PHE  | CA-CB-CG | -8.58  | 105.22      | 113.80   |
| 1   | A     | 411 | ALA  | N-CA-C   | -8.51  | 101.95      | 111.14   |
| 1   | A     | 85  | ASP  | CA-CB-CG | -8.50  | 104.10      | 112.60   |
| 1   | A     | 602 | PHE  | CA-CB-CG | -8.42  | 105.38      | 113.80   |
| 1   | A     | 659 | ASN  | CA-C-N   | 8.38   | 130.31      | 119.84   |
| 1   | A     | 659 | ASN  | C-N-CA   | 8.38   | 130.31      | 119.84   |
| 1   | A     | 261 | PRO  | CB-CA-C  | -8.14  | 100.30      | 111.85   |
| 1   | A     | 318 | ASP  | N-CA-CB  | -8.07  | 99.05       | 111.56   |
| 1   | A     | 458 | VAL  | N-CA-C   | 7.89   | 117.99      | 110.42   |
| 1   | A     | 731 | GLU  | N-CA-C   | -7.70  | 101.81      | 112.12   |
| 1   | A     | 833 | GLU  | N-CA-C   | -7.63  | 103.94      | 113.18   |
| 1   | A     | 369 | GLU  | N-CA-CB  | 7.55   | 122.85      | 110.39   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 734 | SER  | CA-C-N     | 7.54  | 133.36      | 122.35   |
| 1   | A     | 734 | SER  | C-N-CA     | 7.54  | 133.36      | 122.35   |
| 1   | A     | 189 | GLU  | N-CA-C     | -7.52 | 102.78      | 110.97   |
| 1   | A     | 368 | ILE  | CA-C-N     | -7.35 | 112.63      | 122.85   |
| 1   | A     | 368 | ILE  | C-N-CA     | -7.35 | 112.63      | 122.85   |
| 1   | A     | 314 | LYS  | N-CA-C     | -7.34 | 103.35      | 111.36   |
| 1   | A     | 706 | PRO  | CB-CA-C    | -7.31 | 99.92       | 110.75   |
| 1   | A     | 276 | ALA  | CA-C-N     | -7.29 | 111.79      | 122.65   |
| 1   | A     | 276 | ALA  | C-N-CA     | -7.29 | 111.79      | 122.65   |
| 1   | A     | 520 | SER  | N-CA-C     | -7.21 | 103.14      | 112.23   |
| 1   | A     | 756 | ILE  | N-CA-C     | -7.18 | 103.46      | 110.72   |
| 1   | A     | 659 | ASN  | O-C-N      | 7.14  | 127.24      | 121.17   |
| 1   | A     | 542 | THR  | OG1-CB-CG2 | 7.08  | 123.45      | 109.30   |
| 1   | A     | 837 | ASP  | CA-CB-CG   | -6.97 | 105.63      | 112.60   |
| 1   | A     | 572 | ILE  | N-CA-C     | 6.83  | 117.53      | 110.36   |
| 1   | A     | 243 | VAL  | CA-C-N     | -6.76 | 113.50      | 123.11   |
| 1   | A     | 243 | VAL  | C-N-CA     | -6.76 | 113.50      | 123.11   |
| 1   | A     | 648 | VAL  | N-CA-C     | 6.65  | 116.79      | 110.74   |
| 1   | A     | 326 | ILE  | CB-CA-C    | -6.60 | 101.32      | 110.96   |
| 1   | A     | 281 | VAL  | CA-CB-CG1  | 6.60  | 121.62      | 110.40   |
| 1   | A     | 232 | ASP  | N-CA-C     | -6.60 | 104.40      | 114.16   |
| 1   | A     | 652 | VAL  | CB-CA-C    | -6.54 | 103.60      | 111.97   |
| 1   | A     | 321 | ASP  | O-C-N      | -6.51 | 115.30      | 123.05   |
| 1   | A     | 502 | THR  | N-CA-C     | 6.50  | 119.67      | 110.50   |
| 1   | A     | 414 | ALA  | N-CA-C     | -6.49 | 104.28      | 111.36   |
| 1   | A     | 741 | GLY  | CA-C-N     | -6.47 | 111.73      | 122.21   |
| 1   | A     | 741 | GLY  | C-N-CA     | -6.47 | 111.73      | 122.21   |
| 1   | A     | 296 | ASN  | CA-C-N     | 6.34  | 129.60      | 120.79   |
| 1   | A     | 296 | ASN  | C-N-CA     | 6.34  | 129.60      | 120.79   |
| 1   | A     | 455 | HIS  | CA-CB-CG   | 6.30  | 120.10      | 113.80   |
| 1   | A     | 734 | SER  | CA-C-O     | 6.30  | 129.52      | 120.51   |
| 1   | A     | 112 | ASN  | O-C-N      | 6.28  | 129.86      | 123.26   |
| 1   | A     | 136 | PHE  | CA-CB-CG   | -6.28 | 107.52      | 113.80   |
| 1   | A     | 698 | ASP  | N-CA-CB    | 6.27  | 119.19      | 109.85   |
| 1   | A     | 847 | VAL  | O-C-N      | 6.27  | 128.88      | 121.80   |
| 1   | A     | 597 | PHE  | CA-CB-CG   | -6.26 | 107.54      | 113.80   |
| 1   | A     | 376 | LEU  | CB-CA-C    | -6.24 | 98.68       | 110.67   |
| 1   | A     | 428 | ARG  | N-CA-C     | 6.22  | 118.64      | 109.24   |
| 1   | A     | 76  | ASN  | N-CA-C     | 6.21  | 118.94      | 110.06   |
| 1   | A     | 316 | PHE  | CA-CB-CG   | -6.19 | 107.61      | 113.80   |
| 1   | A     | 731 | GLU  | N-CA-CB    | 6.17  | 122.61      | 110.63   |
| 1   | A     | 412 | ASP  | CA-CB-CG   | 6.17  | 118.77      | 112.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 705 | ILE  | CB-CA-C   | -6.16 | 104.12      | 110.71   |
| 1   | A     | 673 | TYR  | O-C-N     | 6.16  | 126.37      | 121.20   |
| 1   | A     | 529 | ASP  | CA-C-N    | -6.15 | 110.39      | 121.14   |
| 1   | A     | 529 | ASP  | C-N-CA    | -6.15 | 110.39      | 121.14   |
| 1   | A     | 281 | VAL  | N-CA-C    | 6.14  | 116.30      | 110.53   |
| 1   | A     | 577 | LYS  | N-CA-C    | -6.13 | 104.52      | 111.14   |
| 1   | A     | 617 | ARG  | CB-CA-C   | 6.13  | 120.12      | 110.19   |
| 1   | A     | 480 | ALA  | N-CA-C    | -6.11 | 105.53      | 114.39   |
| 1   | A     | 244 | PHE  | N-CA-C    | 6.10  | 118.79      | 107.99   |
| 1   | A     | 812 | VAL  | CB-CA-C   | -6.06 | 103.85      | 112.22   |
| 1   | A     | 776 | GLY  | CA-C-N    | -6.03 | 112.20      | 122.33   |
| 1   | A     | 776 | GLY  | C-N-CA    | -6.03 | 112.20      | 122.33   |
| 1   | A     | 529 | ASP  | O-C-N     | -6.03 | 114.57      | 122.59   |
| 1   | A     | 277 | GLN  | N-CA-CB   | 6.00  | 120.41      | 110.52   |
| 1   | A     | 670 | ALA  | CA-C-O    | 5.98  | 126.74      | 119.38   |
| 1   | A     | 467 | CYS  | N-CA-C    | 5.95  | 118.36      | 108.13   |
| 1   | A     | 216 | ASP  | CA-CB-CG  | 5.94  | 118.54      | 112.60   |
| 1   | A     | 768 | ASN  | CA-CB-CG  | -5.93 | 106.67      | 112.60   |
| 1   | A     | 542 | THR  | O-C-N     | 5.92  | 125.50      | 121.71   |
| 1   | A     | 397 | PRO  | N-CA-CB   | 5.91  | 106.67      | 102.65   |
| 1   | A     | 535 | LYS  | N-CA-C    | -5.91 | 102.91      | 110.53   |
| 1   | A     | 735 | ASP  | CB-CA-C   | 5.90  | 119.66      | 111.63   |
| 1   | A     | 473 | GLU  | CA-C-N    | -5.88 | 114.79      | 122.37   |
| 1   | A     | 473 | GLU  | C-N-CA    | -5.88 | 114.79      | 122.37   |
| 1   | A     | 629 | HIS  | CA-C-O    | 5.87  | 125.51      | 119.05   |
| 1   | A     | 476 | ILE  | N-CA-C    | 5.87  | 118.39      | 109.12   |
| 1   | A     | 147 | VAL  | CA-C-N    | 5.87  | 127.17      | 119.84   |
| 1   | A     | 147 | VAL  | C-N-CA    | 5.87  | 127.17      | 119.84   |
| 1   | A     | 269 | TYR  | CA-CB-CG  | 5.87  | 124.46      | 113.90   |
| 1   | A     | 542 | THR  | N-CA-CB   | -5.86 | 100.63      | 111.18   |
| 1   | A     | 872 | ASN  | CA-CB-CG  | -5.85 | 106.75      | 112.60   |
| 1   | A     | 517 | VAL  | N-CA-C    | 5.79  | 121.37      | 109.34   |
| 1   | A     | 440 | HIS  | CA-CB-CG  | -5.77 | 108.03      | 113.80   |
| 1   | A     | 382 | ASN  | CA-CB-CG  | -5.76 | 106.84      | 112.60   |
| 1   | A     | 599 | LYS  | CA-C-O    | 5.76  | 126.41      | 119.61   |
| 1   | A     | 744 | ILE  | N-CA-CB   | 5.74  | 117.86      | 111.89   |
| 1   | A     | 200 | PRO  | N-CA-CB   | 5.73  | 109.26      | 103.25   |
| 1   | A     | 728 | VAL  | CB-CA-C   | 5.70  | 119.88      | 112.24   |
| 1   | A     | 857 | PHE  | N-CA-C    | 5.70  | 118.43      | 111.82   |
| 1   | A     | 806 | THR  | CA-CB-OG1 | -5.68 | 101.08      | 109.60   |
| 1   | A     | 739 | HIS  | CA-C-N    | -5.67 | 115.75      | 123.12   |
| 1   | A     | 739 | HIS  | C-N-CA    | -5.67 | 115.75      | 123.12   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 177 | LYS  | N-CA-C     | -5.65 | 105.50      | 112.90   |
| 1   | A     | 193 | GLY  | N-CA-C     | -5.64 | 107.17      | 115.30   |
| 1   | A     | 495 | TYR  | CA-C-N     | -5.64 | 114.59      | 122.71   |
| 1   | A     | 495 | TYR  | C-N-CA     | -5.64 | 114.59      | 122.71   |
| 1   | A     | 34  | MET  | N-CA-CB    | -5.63 | 103.22      | 110.03   |
| 1   | A     | 855 | SER  | CA-CB-OG   | -5.63 | 99.84       | 111.10   |
| 1   | A     | 805 | GLN  | OE1-CD-NE2 | 5.62  | 128.22      | 122.60   |
| 1   | A     | 65  | ILE  | CB-CA-C    | -5.61 | 104.67      | 112.02   |
| 1   | A     | 445 | ILE  | O-C-N      | 5.61  | 128.86      | 123.14   |
| 1   | A     | 442 | ALA  | N-CA-C     | 5.58  | 118.78      | 110.52   |
| 1   | A     | 719 | ASP  | CA-CB-CG   | -5.56 | 107.04      | 112.60   |
| 1   | A     | 137 | ILE  | N-CA-C     | -5.55 | 105.09      | 110.42   |
| 1   | A     | 99  | MET  | O-C-N      | 5.53  | 127.68      | 121.32   |
| 1   | A     | 58  | THR  | N-CA-C     | 5.53  | 117.67      | 110.43   |
| 1   | A     | 690 | GLU  | CG-CD-OE2  | -5.47 | 105.81      | 118.40   |
| 1   | A     | 658 | PHE  | N-CA-C     | 5.46  | 117.31      | 111.36   |
| 1   | A     | 524 | ILE  | N-CA-C     | -5.44 | 105.30      | 110.42   |
| 1   | A     | 293 | GLN  | CB-CG-CD   | -5.42 | 103.38      | 112.60   |
| 1   | A     | 250 | THR  | CA-CB-CG2  | -5.41 | 101.30      | 110.50   |
| 1   | A     | 409 | PHE  | CA-CB-CG   | -5.41 | 108.39      | 113.80   |
| 1   | A     | 717 | VAL  | N-CA-C     | -5.41 | 105.11      | 111.00   |
| 1   | A     | 295 | GLU  | N-CA-C     | -5.39 | 105.48      | 111.36   |
| 1   | A     | 500 | GLY  | N-CA-C     | -5.38 | 100.43      | 113.18   |
| 1   | A     | 237 | VAL  | CB-CA-C    | -5.36 | 103.15      | 110.77   |
| 1   | A     | 33  | GLY  | CA-C-O     | 5.35  | 124.96      | 118.86   |
| 1   | A     | 800 | PHE  | CB-CA-C    | -5.34 | 100.87      | 110.37   |
| 1   | A     | 195 | GLU  | CB-CA-C    | 5.34  | 119.04      | 110.29   |
| 1   | A     | 35  | PRO  | CB-CA-C    | -5.31 | 102.80      | 111.56   |
| 1   | A     | 698 | ASP  | CA-CB-CG   | -5.30 | 107.30      | 112.60   |
| 1   | A     | 277 | GLN  | CB-CA-C    | 5.30  | 118.39      | 109.48   |
| 1   | A     | 693 | GLU  | CB-CA-C    | -5.30 | 102.79      | 110.96   |
| 1   | A     | 336 | THR  | N-CA-CB    | 5.29  | 119.77      | 111.20   |
| 1   | A     | 457 | ALA  | N-CA-C     | -5.29 | 104.76      | 111.11   |
| 1   | A     | 523 | ARG  | NE-CZ-NH2  | 5.28  | 123.95      | 119.20   |
| 1   | A     | 121 | LYS  | N-CA-CB    | 5.26  | 117.91      | 110.13   |
| 1   | A     | 265 | GLU  | N-CA-C     | 5.25  | 121.98      | 110.80   |
| 1   | A     | 561 | ARG  | CA-C-N     | -5.23 | 114.44      | 122.60   |
| 1   | A     | 561 | ARG  | C-N-CA     | -5.23 | 114.44      | 122.60   |
| 1   | A     | 613 | PRO  | N-CA-CB    | 5.23  | 107.90      | 103.35   |
| 1   | A     | 616 | VAL  | N-CA-CB    | -5.22 | 105.03      | 110.72   |
| 1   | A     | 552 | LEU  | CA-C-O     | 5.22  | 125.79      | 119.11   |
| 1   | A     | 280 | ASP  | CA-CB-CG   | 5.20  | 117.80      | 112.60   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 532 | ARG  | CG-CD-NE | 5.20  | 123.44      | 112.00   |
| 1   | A     | 333 | PHE  | CA-CB-CG | -5.19 | 108.61      | 113.80   |
| 1   | A     | 249 | GLU  | CB-CG-CD | -5.19 | 103.77      | 112.60   |
| 1   | A     | 499 | ASP  | CA-CB-CG | 5.19  | 117.79      | 112.60   |
| 1   | A     | 330 | LYS  | CB-CA-C  | 5.19  | 118.77      | 110.16   |
| 1   | A     | 819 | GLY  | N-CA-C   | -5.17 | 106.46      | 113.24   |
| 1   | A     | 47  | CYS  | N-CA-C   | -5.16 | 105.35      | 110.97   |
| 1   | A     | 264 | GLY  | CA-C-O   | 5.14  | 124.04      | 118.95   |
| 1   | A     | 434 | GLU  | O-C-N    | 5.12  | 127.55      | 122.12   |
| 1   | A     | 251 | SER  | N-CA-C   | -5.11 | 101.59      | 109.52   |
| 1   | A     | 94  | ALA  | CB-CA-C  | -5.11 | 104.73      | 111.42   |
| 1   | A     | 69  | ILE  | CB-CA-C  | -5.09 | 105.37      | 112.04   |
| 1   | A     | 103 | MET  | CB-CA-C  | 5.08  | 118.13      | 109.75   |
| 1   | A     | 84  | GLU  | CB-CG-CD | 5.08  | 121.23      | 112.60   |
| 1   | A     | 80  | PHE  | CB-CA-C  | 5.06  | 120.49      | 110.42   |
| 1   | A     | 249 | GLU  | N-CA-C   | 5.06  | 121.57      | 110.80   |
| 1   | A     | 821 | GLN  | N-CA-C   | -5.05 | 105.86      | 112.23   |
| 1   | A     | 707 | LEU  | CB-CA-C  | -5.04 | 104.74      | 111.89   |
| 1   | A     | 18  | LEU  | CB-CA-C  | -5.04 | 101.35      | 110.56   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 422 | GLU  | Sidechain |
| 1   | A     | 457 | ALA  | Mainchain |

## 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     | 6724  | 0        | 6645     | 799     | 4            |
| 2   | A     | 10    | 0        | 0        | 2       | 0            |
| 3   | A     | 44    | 0        | 0        | 2       | 0            |
| All | All   | 6778  | 0        | 6645     | 799     | 4            |

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 60.

All (799) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:828:CYS:H    | 1:A:850:ASN:ND2  | 1.40                     | 1.19              |
| 1:A:107:LEU:HB3  | 1:A:242:MET:HE1  | 1.15                     | 1.15              |
| 1:A:107:LEU:HD21 | 1:A:279:GLU:HG3  | 1.34                     | 1.10              |
| 1:A:253:THR:HG21 | 1:A:278:GLY:HA2  | 1.37                     | 1.06              |
| 1:A:276:ALA:HB1  | 1:A:281:VAL:HG21 | 1.07                     | 1.03              |
| 1:A:734:SER:HB3  | 1:A:736:MET:H    | 1.26                     | 1.00              |
| 1:A:84:GLU:HG2   | 1:A:118:GLY:HA2  | 1.47                     | 0.96              |
| 1:A:578:MET:HE3  | 1:A:587:ARG:HD3  | 1.48                     | 0.95              |
| 1:A:43:THR:HG22  | 1:A:45:GLU:H     | 1.31                     | 0.94              |
| 1:A:262:SER:HB3  | 1:A:461:ARG:HD2  | 1.48                     | 0.94              |
| 1:A:330:LYS:HD2  | 1:A:331:LEU:N    | 1.84                     | 0.93              |
| 1:A:84:GLU:HA    | 1:A:118:GLY:HA3  | 1.50                     | 0.92              |
| 1:A:146:GLU:HG3  | 1:A:187:TYR:CE1  | 2.04                     | 0.92              |
| 1:A:108:ASN:HD21 | 1:A:277:GLN:HE22 | 1.16                     | 0.91              |
| 1:A:167:PHE:HB3  | 1:A:169:THR:HG22 | 1.51                     | 0.91              |
| 1:A:276:ALA:CB   | 1:A:281:VAL:HG21 | 1.99                     | 0.91              |
| 1:A:578:MET:HG2  | 1:A:587:ARG:HG3  | 1.49                     | 0.90              |
| 1:A:828:CYS:H    | 1:A:850:ASN:HD22 | 1.02                     | 0.89              |
| 1:A:408:TYR:HE1  | 1:A:424:VAL:HG22 | 1.35                     | 0.89              |
| 1:A:57:ILE:HD11  | 1:A:209:LYS:HG3  | 1.53                     | 0.88              |
| 1:A:408:TYR:CE1  | 1:A:424:VAL:HG22 | 2.09                     | 0.87              |
| 1:A:163:LYS:HB3  | 1:A:165:VAL:HG12 | 1.58                     | 0.86              |
| 1:A:253:THR:HG21 | 1:A:278:GLY:CA   | 2.06                     | 0.86              |
| 1:A:165:VAL:HG22 | 1:A:170:ASP:HB3  | 1.58                     | 0.85              |
| 1:A:263:THR:OG1  | 1:A:265:GLU:HB2  | 1.75                     | 0.85              |
| 1:A:342:THR:HG22 | 1:A:345:ALA:CB   | 2.07                     | 0.84              |
| 1:A:400:PRO:HA   | 1:A:499:ASP:HB3  | 1.60                     | 0.84              |
| 1:A:57:ILE:CD1   | 1:A:209:LYS:HG3  | 2.08                     | 0.84              |
| 1:A:565:MET:HE1  | 1:A:602:PHE:CE1  | 2.12                     | 0.83              |
| 1:A:400:PRO:HA   | 1:A:499:ASP:CB   | 2.08                     | 0.83              |
| 1:A:213:ARG:HH11 | 1:A:213:ARG:HB2  | 1.42                     | 0.83              |
| 1:A:43:THR:HG21  | 1:A:45:GLU:HG2   | 1.60                     | 0.83              |
| 1:A:224:ARG:NH1  | 1:A:231:GLY:HA3  | 1.94                     | 0.83              |
| 1:A:107:LEU:HD21 | 1:A:279:GLU:CG   | 2.09                     | 0.82              |
| 1:A:196:PHE:CD1  | 1:A:197:PRO:HD2  | 2.15                     | 0.82              |
| 1:A:318:ASP:HB2  | 1:A:367:ARG:HH12 | 1.43                     | 0.82              |
| 1:A:857:PHE:HB2  | 3:A:918:HOH:O    | 1.78                     | 0.81              |
| 1:A:828:CYS:N    | 1:A:850:ASN:HD22 | 1.79                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:16:ARG:HG3   | 1:A:24:CYS:SG    | 2.20                     | 0.81              |
| 1:A:30:THR:OG1   | 1:A:36:ILE:HD11  | 1.80                     | 0.81              |
| 1:A:149:LYS:HZ3  | 1:A:153:GLU:HG3  | 1.46                     | 0.80              |
| 1:A:179:LEU:HD11 | 1:A:183:PHE:CE1  | 2.16                     | 0.80              |
| 1:A:219:ARG:HG3  | 1:A:436:ILE:HG21 | 1.63                     | 0.80              |
| 1:A:172:THR:HG23 | 1:A:175:ASP:OD2  | 1.80                     | 0.80              |
| 1:A:73:GLU:HG2   | 1:A:79:LYS:HA    | 1.62                     | 0.79              |
| 1:A:43:THR:CG2   | 1:A:45:GLU:HG2   | 2.12                     | 0.79              |
| 1:A:107:LEU:HB3  | 1:A:242:MET:CE   | 2.06                     | 0.79              |
| 1:A:644:THR:HG23 | 1:A:647:GLU:OE1  | 1.82                     | 0.79              |
| 1:A:842:GLU:HG2  | 1:A:846:LYS:HD2  | 1.62                     | 0.79              |
| 1:A:101:GLY:O    | 1:A:102:MET:HE2  | 1.83                     | 0.79              |
| 1:A:159:MET:HE1  | 1:A:179:LEU:HB2  | 1.64                     | 0.78              |
| 1:A:165:VAL:CG2  | 1:A:170:ASP:HB3  | 2.14                     | 0.78              |
| 1:A:119:PHE:O    | 1:A:123:THR:HB   | 1.83                     | 0.78              |
| 1:A:828:CYS:N    | 1:A:850:ASN:ND2  | 2.26                     | 0.78              |
| 1:A:156:ILE:HD11 | 1:A:168:ASP:HB3  | 1.63                     | 0.78              |
| 1:A:99:MET:HG3   | 1:A:103:MET:HE2  | 1.64                     | 0.78              |
| 1:A:102:MET:CE   | 1:A:436:ILE:HD13 | 2.14                     | 0.77              |
| 1:A:519:GLY:O    | 1:A:523:ARG:HG3  | 1.82                     | 0.77              |
| 1:A:277:GLN:O    | 1:A:281:VAL:HG22 | 1.83                     | 0.77              |
| 1:A:345:ALA:O    | 1:A:349:ILE:HG13 | 1.84                     | 0.77              |
| 1:A:542:THR:CG2  | 1:A:545:ASP:H    | 1.96                     | 0.77              |
| 1:A:429:LEU:HD11 | 1:A:449:ARG:HE   | 1.50                     | 0.77              |
| 1:A:42:VAL:HB    | 1:A:237:VAL:HG23 | 1.67                     | 0.77              |
| 1:A:99:MET:CG    | 1:A:103:MET:HE2  | 2.15                     | 0.77              |
| 1:A:381:PHE:CG   | 1:A:386:LEU:HD11 | 2.20                     | 0.76              |
| 1:A:478:GLU:O    | 1:A:481:LYS:HG3  | 1.84                     | 0.76              |
| 1:A:107:LEU:CB   | 1:A:242:MET:HE1  | 2.08                     | 0.76              |
| 1:A:584:VAL:O    | 1:A:588:GLU:HB2  | 1.85                     | 0.76              |
| 1:A:71:TRP:O     | 1:A:75:LEU:HB2   | 1.84                     | 0.75              |
| 1:A:532:ARG:HD2  | 1:A:534:LEU:O    | 1.86                     | 0.75              |
| 1:A:729:LYS:HB3  | 1:A:733:GLY:C    | 2.11                     | 0.75              |
| 1:A:108:ASN:OD1  | 1:A:242:MET:HE2  | 1.86                     | 0.75              |
| 1:A:253:THR:CG2  | 1:A:278:GLY:HA2  | 2.17                     | 0.75              |
| 1:A:330:LYS:HD2  | 1:A:331:LEU:H    | 1.50                     | 0.75              |
| 1:A:5:VAL:HG22   | 1:A:42:VAL:HG22  | 1.67                     | 0.74              |
| 1:A:257:PHE:HD2  | 1:A:269:TYR:HD1  | 1.35                     | 0.74              |
| 1:A:432:SER:HB2  | 1:A:433:PRO:HD2  | 1.69                     | 0.74              |
| 1:A:643:LEU:HD23 | 1:A:643:LEU:N    | 2.02                     | 0.74              |
| 1:A:729:LYS:HD3  | 1:A:734:SER:HB3  | 1.70                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:529:ASP:CG   | 1:A:863:ARG:HH21 | 1.94                     | 0.74              |
| 1:A:106:ILE:HD11 | 1:A:143:VAL:HB   | 1.70                     | 0.74              |
| 1:A:109:LEU:HD23 | 1:A:109:LEU:O    | 1.88                     | 0.74              |
| 1:A:707:LEU:CD2  | 1:A:746:ILE:HD11 | 2.18                     | 0.74              |
| 1:A:349:ILE:HG22 | 1:A:353:LEU:CD1  | 2.19                     | 0.73              |
| 1:A:680:GLN:O    | 1:A:684:VAL:HG23 | 1.87                     | 0.73              |
| 1:A:156:ILE:HD11 | 1:A:168:ASP:CB   | 2.19                     | 0.73              |
| 1:A:733:GLY:O    | 1:A:735:ASP:N    | 2.21                     | 0.73              |
| 1:A:12:ASN:OD1   | 1:A:15:MET:HG3   | 1.89                     | 0.73              |
| 1:A:429:LEU:HA   | 1:A:448:VAL:HB   | 1.69                     | 0.73              |
| 1:A:269:TYR:OH   | 1:A:452:MET:HE3  | 1.88                     | 0.73              |
| 1:A:266:LYS:HD2  | 1:A:267:GLY:H    | 1.53                     | 0.72              |
| 1:A:271:GLU:CG   | 1:A:453:THR:HG23 | 2.19                     | 0.72              |
| 1:A:649:LYS:HG3  | 1:A:650:ALA:N    | 2.02                     | 0.72              |
| 1:A:159:MET:CE   | 1:A:179:LEU:HD13 | 2.19                     | 0.72              |
| 1:A:325:THR:O    | 1:A:332:TYR:N    | 2.22                     | 0.72              |
| 1:A:381:PHE:HB3  | 1:A:386:LEU:CD1  | 2.20                     | 0.72              |
| 1:A:664:HIS:HD2  | 1:A:668:ARG:HB3  | 1.54                     | 0.72              |
| 1:A:156:ILE:HD11 | 1:A:168:ASP:CG   | 2.15                     | 0.72              |
| 1:A:349:ILE:HG22 | 1:A:353:LEU:HD11 | 1.71                     | 0.72              |
| 1:A:147:VAL:HB   | 1:A:190:ALA:CB   | 2.19                     | 0.72              |
| 1:A:285:VAL:HG13 | 1:A:286:ARG:H    | 1.54                     | 0.72              |
| 1:A:342:THR:HG22 | 1:A:345:ALA:HB2  | 1.71                     | 0.71              |
| 1:A:513:GLN:HG3  | 1:A:514:GLU:H    | 1.51                     | 0.71              |
| 1:A:362:GLU:OE1  | 1:A:362:GLU:N    | 2.18                     | 0.71              |
| 1:A:495:TYR:C    | 1:A:496:ILE:HG13 | 2.14                     | 0.71              |
| 1:A:94:ALA:C     | 1:A:235:THR:HG22 | 2.16                     | 0.71              |
| 1:A:196:PHE:CG   | 1:A:197:PRO:HD2  | 2.26                     | 0.71              |
| 1:A:318:ASP:HB2  | 1:A:367:ARG:NH1  | 2.06                     | 0.71              |
| 1:A:662:MET:HG2  | 1:A:773:MET:HE2  | 1.72                     | 0.71              |
| 1:A:131:ASP:HB2  | 1:A:176:LEU:CD1  | 2.19                     | 0.70              |
| 1:A:146:GLU:HG3  | 1:A:187:TYR:HE1  | 1.50                     | 0.70              |
| 1:A:149:LYS:NZ   | 1:A:153:GLU:HG3  | 2.05                     | 0.70              |
| 1:A:278:GLY:O    | 1:A:280:ASP:N    | 2.25                     | 0.70              |
| 1:A:595:ILE:N    | 1:A:596:PRO:HD2  | 2.06                     | 0.70              |
| 1:A:153:GLU:O    | 1:A:157:ASP:HB2  | 1.92                     | 0.70              |
| 1:A:59:GLN:HG2   | 1:A:60:GLU:H     | 1.55                     | 0.70              |
| 1:A:679:MET:O    | 1:A:679:MET:HG2  | 1.92                     | 0.69              |
| 1:A:7:LYS:HB2    | 1:A:10:GLU:HG2   | 1.73                     | 0.69              |
| 1:A:73:GLU:OE2   | 1:A:80:PHE:N     | 2.24                     | 0.69              |
| 1:A:167:PHE:CB   | 1:A:169:THR:HG22 | 2.22                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:429:LEU:HD12 | 1:A:449:ARG:HG2  | 1.72                     | 0.69              |
| 1:A:159:MET:HE1  | 1:A:179:LEU:CB   | 2.21                     | 0.69              |
| 1:A:386:LEU:CD1  | 1:A:510:ILE:HG21 | 2.22                     | 0.69              |
| 1:A:525:MET:HE3  | 1:A:860:PRO:CB   | 2.22                     | 0.69              |
| 1:A:351:CYS:O    | 1:A:354:VAL:HB   | 1.91                     | 0.69              |
| 1:A:532:ARG:HH11 | 1:A:532:ARG:CG   | 2.06                     | 0.69              |
| 1:A:167:PHE:O    | 1:A:170:ASP:HB2  | 1.93                     | 0.69              |
| 1:A:213:ARG:HB2  | 1:A:213:ARG:NH1  | 2.07                     | 0.68              |
| 1:A:377:LEU:HD23 | 1:A:515:ALA:CB   | 2.23                     | 0.68              |
| 1:A:312:LEU:O    | 1:A:315:HIS:N    | 2.27                     | 0.68              |
| 1:A:322:MET:HB3  | 1:A:336:THR:HG23 | 1.74                     | 0.68              |
| 1:A:682:ARG:NH1  | 1:A:728:VAL:HG22 | 2.09                     | 0.68              |
| 1:A:347:LEU:HD22 | 1:A:524:ILE:HG13 | 1.76                     | 0.68              |
| 1:A:688:ALA:O    | 1:A:692:LYS:HB2  | 1.92                     | 0.68              |
| 1:A:97:ALA:HB2   | 1:A:233:TRP:HZ3  | 1.59                     | 0.68              |
| 1:A:588:GLU:O    | 1:A:591:LEU:HB2  | 1.93                     | 0.68              |
| 1:A:690:GLU:O    | 1:A:694:GLU:HG2  | 1.94                     | 0.68              |
| 1:A:99:MET:HE3   | 1:A:102:MET:HG3  | 1.74                     | 0.68              |
| 1:A:156:ILE:O    | 1:A:160:LYS:HG3  | 1.93                     | 0.68              |
| 1:A:159:MET:HE3  | 1:A:179:LEU:HD13 | 1.76                     | 0.68              |
| 1:A:598:GLN:CD   | 1:A:679:MET:HE1  | 2.18                     | 0.68              |
| 1:A:59:GLN:HG2   | 1:A:60:GLU:N     | 2.08                     | 0.67              |
| 1:A:60:GLU:O     | 1:A:64:GLN:HG3   | 1.93                     | 0.67              |
| 1:A:84:GLU:HG2   | 1:A:118:GLY:CA   | 2.22                     | 0.67              |
| 1:A:285:VAL:HG13 | 1:A:286:ARG:N    | 2.09                     | 0.67              |
| 1:A:257:PHE:CD2  | 1:A:269:TYR:HD1  | 2.13                     | 0.67              |
| 1:A:495:TYR:O    | 1:A:496:ILE:HG13 | 1.94                     | 0.67              |
| 1:A:271:GLU:HG2  | 1:A:453:THR:HG23 | 1.77                     | 0.67              |
| 1:A:407:VAL:O    | 1:A:492:GLU:HA   | 1.95                     | 0.67              |
| 1:A:106:ILE:CD1  | 1:A:143:VAL:HB   | 2.25                     | 0.67              |
| 1:A:230:PRO:HG2  | 1:A:233:TRP:NE1  | 2.10                     | 0.67              |
| 1:A:727:GLN:O    | 1:A:730:LYS:HD3  | 1.94                     | 0.67              |
| 1:A:578:MET:CE   | 1:A:587:ARG:HD3  | 2.24                     | 0.67              |
| 1:A:102:MET:HE3  | 1:A:436:ILE:HD13 | 1.76                     | 0.66              |
| 1:A:342:THR:HG22 | 1:A:345:ALA:HB3  | 1.77                     | 0.66              |
| 1:A:384:ALA:HA   | 1:A:387:LYS:HE3  | 1.77                     | 0.66              |
| 1:A:478:GLU:O    | 1:A:481:LYS:N    | 2.28                     | 0.66              |
| 1:A:330:LYS:NZ   | 1:A:331:LEU:O    | 2.26                     | 0.66              |
| 1:A:440:HIS:HA   | 1:A:463:MET:SD   | 2.35                     | 0.66              |
| 1:A:659:ASN:N    | 1:A:660:PRO:HD3  | 2.10                     | 0.66              |
| 1:A:685:MET:HE2  | 1:A:725:ALA:HB1  | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:92:ARG:HH22  | 1:A:279:GLU:CD   | 2.03                     | 0.66              |
| 1:A:116:VAL:HG11 | 1:A:130:TYR:CE1  | 2.30                     | 0.66              |
| 1:A:410:THR:OG1  | 1:A:413:GLU:HG2  | 1.96                     | 0.66              |
| 1:A:471:CYS:SG   | 1:A:474:ILE:HG13 | 2.36                     | 0.66              |
| 1:A:123:THR:HG22 | 1:A:125:ASN:H    | 1.61                     | 0.66              |
| 1:A:285:VAL:HG22 | 1:A:286:ARG:N    | 2.11                     | 0.66              |
| 1:A:673:TYR:O    | 1:A:676:ILE:HG13 | 1.96                     | 0.66              |
| 1:A:842:GLU:CD   | 1:A:873:ASN:HD21 | 2.02                     | 0.66              |
| 1:A:40:PHE:CZ    | 1:A:239:VAL:HB   | 2.31                     | 0.66              |
| 1:A:603:LYS:O    | 1:A:607:LYS:HG3  | 1.96                     | 0.66              |
| 1:A:208:VAL:HA   | 1:A:237:VAL:HG11 | 1.76                     | 0.65              |
| 1:A:261:PRO:HA   | 1:A:319:MET:CE   | 2.26                     | 0.65              |
| 1:A:330:LYS:HD2  | 1:A:330:LYS:C    | 2.17                     | 0.65              |
| 1:A:126:PRO:HB2  | 1:A:173:ALA:HB1  | 1.77                     | 0.65              |
| 1:A:71:TRP:NE1   | 1:A:75:LEU:HD23  | 2.12                     | 0.65              |
| 1:A:349:ILE:O    | 1:A:353:LEU:HD12 | 1.97                     | 0.65              |
| 1:A:165:VAL:HG22 | 1:A:170:ASP:CB   | 2.26                     | 0.65              |
| 1:A:630:THR:O    | 1:A:634:GLN:HG3  | 1.96                     | 0.65              |
| 1:A:380:THR:O    | 1:A:512:THR:HA   | 1.97                     | 0.64              |
| 1:A:381:PHE:CD2  | 1:A:386:LEU:HD21 | 2.32                     | 0.64              |
| 1:A:109:LEU:HB2  | 1:A:136:PHE:CE1  | 2.32                     | 0.64              |
| 1:A:189:GLU:OE1  | 1:A:190:ALA:N    | 2.30                     | 0.64              |
| 1:A:617:ARG:HB2  | 1:A:704:MET:HE2  | 1.80                     | 0.64              |
| 1:A:184:LYS:HZ3  | 1:A:196:PHE:N    | 1.95                     | 0.64              |
| 1:A:347:LEU:O    | 1:A:350:ALA:HB3  | 1.98                     | 0.64              |
| 1:A:102:MET:HE1  | 1:A:436:ILE:HD13 | 1.80                     | 0.63              |
| 1:A:691:VAL:O    | 1:A:695:THR:HG23 | 1.98                     | 0.63              |
| 1:A:729:LYS:HB3  | 1:A:733:GLY:HA2  | 1.79                     | 0.63              |
| 1:A:96:ARG:HG2   | 1:A:96:ARG:O     | 1.98                     | 0.63              |
| 1:A:617:ARG:NH2  | 2:A:902:SO4:O3   | 2.29                     | 0.63              |
| 1:A:726:GLU:OE1  | 1:A:729:LYS:HE3  | 1.99                     | 0.63              |
| 1:A:523:ARG:NE   | 2:A:901:SO4:O3   | 2.30                     | 0.63              |
| 1:A:473:GLU:CD   | 1:A:473:GLU:H    | 2.04                     | 0.63              |
| 1:A:751:LEU:HD23 | 1:A:814:MET:CE   | 2.29                     | 0.63              |
| 1:A:525:MET:HE3  | 1:A:860:PRO:HB3  | 1.79                     | 0.63              |
| 1:A:354:VAL:HG11 | 1:A:527:TRP:CH2  | 2.33                     | 0.63              |
| 1:A:368:ILE:HB   | 1:A:864:LEU:HD11 | 1.81                     | 0.63              |
| 1:A:390:GLU:CB   | 1:A:505:ILE:HG22 | 2.29                     | 0.63              |
| 1:A:515:ALA:O    | 1:A:516:SER:HB3  | 1.97                     | 0.63              |
| 1:A:404:ALA:HB2  | 1:A:496:ILE:HG23 | 1.80                     | 0.62              |
| 1:A:373:LEU:HA   | 1:A:376:LEU:HD23 | 1.80                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:386:LEU:HD11 | 1:A:510:ILE:HG21 | 1.81                     | 0.62              |
| 1:A:159:MET:CE   | 1:A:179:LEU:HB2  | 2.30                     | 0.62              |
| 1:A:479:GLU:OE1  | 1:A:479:GLU:N    | 2.27                     | 0.62              |
| 1:A:376:LEU:N    | 1:A:376:LEU:HD22 | 2.15                     | 0.62              |
| 1:A:418:HIS:HB2  | 1:A:422:GLU:HG3  | 1.81                     | 0.62              |
| 1:A:323:GLU:HB3  | 1:A:334:LEU:HB2  | 1.80                     | 0.62              |
| 1:A:258:THR:HA   | 1:A:268:ILE:HD13 | 1.82                     | 0.62              |
| 1:A:599:LYS:HD3  | 1:A:686:GLU:CB   | 2.30                     | 0.62              |
| 1:A:323:GLU:OE1  | 1:A:335:GLN:NE2  | 2.33                     | 0.62              |
| 1:A:542:THR:HG22 | 1:A:545:ASP:H    | 1.65                     | 0.62              |
| 1:A:147:VAL:CG2  | 1:A:148:PRO:HD2  | 2.28                     | 0.61              |
| 1:A:317:ARG:NH2  | 1:A:363:GLU:OE1  | 2.33                     | 0.61              |
| 1:A:729:LYS:HB3  | 1:A:733:GLY:CA   | 2.30                     | 0.61              |
| 1:A:32:LEU:HD21  | 1:A:315:HIS:CE1  | 2.35                     | 0.61              |
| 1:A:163:LYS:O    | 1:A:165:VAL:N    | 2.32                     | 0.61              |
| 1:A:644:THR:H    | 1:A:647:GLU:HB2  | 1.65                     | 0.61              |
| 1:A:191:MET:C    | 1:A:193:GLY:H    | 2.07                     | 0.61              |
| 1:A:99:MET:HE2   | 1:A:102:MET:CB   | 2.30                     | 0.61              |
| 1:A:147:VAL:HB   | 1:A:190:ALA:HB3  | 1.80                     | 0.61              |
| 1:A:211:VAL:O    | 1:A:214:SER:N    | 2.33                     | 0.61              |
| 1:A:732:LYS:O    | 1:A:732:LYS:HG2  | 1.98                     | 0.61              |
| 1:A:658:PHE:C    | 1:A:660:PRO:HD3  | 2.25                     | 0.61              |
| 1:A:285:VAL:HG22 | 1:A:286:ARG:H    | 1.66                     | 0.61              |
| 1:A:84:GLU:OE1   | 1:A:122:LYS:HG2  | 2.01                     | 0.61              |
| 1:A:478:GLU:C    | 1:A:481:LYS:H    | 2.08                     | 0.61              |
| 1:A:599:LYS:CD   | 1:A:686:GLU:HB3  | 2.30                     | 0.61              |
| 1:A:73:GLU:CG    | 1:A:80:PHE:H     | 2.13                     | 0.60              |
| 1:A:196:PHE:O    | 1:A:198:GLN:HG2  | 2.00                     | 0.60              |
| 1:A:43:THR:HG22  | 1:A:45:GLU:N     | 2.10                     | 0.60              |
| 1:A:86:PRO:HG3   | 1:A:115:ALA:HB1  | 1.82                     | 0.60              |
| 1:A:5:VAL:HG11   | 1:A:68:ALA:HB2   | 1.83                     | 0.60              |
| 1:A:16:ARG:HG3   | 1:A:21:GLY:HA2   | 1.83                     | 0.60              |
| 1:A:99:MET:HE2   | 1:A:102:MET:HB2  | 1.82                     | 0.60              |
| 1:A:199:GLU:OE2  | 1:A:201:LYS:HB2  | 2.01                     | 0.60              |
| 1:A:423:ARG:HA   | 1:A:443:GLU:HG2  | 1.83                     | 0.60              |
| 1:A:420:LYS:HA   | 1:A:441:ALA:O    | 2.01                     | 0.60              |
| 1:A:424:VAL:O    | 1:A:425:ILE:HD13 | 2.01                     | 0.60              |
| 1:A:326:ILE:HA   | 1:A:330:LYS:O    | 2.01                     | 0.60              |
| 1:A:93:SER:HB2   | 1:A:235:THR:HG21 | 1.83                     | 0.60              |
| 1:A:549:ALA:HB1  | 1:A:554:ALA:HB2  | 1.83                     | 0.60              |
| 1:A:363:GLU:O    | 1:A:367:ARG:HG3  | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:591:LEU:HD12 | 1:A:675:GLU:HB3  | 1.84                     | 0.60              |
| 1:A:381:PHE:HB3  | 1:A:386:LEU:HD11 | 1.82                     | 0.59              |
| 1:A:637:LEU:O    | 1:A:641:MET:HG3  | 2.01                     | 0.59              |
| 1:A:649:LYS:O    | 1:A:653:ASP:OD1  | 2.20                     | 0.59              |
| 1:A:73:GLU:HG2   | 1:A:80:PHE:H     | 1.66                     | 0.59              |
| 1:A:869:ALA:O    | 1:A:873:ASN:ND2  | 2.34                     | 0.59              |
| 1:A:396:LEU:HB2  | 1:A:469:SER:O    | 2.01                     | 0.59              |
| 1:A:347:LEU:CD2  | 1:A:524:ILE:HG13 | 2.33                     | 0.59              |
| 1:A:360:THR:OG1  | 1:A:363:GLU:HG3  | 2.03                     | 0.59              |
| 1:A:109:LEU:HB2  | 1:A:136:PHE:HE1  | 1.65                     | 0.59              |
| 1:A:419:GLU:HA   | 1:A:441:ALA:HB1  | 1.84                     | 0.59              |
| 1:A:779:ARG:NH2  | 1:A:833:GLU:OE2  | 2.35                     | 0.59              |
| 1:A:79:LYS:HB3   | 1:A:82:ASP:HB2   | 1.85                     | 0.59              |
| 1:A:599:LYS:HD3  | 1:A:686:GLU:HB3  | 1.83                     | 0.59              |
| 1:A:726:GLU:OE1  | 1:A:726:GLU:HA   | 2.02                     | 0.59              |
| 1:A:781:ASP:O    | 1:A:784:LYS:HG2  | 2.02                     | 0.59              |
| 1:A:163:LYS:C    | 1:A:165:VAL:H    | 2.11                     | 0.59              |
| 1:A:707:LEU:HD22 | 1:A:746:ILE:HD11 | 1.83                     | 0.59              |
| 1:A:121:LYS:C    | 1:A:123:THR:H    | 2.09                     | 0.59              |
| 1:A:131:ASP:HA   | 1:A:176:LEU:HD13 | 1.85                     | 0.59              |
| 1:A:525:MET:HE3  | 1:A:860:PRO:CA   | 2.33                     | 0.59              |
| 1:A:276:ALA:HB2  | 1:A:286:ARG:HH22 | 1.68                     | 0.58              |
| 1:A:278:GLY:HA3  | 3:A:930:HOH:O    | 2.02                     | 0.58              |
| 1:A:420:LYS:HB3  | 1:A:440:HIS:O    | 2.02                     | 0.58              |
| 1:A:84:GLU:CG    | 1:A:118:GLY:HA2  | 2.28                     | 0.58              |
| 1:A:429:LEU:CD1  | 1:A:449:ARG:HG2  | 2.33                     | 0.58              |
| 1:A:440:HIS:HB2  | 1:A:463:MET:HE1  | 1.85                     | 0.58              |
| 1:A:572:ILE:O    | 1:A:575:ILE:HG22 | 2.03                     | 0.58              |
| 1:A:100:PRO:HB3  | 1:A:458:VAL:HG12 | 1.85                     | 0.58              |
| 1:A:730:LYS:HG3  | 1:A:730:LYS:O    | 2.04                     | 0.58              |
| 1:A:219:ARG:HD3  | 1:A:436:ILE:HG22 | 1.86                     | 0.58              |
| 1:A:131:ASP:CA   | 1:A:176:LEU:HD13 | 2.33                     | 0.57              |
| 1:A:68:ALA:O     | 1:A:71:TRP:HB3   | 2.04                     | 0.57              |
| 1:A:73:GLU:OE2   | 1:A:79:LYS:HG2   | 2.04                     | 0.57              |
| 1:A:108:ASN:HB2  | 1:A:136:PHE:HB2  | 1.86                     | 0.57              |
| 1:A:215:TRP:HH2  | 1:A:232:ASP:N    | 2.03                     | 0.57              |
| 1:A:274:ILE:HD11 | 1:A:298:MET:HE3  | 1.86                     | 0.57              |
| 1:A:396:LEU:O    | 1:A:468:VAL:HA   | 2.04                     | 0.57              |
| 1:A:403:ALA:O    | 1:A:496:ILE:HG23 | 2.03                     | 0.57              |
| 1:A:572:ILE:O    | 1:A:576:ARG:HG3  | 2.03                     | 0.57              |
| 1:A:46:ALA:HA    | 1:A:49:GLU:HB3   | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:168:ASP:OD1  | 1:A:168:ASP:N    | 2.37                     | 0.57              |
| 1:A:183:PHE:HA   | 1:A:186:VAL:HG23 | 1.87                     | 0.57              |
| 1:A:84:GLU:OE2   | 1:A:121:LYS:HB2  | 2.05                     | 0.57              |
| 1:A:262:SER:O    | 1:A:342:THR:HG21 | 2.05                     | 0.57              |
| 1:A:529:ASP:OD2  | 1:A:863:ARG:NH2  | 2.35                     | 0.57              |
| 1:A:449:ARG:HG3  | 1:A:449:ARG:O    | 2.04                     | 0.57              |
| 1:A:140:TYR:O    | 1:A:144:VAL:HB   | 2.05                     | 0.57              |
| 1:A:51:TYR:OH    | 1:A:216:ASP:HB2  | 2.03                     | 0.57              |
| 1:A:104:ASP:HB3  | 1:A:143:VAL:HG13 | 1.87                     | 0.57              |
| 1:A:392:ILE:CD1  | 1:A:490:PHE:HZ   | 2.18                     | 0.57              |
| 1:A:460:ALA:O    | 1:A:464:GLY:N    | 2.37                     | 0.57              |
| 1:A:318:ASP:CG   | 1:A:341:ARG:HH22 | 2.13                     | 0.56              |
| 1:A:565:MET:HE1  | 1:A:602:PHE:CZ   | 2.39                     | 0.56              |
| 1:A:141:SER:CB   | 1:A:187:TYR:HD1  | 2.18                     | 0.56              |
| 1:A:343:ALA:HB3  | 1:A:344:PRO:HD3  | 1.86                     | 0.56              |
| 1:A:371:LYS:HG2  | 1:A:838:PRO:HG2  | 1.85                     | 0.56              |
| 1:A:595:ILE:N    | 1:A:596:PRO:CD   | 2.69                     | 0.56              |
| 1:A:631:GLU:O    | 1:A:631:GLU:HG3  | 2.04                     | 0.56              |
| 1:A:4:TRP:H      | 1:A:64:GLN:NE2   | 2.02                     | 0.56              |
| 1:A:390:GLU:HB3  | 1:A:505:ILE:HG22 | 1.87                     | 0.56              |
| 1:A:131:ASP:OD1  | 1:A:134:ARG:NH1  | 2.39                     | 0.56              |
| 1:A:376:LEU:H    | 1:A:376:LEU:CD2  | 2.17                     | 0.56              |
| 1:A:398:ALA:HB1  | 1:A:457:ALA:HA   | 1.88                     | 0.56              |
| 1:A:729:LYS:CB   | 1:A:733:GLY:HA2  | 2.35                     | 0.56              |
| 1:A:140:TYR:CD2  | 1:A:144:VAL:HG21 | 2.41                     | 0.56              |
| 1:A:840:SER:O    | 1:A:843:PHE:HB3  | 2.05                     | 0.56              |
| 1:A:111:LEU:HB3  | 1:A:133:TYR:HD1  | 1.70                     | 0.56              |
| 1:A:148:PRO:O    | 1:A:150:SER:N    | 2.39                     | 0.56              |
| 1:A:66:PHE:CE1   | 1:A:201:LYS:HG2  | 2.41                     | 0.55              |
| 1:A:386:LEU:HD12 | 1:A:510:ILE:HG21 | 1.87                     | 0.55              |
| 1:A:711:LYS:HE3  | 1:A:758:GLU:OE1  | 2.05                     | 0.55              |
| 1:A:178:GLU:O    | 1:A:181:GLU:HB3  | 2.07                     | 0.55              |
| 1:A:432:SER:O    | 1:A:435:ASP:N    | 2.39                     | 0.55              |
| 1:A:495:TYR:OH   | 1:A:503:GLY:HA3  | 2.06                     | 0.55              |
| 1:A:126:PRO:HB2  | 1:A:173:ALA:CB   | 2.36                     | 0.55              |
| 1:A:184:LYS:HZ3  | 1:A:196:PHE:H    | 1.55                     | 0.55              |
| 1:A:260:ASN:OD1  | 1:A:261:PRO:HD2  | 2.07                     | 0.55              |
| 1:A:603:LYS:HE3  | 1:A:690:GLU:HB3  | 1.89                     | 0.55              |
| 1:A:615:THR:OG1  | 1:A:702:GLU:OE1  | 2.24                     | 0.55              |
| 1:A:744:ILE:HD13 | 1:A:744:ILE:N    | 2.22                     | 0.55              |
| 1:A:9:GLU:OE1    | 1:A:38:GLN:OE1   | 2.25                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:12:ASN:O     | 1:A:24:CYS:HB2   | 2.07                     | 0.55              |
| 1:A:244:PHE:HB2  | 1:A:247:LYS:HG2  | 1.89                     | 0.55              |
| 1:A:782:ALA:HB1  | 1:A:786:LEU:HD22 | 1.88                     | 0.55              |
| 1:A:109:LEU:HD23 | 1:A:109:LEU:C    | 2.32                     | 0.55              |
| 1:A:513:GLN:HG3  | 1:A:514:GLU:N    | 2.22                     | 0.55              |
| 1:A:76:ASN:HD22  | 1:A:76:ASN:C     | 2.15                     | 0.54              |
| 1:A:391:VAL:HA   | 1:A:504:LYS:HB3  | 1.88                     | 0.54              |
| 1:A:569:ALA:C    | 1:A:571:ARG:H    | 2.15                     | 0.54              |
| 1:A:728:VAL:O    | 1:A:730:LYS:N    | 2.39                     | 0.54              |
| 1:A:787:ASP:HA   | 1:A:790:TYR:HD2  | 1.72                     | 0.54              |
| 1:A:376:LEU:HD22 | 1:A:376:LEU:H    | 1.72                     | 0.54              |
| 1:A:542:THR:HG22 | 1:A:545:ASP:HB2  | 1.88                     | 0.54              |
| 1:A:381:PHE:CB   | 1:A:386:LEU:HD11 | 2.37                     | 0.54              |
| 1:A:106:ILE:HD11 | 1:A:143:VAL:CB   | 2.36                     | 0.54              |
| 1:A:618:TYR:CE1  | 1:A:703:ILE:HG23 | 2.42                     | 0.54              |
| 1:A:842:GLU:CG   | 1:A:873:ASN:HD21 | 2.19                     | 0.54              |
| 1:A:392:ILE:HD11 | 1:A:495:TYR:HE2  | 1.73                     | 0.54              |
| 1:A:638:ALA:HB2  | 1:A:648:VAL:HG21 | 1.89                     | 0.54              |
| 1:A:849:LEU:N    | 1:A:849:LEU:HD23 | 2.22                     | 0.54              |
| 1:A:215:TRP:CZ2  | 1:A:234:GLY:N    | 2.76                     | 0.54              |
| 1:A:221:ILE:HG12 | 1:A:224:ARG:NH2  | 2.22                     | 0.54              |
| 1:A:385:ALA:HB1  | 1:A:510:ILE:HG23 | 1.89                     | 0.53              |
| 1:A:411:ALA:O    | 1:A:413:GLU:N    | 2.40                     | 0.53              |
| 1:A:174:ASP:O    | 1:A:177:LYS:N    | 2.40                     | 0.53              |
| 1:A:190:ALA:O    | 1:A:191:MET:HG2  | 2.07                     | 0.53              |
| 1:A:699:ILE:HG22 | 1:A:700:VAL:N    | 2.23                     | 0.53              |
| 1:A:43:THR:HG22  | 1:A:44:THR:N     | 2.22                     | 0.53              |
| 1:A:408:TYR:HD1  | 1:A:424:VAL:HG13 | 1.73                     | 0.53              |
| 1:A:390:GLU:HB2  | 1:A:505:ILE:HG22 | 1.90                     | 0.53              |
| 1:A:418:HIS:HB2  | 1:A:422:GLU:CG   | 2.38                     | 0.53              |
| 1:A:248:GLY:C    | 1:A:275:ASN:HB2  | 2.34                     | 0.53              |
| 1:A:55:LYS:HD2   | 1:A:213:ARG:HH22 | 1.74                     | 0.53              |
| 1:A:197:PRO:O    | 1:A:203:GLN:NE2  | 2.42                     | 0.53              |
| 1:A:73:GLU:CD    | 1:A:80:PHE:H     | 2.16                     | 0.53              |
| 1:A:219:ARG:NH2  | 1:A:437:GLU:OE1  | 2.42                     | 0.53              |
| 1:A:436:ILE:HG23 | 1:A:437:GLU:N    | 2.24                     | 0.53              |
| 1:A:525:MET:HE1  | 1:A:860:PRO:O    | 2.08                     | 0.53              |
| 1:A:422:GLU:OE1  | 1:A:422:GLU:O    | 2.26                     | 0.52              |
| 1:A:16:ARG:CG    | 1:A:21:GLY:HA2   | 2.39                     | 0.52              |
| 1:A:38:GLN:O     | 1:A:241:THR:HG22 | 2.08                     | 0.52              |
| 1:A:101:GLY:C    | 1:A:102:MET:HE2  | 2.35                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:667:CYS:HB3  | 1:A:706:PRO:O    | 2.09                     | 0.52              |
| 1:A:386:LEU:HA   | 1:A:510:ILE:CD1  | 2.40                     | 0.52              |
| 1:A:514:GLU:O    | 1:A:515:ALA:O    | 2.28                     | 0.52              |
| 1:A:563:GLU:CG   | 1:A:621:PRO:HD3  | 2.40                     | 0.52              |
| 1:A:199:GLU:O    | 1:A:202:ASP:N    | 2.42                     | 0.52              |
| 1:A:271:GLU:HB2  | 1:A:288:PRO:HB2  | 1.91                     | 0.52              |
| 1:A:273:LEU:HD11 | 1:A:286:ARG:O    | 2.10                     | 0.52              |
| 1:A:439:MET:HE1  | 1:A:455:HIS:CE1  | 2.45                     | 0.52              |
| 1:A:447:THR:OG1  | 1:A:469:SER:HA   | 2.09                     | 0.52              |
| 1:A:599:LYS:HG3  | 1:A:687:ALA:HB2  | 1.90                     | 0.52              |
| 1:A:133:TYR:CE2  | 1:A:137:ILE:HD11 | 2.45                     | 0.52              |
| 1:A:188:LYS:HA   | 1:A:191:MET:HB2  | 1.92                     | 0.52              |
| 1:A:525:MET:O    | 1:A:528:ALA:HB3  | 2.09                     | 0.52              |
| 1:A:597:PHE:CD1  | 1:A:597:PHE:N    | 2.78                     | 0.52              |
| 1:A:159:MET:HE1  | 1:A:179:LEU:HD13 | 1.88                     | 0.52              |
| 1:A:532:ARG:HE   | 1:A:536:VAL:HG23 | 1.73                     | 0.52              |
| 1:A:285:VAL:CG1  | 1:A:286:ARG:H    | 2.17                     | 0.52              |
| 1:A:373:LEU:HA   | 1:A:376:LEU:CD2  | 2.40                     | 0.52              |
| 1:A:360:THR:HG23 | 1:A:363:GLU:OE2  | 2.10                     | 0.52              |
| 1:A:814:MET:HA   | 1:A:817:LYS:HE2  | 1.93                     | 0.51              |
| 1:A:386:LEU:HD12 | 1:A:386:LEU:N    | 2.26                     | 0.51              |
| 1:A:182:LYS:O    | 1:A:185:ALA:HB3  | 2.09                     | 0.51              |
| 1:A:92:ARG:HH11  | 1:A:92:ARG:CB    | 2.24                     | 0.51              |
| 1:A:320:GLN:HB2  | 1:A:322:MET:CE   | 2.41                     | 0.51              |
| 1:A:382:ASN:O    | 1:A:385:ALA:HB3  | 2.10                     | 0.51              |
| 1:A:407:VAL:HG12 | 1:A:425:ILE:HB   | 1.91                     | 0.51              |
| 1:A:771:THR:HA   | 1:A:808:VAL:HG21 | 1.93                     | 0.51              |
| 1:A:219:ARG:HG2  | 1:A:433:PRO:O    | 2.10                     | 0.51              |
| 1:A:352:ASP:O    | 1:A:356:GLU:HG3  | 2.09                     | 0.51              |
| 1:A:377:LEU:HA   | 1:A:515:ALA:HB2  | 1.91                     | 0.51              |
| 1:A:4:TRP:H      | 1:A:64:GLN:HE22  | 1.59                     | 0.51              |
| 1:A:131:ASP:HB2  | 1:A:176:LEU:HD13 | 1.92                     | 0.51              |
| 1:A:261:PRO:HD3  | 1:A:269:TYR:CD1  | 2.46                     | 0.51              |
| 1:A:291:ILE:O    | 1:A:302:TYR:HE1  | 1.93                     | 0.51              |
| 1:A:578:MET:HG2  | 1:A:587:ARG:CG   | 2.32                     | 0.51              |
| 1:A:73:GLU:HA    | 1:A:78:LYS:O     | 2.11                     | 0.51              |
| 1:A:257:PHE:CD2  | 1:A:269:TYR:CD1  | 2.97                     | 0.51              |
| 1:A:593:GLU:O    | 1:A:596:PRO:HD2  | 2.10                     | 0.51              |
| 1:A:621:PRO:HG2  | 1:A:626:PHE:CE2  | 2.45                     | 0.51              |
| 1:A:208:VAL:HG13 | 1:A:237:VAL:HG21 | 1.93                     | 0.51              |
| 1:A:392:ILE:HD11 | 1:A:495:TYR:CE2  | 2.46                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:122:LYS:HE3  | 1:A:122:LYS:CA   | 2.41                     | 0.51              |
| 1:A:557:ILE:HB   | 1:A:614:MET:HA   | 1.93                     | 0.51              |
| 1:A:259:ARG:HD3  | 1:A:266:LYS:HD3  | 1.92                     | 0.50              |
| 1:A:215:TRP:CH2  | 1:A:231:GLY:C    | 2.89                     | 0.50              |
| 1:A:651:LYS:HD2  | 1:A:651:LYS:O    | 2.11                     | 0.50              |
| 1:A:16:ARG:O     | 1:A:20:GLY:N     | 2.44                     | 0.50              |
| 1:A:320:GLN:HB2  | 1:A:322:MET:HE2  | 1.94                     | 0.50              |
| 1:A:734:SER:OG   | 1:A:736:MET:HB2  | 2.11                     | 0.50              |
| 1:A:135:ARG:CD   | 1:A:277:GLN:NE2  | 2.74                     | 0.50              |
| 1:A:187:TYR:O    | 1:A:191:MET:HG2  | 2.11                     | 0.50              |
| 1:A:327:GLU:N    | 1:A:330:LYS:O    | 2.41                     | 0.50              |
| 1:A:350:ALA:O    | 1:A:354:VAL:HG23 | 2.11                     | 0.50              |
| 1:A:135:ARG:HD2  | 1:A:277:GLN:NE2  | 2.26                     | 0.50              |
| 1:A:80:PHE:HA    | 1:A:87:LEU:HB3   | 1.92                     | 0.50              |
| 1:A:349:ILE:HG22 | 1:A:353:LEU:HD12 | 1.92                     | 0.50              |
| 1:A:485:LEU:O    | 1:A:487:GLY:N    | 2.43                     | 0.50              |
| 1:A:141:SER:HB3  | 1:A:187:TYR:HD1  | 1.77                     | 0.50              |
| 1:A:122:LYS:HE3  | 1:A:122:LYS:HA   | 1.92                     | 0.49              |
| 1:A:135:ARG:O    | 1:A:139:MET:HG3  | 2.12                     | 0.49              |
| 1:A:171:LEU:HB3  | 1:A:175:ASP:HB2  | 1.93                     | 0.49              |
| 1:A:699:ILE:HB   | 1:A:736:MET:HE2  | 1.94                     | 0.49              |
| 1:A:100:PRO:O    | 1:A:102:MET:HG2  | 2.12                     | 0.49              |
| 1:A:263:THR:C    | 1:A:265:GLU:H    | 2.19                     | 0.49              |
| 1:A:474:ILE:HG12 | 1:A:485:LEU:CD1  | 2.42                     | 0.49              |
| 1:A:711:LYS:HG3  | 1:A:755:ALA:O    | 2.12                     | 0.49              |
| 1:A:381:PHE:HZ   | 1:A:496:ILE:CG2  | 2.25                     | 0.49              |
| 1:A:498:LEU:N    | 1:A:498:LEU:HD13 | 2.28                     | 0.49              |
| 1:A:510:ILE:CG2  | 1:A:511:GLU:N    | 2.74                     | 0.49              |
| 1:A:563:GLU:HG2  | 1:A:621:PRO:HD3  | 1.94                     | 0.49              |
| 1:A:107:LEU:HG   | 1:A:139:MET:SD   | 2.52                     | 0.49              |
| 1:A:316:PHE:N    | 1:A:316:PHE:CD1  | 2.80                     | 0.49              |
| 1:A:733:GLY:O    | 1:A:735:ASP:OD1  | 2.31                     | 0.49              |
| 1:A:67:GLU:O     | 1:A:70:THR:HG23  | 2.12                     | 0.49              |
| 1:A:140:TYR:C    | 1:A:140:TYR:CD1  | 2.90                     | 0.49              |
| 1:A:141:SER:CB   | 1:A:187:TYR:CD1  | 2.96                     | 0.49              |
| 1:A:175:ASP:O    | 1:A:179:LEU:N    | 2.38                     | 0.49              |
| 1:A:322:MET:SD   | 1:A:333:PHE:HE2  | 2.36                     | 0.49              |
| 1:A:278:GLY:C    | 1:A:280:ASP:H    | 2.21                     | 0.49              |
| 1:A:294:LEU:O    | 1:A:294:LEU:HD23 | 2.13                     | 0.49              |
| 1:A:135:ARG:HH12 | 1:A:281:VAL:CG1  | 2.26                     | 0.49              |
| 1:A:141:SER:HB3  | 1:A:187:TYR:CD1  | 2.47                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:159:MET:HE1  | 1:A:179:LEU:CA   | 2.43                     | 0.49              |
| 1:A:222:VAL:HG11 | 1:A:437:GLU:HG3  | 1.95                     | 0.49              |
| 1:A:376:LEU:N    | 1:A:376:LEU:CD2  | 2.75                     | 0.49              |
| 1:A:491:ALA:O    | 1:A:492:GLU:HB2  | 2.13                     | 0.49              |
| 1:A:496:ILE:HG21 | 1:A:510:ILE:HB   | 1.95                     | 0.49              |
| 1:A:677:ALA:O    | 1:A:681:THR:OG1  | 2.22                     | 0.49              |
| 1:A:444:GLY:HA2  | 1:A:465:THR:HG22 | 1.94                     | 0.49              |
| 1:A:734:SER:CB   | 1:A:736:MET:H    | 2.10                     | 0.49              |
| 1:A:130:TYR:CE1  | 1:A:177:LYS:HD3  | 2.48                     | 0.49              |
| 1:A:177:LYS:HD2  | 1:A:177:LYS:O    | 2.13                     | 0.49              |
| 1:A:542:THR:HG23 | 1:A:544:GLU:HG2  | 1.95                     | 0.49              |
| 1:A:13:ALA:HA    | 1:A:24:CYS:HB2   | 1.95                     | 0.48              |
| 1:A:49:GLU:HG2   | 1:A:61:ILE:HD11  | 1.95                     | 0.48              |
| 1:A:830:ILE:CG2  | 1:A:852:VAL:HG12 | 2.43                     | 0.48              |
| 1:A:99:MET:HB2   | 1:A:223:TYR:CE1  | 2.49                     | 0.48              |
| 1:A:411:ALA:HB1  | 1:A:438:GLY:H    | 1.78                     | 0.48              |
| 1:A:172:THR:C    | 1:A:174:ASP:N    | 2.71                     | 0.48              |
| 1:A:253:THR:HG21 | 1:A:278:GLY:N    | 2.28                     | 0.48              |
| 1:A:448:VAL:HG22 | 1:A:474:ILE:HB   | 1.95                     | 0.48              |
| 1:A:474:ILE:CG2  | 1:A:483:PHE:HB2  | 2.43                     | 0.48              |
| 1:A:498:LEU:N    | 1:A:498:LEU:CD1  | 2.76                     | 0.48              |
| 1:A:563:GLU:OE2  | 1:A:620:ASP:N    | 2.41                     | 0.48              |
| 1:A:578:MET:HE3  | 1:A:587:ARG:CD   | 2.32                     | 0.48              |
| 1:A:42:VAL:HB    | 1:A:237:VAL:CG2  | 2.41                     | 0.48              |
| 1:A:44:THR:O     | 1:A:47:CYS:HB3   | 2.12                     | 0.48              |
| 1:A:73:GLU:HG2   | 1:A:80:PHE:N     | 2.29                     | 0.48              |
| 1:A:184:LYS:NZ   | 1:A:196:PHE:H    | 2.12                     | 0.48              |
| 1:A:594:LEU:C    | 1:A:596:PRO:HD2  | 2.37                     | 0.48              |
| 1:A:187:TYR:HE2  | 1:A:194:GLU:OE1  | 1.96                     | 0.48              |
| 1:A:49:GLU:OE2   | 1:A:53:SER:OG    | 2.30                     | 0.48              |
| 1:A:107:LEU:CD2  | 1:A:279:GLU:HG3  | 2.24                     | 0.48              |
| 1:A:278:GLY:C    | 1:A:280:ASP:N    | 2.71                     | 0.48              |
| 1:A:320:GLN:HB3  | 1:A:336:THR:HG22 | 1.96                     | 0.48              |
| 1:A:377:LEU:HD23 | 1:A:515:ALA:HB2  | 1.93                     | 0.48              |
| 1:A:407:VAL:CG1  | 1:A:495:TYR:HB3  | 2.43                     | 0.48              |
| 1:A:864:LEU:HD13 | 1:A:868:GLN:NE2  | 2.28                     | 0.48              |
| 1:A:319:MET:SD   | 1:A:339:GLY:HA3  | 2.54                     | 0.48              |
| 1:A:143:VAL:C    | 1:A:145:MET:H    | 2.20                     | 0.48              |
| 1:A:147:VAL:HG23 | 1:A:148:PRO:HD2  | 1.94                     | 0.48              |
| 1:A:418:HIS:HB2  | 1:A:422:GLU:CB   | 2.44                     | 0.48              |
| 1:A:71:TRP:O     | 1:A:74:GLU:HG2   | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:97:ALA:HB2   | 1:A:233:TRP:CZ3  | 2.45                     | 0.48              |
| 1:A:400:PRO:HA   | 1:A:499:ASP:HB2  | 1.92                     | 0.48              |
| 1:A:803:LEU:CD2  | 1:A:843:PHE:CD2  | 2.97                     | 0.48              |
| 1:A:384:ALA:HA   | 1:A:387:LYS:HB3  | 1.96                     | 0.48              |
| 1:A:573:MET:O    | 1:A:577:LYS:N    | 2.46                     | 0.48              |
| 1:A:864:LEU:O    | 1:A:867:ALA:HB3  | 2.14                     | 0.48              |
| 1:A:121:LYS:C    | 1:A:123:THR:N    | 2.72                     | 0.47              |
| 1:A:392:ILE:CD1  | 1:A:490:PHE:CZ   | 2.95                     | 0.47              |
| 1:A:649:LYS:O    | 1:A:652:VAL:HB   | 2.14                     | 0.47              |
| 1:A:857:PHE:O    | 1:A:860:PRO:HD2  | 2.14                     | 0.47              |
| 1:A:73:GLU:CG    | 1:A:79:LYS:HA    | 2.39                     | 0.47              |
| 1:A:137:ILE:HD13 | 1:A:184:LYS:HB2  | 1.95                     | 0.47              |
| 1:A:579:ILE:HG12 | 1:A:623:LEU:HD13 | 1.95                     | 0.47              |
| 1:A:754:ASP:O    | 1:A:822:THR:HG21 | 2.13                     | 0.47              |
| 1:A:127:ARG:HD2  | 1:A:171:LEU:O    | 2.13                     | 0.47              |
| 1:A:369:GLU:O    | 1:A:372:SER:OG   | 2.25                     | 0.47              |
| 1:A:43:THR:CG2   | 1:A:44:THR:N     | 2.77                     | 0.47              |
| 1:A:94:ALA:N     | 1:A:235:THR:HG22 | 2.30                     | 0.47              |
| 1:A:99:MET:HG3   | 1:A:99:MET:O     | 2.14                     | 0.47              |
| 1:A:130:TYR:CD1  | 1:A:177:LYS:HB2  | 2.48                     | 0.47              |
| 1:A:520:SER:O    | 1:A:524:ILE:HG12 | 2.15                     | 0.47              |
| 1:A:617:ARG:HB2  | 1:A:704:MET:CE   | 2.44                     | 0.47              |
| 1:A:751:LEU:CD2  | 1:A:814:MET:HE1  | 2.44                     | 0.47              |
| 1:A:142:ASP:O    | 1:A:145:MET:HE2  | 2.15                     | 0.47              |
| 1:A:281:VAL:HG23 | 1:A:282:VAL:N    | 2.28                     | 0.47              |
| 1:A:415:LYS:O    | 1:A:418:HIS:N    | 2.48                     | 0.47              |
| 1:A:429:LEU:HD21 | 1:A:449:ARG:HH21 | 1.79                     | 0.47              |
| 1:A:495:TYR:CD1  | 1:A:496:ILE:N    | 2.82                     | 0.47              |
| 1:A:224:ARG:HH11 | 1:A:231:GLY:HA3  | 1.77                     | 0.47              |
| 1:A:259:ARG:CZ   | 1:A:266:LYS:HD3  | 2.44                     | 0.47              |
| 1:A:381:PHE:CB   | 1:A:386:LEU:HD21 | 2.45                     | 0.47              |
| 1:A:132:SER:O    | 1:A:135:ARG:HB2  | 2.14                     | 0.47              |
| 1:A:159:MET:HE1  | 1:A:179:LEU:CD1  | 2.44                     | 0.47              |
| 1:A:172:THR:C    | 1:A:174:ASP:H    | 2.22                     | 0.47              |
| 1:A:200:PRO:O    | 1:A:203:GLN:HB2  | 2.13                     | 0.47              |
| 1:A:258:THR:O    | 1:A:259:ARG:HG2  | 2.14                     | 0.47              |
| 1:A:429:LEU:HD11 | 1:A:449:ARG:NE   | 2.25                     | 0.47              |
| 1:A:538:THR:HG21 | 1:A:549:ALA:CB   | 2.44                     | 0.47              |
| 1:A:747:PRO:O    | 1:A:751:LEU:HG   | 2.15                     | 0.47              |
| 1:A:864:LEU:HD23 | 1:A:864:LEU:HA   | 1.71                     | 0.47              |
| 1:A:72:LEU:O     | 1:A:75:LEU:HB3   | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:160:LYS:HD2  | 1:A:166:HIS:C    | 2.40                     | 0.47              |
| 1:A:40:PHE:CE2   | 1:A:239:VAL:HB   | 2.50                     | 0.47              |
| 1:A:97:ALA:CB    | 1:A:233:TRP:HZ3  | 2.25                     | 0.47              |
| 1:A:342:THR:HG23 | 1:A:344:PRO:HD2  | 1.96                     | 0.47              |
| 1:A:347:LEU:HD12 | 1:A:376:LEU:HD11 | 1.96                     | 0.47              |
| 1:A:633:GLU:O    | 1:A:633:GLU:OE1  | 2.33                     | 0.47              |
| 1:A:811:LEU:HD23 | 1:A:814:MET:CE   | 2.45                     | 0.47              |
| 1:A:84:GLU:HA    | 1:A:118:GLY:CA   | 2.33                     | 0.47              |
| 1:A:271:GLU:CG   | 1:A:453:THR:CG2  | 2.92                     | 0.47              |
| 1:A:381:PHE:HD2  | 1:A:386:LEU:HD21 | 1.79                     | 0.47              |
| 1:A:149:LYS:HG2  | 1:A:149:LYS:O    | 2.15                     | 0.46              |
| 1:A:729:LYS:HD3  | 1:A:734:SER:CB   | 2.44                     | 0.46              |
| 1:A:732:LYS:C    | 1:A:734:SER:N    | 2.68                     | 0.46              |
| 1:A:277:GLN:H    | 1:A:281:VAL:CG1  | 2.28                     | 0.46              |
| 1:A:381:PHE:HB3  | 1:A:386:LEU:HD13 | 1.95                     | 0.46              |
| 1:A:734:SER:HB3  | 1:A:736:MET:N    | 2.10                     | 0.46              |
| 1:A:855:SER:HB3  | 1:A:856:PRO:HD2  | 1.96                     | 0.46              |
| 1:A:99:MET:SD    | 1:A:103:MET:HE2  | 2.55                     | 0.46              |
| 1:A:695:THR:OG1  | 1:A:696:GLY:N    | 2.48                     | 0.46              |
| 1:A:373:LEU:O    | 1:A:376:LEU:HD23 | 2.15                     | 0.46              |
| 1:A:420:LYS:NZ   | 1:A:420:LYS:CB   | 2.79                     | 0.46              |
| 1:A:521:PHE:CD1  | 1:A:521:PHE:C    | 2.94                     | 0.46              |
| 1:A:587:ARG:HD2  | 1:A:675:GLU:OE1  | 2.15                     | 0.46              |
| 1:A:601:ASP:O    | 1:A:605:MET:HG2  | 2.16                     | 0.46              |
| 1:A:668:ARG:HH11 | 1:A:668:ARG:CG   | 2.28                     | 0.46              |
| 1:A:842:GLU:HG3  | 1:A:873:ASN:HD21 | 1.79                     | 0.46              |
| 1:A:52:ASN:C     | 1:A:54:GLY:H     | 2.24                     | 0.46              |
| 1:A:230:PRO:HG2  | 1:A:233:TRP:CE2  | 2.50                     | 0.46              |
| 1:A:65:ILE:CG2   | 1:A:204:LEU:HD21 | 2.45                     | 0.46              |
| 1:A:65:ILE:HG21  | 1:A:205:MET:HE1  | 1.96                     | 0.46              |
| 1:A:100:PRO:HD2  | 1:A:223:TYR:OH   | 2.15                     | 0.46              |
| 1:A:627:VAL:HB   | 1:A:628:PRO:HD2  | 1.97                     | 0.46              |
| 1:A:782:ALA:HA   | 1:A:785:PHE:CZ   | 2.50                     | 0.46              |
| 1:A:108:ASN:ND2  | 1:A:277:GLN:HE22 | 1.98                     | 0.46              |
| 1:A:111:LEU:HB3  | 1:A:133:TYR:CD1  | 2.49                     | 0.46              |
| 1:A:391:VAL:O    | 1:A:391:VAL:HG12 | 2.15                     | 0.46              |
| 1:A:532:ARG:CG   | 1:A:532:ARG:NH1  | 2.76                     | 0.46              |
| 1:A:599:LYS:HD3  | 1:A:686:GLU:HB2  | 1.96                     | 0.46              |
| 1:A:92:ARG:HH11  | 1:A:92:ARG:HB3   | 1.81                     | 0.46              |
| 1:A:117:GLU:O    | 1:A:121:LYS:HG2  | 2.16                     | 0.46              |
| 1:A:199:GLU:HA   | 1:A:200:PRO:HD2  | 1.80                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:482:THR:HA   | 1:A:490:PHE:O    | 2.16                     | 0.46              |
| 1:A:543:PRO:O    | 1:A:546:THR:HB   | 2.15                     | 0.46              |
| 1:A:205:MET:O    | 1:A:209:LYS:HB2  | 2.15                     | 0.46              |
| 1:A:214:SER:O    | 1:A:217:ASN:HB2  | 2.16                     | 0.46              |
| 1:A:321:ASP:HB2  | 1:A:339:GLY:HA2  | 1.98                     | 0.46              |
| 1:A:603:LYS:HE3  | 1:A:690:GLU:CB   | 2.46                     | 0.46              |
| 1:A:221:ILE:CG1  | 1:A:224:ARG:NH2  | 2.78                     | 0.46              |
| 1:A:445:ILE:HD13 | 1:A:460:ALA:HB2  | 1.97                     | 0.46              |
| 1:A:476:ILE:HG22 | 1:A:477:ASN:N    | 2.31                     | 0.46              |
| 1:A:624:HIS:CE1  | 1:A:629:HIS:CD2  | 3.04                     | 0.46              |
| 1:A:710:GLU:O    | 1:A:713:GLU:HB3  | 2.14                     | 0.45              |
| 1:A:527:TRP:O    | 1:A:531:PHE:CD2  | 2.69                     | 0.45              |
| 1:A:404:ALA:HB1  | 1:A:496:ILE:HG12 | 1.98                     | 0.45              |
| 1:A:649:LYS:HG3  | 1:A:650:ALA:H    | 1.76                     | 0.45              |
| 1:A:707:LEU:HD21 | 1:A:746:ILE:HD11 | 1.94                     | 0.45              |
| 1:A:537:ARG:HH22 | 1:A:702:GLU:CD   | 2.25                     | 0.45              |
| 1:A:627:VAL:HB   | 1:A:628:PRO:CD   | 2.46                     | 0.45              |
| 1:A:117:GLU:OE1  | 1:A:117:GLU:HA   | 2.16                     | 0.45              |
| 1:A:189:GLU:OE1  | 1:A:190:ALA:HB2  | 2.17                     | 0.45              |
| 1:A:285:VAL:CG2  | 1:A:286:ARG:H    | 2.25                     | 0.45              |
| 1:A:436:ILE:CG2  | 1:A:437:GLU:N    | 2.79                     | 0.45              |
| 1:A:591:LEU:HA   | 1:A:591:LEU:HD23 | 1.62                     | 0.45              |
| 1:A:842:GLU:HG3  | 1:A:873:ASN:ND2  | 2.32                     | 0.45              |
| 1:A:4:TRP:CB     | 1:A:61:ILE:HG12  | 2.46                     | 0.45              |
| 1:A:189:GLU:CD   | 1:A:190:ALA:N    | 2.75                     | 0.45              |
| 1:A:542:THR:CG2  | 1:A:544:GLU:HG2  | 2.46                     | 0.45              |
| 1:A:557:ILE:HG22 | 1:A:559:LEU:H    | 1.82                     | 0.45              |
| 1:A:643:LEU:HD23 | 1:A:643:LEU:H    | 1.78                     | 0.45              |
| 1:A:163:LYS:C    | 1:A:165:VAL:N    | 2.75                     | 0.45              |
| 1:A:165:VAL:HG21 | 1:A:170:ASP:HB3  | 1.96                     | 0.45              |
| 1:A:217:ASN:OD1  | 1:A:218:PRO:HD2  | 2.17                     | 0.45              |
| 1:A:102:MET:SD   | 1:A:223:TYR:CD2  | 3.10                     | 0.45              |
| 1:A:159:MET:O    | 1:A:163:LYS:HB2  | 2.16                     | 0.45              |
| 1:A:69:ILE:HA    | 1:A:69:ILE:HD13  | 1.51                     | 0.45              |
| 1:A:148:PRO:C    | 1:A:150:SER:H    | 2.25                     | 0.45              |
| 1:A:290:PRO:O    | 1:A:292:THR:N    | 2.50                     | 0.45              |
| 1:A:381:PHE:CZ   | 1:A:496:ILE:CG2  | 3.00                     | 0.45              |
| 1:A:386:LEU:HD12 | 1:A:510:ILE:HD13 | 1.99                     | 0.45              |
| 1:A:406:LYS:O    | 1:A:424:VAL:HA   | 2.16                     | 0.45              |
| 1:A:699:ILE:HB   | 1:A:736:MET:CE   | 2.46                     | 0.45              |
| 1:A:127:ARG:O    | 1:A:176:LEU:HD12 | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:386:LEU:CD1  | 1:A:386:LEU:N    | 2.80                     | 0.44              |
| 1:A:418:HIS:HB2  | 1:A:422:GLU:HB2  | 1.98                     | 0.44              |
| 1:A:559:LEU:CD1  | 1:A:617:ARG:HB3  | 2.46                     | 0.44              |
| 1:A:222:VAL:HG22 | 1:A:222:VAL:O    | 2.17                     | 0.44              |
| 1:A:258:THR:HG23 | 1:A:322:MET:CE   | 2.47                     | 0.44              |
| 1:A:268:ILE:HD13 | 1:A:268:ILE:HA   | 1.41                     | 0.44              |
| 1:A:342:THR:CG2  | 1:A:345:ALA:H    | 2.30                     | 0.44              |
| 1:A:432:SER:OG   | 1:A:434:GLU:HG2  | 2.17                     | 0.44              |
| 1:A:639:LYS:C    | 1:A:641:MET:H    | 2.25                     | 0.44              |
| 1:A:753:ALA:HB1  | 1:A:763:PHE:CE2  | 2.52                     | 0.44              |
| 1:A:99:MET:HA    | 1:A:100:PRO:HD2  | 1.54                     | 0.44              |
| 1:A:106:ILE:HD11 | 1:A:143:VAL:CG1  | 2.47                     | 0.44              |
| 1:A:266:LYS:HD2  | 1:A:267:GLY:N    | 2.26                     | 0.44              |
| 1:A:649:LYS:CB   | 1:A:649:LYS:NZ   | 2.80                     | 0.44              |
| 1:A:259:ARG:HB2  | 1:A:319:MET:HG3  | 2.00                     | 0.44              |
| 1:A:309:ALA:O    | 1:A:312:LEU:HB2  | 2.17                     | 0.44              |
| 1:A:72:LEU:HB3   | 1:A:87:LEU:HD21  | 1.98                     | 0.44              |
| 1:A:219:ARG:CG   | 1:A:436:ILE:HG21 | 2.40                     | 0.44              |
| 1:A:381:PHE:CE2  | 1:A:498:LEU:HB3  | 2.53                     | 0.44              |
| 1:A:747:PRO:HB3  | 1:A:811:LEU:HD13 | 1.98                     | 0.44              |
| 1:A:281:VAL:CG2  | 1:A:282:VAL:N    | 2.80                     | 0.44              |
| 1:A:353:LEU:CD2  | 1:A:358:MET:SD   | 3.05                     | 0.44              |
| 1:A:411:ALA:HA   | 1:A:438:GLY:HA3  | 1.99                     | 0.44              |
| 1:A:72:LEU:HD23  | 1:A:72:LEU:HA    | 1.91                     | 0.44              |
| 1:A:557:ILE:HD13 | 1:A:557:ILE:HG21 | 1.61                     | 0.44              |
| 1:A:573:MET:O    | 1:A:577:LYS:HG3  | 2.17                     | 0.44              |
| 1:A:262:SER:CB   | 1:A:461:ARG:HD2  | 2.33                     | 0.44              |
| 1:A:150:SER:HB2  | 1:A:151:HIS:ND1  | 2.33                     | 0.44              |
| 1:A:474:ILE:HG12 | 1:A:485:LEU:HD11 | 2.00                     | 0.44              |
| 1:A:50:TYR:OH    | 1:A:213:ARG:NH1  | 2.51                     | 0.43              |
| 1:A:147:VAL:HA   | 1:A:148:PRO:HD3  | 1.46                     | 0.43              |
| 1:A:390:GLU:HB3  | 1:A:505:ILE:CG2  | 2.48                     | 0.43              |
| 1:A:418:HIS:O    | 1:A:419:GLU:O    | 2.36                     | 0.43              |
| 1:A:577:LYS:NZ   | 1:A:577:LYS:HB3  | 2.33                     | 0.43              |
| 1:A:643:LEU:N    | 1:A:643:LEU:CD2  | 2.75                     | 0.43              |
| 1:A:704:MET:HE3  | 1:A:743:MET:HE2  | 2.00                     | 0.43              |
| 1:A:4:TRP:CG     | 1:A:61:ILE:HG12  | 2.52                     | 0.43              |
| 1:A:261:PRO:HA   | 1:A:319:MET:HE1  | 1.96                     | 0.43              |
| 1:A:372:SER:H    | 1:A:372:SER:HG   | 1.39                     | 0.43              |
| 1:A:382:ASN:O    | 1:A:386:LEU:HD13 | 2.18                     | 0.43              |
| 1:A:429:LEU:O    | 1:A:449:ARG:HG2  | 2.17                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:537:ARG:NH2  | 1:A:702:GLU:OE1  | 2.46                     | 0.43              |
| 1:A:716:PHE:CD1  | 1:A:716:PHE:C    | 2.96                     | 0.43              |
| 1:A:160:LYS:O    | 1:A:165:VAL:O    | 2.36                     | 0.43              |
| 1:A:290:PRO:C    | 1:A:292:THR:N    | 2.76                     | 0.43              |
| 1:A:382:ASN:OD1  | 1:A:383:PRO:HD2  | 2.17                     | 0.43              |
| 1:A:465:THR:HG22 | 1:A:466:CYS:N    | 2.33                     | 0.43              |
| 1:A:145:MET:O    | 1:A:145:MET:HG3  | 2.18                     | 0.43              |
| 1:A:496:ILE:HD13 | 1:A:510:ILE:N    | 2.33                     | 0.43              |
| 1:A:621:PRO:HB2  | 1:A:622:PRO:HD2  | 2.01                     | 0.43              |
| 1:A:274:ILE:HD11 | 1:A:298:MET:CE   | 2.48                     | 0.43              |
| 1:A:547:LEU:HD23 | 1:A:547:LEU:HA   | 1.70                     | 0.43              |
| 1:A:722:VAL:HG12 | 1:A:723:GLU:N    | 2.32                     | 0.43              |
| 1:A:782:ALA:HA   | 1:A:785:PHE:CE2  | 2.53                     | 0.43              |
| 1:A:477:ASN:O    | 1:A:481:LYS:N    | 2.52                     | 0.43              |
| 1:A:445:ILE:HD12 | 1:A:466:CYS:O    | 2.19                     | 0.43              |
| 1:A:92:ARG:HB3   | 1:A:92:ARG:NH1   | 2.34                     | 0.43              |
| 1:A:312:LEU:O    | 1:A:315:HIS:HB3  | 2.19                     | 0.43              |
| 1:A:381:PHE:HD1  | 1:A:381:PHE:HA   | 1.69                     | 0.43              |
| 1:A:747:PRO:HB3  | 1:A:811:LEU:CD1  | 2.49                     | 0.43              |
| 1:A:87:LEU:HD12  | 1:A:87:LEU:HA    | 1.92                     | 0.42              |
| 1:A:112:ASN:HA   | 1:A:133:TYR:HE1  | 1.84                     | 0.42              |
| 1:A:215:TRP:CE2  | 1:A:234:GLY:HA2  | 2.53                     | 0.42              |
| 1:A:390:GLU:CB   | 1:A:505:ILE:CG2  | 2.95                     | 0.42              |
| 1:A:399:SER:HB3  | 1:A:461:ARG:HG3  | 2.01                     | 0.42              |
| 1:A:641:MET:O    | 1:A:643:LEU:HD23 | 2.19                     | 0.42              |
| 1:A:253:THR:O    | 1:A:282:VAL:HG21 | 2.19                     | 0.42              |
| 1:A:411:ALA:HB1  | 1:A:438:GLY:HA3  | 2.01                     | 0.42              |
| 1:A:474:ILE:HA   | 1:A:484:GLU:O    | 2.19                     | 0.42              |
| 1:A:478:GLU:O    | 1:A:480:ALA:N    | 2.52                     | 0.42              |
| 1:A:733:GLY:C    | 1:A:735:ASP:N    | 2.77                     | 0.42              |
| 1:A:751:LEU:HD23 | 1:A:814:MET:HE3  | 1.99                     | 0.42              |
| 1:A:95:ALA:N     | 1:A:235:THR:CG2  | 2.82                     | 0.42              |
| 1:A:187:TYR:CD2  | 1:A:187:TYR:C    | 2.95                     | 0.42              |
| 1:A:514:GLU:HG2  | 1:A:515:ALA:N    | 2.33                     | 0.42              |
| 1:A:43:THR:O     | 1:A:46:ALA:HB3   | 2.19                     | 0.42              |
| 1:A:217:ASN:CG   | 1:A:218:PRO:HD2  | 2.45                     | 0.42              |
| 1:A:385:ALA:C    | 1:A:510:ILE:HD13 | 2.44                     | 0.42              |
| 1:A:386:LEU:HD12 | 1:A:510:ILE:CG2  | 2.50                     | 0.42              |
| 1:A:411:ALA:C    | 1:A:413:GLU:N    | 2.76                     | 0.42              |
| 1:A:594:LEU:HB2  | 1:A:679:MET:HE3  | 2.01                     | 0.42              |
| 1:A:599:LYS:HD2  | 1:A:686:GLU:HB3  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:61:ILE:HG22  | 1:A:62:GLN:N     | 2.35                     | 0.42              |
| 1:A:135:ARG:HD3  | 1:A:277:GLN:HE21 | 1.84                     | 0.42              |
| 1:A:373:LEU:CA   | 1:A:376:LEU:HD23 | 2.49                     | 0.42              |
| 1:A:409:PHE:O    | 1:A:410:THR:HG22 | 2.19                     | 0.42              |
| 1:A:446:LEU:HD23 | 1:A:446:LEU:HA   | 1.53                     | 0.42              |
| 1:A:729:LYS:NZ   | 1:A:736:MET:O    | 2.50                     | 0.42              |
| 1:A:750:ALA:HB1  | 1:A:811:LEU:O    | 2.19                     | 0.42              |
| 1:A:830:ILE:HG22 | 1:A:852:VAL:HA   | 2.02                     | 0.42              |
| 1:A:130:TYR:CE1  | 1:A:177:LYS:HB2  | 2.55                     | 0.42              |
| 1:A:143:VAL:C    | 1:A:145:MET:N    | 2.78                     | 0.42              |
| 1:A:147:VAL:HB   | 1:A:190:ALA:HB1  | 1.98                     | 0.42              |
| 1:A:640:ASN:O    | 1:A:641:MET:HG2  | 2.20                     | 0.42              |
| 1:A:842:GLU:CG   | 1:A:846:LYS:HD2  | 2.42                     | 0.42              |
| 1:A:131:ASP:CB   | 1:A:176:LEU:HD13 | 2.49                     | 0.42              |
| 1:A:148:PRO:C    | 1:A:150:SER:N    | 2.78                     | 0.42              |
| 1:A:261:PRO:HG3  | 1:A:269:TYR:CE1  | 2.55                     | 0.42              |
| 1:A:293:GLN:C    | 1:A:295:GLU:N    | 2.77                     | 0.42              |
| 1:A:557:ILE:HB   | 1:A:614:MET:HB2  | 2.02                     | 0.42              |
| 1:A:182:LYS:O    | 1:A:185:ALA:N    | 2.46                     | 0.42              |
| 1:A:183:PHE:O    | 1:A:186:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:463:MET:HG3  | 1:A:465:THR:OG1  | 2.20                     | 0.42              |
| 1:A:478:GLU:C    | 1:A:480:ALA:N    | 2.76                     | 0.42              |
| 1:A:219:ARG:O    | 1:A:222:VAL:HG12 | 2.20                     | 0.42              |
| 1:A:219:ARG:CD   | 1:A:436:ILE:HG22 | 2.50                     | 0.42              |
| 1:A:259:ARG:CD   | 1:A:266:LYS:HD3  | 2.50                     | 0.42              |
| 1:A:309:ALA:HA   | 1:A:312:LEU:HD12 | 2.02                     | 0.42              |
| 1:A:706:PRO:HA   | 1:A:743:MET:HB2  | 2.02                     | 0.42              |
| 1:A:767:THR:HA   | 1:A:770:LEU:HB3  | 2.02                     | 0.42              |
| 1:A:71:TRP:HA    | 1:A:74:GLU:HG2   | 2.02                     | 0.42              |
| 1:A:257:PHE:HA   | 1:A:320:GLN:O    | 2.20                     | 0.42              |
| 1:A:293:GLN:O    | 1:A:296:ASN:HB2  | 2.20                     | 0.42              |
| 1:A:497:SER:O    | 1:A:498:LEU:HB3  | 2.19                     | 0.42              |
| 1:A:587:ARG:O    | 1:A:591:LEU:HG   | 2.20                     | 0.42              |
| 1:A:675:GLU:H    | 1:A:675:GLU:HG3  | 1.41                     | 0.42              |
| 1:A:4:TRP:HB3    | 1:A:61:ILE:HG12  | 2.02                     | 0.41              |
| 1:A:37:PRO:HB2   | 1:A:240:GLN:HG2  | 2.02                     | 0.41              |
| 1:A:51:TYR:CZ    | 1:A:216:ASP:HB2  | 2.55                     | 0.41              |
| 1:A:84:GLU:CD    | 1:A:121:LYS:HB2  | 2.45                     | 0.41              |
| 1:A:168:ASP:C    | 1:A:170:ASP:H    | 2.28                     | 0.41              |
| 1:A:387:LYS:HE3  | 1:A:387:LYS:HB3  | 1.63                     | 0.41              |
| 1:A:396:LEU:HA   | 1:A:397:PRO:HD2  | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:543:PRO:HA   | 1:A:546:THR:HB   | 2.02                     | 0.41              |
| 1:A:34:MET:HB3   | 1:A:34:MET:HE3   | 1.40                     | 0.41              |
| 1:A:140:TYR:CE2  | 1:A:144:VAL:HG21 | 2.55                     | 0.41              |
| 1:A:303:LYS:NZ   | 1:A:303:LYS:CB   | 2.84                     | 0.41              |
| 1:A:729:LYS:HD3  | 1:A:735:ASP:H    | 1.85                     | 0.41              |
| 1:A:121:LYS:O    | 1:A:123:THR:N    | 2.53                     | 0.41              |
| 1:A:188:LYS:HB3  | 1:A:194:GLU:O    | 2.20                     | 0.41              |
| 1:A:276:ALA:HB2  | 1:A:286:ARG:NH2  | 2.32                     | 0.41              |
| 1:A:477:ASN:OD1  | 1:A:479:GLU:HB2  | 2.20                     | 0.41              |
| 1:A:565:MET:O    | 1:A:571:ARG:HD3  | 2.21                     | 0.41              |
| 1:A:673:TYR:N    | 1:A:674:PRO:HD3  | 2.35                     | 0.41              |
| 1:A:591:LEU:CD1  | 1:A:675:GLU:CB   | 2.98                     | 0.41              |
| 1:A:390:GLU:HA   | 1:A:390:GLU:OE1  | 2.21                     | 0.41              |
| 1:A:440:HIS:ND1  | 1:A:440:HIS:C    | 2.77                     | 0.41              |
| 1:A:662:MET:HG2  | 1:A:773:MET:CE   | 2.47                     | 0.41              |
| 1:A:36:ILE:HG21  | 1:A:36:ILE:HD13  | 1.65                     | 0.41              |
| 1:A:274:ILE:CD1  | 1:A:298:MET:CE   | 2.98                     | 0.41              |
| 1:A:5:VAL:HG13   | 1:A:40:PHE:HB2   | 2.02                     | 0.41              |
| 1:A:18:LEU:HD23  | 1:A:18:LEU:HA    | 1.76                     | 0.41              |
| 1:A:569:ALA:C    | 1:A:571:ARG:N    | 2.77                     | 0.41              |
| 1:A:619:LEU:HD12 | 1:A:619:LEU:HA   | 1.81                     | 0.41              |
| 1:A:729:LYS:C    | 1:A:733:GLY:HA2  | 2.45                     | 0.41              |
| 1:A:127:ARG:HA   | 1:A:173:ALA:HA   | 2.02                     | 0.41              |
| 1:A:320:GLN:CB   | 1:A:322:MET:HE2  | 2.50                     | 0.41              |
| 1:A:643:LEU:HB3  | 1:A:647:GLU:CB   | 2.51                     | 0.41              |
| 1:A:659:ASN:HA   | 1:A:660:PRO:HD2  | 1.88                     | 0.41              |
| 1:A:742:THR:N    | 1:A:762:PHE:O    | 2.50                     | 0.41              |
| 1:A:62:GLN:CD    | 1:A:66:PHE:CE2   | 2.99                     | 0.41              |
| 1:A:99:MET:CE    | 1:A:102:MET:CB   | 2.99                     | 0.41              |
| 1:A:141:SER:HB2  | 1:A:187:TYR:CD1  | 2.56                     | 0.41              |
| 1:A:293:GLN:C    | 1:A:295:GLU:H    | 2.28                     | 0.41              |
| 1:A:542:THR:HG22 | 1:A:545:ASP:CB   | 2.50                     | 0.41              |
| 1:A:649:LYS:NZ   | 1:A:649:LYS:HB3  | 2.36                     | 0.41              |
| 1:A:782:ALA:O    | 1:A:784:LYS:N    | 2.54                     | 0.41              |
| 1:A:847:VAL:HG12 | 1:A:849:LEU:HD23 | 2.03                     | 0.41              |
| 1:A:7:LYS:HB2    | 1:A:10:GLU:CG    | 2.45                     | 0.41              |
| 1:A:107:LEU:HD11 | 1:A:279:GLU:HG2  | 2.03                     | 0.41              |
| 1:A:95:ALA:N     | 1:A:235:THR:HG22 | 2.36                     | 0.40              |
| 1:A:163:LYS:HB2  | 1:A:163:LYS:HE3  | 1.83                     | 0.40              |
| 1:A:304:GLN:OE1  | 1:A:331:LEU:HB3  | 2.21                     | 0.40              |
| 1:A:431:THR:HA   | 1:A:435:ASP:OD2  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:657:GLU:CD   | 1:A:663:GLY:HA3  | 2.46                     | 0.40              |
| 1:A:482:THR:HB   | 1:A:490:PHE:O    | 2.20                     | 0.40              |
| 1:A:623:LEU:HA   | 1:A:623:LEU:HD23 | 1.70                     | 0.40              |
| 1:A:746:ILE:HD13 | 1:A:773:MET:SD   | 2.61                     | 0.40              |
| 1:A:37:PRO:O     | 1:A:240:GLN:HG3  | 2.21                     | 0.40              |
| 1:A:67:GLU:HA    | 1:A:70:THR:HG23  | 2.03                     | 0.40              |
| 1:A:149:LYS:NZ   | 1:A:153:GLU:CG   | 2.81                     | 0.40              |
| 1:A:179:LEU:CD1  | 1:A:183:PHE:CE1  | 2.97                     | 0.40              |
| 1:A:225:ARG:C    | 1:A:227:ASN:N    | 2.79                     | 0.40              |
| 1:A:444:GLY:HA3  | 1:A:466:CYS:HB3  | 2.02                     | 0.40              |
| 1:A:187:TYR:CE2  | 1:A:191:MET:HG3  | 2.57                     | 0.40              |
| 1:A:353:LEU:O    | 1:A:358:MET:N    | 2.48                     | 0.40              |
| 1:A:365:VAL:HG13 | 1:A:864:LEU:CD2  | 2.51                     | 0.40              |
| 1:A:543:PRO:O    | 1:A:547:LEU:N    | 2.48                     | 0.40              |
| 1:A:584:VAL:H    | 1:A:584:VAL:HG23 | 1.63                     | 0.40              |
| 1:A:598:GLN:OE1  | 1:A:679:MET:HE1  | 2.20                     | 0.40              |
| 1:A:599:LYS:O    | 1:A:603:LYS:HG3  | 2.22                     | 0.40              |
| 1:A:669:LEU:HD23 | 1:A:669:LEU:HA   | 1.65                     | 0.40              |
| 1:A:707:LEU:HA   | 1:A:707:LEU:HD23 | 1.66                     | 0.40              |
| 1:A:106:ILE:HD12 | 1:A:140:TYR:HA   | 2.04                     | 0.40              |
| 1:A:159:MET:HE1  | 1:A:179:LEU:HA   | 2.03                     | 0.40              |
| 1:A:415:LYS:NZ   | 1:A:437:GLU:OE2  | 2.45                     | 0.40              |
| 1:A:751:LEU:HD23 | 1:A:814:MET:HE1  | 2.02                     | 0.40              |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 1:A:121:LYS:CE  | 1:A:732:LYS:NZ[1_554] | 1.65                     | 0.55              |
| 1:A:117:GLU:CG  | 1:A:732:LYS:CG[1_554] | 1.79                     | 0.41              |
| 1:A:117:GLU:OE1 | 1:A:732:LYS:CE[1_554] | 1.84                     | 0.36              |
| 1:A:117:GLU:CD  | 1:A:732:LYS:CD[1_554] | 2.00                     | 0.20              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 1   | A     | 865/873 (99%) | 732 (85%) | 93 (11%) | 40 (5%)  | 2           | 2 |

All (40) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 113 | ASP  |
| 1   | A     | 145 | MET  |
| 1   | A     | 265 | GLU  |
| 1   | A     | 279 | GLU  |
| 1   | A     | 419 | GLU  |
| 1   | A     | 420 | LYS  |
| 1   | A     | 515 | ALA  |
| 1   | A     | 516 | SER  |
| 1   | A     | 734 | SER  |
| 1   | A     | 77  | GLY  |
| 1   | A     | 149 | LYS  |
| 1   | A     | 215 | TRP  |
| 1   | A     | 266 | LYS  |
| 1   | A     | 278 | GLY  |
| 1   | A     | 285 | VAL  |
| 1   | A     | 412 | ASP  |
| 1   | A     | 436 | ILE  |
| 1   | A     | 473 | GLU  |
| 1   | A     | 493 | GLY  |
| 1   | A     | 3   | LYS  |
| 1   | A     | 275 | ASN  |
| 1   | A     | 286 | ARG  |
| 1   | A     | 500 | GLY  |
| 1   | A     | 618 | TYR  |
| 1   | A     | 80  | PHE  |
| 1   | A     | 148 | PRO  |
| 1   | A     | 398 | ALA  |
| 1   | A     | 418 | HIS  |
| 1   | A     | 487 | GLY  |
| 1   | A     | 518 | SER  |
| 1   | A     | 529 | ASP  |
| 1   | A     | 152 | PHE  |
| 1   | A     | 249 | GLU  |
| 1   | A     | 479 | GLU  |
| 1   | A     | 20  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 421 | GLY  |
| 1   | A     | 620 | ASP  |
| 1   | A     | 783 | GLY  |
| 1   | A     | 164 | GLY  |
| 1   | A     | 517 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles       |
|-----|-------|----------------|-----------|-----------|-------------------|
| 1   | A     | 710/713 (100%) | 586 (82%) | 124 (18%) | <b>2</b> <b>3</b> |

All (124) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 31  | ILE  |
| 1   | A     | 34  | MET  |
| 1   | A     | 36  | ILE  |
| 1   | A     | 59  | GLN  |
| 1   | A     | 67  | GLU  |
| 1   | A     | 69  | ILE  |
| 1   | A     | 70  | THR  |
| 1   | A     | 75  | LEU  |
| 1   | A     | 76  | ASN  |
| 1   | A     | 78  | LYS  |
| 1   | A     | 84  | GLU  |
| 1   | A     | 92  | ARG  |
| 1   | A     | 104 | ASP  |
| 1   | A     | 106 | ILE  |
| 1   | A     | 109 | LEU  |
| 1   | A     | 116 | VAL  |
| 1   | A     | 121 | LYS  |
| 1   | A     | 123 | THR  |
| 1   | A     | 134 | ARG  |
| 1   | A     | 140 | TYR  |
| 1   | A     | 142 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 151 | HIS  |
| 1   | A     | 157 | ASP  |
| 1   | A     | 161 | GLU  |
| 1   | A     | 163 | LYS  |
| 1   | A     | 168 | ASP  |
| 1   | A     | 171 | LEU  |
| 1   | A     | 172 | THR  |
| 1   | A     | 186 | VAL  |
| 1   | A     | 189 | GLU  |
| 1   | A     | 194 | GLU  |
| 1   | A     | 195 | GLU  |
| 1   | A     | 199 | GLU  |
| 1   | A     | 205 | MET  |
| 1   | A     | 213 | ARG  |
| 1   | A     | 216 | ASP  |
| 1   | A     | 219 | ARG  |
| 1   | A     | 235 | THR  |
| 1   | A     | 237 | VAL  |
| 1   | A     | 241 | THR  |
| 1   | A     | 249 | GLU  |
| 1   | A     | 268 | ILE  |
| 1   | A     | 274 | ILE  |
| 1   | A     | 277 | GLN  |
| 1   | A     | 280 | ASP  |
| 1   | A     | 281 | VAL  |
| 1   | A     | 287 | THR  |
| 1   | A     | 303 | LYS  |
| 1   | A     | 307 | ASP  |
| 1   | A     | 325 | THR  |
| 1   | A     | 330 | LYS  |
| 1   | A     | 336 | THR  |
| 1   | A     | 340 | LYS  |
| 1   | A     | 342 | THR  |
| 1   | A     | 349 | ILE  |
| 1   | A     | 354 | VAL  |
| 1   | A     | 363 | GLU  |
| 1   | A     | 366 | VAL  |
| 1   | A     | 371 | LYS  |
| 1   | A     | 374 | ASP  |
| 1   | A     | 376 | LEU  |
| 1   | A     | 381 | PHE  |
| 1   | A     | 390 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 410 | THR  |
| 1   | A     | 415 | LYS  |
| 1   | A     | 419 | GLU  |
| 1   | A     | 420 | LYS  |
| 1   | A     | 440 | HIS  |
| 1   | A     | 446 | LEU  |
| 1   | A     | 452 | MET  |
| 1   | A     | 463 | MET  |
| 1   | A     | 473 | GLU  |
| 1   | A     | 475 | LYS  |
| 1   | A     | 485 | LEU  |
| 1   | A     | 498 | LEU  |
| 1   | A     | 499 | ASP  |
| 1   | A     | 502 | THR  |
| 1   | A     | 504 | LYS  |
| 1   | A     | 505 | ILE  |
| 1   | A     | 510 | ILE  |
| 1   | A     | 520 | SER  |
| 1   | A     | 525 | MET  |
| 1   | A     | 532 | ARG  |
| 1   | A     | 542 | THR  |
| 1   | A     | 544 | GLU  |
| 1   | A     | 578 | MET  |
| 1   | A     | 584 | VAL  |
| 1   | A     | 588 | GLU  |
| 1   | A     | 589 | GLU  |
| 1   | A     | 614 | MET  |
| 1   | A     | 617 | ARG  |
| 1   | A     | 632 | GLU  |
| 1   | A     | 633 | GLU  |
| 1   | A     | 636 | GLU  |
| 1   | A     | 643 | LEU  |
| 1   | A     | 649 | LYS  |
| 1   | A     | 655 | LEU  |
| 1   | A     | 668 | ARG  |
| 1   | A     | 675 | GLU  |
| 1   | A     | 676 | ILE  |
| 1   | A     | 679 | MET  |
| 1   | A     | 694 | GLU  |
| 1   | A     | 697 | ILE  |
| 1   | A     | 711 | LYS  |
| 1   | A     | 721 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 722 | VAL  |
| 1   | A     | 734 | SER  |
| 1   | A     | 737 | GLN  |
| 1   | A     | 744 | ILE  |
| 1   | A     | 767 | THR  |
| 1   | A     | 769 | ASP  |
| 1   | A     | 771 | THR  |
| 1   | A     | 784 | LYS  |
| 1   | A     | 786 | LEU  |
| 1   | A     | 796 | GLU  |
| 1   | A     | 797 | SER  |
| 1   | A     | 812 | VAL  |
| 1   | A     | 814 | MET  |
| 1   | A     | 826 | LEU  |
| 1   | A     | 839 | SER  |
| 1   | A     | 847 | VAL  |
| 1   | A     | 849 | LEU  |
| 1   | A     | 855 | SER  |
| 1   | A     | 864 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 52  | ASN  |
| 1   | A     | 59  | GLN  |
| 1   | A     | 64  | GLN  |
| 1   | A     | 76  | ASN  |
| 1   | A     | 227 | ASN  |
| 1   | A     | 275 | ASN  |
| 1   | A     | 277 | GLN  |
| 1   | A     | 335 | GLN  |
| 1   | A     | 378 | HIS  |
| 1   | A     | 624 | HIS  |
| 1   | A     | 664 | HIS  |
| 1   | A     | 737 | GLN  |
| 1   | A     | 739 | HIS  |
| 1   | A     | 821 | GLN  |
| 1   | A     | 845 | HIS  |
| 1   | A     | 850 | ASN  |
| 1   | A     | 873 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | SO4  | A     | 902 | -    | 4,4,4        | 2.30 | 2 (50%)     | 6,6,6       | 0.58 | 0           |
| 2   | SO4  | A     | 901 | -    | 4,4,4        | 0.94 | 0           | 6,6,6       | 0.32 | 0           |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | A     | 902 | SO4  | O1-S  | 3.62 | 1.66        | 1.44     |
| 2   | A     | 902 | SO4  | O4-S  | 2.26 | 1.66        | 1.48     |

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 902 | SO4  | 1       | 0            |
| 2   | A     | 901 | SO4  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.