



## Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 09:01 PM UTC

PDB ID : 4UWA / pdb\_00004uwa  
EMDB ID : EMD-2751  
Title : Structure of the ryanodine receptor at resolution of 6.1 Å in closed state  
Authors : Efremov, R.G.; Leitner, A.; Aebersold, R.; Raunser, S.  
Deposited on : 2014-08-11  
Resolution : 6.10 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

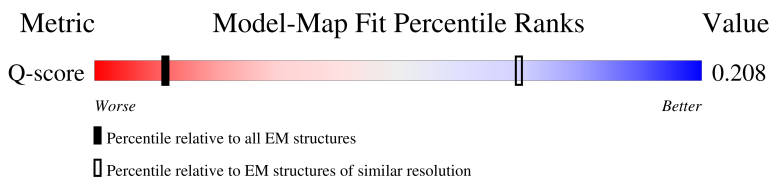
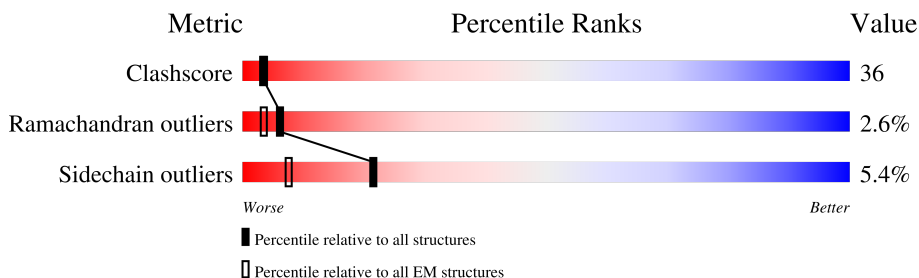
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 531 ( 5.60 - 6.60 )                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|-------------------|
| 1   | A     | 5037   | <br>52% 12% • 34% |
| 1   | B     | 5037   | <br>52% 12% • 34% |
| 1   | C     | 5037   | <br>52% 12% • 34% |
| 1   | D     | 5037   | <br>52% 12% • 34% |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 81640 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RYANODINE RECEPTOR 1.

| Mol | Chain | Residues | Atoms |       |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|----|---------|-------|
| 1   | A     | 3324     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 20410 | 12590 | 3818 | 3946 | 56 |         |       |
| 1   | B     | 3324     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 20410 | 12590 | 3818 | 3946 | 56 |         |       |
| 1   | C     | 3324     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 20410 | 12590 | 3818 | 3946 | 56 |         |       |
| 1   | D     | 3324     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 20410 | 12590 | 3818 | 3946 | 56 |         |       |

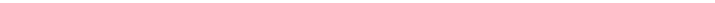


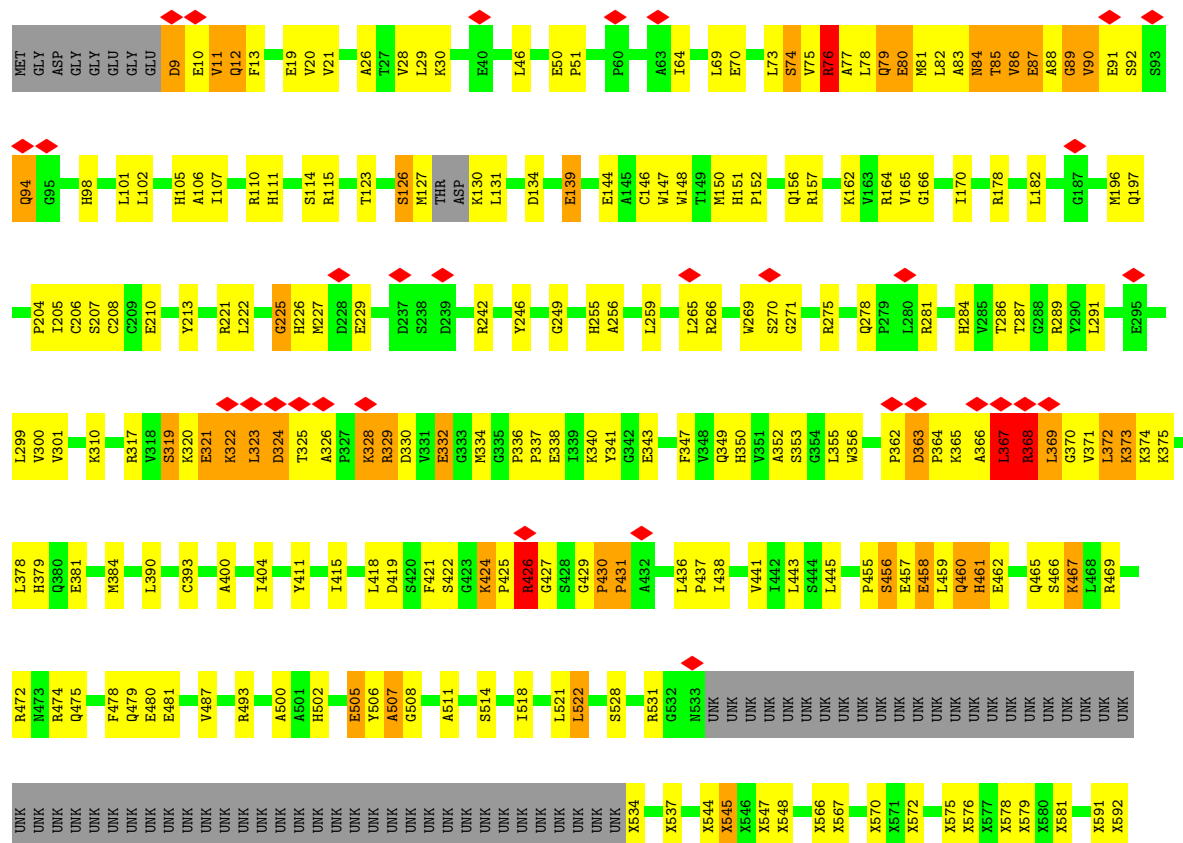




[illegible]

- Molecule 1: RYANODINE RECEPTOR 1

Chain B:  52% 12% 34%





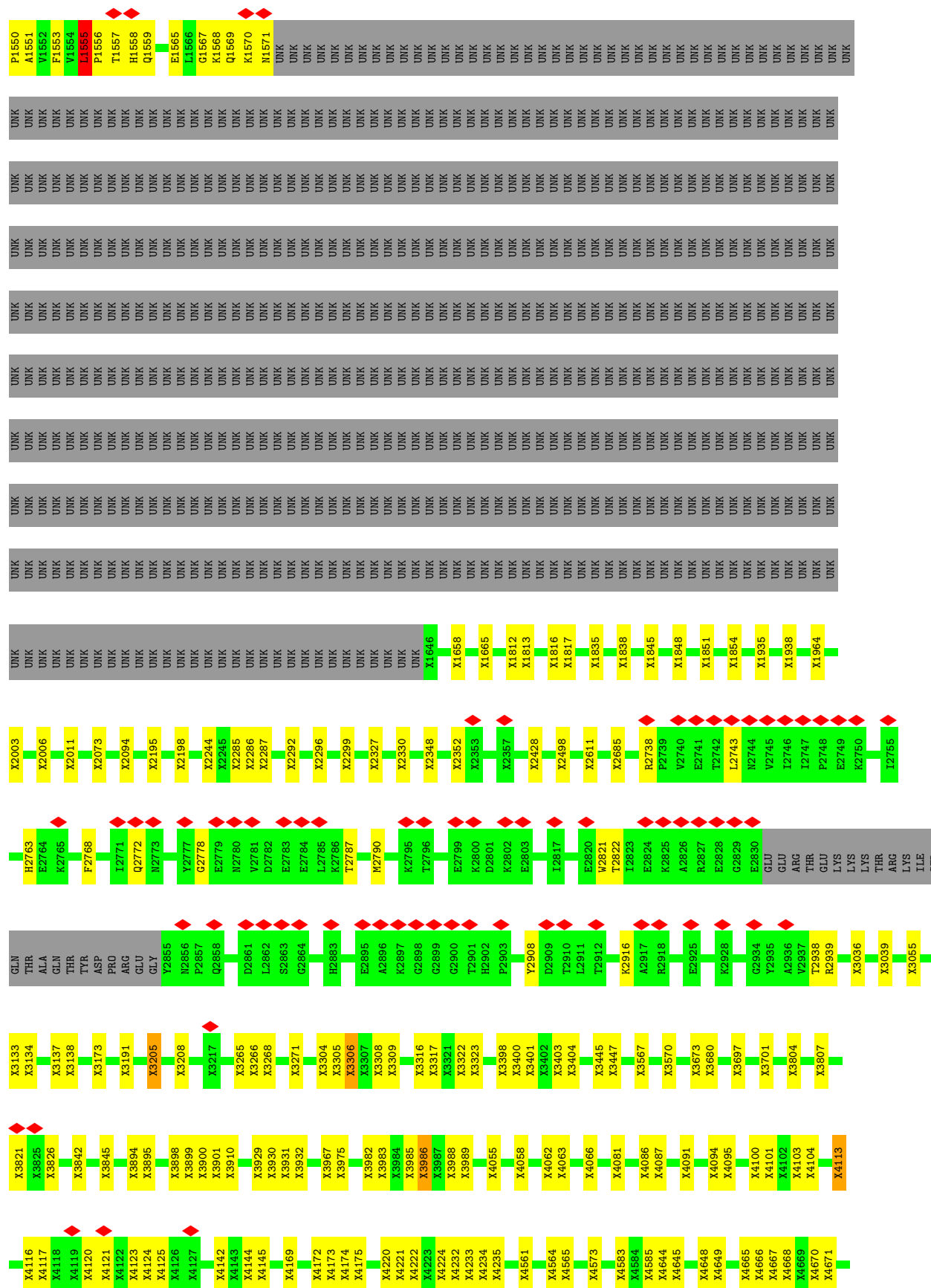


- Molecule 1: RYANODINE RECEPTOR 1

| Frequency | Percentage |
|-----------|------------|
| Daily     | 52%        |
| Weekly    | 12%        |
| Monthly   | 34%        |









|      |      |      |      |      |      |      |      |      |      |      |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |
|------|------|------|------|------|------|------|------|------|------|------|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|
| L101 | H105 | A106 | I107 | R110 | H111 | S114 | R115 | T123 | S126 | M127 | THR | ASP | K130 | L131 | D134 | E139 | E144 | A145 | C146 | M147 | W148 | T149 | M150 | H151 | P152 | Q156 | R157 | K162 | R163 | R164 | V165 | I170 | R178 | L182 | G187 | M196 | Q197 | P204 | C205 | C206 | S207 | C208 |     |     |     |     |     |     |     |     |
| MET  | GLY  | ASP  | GLY  | GLY  | GLU  | GLY  | GLY  | D9   | E10  | V11  | Q12 | F13 | E19  | V20  | V21  | A26  | T27  | V28  | L29  | K30  | E40  | P60  | A63  | I64  | L69  | E70  | L73  | S74  | V75  | R76  | A77  | L78  | Q79  | E80  | M81  | L82  | A83  | N84  | T85  | V86  | E87  | A88  | G89 | V90 | E91 | S92 | G93 | Q94 | G95 | H98 |





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## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, C4                       | Depositor |
| Number of particles used             | 25000                           | Depositor |
| Resolution determination method      | Not provided                    |           |
| CTF correction method                | FULL CORRECTION                 | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 20                              | Depositor |
| Minimum defocus (nm)                 | 1000                            | Depositor |
| Maximum defocus (nm)                 | 3000                            | Depositor |
| Magnification                        | 47992                           | Depositor |
| Image detector                       | FEI FALCON II (4k x 4k)         | Depositor |
| Maximum map value                    | 3.862                           | Depositor |
| Minimum map value                    | -2.497                          | Depositor |
| Average map value                    | 0.010                           | Depositor |
| Map value standard deviation         | 0.118                           | Depositor |
| Recommended contour level            | 0.443                           | Depositor |
| Map size ( $\text{\AA}$ )            | 545.27997, 545.27997, 545.27997 | wwPDB     |
| Map dimensions                       | 384, 384, 384                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.42, 1.42, 1.42                | Depositor |

## 5 Model quality [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 1   | A     | 0.43         | 0/10556 | 0.90        | 30/14313 (0.2%)  |
| 1   | B     | 0.43         | 0/10556 | 0.90        | 30/14313 (0.2%)  |
| 1   | C     | 0.43         | 0/10556 | 0.90        | 30/14313 (0.2%)  |
| 1   | D     | 0.43         | 0/10556 | 0.90        | 30/14313 (0.2%)  |
| All | All   | 0.43         | 0/42224 | 0.90        | 120/57252 (0.2%) |

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                   | 10                  |
| 1   | B     | 0                   | 10                  |
| 1   | C     | 0                   | 10                  |
| 1   | D     | 0                   | 10                  |
| All | All   | 0                   | 40                  |

There are no bond length outliers.

All (120) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 1195 | GLY  | CA-C-N | 9.05  | 131.15      | 119.84   |
| 1   | A     | 1195 | GLY  | C-N-CA | 9.05  | 131.15      | 119.84   |
| 1   | D     | 1195 | GLY  | CA-C-N | 9.04  | 131.13      | 119.84   |
| 1   | D     | 1195 | GLY  | C-N-CA | 9.04  | 131.13      | 119.84   |
| 1   | C     | 1195 | GLY  | CA-C-N | 9.01  | 131.10      | 119.84   |
| 1   | C     | 1195 | GLY  | C-N-CA | 9.01  | 131.10      | 119.84   |
| 1   | B     | 1195 | GLY  | CA-C-N | 8.99  | 131.07      | 119.84   |
| 1   | B     | 1195 | GLY  | C-N-CA | 8.99  | 131.07      | 119.84   |
| 1   | D     | 85   | THR  | N-CA-C | -8.05 | 102.50      | 111.28   |
| 1   | B     | 85   | THR  | N-CA-C | -8.01 | 102.56      | 111.28   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 85   | THR  | N-CA-C   | -7.95 | 102.61      | 111.28   |
| 1   | C     | 85   | THR  | N-CA-C   | -7.93 | 102.63      | 111.28   |
| 1   | C     | 728  | ARG  | C-N-CD   | 7.68  | 137.50      | 120.60   |
| 1   | B     | 728  | ARG  | C-N-CD   | 7.65  | 137.43      | 120.60   |
| 1   | A     | 728  | ARG  | C-N-CD   | 7.65  | 137.43      | 120.60   |
| 1   | D     | 728  | ARG  | C-N-CD   | 7.65  | 137.43      | 120.60   |
| 1   | B     | 954  | LYS  | N-CA-C   | 7.57  | 119.53      | 111.28   |
| 1   | A     | 954  | LYS  | N-CA-C   | 7.53  | 119.49      | 111.28   |
| 1   | D     | 954  | LYS  | N-CA-C   | 7.53  | 119.49      | 111.28   |
| 1   | C     | 954  | LYS  | N-CA-C   | 7.51  | 119.47      | 111.28   |
| 1   | A     | 367  | LEU  | CA-CB-CG | 7.38  | 142.14      | 116.30   |
| 1   | D     | 367  | LEU  | CA-CB-CG | 7.38  | 142.11      | 116.30   |
| 1   | C     | 367  | LEU  | CA-CB-CG | 7.37  | 142.10      | 116.30   |
| 1   | B     | 367  | LEU  | CA-CB-CG | 7.36  | 142.06      | 116.30   |
| 1   | A     | 751  | SER  | N-CA-C   | 7.34  | 119.28      | 111.28   |
| 1   | D     | 751  | SER  | N-CA-C   | 7.29  | 119.23      | 111.28   |
| 1   | C     | 751  | SER  | N-CA-C   | 7.27  | 119.21      | 111.28   |
| 1   | B     | 751  | SER  | N-CA-C   | 7.26  | 119.20      | 111.28   |
| 1   | A     | 752  | VAL  | C-N-CD   | 7.18  | 136.41      | 120.60   |
| 1   | C     | 752  | VAL  | C-N-CD   | 7.18  | 136.41      | 120.60   |
| 1   | D     | 752  | VAL  | C-N-CD   | 7.18  | 136.40      | 120.60   |
| 1   | B     | 752  | VAL  | C-N-CD   | 7.18  | 136.39      | 120.60   |
| 1   | A     | 1444 | GLU  | C-N-CD   | 7.14  | 136.32      | 120.60   |
| 1   | C     | 1444 | GLU  | C-N-CD   | 7.12  | 136.27      | 120.60   |
| 1   | D     | 1444 | GLU  | C-N-CD   | 7.12  | 136.26      | 120.60   |
| 1   | B     | 1444 | GLU  | C-N-CD   | 7.12  | 136.25      | 120.60   |
| 1   | C     | 992  | GLY  | N-CA-C   | -6.57 | 104.54      | 113.27   |
| 1   | D     | 992  | GLY  | N-CA-C   | -6.55 | 104.56      | 113.27   |
| 1   | B     | 992  | GLY  | N-CA-C   | -6.53 | 104.58      | 113.27   |
| 1   | A     | 992  | GLY  | N-CA-C   | -6.50 | 104.62      | 113.27   |
| 1   | A     | 363  | ASP  | C-N-CD   | -6.26 | 106.84      | 120.60   |
| 1   | D     | 363  | ASP  | C-N-CD   | -6.22 | 106.92      | 120.60   |
| 1   | B     | 363  | ASP  | C-N-CD   | -6.22 | 106.93      | 120.60   |
| 1   | C     | 363  | ASP  | C-N-CD   | -6.21 | 106.94      | 120.60   |
| 1   | A     | 1426 | ILE  | N-CA-C   | 6.08  | 116.55      | 110.23   |
| 1   | B     | 1426 | ILE  | N-CA-C   | 6.03  | 116.50      | 110.23   |
| 1   | C     | 1426 | ILE  | N-CA-C   | 6.03  | 116.50      | 110.23   |
| 1   | D     | 1426 | ILE  | N-CA-C   | 5.99  | 116.46      | 110.23   |
| 1   | C     | 658  | GLN  | N-CA-C   | 5.98  | 117.80      | 111.28   |
| 1   | C     | 904  | HIS  | CA-C-N   | 5.97  | 127.31      | 119.84   |
| 1   | C     | 904  | HIS  | C-N-CA   | 5.97  | 127.31      | 119.84   |
| 1   | A     | 904  | HIS  | CA-C-N   | 5.97  | 127.30      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 904  | HIS  | C-N-CA | 5.97  | 127.30      | 119.84   |
| 1   | B     | 904  | HIS  | CA-C-N | 5.96  | 127.29      | 119.84   |
| 1   | B     | 904  | HIS  | C-N-CA | 5.96  | 127.29      | 119.84   |
| 1   | D     | 904  | HIS  | CA-C-N | 5.95  | 127.28      | 119.84   |
| 1   | D     | 904  | HIS  | C-N-CA | 5.95  | 127.28      | 119.84   |
| 1   | D     | 76   | ARG  | N-CA-C | -5.93 | 104.72      | 111.07   |
| 1   | A     | 658  | GLN  | N-CA-C | 5.91  | 117.72      | 111.28   |
| 1   | A     | 76   | ARG  | N-CA-C | -5.90 | 104.76      | 111.07   |
| 1   | B     | 76   | ARG  | N-CA-C | -5.89 | 104.77      | 111.07   |
| 1   | B     | 658  | GLN  | N-CA-C | 5.89  | 117.70      | 111.28   |
| 1   | D     | 658  | GLN  | N-CA-C | 5.88  | 117.69      | 111.28   |
| 1   | C     | 76   | ARG  | N-CA-C | -5.87 | 104.79      | 111.07   |
| 1   | A     | 363  | ASP  | CA-C-N | 5.69  | 140.66      | 127.00   |
| 1   | A     | 363  | ASP  | C-N-CA | 5.69  | 140.66      | 127.00   |
| 1   | B     | 363  | ASP  | CA-C-N | 5.68  | 140.64      | 127.00   |
| 1   | B     | 363  | ASP  | C-N-CA | 5.68  | 140.64      | 127.00   |
| 1   | C     | 363  | ASP  | CA-C-N | 5.67  | 140.60      | 127.00   |
| 1   | C     | 363  | ASP  | C-N-CA | 5.67  | 140.60      | 127.00   |
| 1   | D     | 363  | ASP  | CA-C-N | 5.66  | 140.59      | 127.00   |
| 1   | D     | 363  | ASP  | C-N-CA | 5.66  | 140.59      | 127.00   |
| 1   | C     | 1555 | LEU  | CA-C-N | -5.65 | 114.14      | 119.85   |
| 1   | C     | 1555 | LEU  | C-N-CA | -5.65 | 114.14      | 119.85   |
| 1   | A     | 1555 | LEU  | CA-C-N | -5.61 | 114.18      | 119.85   |
| 1   | A     | 1555 | LEU  | C-N-CA | -5.61 | 114.18      | 119.85   |
| 1   | C     | 507  | ALA  | N-CA-C | -5.60 | 98.86       | 110.80   |
| 1   | B     | 1555 | LEU  | CA-C-N | -5.60 | 114.19      | 119.85   |
| 1   | B     | 1555 | LEU  | C-N-CA | -5.60 | 114.19      | 119.85   |
| 1   | D     | 1555 | LEU  | CA-C-N | -5.58 | 114.21      | 119.85   |
| 1   | D     | 1555 | LEU  | C-N-CA | -5.58 | 114.21      | 119.85   |
| 1   | A     | 507  | ALA  | N-CA-C | -5.57 | 98.94       | 110.80   |
| 1   | B     | 507  | ALA  | N-CA-C | -5.56 | 98.95       | 110.80   |
| 1   | D     | 507  | ALA  | N-CA-C | -5.55 | 98.99       | 110.80   |
| 1   | A     | 958  | THR  | N-CA-C | 5.50  | 120.09      | 113.17   |
| 1   | A     | 1549 | PHE  | CA-C-N | -5.50 | 114.27      | 119.76   |
| 1   | A     | 1549 | PHE  | C-N-CA | -5.50 | 114.27      | 119.76   |
| 1   | D     | 1473 | THR  | N-CA-C | 5.47  | 118.37      | 108.69   |
| 1   | B     | 958  | THR  | N-CA-C | 5.46  | 120.05      | 113.17   |
| 1   | C     | 958  | THR  | N-CA-C | 5.46  | 120.05      | 113.17   |
| 1   | D     | 958  | THR  | N-CA-C | 5.46  | 120.05      | 113.17   |
| 1   | C     | 1473 | THR  | N-CA-C | 5.45  | 118.34      | 108.69   |
| 1   | A     | 1473 | THR  | N-CA-C | 5.45  | 118.34      | 108.69   |
| 1   | B     | 1549 | PHE  | CA-C-N | -5.45 | 114.31      | 119.76   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | B     | 1549 | PHE  | C-N-CA | -5.45 | 114.31      | 119.76   |
| 1   | C     | 955  | LEU  | N-CA-C | 5.44  | 118.52      | 108.94   |
| 1   | C     | 1549 | PHE  | CA-C-N | -5.44 | 114.32      | 119.76   |
| 1   | C     | 1549 | PHE  | C-N-CA | -5.44 | 114.32      | 119.76   |
| 1   | B     | 1473 | THR  | N-CA-C | 5.43  | 118.31      | 108.69   |
| 1   | D     | 1549 | PHE  | CA-C-N | -5.43 | 114.33      | 119.76   |
| 1   | D     | 1549 | PHE  | C-N-CA | -5.43 | 114.33      | 119.76   |
| 1   | B     | 955  | LEU  | N-CA-C | 5.42  | 118.48      | 108.94   |
| 1   | A     | 955  | LEU  | N-CA-C | 5.41  | 118.47      | 108.94   |
| 1   | D     | 955  | LEU  | N-CA-C | 5.41  | 118.46      | 108.94   |
| 1   | A     | 80   | GLU  | N-CA-C | -5.34 | 105.46      | 111.28   |
| 1   | B     | 80   | GLU  | N-CA-C | -5.34 | 105.46      | 111.28   |
| 1   | A     | 864  | PRO  | O-C-N  | 5.32  | 123.65      | 121.15   |
| 1   | C     | 80   | GLU  | N-CA-C | -5.28 | 105.53      | 111.28   |
| 1   | D     | 864  | PRO  | O-C-N  | 5.27  | 123.63      | 121.15   |
| 1   | D     | 750  | LEU  | N-CA-C | 5.27  | 117.11      | 111.36   |
| 1   | C     | 864  | PRO  | O-C-N  | 5.26  | 123.62      | 121.15   |
| 1   | D     | 80   | GLU  | N-CA-C | -5.24 | 105.57      | 111.28   |
| 1   | A     | 750  | LEU  | N-CA-C | 5.24  | 117.07      | 111.36   |
| 1   | B     | 750  | LEU  | N-CA-C | 5.23  | 117.06      | 111.36   |
| 1   | C     | 750  | LEU  | N-CA-C | 5.22  | 117.05      | 111.36   |
| 1   | B     | 864  | PRO  | O-C-N  | 5.20  | 123.59      | 121.15   |
| 1   | B     | 430  | PRO  | N-CA-C | 5.10  | 116.92      | 110.70   |
| 1   | D     | 430  | PRO  | N-CA-C | 5.08  | 116.89      | 110.70   |
| 1   | A     | 430  | PRO  | N-CA-C | 5.04  | 116.85      | 110.70   |
| 1   | C     | 430  | PRO  | N-CA-C | 5.01  | 116.81      | 110.70   |

There are no chirality outliers.

All (40) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 3055 | UNK  | Peptide |
| 1   | A     | 3205 | UNK  | Peptide |
| 1   | A     | 3306 | UNK  | Peptide |
| 1   | A     | 3986 | UNK  | Peptide |
| 1   | A     | 4081 | UNK  | Peptide |
| 1   | A     | 4113 | UNK  | Peptide |
| 1   | A     | 4729 | UNK  | Peptide |
| 1   | A     | 4898 | UNK  | Peptide |
| 1   | A     | 545  | UNK  | Peptide |
| 1   | A     | 88   | ALA  | Peptide |
| 1   | B     | 3055 | UNK  | Peptide |

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| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | B     | 3205 | UNK  | Peptide |
| 1   | B     | 3306 | UNK  | Peptide |
| 1   | B     | 3986 | UNK  | Peptide |
| 1   | B     | 4081 | UNK  | Peptide |
| 1   | B     | 4113 | UNK  | Peptide |
| 1   | B     | 4729 | UNK  | Peptide |
| 1   | B     | 4898 | UNK  | Peptide |
| 1   | B     | 545  | UNK  | Peptide |
| 1   | B     | 88   | ALA  | Peptide |
| 1   | C     | 3055 | UNK  | Peptide |
| 1   | C     | 3205 | UNK  | Peptide |
| 1   | C     | 3306 | UNK  | Peptide |
| 1   | C     | 3986 | UNK  | Peptide |
| 1   | C     | 4081 | UNK  | Peptide |
| 1   | C     | 4113 | UNK  | Peptide |
| 1   | C     | 4729 | UNK  | Peptide |
| 1   | C     | 4898 | UNK  | Peptide |
| 1   | C     | 545  | UNK  | Peptide |
| 1   | C     | 88   | ALA  | Peptide |
| 1   | D     | 3055 | UNK  | Peptide |
| 1   | D     | 3205 | UNK  | Peptide |
| 1   | D     | 3306 | UNK  | Peptide |
| 1   | D     | 3986 | UNK  | Peptide |
| 1   | D     | 4081 | UNK  | Peptide |
| 1   | D     | 4113 | UNK  | Peptide |
| 1   | D     | 4729 | UNK  | Peptide |
| 1   | D     | 4898 | UNK  | Peptide |
| 1   | D     | 545  | UNK  | Peptide |
| 1   | D     | 88   | ALA  | Peptide |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 20410 | 0        | 12266    | 1195    | 0            |
| 1   | B     | 20410 | 0        | 12265    | 1181    | 0            |
| 1   | C     | 20410 | 0        | 12266    | 1184    | 0            |
| 1   | D     | 20410 | 0        | 12266    | 1174    | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 81640 | 0        | 49063    | 4677    | 0            |

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

All (4677) 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:C:657:THR:HG21 | 1:C:662:TRP:CE3  | 1.15                     | 1.68              |
| 1:B:956:PRO:HG3  | 1:B:959:TYR:CZ   | 1.25                     | 1.65              |
| 1:A:956:PRO:HG3  | 1:A:959:TYR:CE1  | 1.30                     | 1.65              |
| 1:D:956:PRO:HG3  | 1:D:959:TYR:CE1  | 1.31                     | 1.65              |
| 1:D:956:PRO:CD   | 1:D:959:TYR:CD2  | 1.74                     | 1.64              |
| 1:B:956:PRO:CD   | 1:B:959:TYR:CD2  | 1.74                     | 1.64              |
| 1:A:956:PRO:HG3  | 1:A:959:TYR:CZ   | 1.25                     | 1.63              |
| 1:C:956:PRO:HG3  | 1:C:959:TYR:CZ   | 1.25                     | 1.63              |
| 1:A:956:PRO:CD   | 1:A:959:TYR:CD2  | 1.74                     | 1.63              |
| 1:A:657:THR:HG21 | 1:A:662:TRP:CE3  | 1.15                     | 1.63              |
| 1:B:657:THR:HG21 | 1:B:662:TRP:CE3  | 1.15                     | 1.63              |
| 1:C:657:THR:HG21 | 1:C:662:TRP:CD2  | 1.31                     | 1.61              |
| 1:D:657:THR:HG21 | 1:D:662:TRP:CE3  | 1.15                     | 1.61              |
| 1:C:753:PRO:HG3  | 1:C:773:LEU:CD1  | 1.28                     | 1.61              |
| 1:D:956:PRO:HG3  | 1:D:959:TYR:CZ   | 1.25                     | 1.60              |
| 1:D:753:PRO:HG3  | 1:D:773:LEU:CD1  | 1.28                     | 1.60              |
| 1:C:956:PRO:HG3  | 1:C:959:TYR:CE1  | 1.31                     | 1.59              |
| 1:B:956:PRO:HG3  | 1:B:959:TYR:CE1  | 1.31                     | 1.59              |
| 1:D:657:THR:HG21 | 1:D:662:TRP:CD2  | 1.31                     | 1.59              |
| 1:A:657:THR:HG21 | 1:A:662:TRP:CD2  | 1.31                     | 1.58              |
| 1:C:956:PRO:CD   | 1:C:959:TYR:CD2  | 1.74                     | 1.58              |
| 1:A:753:PRO:HG3  | 1:A:773:LEU:CD1  | 1.28                     | 1.58              |
| 1:C:1007:TYR:CD1 | 1:C:1016:ARG:NH2 | 1.70                     | 1.57              |
| 1:A:1007:TYR:CD1 | 1:A:1016:ARG:NH2 | 1.70                     | 1.56              |
| 1:B:657:THR:HG21 | 1:B:662:TRP:CD2  | 1.31                     | 1.56              |
| 1:D:1007:TYR:CD1 | 1:D:1016:ARG:NH2 | 1.70                     | 1.56              |
| 1:B:753:PRO:HG3  | 1:B:773:LEU:CD1  | 1.28                     | 1.56              |
| 1:B:1007:TYR:CD1 | 1:B:1016:ARG:NH2 | 1.70                     | 1.55              |
| 1:B:956:PRO:CD   | 1:B:959:TYR:CG   | 1.92                     | 1.52              |
| 1:C:956:PRO:HD3  | 1:C:959:TYR:CG   | 1.45                     | 1.52              |
| 1:A:956:PRO:CD   | 1:A:959:TYR:CG   | 1.92                     | 1.51              |
| 1:D:956:PRO:CD   | 1:D:959:TYR:CG   | 1.92                     | 1.51              |
| 1:D:956:PRO:HD3  | 1:D:959:TYR:CG   | 1.45                     | 1.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1004:GLY:HA2 | 1:D:1007:TYR:CE1  | 1.46                     | 1.50              |
| 1:C:996:TRP:CZ2  | 1:C:1021:LEU:HD13 | 1.45                     | 1.50              |
| 1:B:996:TRP:CZ2  | 1:B:1021:LEU:HD13 | 1.45                     | 1.50              |
| 1:B:3316:UNK:CB  | 1:B:3322:UNK:CB   | 1.91                     | 1.49              |
| 1:A:996:TRP:CZ2  | 1:A:1021:LEU:HD13 | 1.45                     | 1.49              |
| 1:D:996:TRP:CZ2  | 1:D:1021:LEU:HD13 | 1.45                     | 1.49              |
| 1:C:3316:UNK:CB  | 1:C:3322:UNK:CB   | 1.91                     | 1.48              |
| 1:B:1004:GLY:HA2 | 1:B:1007:TYR:CE1  | 1.46                     | 1.48              |
| 1:C:956:PRO:CD   | 1:C:959:TYR:CG    | 1.92                     | 1.48              |
| 1:C:1004:GLY:HA2 | 1:C:1007:TYR:CE1  | 1.47                     | 1.48              |
| 1:A:1004:GLY:HA2 | 1:A:1007:TYR:CE1  | 1.46                     | 1.47              |
| 1:A:956:PRO:HD3  | 1:A:959:TYR:CG    | 1.45                     | 1.46              |
| 1:A:3316:UNK:CB  | 1:A:3322:UNK:CB   | 1.91                     | 1.46              |
| 1:B:956:PRO:HD3  | 1:B:959:TYR:CG    | 1.45                     | 1.46              |
| 1:C:1018:ASN:HB2 | 1:C:1021:LEU:CD2  | 1.46                     | 1.45              |
| 1:C:953:THR:O    | 1:C:959:TYR:CD2   | 1.69                     | 1.45              |
| 1:D:3316:UNK:CB  | 1:D:3322:UNK:CB   | 1.91                     | 1.45              |
| 1:D:728:ARG:HB2  | 1:D:1134:LEU:CD2  | 1.47                     | 1.45              |
| 1:D:1018:ASN:HB2 | 1:D:1021:LEU:CD2  | 1.46                     | 1.45              |
| 1:A:1018:ASN:HB2 | 1:A:1021:LEU:CD2  | 1.46                     | 1.44              |
| 1:B:1018:ASN:HB2 | 1:B:1021:LEU:CD2  | 1.46                     | 1.44              |
| 1:A:728:ARG:HB2  | 1:A:1134:LEU:CD2  | 1.47                     | 1.44              |
| 1:C:1434:TYR:CE1 | 1:C:1570:LYS:HD2  | 1.53                     | 1.43              |
| 1:B:953:THR:O    | 1:B:959:TYR:CD2   | 1.69                     | 1.42              |
| 1:D:317:ARG:CZ   | 1:D:322:LYS:HA    | 1.46                     | 1.42              |
| 1:D:657:THR:CG2  | 1:D:662:TRP:CE3   | 2.02                     | 1.42              |
| 1:D:953:THR:O    | 1:D:959:TYR:CD2   | 1.69                     | 1.42              |
| 1:B:317:ARG:CZ   | 1:B:322:LYS:HA    | 1.46                     | 1.42              |
| 1:C:657:THR:CG2  | 1:C:662:TRP:CE3   | 2.02                     | 1.42              |
| 1:A:317:ARG:CZ   | 1:A:322:LYS:HA    | 1.46                     | 1.42              |
| 1:A:953:THR:O    | 1:A:959:TYR:CD2   | 1.69                     | 1.42              |
| 1:C:1018:ASN:CB  | 1:C:1021:LEU:HD21 | 1.49                     | 1.42              |
| 1:B:1018:ASN:CB  | 1:B:1021:LEU:HD21 | 1.49                     | 1.41              |
| 1:C:728:ARG:HB2  | 1:C:1134:LEU:CD2  | 1.47                     | 1.41              |
| 1:A:1434:TYR:CE1 | 1:A:1570:LYS:HD2  | 1.53                     | 1.41              |
| 1:C:317:ARG:CZ   | 1:C:322:LYS:HA    | 1.46                     | 1.41              |
| 1:B:728:ARG:HB2  | 1:B:1134:LEU:CD2  | 1.47                     | 1.41              |
| 1:B:1020:ARG:NH1 | 1:B:1024:TYR:HA   | 1.34                     | 1.40              |
| 1:B:1434:TYR:CE1 | 1:B:1570:LYS:HD2  | 1.53                     | 1.40              |
| 1:D:1018:ASN:CB  | 1:D:1021:LEU:HD21 | 1.49                     | 1.40              |
| 1:A:657:THR:CG2  | 1:A:662:TRP:CE3   | 2.02                     | 1.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1434:TYR:CE1 | 1:D:1570:LYS:HD2  | 1.53                     | 1.40              |
| 1:C:3967:UNK:O   | 1:C:3975:UNK:CB   | 1.71                     | 1.39              |
| 1:A:2296:UNK:HA  | 1:A:2352:UNK:CB   | 1.53                     | 1.39              |
| 1:B:657:THR:CG2  | 1:B:662:TRP:CE3   | 2.02                     | 1.38              |
| 1:B:2296:UNK:HA  | 1:B:2352:UNK:CB   | 1.53                     | 1.38              |
| 1:D:2296:UNK:HA  | 1:D:2352:UNK:CB   | 1.53                     | 1.38              |
| 1:C:2296:UNK:HA  | 1:C:2352:UNK:CB   | 1.53                     | 1.38              |
| 1:C:752:VAL:HG11 | 1:C:769:GLU:CG    | 1.53                     | 1.38              |
| 1:D:752:VAL:HG11 | 1:D:769:GLU:CG    | 1.53                     | 1.38              |
| 1:B:3967:UNK:O   | 1:B:3975:UNK:CB   | 1.71                     | 1.38              |
| 1:C:1020:ARG:NH1 | 1:C:1024:TYR:HA   | 1.34                     | 1.38              |
| 1:A:1020:ARG:NH1 | 1:A:1024:TYR:HA   | 1.34                     | 1.37              |
| 1:B:3900:UNK:HA  | 1:B:3910:UNK:CB   | 1.53                     | 1.37              |
| 1:D:3967:UNK:O   | 1:D:3975:UNK:CB   | 1.71                     | 1.37              |
| 1:A:1018:ASN:CB  | 1:A:1021:LEU:HD21 | 1.49                     | 1.37              |
| 1:D:1020:ARG:NH1 | 1:D:1024:TYR:HA   | 1.34                     | 1.37              |
| 1:B:317:ARG:NH1  | 1:B:322:LYS:HA    | 1.38                     | 1.36              |
| 1:B:752:VAL:HG11 | 1:B:769:GLU:CG    | 1.53                     | 1.36              |
| 1:B:956:PRO:CG   | 1:B:959:TYR:CE1   | 2.08                     | 1.36              |
| 1:C:956:PRO:CG   | 1:C:959:TYR:CE1   | 2.08                     | 1.36              |
| 1:A:3900:UNK:HA  | 1:A:3910:UNK:CB   | 1.53                     | 1.35              |
| 1:A:3930:UNK:C   | 1:D:76:ARG:HH12   | 1.38                     | 1.35              |
| 1:C:317:ARG:NH1  | 1:C:322:LYS:HA    | 1.38                     | 1.35              |
| 1:C:1452:TRP:CZ3 | 1:C:1527:MET:HB3  | 1.42                     | 1.35              |
| 1:B:76:ARG:HH12  | 1:C:3930:UNK:C    | 1.38                     | 1.35              |
| 1:D:956:PRO:CG   | 1:D:959:TYR:CE1   | 2.08                     | 1.35              |
| 1:D:3900:UNK:HA  | 1:D:3910:UNK:CB   | 1.53                     | 1.35              |
| 1:A:76:ARG:HH12  | 1:B:3930:UNK:C    | 1.38                     | 1.35              |
| 1:A:956:PRO:HD3  | 1:A:959:TYR:CD2   | 0.82                     | 1.35              |
| 1:A:3967:UNK:O   | 1:A:3975:UNK:CB   | 1.71                     | 1.35              |
| 1:C:753:PRO:CG   | 1:C:773:LEU:CD1   | 2.05                     | 1.35              |
| 1:C:3900:UNK:HA  | 1:C:3910:UNK:CB   | 1.53                     | 1.34              |
| 1:A:317:ARG:NH1  | 1:A:322:LYS:HA    | 1.38                     | 1.34              |
| 1:A:2292:UNK:C   | 1:A:2348:UNK:CB   | 2.05                     | 1.34              |
| 1:B:956:PRO:HD3  | 1:B:959:TYR:CD2   | 0.82                     | 1.34              |
| 1:C:956:PRO:HD3  | 1:C:959:TYR:CD2   | 0.82                     | 1.34              |
| 1:A:752:VAL:HG11 | 1:A:769:GLU:CG    | 1.53                     | 1.34              |
| 1:A:956:PRO:CG   | 1:A:959:TYR:CE1   | 2.08                     | 1.34              |
| 1:D:2292:UNK:O   | 1:D:2348:UNK:CB   | 1.76                     | 1.34              |
| 1:D:317:ARG:NH1  | 1:D:322:LYS:HA    | 1.38                     | 1.34              |
| 1:B:2292:UNK:C   | 1:B:2348:UNK:CB   | 2.05                     | 1.33              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:2292:UNK:C   | 1:C:2348:UNK:CB  | 2.05                     | 1.33              |
| 1:C:76:ARG:HH12  | 1:D:3930:UNK:C   | 1.40                     | 1.33              |
| 1:D:753:PRO:CG   | 1:D:773:LEU:CD1  | 2.05                     | 1.33              |
| 1:D:956:PRO:HD3  | 1:D:959:TYR:CD2  | 0.82                     | 1.33              |
| 1:A:207:SER:CA   | 1:A:269:TRP:HZ3  | 1.42                     | 1.32              |
| 1:D:207:SER:CA   | 1:D:269:TRP:HZ3  | 1.42                     | 1.32              |
| 1:D:1463:ASN:O   | 1:D:1468:LYS:NZ  | 1.62                     | 1.32              |
| 1:A:2292:UNK:O   | 1:A:2348:UNK:CB  | 1.76                     | 1.32              |
| 1:B:207:SER:CA   | 1:B:269:TRP:HZ3  | 1.42                     | 1.32              |
| 1:B:753:PRO:CG   | 1:B:773:LEU:CD1  | 2.05                     | 1.32              |
| 1:B:2292:UNK:O   | 1:B:2348:UNK:CB  | 1.76                     | 1.31              |
| 1:A:753:PRO:CG   | 1:A:773:LEU:CD1  | 2.05                     | 1.31              |
| 1:D:2292:UNK:C   | 1:D:2348:UNK:CB  | 2.05                     | 1.31              |
| 1:A:1463:ASN:O   | 1:A:1468:LYS:NZ  | 1.62                     | 1.31              |
| 1:B:1463:ASN:O   | 1:B:1468:LYS:NZ  | 1.62                     | 1.30              |
| 1:C:2292:UNK:O   | 1:C:2348:UNK:CB  | 1.76                     | 1.30              |
| 1:B:426:ARG:NH2  | 1:B:796:ARG:NH1  | 1.80                     | 1.30              |
| 1:B:1452:TRP:CZ3 | 1:B:1527:MET:HB3 | 1.42                     | 1.30              |
| 1:C:207:SER:CA   | 1:C:269:TRP:HZ3  | 1.42                     | 1.30              |
| 1:D:1452:TRP:CZ3 | 1:D:1527:MET:HB3 | 1.42                     | 1.29              |
| 1:C:426:ARG:NH2  | 1:C:796:ARG:NH1  | 1.80                     | 1.29              |
| 1:C:1463:ASN:O   | 1:C:1468:LYS:NZ  | 1.62                     | 1.29              |
| 1:B:426:ARG:HH22 | 1:B:796:ARG:CZ   | 1.45                     | 1.29              |
| 1:C:426:ARG:HH22 | 1:C:796:ARG:CZ   | 1.45                     | 1.29              |
| 1:D:426:ARG:HH22 | 1:D:796:ARG:CZ   | 1.45                     | 1.28              |
| 1:A:426:ARG:HH22 | 1:A:796:ARG:CZ   | 1.45                     | 1.28              |
| 1:A:1002:ALA:HA  | 1:A:1005:TRP:CD1 | 1.68                     | 1.28              |
| 1:B:1002:ALA:HA  | 1:B:1005:TRP:CD1 | 1.68                     | 1.28              |
| 1:A:426:ARG:NH2  | 1:A:796:ARG:NH1  | 1.80                     | 1.28              |
| 1:D:426:ARG:NH2  | 1:D:796:ARG:NH1  | 1.80                     | 1.27              |
| 1:A:1007:TYR:CE1 | 1:A:1016:ARG:NH2 | 1.85                     | 1.27              |
| 1:D:1002:ALA:HA  | 1:D:1005:TRP:CD1 | 1.68                     | 1.27              |
| 1:C:1002:ALA:HA  | 1:C:1005:TRP:CD1 | 1.68                     | 1.26              |
| 1:A:956:PRO:O    | 1:A:958:THR:N    | 1.69                     | 1.26              |
| 1:C:657:THR:CG2  | 1:C:662:TRP:CD2  | 2.16                     | 1.26              |
| 1:D:657:THR:CG2  | 1:D:662:TRP:CD2  | 2.16                     | 1.26              |
| 1:A:1452:TRP:CZ3 | 1:A:1527:MET:HB3 | 1.42                     | 1.26              |
| 1:B:956:PRO:O    | 1:B:958:THR:N    | 1.68                     | 1.26              |
| 1:C:1007:TYR:CE1 | 1:C:1016:ARG:NH2 | 1.85                     | 1.25              |
| 1:C:657:THR:CG2  | 1:C:662:TRP:CZ3  | 2.20                     | 1.25              |
| 1:B:956:PRO:CG   | 1:B:959:TYR:CZ   | 2.19                     | 1.25              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:657:THR:CG2  | 1:D:662:TRP:CZ3  | 2.20                     | 1.25              |
| 1:A:1452:TRP:CH2 | 1:A:1527:MET:HB3 | 1.72                     | 1.24              |
| 1:B:1007:TYR:CE1 | 1:B:1016:ARG:NH2 | 1.85                     | 1.24              |
| 1:A:956:PRO:CG   | 1:A:959:TYR:CZ   | 2.19                     | 1.24              |
| 1:B:657:THR:CG2  | 1:B:662:TRP:CD2  | 2.16                     | 1.24              |
| 1:B:657:THR:CG2  | 1:B:662:TRP:CZ3  | 2.20                     | 1.24              |
| 1:D:426:ARG:NH2  | 1:D:796:ARG:CZ   | 2.01                     | 1.24              |
| 1:C:956:PRO:O    | 1:C:958:THR:N    | 1.69                     | 1.23              |
| 1:C:1452:TRP:CH2 | 1:C:1527:MET:HB3 | 1.72                     | 1.23              |
| 1:A:657:THR:CG2  | 1:A:662:TRP:CZ3  | 2.20                     | 1.23              |
| 1:C:956:PRO:CG   | 1:C:959:TYR:CD1  | 2.22                     | 1.23              |
| 1:D:956:PRO:O    | 1:D:958:THR:N    | 1.69                     | 1.23              |
| 1:A:426:ARG:NH2  | 1:A:796:ARG:CZ   | 2.01                     | 1.23              |
| 1:B:956:PRO:CG   | 1:B:959:TYR:CD1  | 2.22                     | 1.23              |
| 1:D:956:PRO:CG   | 1:D:959:TYR:CZ   | 2.19                     | 1.23              |
| 1:C:998:ARG:HH22 | 1:C:1002:ALA:CB  | 1.52                     | 1.22              |
| 1:D:1452:TRP:CH2 | 1:D:1527:MET:HB3 | 1.72                     | 1.22              |
| 1:A:657:THR:CG2  | 1:A:662:TRP:CD2  | 2.16                     | 1.22              |
| 1:A:956:PRO:CG   | 1:A:959:TYR:CD1  | 2.22                     | 1.22              |
| 1:B:1452:TRP:CH2 | 1:B:1527:MET:HB3 | 1.72                     | 1.22              |
| 1:A:752:VAL:CG1  | 1:A:769:GLU:HB3  | 1.69                     | 1.22              |
| 1:D:998:ARG:HH22 | 1:D:1002:ALA:CB  | 1.52                     | 1.22              |
| 1:D:956:PRO:CG   | 1:D:959:TYR:CD1  | 2.22                     | 1.22              |
| 1:A:1016:ARG:NH1 | 1:A:1016:ARG:HB3 | 1.55                     | 1.21              |
| 1:D:752:VAL:CG1  | 1:D:769:GLU:HB3  | 1.69                     | 1.21              |
| 1:D:1016:ARG:NH1 | 1:D:1016:ARG:HB3 | 1.55                     | 1.21              |
| 1:A:4796:UNK:CB  | 1:A:4804:UNK:CB  | 2.18                     | 1.21              |
| 1:B:752:VAL:CG1  | 1:B:769:GLU:HB3  | 1.69                     | 1.21              |
| 1:B:998:ARG:HH22 | 1:B:1002:ALA:CB  | 1.52                     | 1.21              |
| 1:B:1004:GLY:HA3 | 1:B:1015:ALA:CB  | 1.71                     | 1.20              |
| 1:C:752:VAL:CG1  | 1:C:769:GLU:HB3  | 1.69                     | 1.20              |
| 1:A:752:VAL:HG11 | 1:A:769:GLU:CD   | 1.67                     | 1.20              |
| 1:B:752:VAL:HG11 | 1:B:769:GLU:CD   | 1.67                     | 1.20              |
| 1:B:4796:UNK:CB  | 1:B:4804:UNK:CB  | 2.18                     | 1.20              |
| 1:C:1016:ARG:HB3 | 1:C:1016:ARG:NH1 | 1.55                     | 1.20              |
| 1:D:4796:UNK:CB  | 1:D:4804:UNK:CB  | 2.18                     | 1.20              |
| 1:A:998:ARG:HH22 | 1:A:1002:ALA:CB  | 1.52                     | 1.20              |
| 1:B:426:ARG:NH2  | 1:B:796:ARG:NH2  | 1.90                     | 1.20              |
| 1:C:752:VAL:HG11 | 1:C:769:GLU:CD   | 1.67                     | 1.20              |
| 1:C:4796:UNK:CB  | 1:C:4804:UNK:CB  | 2.18                     | 1.20              |
| 1:A:1439:VAL:N   | 1:A:1515:VAL:HA  | 1.57                     | 1.20              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:426:ARG:NH2   | 1:D:796:ARG:NH2  | 1.90                     | 1.20              |
| 1:A:1465:ASP:HA   | 1:A:1553:PHE:CG  | 1.77                     | 1.20              |
| 1:B:1439:VAL:N    | 1:B:1515:VAL:HA  | 1.57                     | 1.20              |
| 1:D:956:PRO:HD3   | 1:D:959:TYR:CE2  | 1.77                     | 1.20              |
| 1:B:426:ARG:NH2   | 1:B:796:ARG:CZ   | 2.01                     | 1.19              |
| 1:D:1004:GLY:HA3  | 1:D:1015:ALA:CB  | 1.71                     | 1.19              |
| 1:B:1016:ARG:NH1  | 1:B:1016:ARG:HB3 | 1.55                     | 1.19              |
| 1:D:1439:VAL:N    | 1:D:1515:VAL:HA  | 1.57                     | 1.19              |
| 1:B:426:ARG:HH21  | 1:B:796:ARG:NH1  | 1.37                     | 1.19              |
| 1:C:426:ARG:NH2   | 1:C:796:ARG:NH2  | 1.90                     | 1.19              |
| 1:A:1004:GLY:HA3  | 1:A:1015:ALA:CB  | 1.71                     | 1.19              |
| 1:C:956:PRO:CG    | 1:C:959:TYR:CZ   | 2.19                     | 1.19              |
| 1:C:993:HIS:CA    | 1:C:996:TRP:HE3  | 1.55                     | 1.19              |
| 1:C:1004:GLY:HA3  | 1:C:1015:ALA:CB  | 1.71                     | 1.19              |
| 1:A:426:ARG:NH2   | 1:A:796:ARG:NH2  | 1.90                     | 1.19              |
| 1:B:993:HIS:CA    | 1:B:996:TRP:HE3  | 1.55                     | 1.19              |
| 1:D:1465:ASP:HA   | 1:D:1553:PHE:CG  | 1.77                     | 1.19              |
| 1:A:956:PRO:HD3   | 1:A:959:TYR:CE2  | 1.77                     | 1.18              |
| 1:B:1465:ASP:HA   | 1:B:1553:PHE:CG  | 1.77                     | 1.18              |
| 1:C:426:ARG:NH2   | 1:C:796:ARG:CZ   | 2.01                     | 1.18              |
| 1:C:956:PRO:HD3   | 1:C:959:TYR:CE2  | 1.77                     | 1.18              |
| 1:A:1001:VAL:HG13 | 1:A:1005:TRP:NE1 | 1.58                     | 1.18              |
| 1:A:4221:UNK:O    | 1:A:4232:UNK:C   | 1.91                     | 1.18              |
| 1:C:426:ARG:HH22  | 1:C:796:ARG:NH2  | 1.41                     | 1.18              |
| 1:D:753:PRO:HG3   | 1:D:773:LEU:HD12 | 1.19                     | 1.18              |
| 1:D:4221:UNK:O    | 1:D:4232:UNK:C   | 1.91                     | 1.18              |
| 1:A:317:ARG:CZ    | 1:A:322:LYS:CA   | 2.22                     | 1.17              |
| 1:B:207:SER:N     | 1:B:269:TRP:CZ3  | 2.12                     | 1.17              |
| 1:C:1465:ASP:HA   | 1:C:1553:PHE:CG  | 1.78                     | 1.17              |
| 1:B:956:PRO:HD3   | 1:B:959:TYR:CE2  | 1.77                     | 1.17              |
| 1:D:426:ARG:HH22  | 1:D:796:ARG:NH2  | 1.42                     | 1.17              |
| 1:D:207:SER:N     | 1:D:269:TRP:CZ3  | 2.12                     | 1.17              |
| 1:C:1001:VAL:HG13 | 1:C:1005:TRP:NE1 | 1.58                     | 1.17              |
| 1:C:4221:UNK:O    | 1:C:4232:UNK:C   | 1.91                     | 1.17              |
| 1:D:317:ARG:CZ    | 1:D:322:LYS:CA   | 2.22                     | 1.17              |
| 1:D:752:VAL:HG11  | 1:D:769:GLU:CD   | 1.67                     | 1.17              |
| 1:C:207:SER:N     | 1:C:269:TRP:CZ3  | 2.12                     | 1.17              |
| 1:C:317:ARG:CZ    | 1:C:322:LYS:CA   | 2.22                     | 1.17              |
| 1:A:753:PRO:CG    | 1:A:773:LEU:HD11 | 1.68                     | 1.16              |
| 1:B:426:ARG:HH22  | 1:B:796:ARG:NH2  | 1.41                     | 1.16              |
| 1:B:4221:UNK:O    | 1:B:4232:UNK:C   | 1.91                     | 1.16              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:317:ARG:CZ    | 1:B:322:LYS:CA    | 2.22                     | 1.16              |
| 1:C:1439:VAL:N    | 1:C:1515:VAL:HA   | 1.57                     | 1.16              |
| 1:D:993:HIS:CA    | 1:D:996:TRP:HE3   | 1.55                     | 1.16              |
| 1:D:1007:TYR:CE1  | 1:D:1016:ARG:NH2  | 1.85                     | 1.16              |
| 1:A:207:SER:N     | 1:A:269:TRP:CZ3   | 2.12                     | 1.16              |
| 1:A:426:ARG:HH22  | 1:A:796:ARG:NH2   | 1.41                     | 1.16              |
| 1:B:753:PRO:CG    | 1:B:773:LEU:HD11  | 1.68                     | 1.16              |
| 1:B:728:ARG:HB2   | 1:B:1134:LEU:HD22 | 1.21                     | 1.16              |
| 1:B:1001:VAL:HG13 | 1:B:1005:TRP:NE1  | 1.58                     | 1.16              |
| 1:D:728:ARG:HB2   | 1:D:1134:LEU:HD22 | 1.21                     | 1.16              |
| 1:A:426:ARG:HH21  | 1:A:796:ARG:NH1   | 1.37                     | 1.16              |
| 1:B:1465:ASP:HA   | 1:B:1553:PHE:CD2  | 1.81                     | 1.16              |
| 1:D:1452:TRP:CZ3  | 1:D:1527:MET:CB   | 2.19                     | 1.16              |
| 1:A:2428:UNK:CB   | 1:A:2498:UNK:CB   | 2.24                     | 1.15              |
| 1:C:426:ARG:HH21  | 1:C:796:ARG:NH1   | 1.37                     | 1.15              |
| 1:D:1432:THR:OG1  | 1:D:1523:ALA:HB2  | 1.46                     | 1.15              |
| 1:A:753:PRO:HG3   | 1:A:773:LEU:HD12  | 1.19                     | 1.15              |
| 1:D:2073:UNK:CB   | 1:D:2094:UNK:CB   | 2.25                     | 1.15              |
| 1:B:1452:TRP:CZ3  | 1:B:1527:MET:CB   | 2.19                     | 1.15              |
| 1:B:2073:UNK:CB   | 1:B:2094:UNK:CB   | 2.25                     | 1.15              |
| 1:C:1432:THR:OG1  | 1:C:1523:ALA:HB2  | 1.46                     | 1.15              |
| 1:C:2428:UNK:CB   | 1:C:2498:UNK:CB   | 2.24                     | 1.15              |
| 1:D:1004:GLY:HA2  | 1:D:1007:TYR:CZ   | 1.82                     | 1.15              |
| 1:A:1432:THR:OG1  | 1:A:1523:ALA:HB2  | 1.46                     | 1.14              |
| 1:A:1465:ASP:HA   | 1:A:1553:PHE:CD2  | 1.81                     | 1.14              |
| 1:B:2428:UNK:CB   | 1:B:2498:UNK:CB   | 2.24                     | 1.14              |
| 1:D:1001:VAL:HG13 | 1:D:1005:TRP:NE1  | 1.58                     | 1.14              |
| 1:D:1476:MET:HE1  | 1:D:1516:ILE:HD11 | 1.29                     | 1.14              |
| 1:A:2073:UNK:CB   | 1:A:2094:UNK:CB   | 2.25                     | 1.14              |
| 1:C:2073:UNK:CB   | 1:C:2094:UNK:CB   | 2.25                     | 1.14              |
| 1:D:2244:UNK:CB   | 1:D:2287:UNK:CB   | 2.26                     | 1.14              |
| 1:D:2428:UNK:CB   | 1:D:2498:UNK:CB   | 2.24                     | 1.14              |
| 1:A:1476:MET:HE1  | 1:A:1516:ILE:HD11 | 1.29                     | 1.14              |
| 1:A:2244:UNK:CB   | 1:A:2287:UNK:CB   | 2.25                     | 1.14              |
| 1:A:953:THR:O     | 1:A:959:TYR:CG    | 2.01                     | 1.14              |
| 1:B:1432:THR:OG1  | 1:B:1523:ALA:HB2  | 1.45                     | 1.14              |
| 1:D:657:THR:HG21  | 1:D:662:TRP:CZ3   | 1.82                     | 1.14              |
| 1:D:1465:ASP:HA   | 1:D:1553:PHE:CD2  | 1.81                     | 1.14              |
| 1:A:222:LEU:HD23  | 1:A:390:LEU:HD21  | 1.30                     | 1.14              |
| 1:D:953:THR:O     | 1:D:959:TYR:CG    | 2.01                     | 1.14              |
| 1:D:990:GLU:O     | 1:D:993:HIS:HB2   | 1.48                     | 1.14              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1016:ARG:HB3  | 1:A:1016:ARG:CZ  | 1.70                     | 1.13              |
| 1:A:1452:TRP:CZ3  | 1:A:1527:MET:CB  | 2.19                     | 1.13              |
| 1:B:1016:ARG:HB3  | 1:B:1016:ARG:CZ  | 1.70                     | 1.13              |
| 1:B:2244:UNK:CB   | 1:B:2287:UNK:CB  | 2.26                     | 1.13              |
| 1:D:426:ARG:HH21  | 1:D:796:ARG:NH1  | 1.37                     | 1.13              |
| 1:A:1004:GLY:HA2  | 1:A:1007:TYR:CZ  | 1.82                     | 1.13              |
| 1:A:1020:ARG:HA   | 1:A:1020:ARG:NE  | 1.63                     | 1.13              |
| 1:C:1465:ASP:HA   | 1:C:1553:PHE:CD2 | 1.81                     | 1.13              |
| 1:C:222:LEU:HD23  | 1:C:390:LEU:HD21 | 1.30                     | 1.13              |
| 1:C:753:PRO:CG    | 1:C:773:LEU:HD11 | 1.68                     | 1.13              |
| 1:C:1004:GLY:HA2  | 1:C:1007:TYR:CZ  | 1.82                     | 1.13              |
| 1:B:953:THR:O     | 1:B:959:TYR:CG   | 2.01                     | 1.13              |
| 1:C:2244:UNK:CB   | 1:C:2287:UNK:CB  | 2.25                     | 1.13              |
| 1:A:956:PRO:HG3   | 1:A:959:TYR:CE2  | 1.84                     | 1.12              |
| 1:C:953:THR:O     | 1:C:959:TYR:CG   | 2.01                     | 1.13              |
| 1:C:1434:TYR:O    | 1:C:1568:LYS:O   | 1.67                     | 1.12              |
| 1:A:657:THR:HB    | 1:A:662:TRP:CE2  | 1.85                     | 1.12              |
| 1:B:1004:GLY:HA2  | 1:B:1007:TYR:CZ  | 1.82                     | 1.12              |
| 1:D:657:THR:HB    | 1:D:662:TRP:CE2  | 1.84                     | 1.12              |
| 1:D:1434:TYR:O    | 1:D:1568:LYS:O   | 1.67                     | 1.12              |
| 1:A:956:PRO:CD    | 1:A:959:TYR:CE2  | 2.32                     | 1.12              |
| 1:A:993:HIS:CA    | 1:A:996:TRP:HE3  | 1.55                     | 1.12              |
| 1:B:657:THR:HB    | 1:B:662:TRP:CE2  | 1.85                     | 1.12              |
| 1:C:752:VAL:HG11  | 1:C:769:GLU:CB   | 1.79                     | 1.12              |
| 1:A:657:THR:HG21  | 1:A:662:TRP:CZ3  | 1.82                     | 1.12              |
| 1:C:990:GLU:O     | 1:C:993:HIS:HB2  | 1.48                     | 1.12              |
| 1:D:752:VAL:HG11  | 1:D:769:GLU:CB   | 1.79                     | 1.12              |
| 1:D:956:PRO:HG3   | 1:D:959:TYR:CE2  | 1.84                     | 1.12              |
| 1:A:1429:ASN:OD1  | 1:A:1546:THR:O   | 1.68                     | 1.12              |
| 1:A:1439:VAL:H    | 1:A:1515:VAL:HA  | 0.99                     | 1.12              |
| 1:B:990:GLU:O     | 1:B:993:HIS:HB2  | 1.48                     | 1.12              |
| 1:C:1452:TRP:CZ3  | 1:C:1527:MET:CB  | 2.19                     | 1.12              |
| 1:B:222:LEU:HD23  | 1:B:390:LEU:CD2  | 1.80                     | 1.11              |
| 1:C:753:PRO:HG3   | 1:C:773:LEU:HD12 | 1.19                     | 1.11              |
| 1:C:1429:ASN:OD1  | 1:C:1546:THR:O   | 1.68                     | 1.11              |
| 1:A:657:THR:HG22  | 1:A:662:TRP:CH2  | 1.86                     | 1.11              |
| 1:B:752:VAL:HG11  | 1:B:769:GLU:CB   | 1.79                     | 1.11              |
| 1:B:956:PRO:HG3   | 1:B:959:TYR:CE2  | 1.84                     | 1.11              |
| 1:A:752:VAL:HG11  | 1:A:769:GLU:CB   | 1.79                     | 1.11              |
| 1:A:1472:VAL:HG22 | 1:A:1496:TRP:CD1 | 1.86                     | 1.11              |
| 1:B:1429:ASN:OD1  | 1:B:1546:THR:O   | 1.68                     | 1.11              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:657:THR:HG22  | 1:C:662:TRP:CH2   | 1.86                     | 1.11              |
| 1:D:1472:VAL:HG22 | 1:D:1496:TRP:CD1  | 1.86                     | 1.11              |
| 1:C:956:PRO:HG3   | 1:C:959:TYR:CE2   | 1.84                     | 1.11              |
| 1:D:753:PRO:CG    | 1:D:773:LEU:HD11  | 1.68                     | 1.11              |
| 1:A:990:GLU:O     | 1:A:993:HIS:HB2   | 1.48                     | 1.10              |
| 1:A:1007:TYR:CG   | 1:A:1016:ARG:NH2  | 2.19                     | 1.10              |
| 1:C:1439:VAL:H    | 1:C:1515:VAL:HA   | 0.99                     | 1.10              |
| 1:A:4585:UNK:CB   | 1:D:4884:UNK:O    | 1.99                     | 1.10              |
| 1:B:207:SER:CA    | 1:B:269:TRP:CZ3   | 2.34                     | 1.10              |
| 1:B:1434:TYR:O    | 1:B:1568:LYS:O    | 1.67                     | 1.10              |
| 1:C:657:THR:HB    | 1:C:662:TRP:CE2   | 1.84                     | 1.10              |
| 1:C:956:PRO:CD    | 1:C:959:TYR:CE2   | 2.32                     | 1.10              |
| 1:A:222:LEU:HD23  | 1:A:390:LEU:CD2   | 1.80                     | 1.10              |
| 1:B:753:PRO:HG3   | 1:B:773:LEU:HD12  | 1.19                     | 1.10              |
| 1:B:1007:TYR:CG   | 1:B:1016:ARG:NH2  | 2.19                     | 1.10              |
| 1:C:1007:TYR:CG   | 1:C:1016:ARG:NH2  | 2.19                     | 1.10              |
| 1:D:207:SER:CA    | 1:D:269:TRP:CZ3   | 2.34                     | 1.10              |
| 1:D:222:LEU:HD23  | 1:D:390:LEU:CD2   | 1.80                     | 1.10              |
| 1:D:956:PRO:CD    | 1:D:959:TYR:CE2   | 2.32                     | 1.10              |
| 1:D:1429:ASN:OD1  | 1:D:1546:THR:O    | 1.68                     | 1.10              |
| 1:A:728:ARG:HB2   | 1:A:1134:LEU:HD23 | 1.32                     | 1.10              |
| 1:A:1022:VAL:O    | 1:A:1023:PRO:O    | 1.69                     | 1.10              |
| 1:B:1439:VAL:H    | 1:B:1515:VAL:HA   | 0.99                     | 1.10              |
| 1:C:222:LEU:HD23  | 1:C:390:LEU:CD2   | 1.80                     | 1.10              |
| 1:C:1004:GLY:CA   | 1:C:1015:ALA:HB1  | 1.82                     | 1.10              |
| 1:C:1022:VAL:O    | 1:C:1023:PRO:O    | 1.69                     | 1.10              |
| 1:C:1476:MET:HE1  | 1:C:1516:ILE:HD11 | 1.29                     | 1.10              |
| 1:C:1472:VAL:HG22 | 1:C:1496:TRP:CD1  | 1.86                     | 1.09              |
| 1:A:728:ARG:HB2   | 1:A:1134:LEU:HD22 | 1.21                     | 1.09              |
| 1:A:1004:GLY:CA   | 1:A:1015:ALA:HB1  | 1.82                     | 1.09              |
| 1:B:752:VAL:HG12  | 1:B:769:GLU:HB3   | 1.34                     | 1.09              |
| 1:B:1437:VAL:O    | 1:B:1516:ILE:O    | 1.70                     | 1.09              |
| 1:B:1472:VAL:HG22 | 1:B:1496:TRP:CD1  | 1.86                     | 1.09              |
| 1:C:205:ILE:O     | 1:C:269:TRP:HA    | 1.51                     | 1.09              |
| 1:D:657:THR:HG22  | 1:D:662:TRP:CH2   | 1.86                     | 1.09              |
| 1:A:207:SER:CA    | 1:A:269:TRP:CZ3   | 2.34                     | 1.09              |
| 1:A:1434:TYR:O    | 1:A:1568:LYS:O    | 1.67                     | 1.09              |
| 1:B:657:THR:HG21  | 1:B:662:TRP:CZ3   | 1.82                     | 1.09              |
| 1:B:657:THR:HG22  | 1:B:662:TRP:CH2   | 1.86                     | 1.09              |
| 1:C:657:THR:HG21  | 1:C:662:TRP:CZ3   | 1.82                     | 1.09              |
| 1:C:1016:ARG:HB3  | 1:C:1016:ARG:CZ   | 1.70                     | 1.09              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:426:ARG:NH2   | 1:D:796:ARG:HH12  | 1.42                     | 1.09              |
| 1:D:1007:TYR:CG   | 1:D:1016:ARG:NH2  | 2.19                     | 1.09              |
| 1:D:1016:ARG:HB3  | 1:D:1016:ARG:CZ   | 1.70                     | 1.09              |
| 1:D:1020:ARG:HA   | 1:D:1020:ARG:NE   | 1.63                     | 1.09              |
| 1:D:1437:VAL:O    | 1:D:1516:ILE:O    | 1.70                     | 1.09              |
| 1:B:1476:MET:HE1  | 1:B:1516:ILE:HD11 | 1.29                     | 1.09              |
| 1:C:1004:GLY:HA3  | 1:C:1015:ALA:HB1  | 1.09                     | 1.09              |
| 1:D:1439:VAL:H    | 1:D:1515:VAL:HA   | 0.99                     | 1.09              |
| 1:A:426:ARG:NH2   | 1:A:796:ARG:HH12  | 1.42                     | 1.09              |
| 1:B:329:ARG:HH11  | 1:B:329:ARG:HG3   | 1.17                     | 1.09              |
| 1:D:1438:ARG:HA   | 1:D:1515:VAL:HG13 | 1.10                     | 1.09              |
| 1:B:998:ARG:NH2   | 1:B:1002:ALA:HB2  | 1.67                     | 1.08              |
| 1:B:1450:VAL:O    | 1:B:1529:PHE:HZ   | 1.36                     | 1.08              |
| 1:B:4884:UNK:O    | 1:C:4585:UNK:CB   | 2.01                     | 1.08              |
| 1:C:368:ARG:HG2   | 1:C:368:ARG:HH11  | 1.16                     | 1.08              |
| 1:D:205:ILE:O     | 1:D:269:TRP:HA    | 1.51                     | 1.08              |
| 1:D:996:TRP:CZ2   | 1:D:1021:LEU:CD1  | 2.36                     | 1.08              |
| 1:D:1022:VAL:O    | 1:D:1023:PRO:O    | 1.69                     | 1.08              |
| 1:A:1472:VAL:HG22 | 1:A:1496:TRP:HD1  | 1.16                     | 1.08              |
| 1:B:1004:GLY:CA   | 1:B:1015:ALA:HB1  | 1.82                     | 1.08              |
| 1:B:1438:ARG:HA   | 1:B:1515:VAL:HG13 | 1.10                     | 1.08              |
| 1:C:1438:ARG:HA   | 1:C:1515:VAL:HG13 | 1.10                     | 1.08              |
| 1:A:1450:VAL:O    | 1:A:1529:PHE:HZ   | 1.36                     | 1.08              |
| 1:B:728:ARG:HB2   | 1:B:1134:LEU:HD23 | 1.32                     | 1.08              |
| 1:B:1020:ARG:NE   | 1:B:1020:ARG:HA   | 1.63                     | 1.08              |
| 1:C:207:SER:CA    | 1:C:269:TRP:CZ3   | 2.34                     | 1.08              |
| 1:C:329:ARG:HH11  | 1:C:329:ARG:HG3   | 1.17                     | 1.08              |
| 1:C:996:TRP:CZ2   | 1:C:1021:LEU:CD1  | 2.36                     | 1.08              |
| 1:D:1004:GLY:CA   | 1:D:1007:TYR:CE1  | 2.37                     | 1.08              |
| 1:A:21:VAL:HG13   | 1:A:205:ILE:HD11  | 1.08                     | 1.08              |
| 1:B:21:VAL:HG13   | 1:B:205:ILE:HD11  | 1.08                     | 1.08              |
| 1:B:657:THR:HG22  | 1:B:662:TRP:CZ3   | 1.87                     | 1.08              |
| 1:B:1004:GLY:CA   | 1:B:1007:TYR:CE1  | 2.37                     | 1.08              |
| 1:B:1022:VAL:O    | 1:B:1023:PRO:O    | 1.69                     | 1.08              |
| 1:C:998:ARG:NH2   | 1:C:1002:ALA:HB2  | 1.67                     | 1.08              |
| 1:A:993:HIS:HA    | 1:A:996:TRP:HE3   | 0.91                     | 1.07              |
| 1:A:996:TRP:CZ2   | 1:A:1021:LEU:CD1  | 2.36                     | 1.07              |
| 1:A:998:ARG:NH2   | 1:A:1002:ALA:HB2  | 1.67                     | 1.07              |
| 1:A:1437:VAL:O    | 1:A:1516:ILE:O    | 1.70                     | 1.07              |
| 1:A:4855:UNK:O    | 1:A:4859:UNK:N    | 1.87                     | 1.07              |
| 1:B:205:ILE:O     | 1:B:269:TRP:HA    | 1.51                     | 1.07              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:993:HIS:HA    | 1:B:996:TRP:HE3  | 0.91                     | 1.07              |
| 1:B:4855:UNK:O    | 1:B:4859:UNK:N   | 1.87                     | 1.07              |
| 1:C:1017:ARG:HD2  | 1:C:1017:ARG:N   | 1.69                     | 1.07              |
| 1:B:80:GLU:O      | 1:B:84:ASN:ND2   | 1.88                     | 1.07              |
| 1:B:222:LEU:HD23  | 1:B:390:LEU:HD21 | 1.30                     | 1.07              |
| 1:B:996:TRP:CZ2   | 1:B:1021:LEU:CD1 | 2.36                     | 1.07              |
| 1:D:998:ARG:NH2   | 1:D:1002:ALA:HB2 | 1.67                     | 1.07              |
| 1:A:205:ILE:O     | 1:A:269:TRP:HA   | 1.51                     | 1.07              |
| 1:B:956:PRO:CD    | 1:B:959:TYR:CE2  | 2.32                     | 1.07              |
| 1:C:80:GLU:O      | 1:C:84:ASN:ND2   | 1.88                     | 1.07              |
| 1:D:80:GLU:O      | 1:D:84:ASN:ND2   | 1.88                     | 1.07              |
| 1:D:1004:GLY:CA   | 1:D:1015:ALA:HB1 | 1.82                     | 1.07              |
| 1:D:1450:VAL:O    | 1:D:1529:PHE:HZ  | 1.36                     | 1.07              |
| 1:D:4855:UNK:O    | 1:D:4859:UNK:N   | 1.87                     | 1.07              |
| 1:A:1450:VAL:C    | 1:A:1529:PHE:HZ  | 1.63                     | 1.07              |
| 1:B:1004:GLY:HA3  | 1:B:1015:ALA:HB1 | 1.09                     | 1.07              |
| 1:B:1450:VAL:C    | 1:B:1529:PHE:HZ  | 1.63                     | 1.07              |
| 1:B:1472:VAL:HG22 | 1:B:1496:TRP:HD1 | 1.16                     | 1.07              |
| 1:C:1004:GLY:CA   | 1:C:1007:TYR:CE1 | 2.37                     | 1.07              |
| 1:C:1450:VAL:O    | 1:C:1529:PHE:HZ  | 1.36                     | 1.07              |
| 1:A:1004:GLY:CA   | 1:A:1007:TYR:CE1 | 2.37                     | 1.07              |
| 1:B:80:GLU:OE1    | 1:C:3932:UNK:CB  | 2.04                     | 1.06              |
| 1:B:4787:UNK:O    | 1:B:4791:UNK:N   | 1.88                     | 1.06              |
| 1:C:1020:ARG:NE   | 1:C:1020:ARG:HA  | 1.63                     | 1.06              |
| 1:C:1437:VAL:O    | 1:C:1516:ILE:O   | 1.70                     | 1.06              |
| 1:D:222:LEU:HD23  | 1:D:390:LEU:HD21 | 1.30                     | 1.06              |
| 1:D:993:HIS:HA    | 1:D:996:TRP:CE3  | 1.82                     | 1.06              |
| 1:A:80:GLU:O      | 1:A:84:ASN:ND2   | 1.88                     | 1.06              |
| 1:A:752:VAL:HG12  | 1:A:769:GLU:HB3  | 1.34                     | 1.06              |
| 1:B:752:VAL:CG2   | 1:B:754:SER:HB2  | 1.86                     | 1.06              |
| 1:C:993:HIS:HA    | 1:C:996:TRP:CE3  | 1.82                     | 1.06              |
| 1:C:998:ARG:HD3   | 1:C:999:ASP:N    | 1.70                     | 1.06              |
| 1:D:657:THR:HG22  | 1:D:662:TRP:CZ3  | 1.87                     | 1.06              |
| 1:D:4787:UNK:O    | 1:D:4791:UNK:N   | 1.88                     | 1.06              |
| 1:C:21:VAL:HG13   | 1:C:205:ILE:HD11 | 1.08                     | 1.06              |
| 1:C:657:THR:HG22  | 1:C:662:TRP:CZ3  | 1.87                     | 1.06              |
| 1:C:4855:UNK:O    | 1:C:4859:UNK:N   | 1.87                     | 1.06              |
| 1:D:998:ARG:HD3   | 1:D:999:ASP:N    | 1.70                     | 1.06              |
| 1:D:3317:UNK:CB   | 1:D:3323:UNK:N   | 2.19                     | 1.06              |
| 1:D:1450:VAL:C    | 1:D:1529:PHE:HZ  | 1.63                     | 1.06              |
| 1:A:4787:UNK:O    | 1:A:4791:UNK:N   | 1.88                     | 1.06              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1450:VAL:C    | 1:C:1529:PHE:HZ   | 1.63                     | 1.06              |
| 1:C:3317:UNK:CB   | 1:C:3323:UNK:N    | 2.19                     | 1.06              |
| 1:D:1004:GLY:HA3  | 1:D:1015:ALA:HB1  | 1.09                     | 1.06              |
| 1:D:728:ARG:HB2   | 1:D:1134:LEU:HD23 | 1.32                     | 1.05              |
| 1:A:752:VAL:CG2   | 1:A:754:SER:HB2   | 1.86                     | 1.05              |
| 1:C:728:ARG:HB2   | 1:C:1134:LEU:HD22 | 1.21                     | 1.05              |
| 1:D:21:VAL:HG13   | 1:D:205:ILE:HD11  | 1.08                     | 1.05              |
| 1:A:1004:GLY:HA3  | 1:A:1015:ALA:HB1  | 1.09                     | 1.05              |
| 1:A:3317:UNK:CB   | 1:A:3323:UNK:N    | 2.19                     | 1.05              |
| 1:C:1466:LEU:HD22 | 1:C:1551:ALA:O    | 1.57                     | 1.05              |
| 1:C:4787:UNK:O    | 1:C:4791:UNK:N    | 1.88                     | 1.05              |
| 1:D:993:HIS:HA    | 1:D:996:TRP:HE3   | 0.91                     | 1.05              |
| 1:A:1438:ARG:HA   | 1:A:1515:VAL:HG13 | 1.10                     | 1.05              |
| 1:B:368:ARG:HG2   | 1:B:368:ARG:HH11  | 1.16                     | 1.05              |
| 1:B:998:ARG:HD3   | 1:B:999:ASP:N     | 1.70                     | 1.05              |
| 1:C:426:ARG:NH2   | 1:C:796:ARG:HH12  | 1.42                     | 1.05              |
| 1:C:728:ARG:HB2   | 1:C:1134:LEU:HD23 | 1.32                     | 1.05              |
| 1:C:752:VAL:CG2   | 1:C:754:SER:HB2   | 1.86                     | 1.05              |
| 1:C:993:HIS:HA    | 1:C:996:TRP:HE3   | 0.91                     | 1.05              |
| 1:D:368:ARG:HG2   | 1:D:368:ARG:HH11  | 1.16                     | 1.05              |
| 1:A:3932:UNK:CB   | 1:D:80:GLU:OE1    | 2.05                     | 1.04              |
| 1:A:657:THR:HG22  | 1:A:662:TRP:CZ3   | 1.87                     | 1.04              |
| 1:B:1466:LEU:HD22 | 1:B:1551:ALA:O    | 1.57                     | 1.04              |
| 1:C:80:GLU:OE1    | 1:D:3932:UNK:CB   | 2.05                     | 1.04              |
| 1:D:752:VAL:CG2   | 1:D:754:SER:HB2   | 1.86                     | 1.04              |
| 1:D:1001:VAL:HG13 | 1:D:1005:TRP:HE1  | 0.91                     | 1.04              |
| 1:A:80:GLU:OE1    | 1:B:3932:UNK:CB   | 2.04                     | 1.04              |
| 1:A:329:ARG:HH11  | 1:A:329:ARG:HG3   | 1.17                     | 1.04              |
| 1:B:426:ARG:NH2   | 1:B:796:ARG:HH12  | 1.42                     | 1.04              |
| 1:B:956:PRO:CG    | 1:B:959:TYR:CE2   | 2.40                     | 1.04              |
| 1:B:3317:UNK:CB   | 1:B:3323:UNK:N    | 2.19                     | 1.04              |
| 1:B:998:ARG:HH22  | 1:B:1002:ALA:HB2  | 1.18                     | 1.04              |
| 1:C:752:VAL:HG12  | 1:C:769:GLU:HB3   | 1.34                     | 1.04              |
| 1:A:1017:ARG:N    | 1:A:1017:ARG:HD2  | 1.70                     | 1.04              |
| 1:A:4884:UNK:O    | 1:B:4585:UNK:CB   | 2.02                     | 1.04              |
| 1:C:753:PRO:HG3   | 1:C:773:LEU:HD13  | 1.38                     | 1.04              |
| 1:C:4884:UNK:O    | 1:D:4585:UNK:CB   | 2.01                     | 1.04              |
| 1:A:753:PRO:HG3   | 1:A:773:LEU:HD13  | 1.38                     | 1.03              |
| 1:A:1001:VAL:HG13 | 1:A:1005:TRP:HE1  | 0.91                     | 1.03              |
| 1:D:956:PRO:CG    | 1:D:959:TYR:CE2   | 2.40                     | 1.03              |
| 1:A:998:ARG:HD3   | 1:A:999:ASP:N     | 1.70                     | 1.03              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:956:PRO:CG    | 1:C:959:TYR:CE2   | 2.40                     | 1.03              |
| 1:C:1001:VAL:HG13 | 1:C:1005:TRP:HE1  | 0.91                     | 1.03              |
| 1:D:1466:LEU:HD22 | 1:D:1551:ALA:O    | 1.57                     | 1.03              |
| 1:D:3899:UNK:O    | 1:D:3910:UNK:N    | 1.92                     | 1.03              |
| 1:A:956:PRO:CG    | 1:A:959:TYR:CE2   | 2.40                     | 1.03              |
| 1:A:1434:TYR:CE1  | 1:A:1570:LYS:CD   | 2.41                     | 1.03              |
| 1:A:1466:LEU:HD22 | 1:A:1551:ALA:O    | 1.57                     | 1.03              |
| 1:B:1001:VAL:HG13 | 1:B:1005:TRP:HE1  | 0.91                     | 1.03              |
| 1:D:752:VAL:HG12  | 1:D:769:GLU:HB3   | 1.34                     | 1.03              |
| 1:D:1017:ARG:N    | 1:D:1017:ARG:HD2  | 1.69                     | 1.03              |
| 1:D:1434:TYR:CE1  | 1:D:1570:LYS:CD   | 2.41                     | 1.03              |
| 1:A:998:ARG:HH22  | 1:A:1002:ALA:HB2  | 1.18                     | 1.03              |
| 1:B:1434:TYR:CE1  | 1:B:1570:LYS:CD   | 2.41                     | 1.03              |
| 1:D:329:ARG:HH11  | 1:D:329:ARG:HG3   | 1.17                     | 1.03              |
| 1:D:998:ARG:HH22  | 1:D:1002:ALA:HB2  | 1.18                     | 1.02              |
| 1:A:368:ARG:HG2   | 1:A:368:ARG:HH11  | 1.16                     | 1.02              |
| 1:A:1000:ARG:NE   | 1:A:1016:ARG:HD2  | 1.75                     | 1.02              |
| 1:B:753:PRO:HG3   | 1:B:773:LEU:HD13  | 1.39                     | 1.02              |
| 1:C:1000:ARG:NE   | 1:C:1016:ARG:HD2  | 1.75                     | 1.02              |
| 1:C:1434:TYR:CE1  | 1:C:1570:LYS:CD   | 2.41                     | 1.02              |
| 1:B:954:LYS:HB3   | 1:B:971:ASP:CG    | 1.85                     | 1.02              |
| 1:D:426:ARG:NH2   | 1:D:796:ARG:HH22  | 1.55                     | 1.02              |
| 1:D:1472:VAL:HG22 | 1:D:1496:TRP:HD1  | 1.16                     | 1.02              |
| 1:A:76:ARG:NH1    | 1:B:3930:UNK:C    | 2.22                     | 1.01              |
| 1:A:753:PRO:HG2   | 1:A:773:LEU:HD11  | 1.43                     | 1.01              |
| 1:B:1000:ARG:NE   | 1:B:1016:ARG:HD2  | 1.75                     | 1.01              |
| 1:B:1476:MET:HE1  | 1:B:1516:ILE:CD1  | 1.90                     | 1.01              |
| 1:B:3316:UNK:C    | 1:B:3322:UNK:CB   | 2.38                     | 1.01              |
| 1:C:1472:VAL:HG22 | 1:C:1496:TRP:HD1  | 1.16                     | 1.01              |
| 1:D:1432:THR:O    | 1:D:1570:LYS:O    | 1.78                     | 1.01              |
| 1:A:956:PRO:HD3   | 1:A:959:TYR:HD2   | 1.19                     | 1.01              |
| 1:A:3316:UNK:C    | 1:A:3322:UNK:CB   | 2.38                     | 1.01              |
| 1:A:3930:UNK:C    | 1:D:76:ARG:NH1    | 2.22                     | 1.01              |
| 1:B:1017:ARG:N    | 1:B:1017:ARG:HD2  | 1.69                     | 1.01              |
| 1:B:3899:UNK:O    | 1:B:3910:UNK:N    | 1.92                     | 1.01              |
| 1:C:1021:LEU:O    | 1:C:1022:VAL:HG13 | 1.61                     | 1.01              |
| 1:A:1017:ARG:HH11 | 1:A:1017:ARG:CG   | 1.74                     | 1.01              |
| 1:A:1452:TRP:CH2  | 1:A:1527:MET:CB   | 2.42                     | 1.01              |
| 1:C:998:ARG:HH22  | 1:C:1002:ALA:HB2  | 1.18                     | 1.01              |
| 1:C:1021:LEU:O    | 1:C:1022:VAL:HG22 | 1.61                     | 1.01              |
| 1:C:1476:MET:HE1  | 1:C:1516:ILE:CD1  | 1.90                     | 1.01              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1000:ARG:NH2  | 1:D:1016:ARG:CG   | 2.24                     | 1.01              |
| 1:D:1021:LEU:O    | 1:D:1022:VAL:HG13 | 1.61                     | 1.01              |
| 1:C:752:VAL:HG21  | 1:C:754:SER:HB2   | 1.42                     | 1.01              |
| 1:C:1432:THR:O    | 1:C:1570:LYS:O    | 1.78                     | 1.01              |
| 1:D:1017:ARG:HH11 | 1:D:1017:ARG:CG   | 1.74                     | 1.01              |
| 1:D:1452:TRP:CH2  | 1:D:1527:MET:CB   | 2.42                     | 1.01              |
| 1:D:1476:MET:HE1  | 1:D:1516:ILE:CD1  | 1.90                     | 1.01              |
| 1:D:3316:UNK:C    | 1:D:3322:UNK:CB   | 2.38                     | 1.01              |
| 1:A:4091:UNK:O    | 1:A:4095:UNK:N    | 1.94                     | 1.00              |
| 1:B:657:THR:CB    | 1:B:662:TRP:CE2   | 2.45                     | 1.00              |
| 1:B:1000:ARG:NH2  | 1:B:1016:ARG:CG   | 2.24                     | 1.00              |
| 1:C:3899:UNK:O    | 1:C:3910:UNK:N    | 1.92                     | 1.00              |
| 1:A:1021:LEU:O    | 1:A:1022:VAL:HG13 | 1.61                     | 1.00              |
| 1:A:1021:LEU:O    | 1:A:1022:VAL:HG22 | 1.61                     | 1.00              |
| 1:A:1432:THR:O    | 1:A:1570:LYS:O    | 1.78                     | 1.00              |
| 1:A:1476:MET:HE1  | 1:A:1516:ILE:CD1  | 1.90                     | 1.00              |
| 1:A:3899:UNK:O    | 1:A:3910:UNK:N    | 1.92                     | 1.00              |
| 1:B:76:ARG:NH1    | 1:C:3930:UNK:C    | 2.22                     | 1.00              |
| 1:C:657:THR:CB    | 1:C:662:TRP:CE2   | 2.45                     | 1.00              |
| 1:A:954:LYS:HB3   | 1:A:971:ASP:CG    | 1.85                     | 1.00              |
| 1:B:222:LEU:CD2   | 1:B:390:LEU:HD21  | 1.92                     | 1.00              |
| 1:B:1021:LEU:O    | 1:B:1022:VAL:HG22 | 1.61                     | 1.00              |
| 1:C:954:LYS:HB3   | 1:C:971:ASP:CG    | 1.85                     | 1.00              |
| 1:C:4113:UNK:HA   | 1:C:4116:UNK:CB   | 1.92                     | 1.00              |
| 1:D:4113:UNK:HA   | 1:D:4116:UNK:CB   | 1.92                     | 1.00              |
| 1:B:753:PRO:HG2   | 1:B:773:LEU:HD11  | 1.43                     | 1.00              |
| 1:D:84:ASN:HA     | 1:D:87:GLU:CB     | 1.91                     | 1.00              |
| 1:D:1000:ARG:NE   | 1:D:1016:ARG:HD2  | 1.75                     | 1.00              |
| 1:A:1000:ARG:NH2  | 1:A:1016:ARG:CG   | 2.24                     | 1.00              |
| 1:B:4848:UNK:O    | 1:B:4852:UNK:N    | 1.95                     | 1.00              |
| 1:C:728:ARG:CB    | 1:C:1134:LEU:CD2  | 2.40                     | 1.00              |
| 1:D:4091:UNK:O    | 1:D:4095:UNK:N    | 1.94                     | 1.00              |
| 1:A:4848:UNK:O    | 1:A:4852:UNK:N    | 1.95                     | 1.00              |
| 1:B:4831:UNK:O    | 1:B:4835:UNK:N    | 1.95                     | 1.00              |
| 1:C:222:LEU:CD2   | 1:C:390:LEU:HD21  | 1.92                     | 1.00              |
| 1:B:4091:UNK:O    | 1:B:4095:UNK:N    | 1.94                     | 1.00              |
| 1:D:84:ASN:HA     | 1:D:87:GLU:HB2    | 1.00                     | 1.00              |
| 1:D:728:ARG:CB    | 1:D:1134:LEU:CD2  | 2.40                     | 1.00              |
| 1:D:753:PRO:HG2   | 1:D:773:LEU:HD11  | 1.43                     | 1.00              |
| 1:D:4848:UNK:O    | 1:D:4852:UNK:N    | 1.95                     | 1.00              |
| 1:A:84:ASN:HA     | 1:A:87:GLU:CB     | 1.91                     | 0.99              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:222:LEU:CD2   | 1:A:390:LEU:HD21  | 1.92                     | 0.99              |
| 1:A:752:VAL:HG21  | 1:A:754:SER:HB2   | 1.42                     | 0.99              |
| 1:B:956:PRO:HD3   | 1:B:959:TYR:HD2   | 1.19                     | 0.99              |
| 1:C:3316:UNK:C    | 1:C:3322:UNK:CB   | 2.38                     | 0.99              |
| 1:C:4091:UNK:O    | 1:C:4095:UNK:N    | 1.94                     | 0.99              |
| 1:A:1452:TRP:HZ3  | 1:A:1527:MET:HB3  | 1.21                     | 0.99              |
| 1:B:84:ASN:HA     | 1:B:87:GLU:CB     | 1.92                     | 0.99              |
| 1:B:993:HIS:HA    | 1:B:996:TRP:CE3   | 1.82                     | 0.99              |
| 1:D:956:PRO:HD2   | 1:D:959:TYR:CG    | 1.97                     | 0.99              |
| 1:A:426:ARG:NH2   | 1:A:796:ARG:HH22  | 1.55                     | 0.99              |
| 1:C:1444:GLU:OE1  | 1:C:1478:ASP:HB2  | 1.61                     | 0.99              |
| 1:D:222:LEU:CD2   | 1:D:390:LEU:HD21  | 1.92                     | 0.99              |
| 1:D:479:GLN:NE2   | 1:D:534:UNK:N     | 2.09                     | 0.99              |
| 1:D:954:LYS:HB3   | 1:D:971:ASP:CG    | 1.85                     | 0.99              |
| 1:A:4831:UNK:O    | 1:A:4835:UNK:N    | 1.95                     | 0.99              |
| 1:C:76:ARG:NH1    | 1:D:3930:UNK:C    | 2.24                     | 0.99              |
| 1:C:1000:ARG:NH2  | 1:C:1016:ARG:CG   | 2.24                     | 0.99              |
| 1:B:4113:UNK:HA   | 1:B:4116:UNK:CB   | 1.92                     | 0.99              |
| 1:D:753:PRO:HG3   | 1:D:773:LEU:HD13  | 1.38                     | 0.99              |
| 1:C:1438:ARG:CA   | 1:C:1515:VAL:HG13 | 1.92                     | 0.99              |
| 1:C:4848:UNK:O    | 1:C:4852:UNK:N    | 1.95                     | 0.99              |
| 1:D:1438:ARG:CA   | 1:D:1515:VAL:HG13 | 1.92                     | 0.99              |
| 1:D:1444:GLU:OE1  | 1:D:1478:ASP:HB2  | 1.61                     | 0.99              |
| 1:A:1444:GLU:OE1  | 1:A:1478:ASP:HB2  | 1.61                     | 0.99              |
| 1:B:4884:UNK:CB   | 1:C:4583:UNK:O    | 2.07                     | 0.99              |
| 1:C:207:SER:HA    | 1:C:269:TRP:HZ3   | 1.27                     | 0.99              |
| 1:C:657:THR:CG2   | 1:C:662:TRP:CE2   | 2.46                     | 0.99              |
| 1:C:1474:VAL:HG23 | 1:C:1540:PHE:HE2  | 1.28                     | 0.99              |
| 1:B:1432:THR:O    | 1:B:1570:LYS:O    | 1.78                     | 0.99              |
| 1:B:1438:ARG:CA   | 1:B:1515:VAL:HG13 | 1.92                     | 0.99              |
| 1:C:479:GLN:NE2   | 1:C:534:UNK:N     | 2.09                     | 0.99              |
| 1:A:728:ARG:CB    | 1:A:1134:LEU:CD2  | 2.40                     | 0.99              |
| 1:A:993:HIS:HA    | 1:A:996:TRP:CE3   | 1.82                     | 0.99              |
| 1:A:4113:UNK:HA   | 1:A:4116:UNK:CB   | 1.92                     | 0.99              |
| 1:B:728:ARG:CB    | 1:B:1134:LEU:CD2  | 2.40                     | 0.99              |
| 1:B:728:ARG:HD2   | 1:B:1134:LEU:HB2  | 1.45                     | 0.99              |
| 1:B:1021:LEU:O    | 1:B:1022:VAL:HG13 | 1.61                     | 0.99              |
| 1:B:1444:GLU:OE1  | 1:B:1478:ASP:HB2  | 1.61                     | 0.99              |
| 1:D:317:ARG:NH2   | 1:D:322:LYS:CA    | 2.20                     | 0.99              |
| 1:D:657:THR:CB    | 1:D:662:TRP:CE2   | 2.45                     | 0.99              |
| 1:B:84:ASN:HA     | 1:B:87:GLU:HB2    | 1.00                     | 0.98              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1021:LEU:O    | 1:D:1022:VAL:HG22 | 1.61                     | 0.98              |
| 1:A:207:SER:OG    | 1:A:269:TRP:CZ3   | 2.16                     | 0.98              |
| 1:A:479:GLN:NE2   | 1:A:534:UNK:N     | 2.09                     | 0.98              |
| 1:B:1000:ARG:HE   | 1:B:1016:ARG:HG2  | 1.27                     | 0.98              |
| 1:B:1000:ARG:CZ   | 1:B:1007:TYR:OH   | 2.11                     | 0.98              |
| 1:C:1018:ASN:O    | 1:C:1021:LEU:HD22 | 1.64                     | 0.98              |
| 1:D:657:THR:CG2   | 1:D:662:TRP:CE2   | 2.46                     | 0.98              |
| 1:A:657:THR:CB    | 1:A:662:TRP:CE2   | 2.45                     | 0.98              |
| 1:D:956:PRO:CG    | 1:D:959:TYR:CG    | 2.44                     | 0.98              |
| 1:B:1022:VAL:O    | 1:B:1022:VAL:HG23 | 1.63                     | 0.98              |
| 1:C:753:PRO:HG2   | 1:C:773:LEU:HD11  | 1.42                     | 0.98              |
| 1:A:84:ASN:HA     | 1:A:87:GLU:HB2    | 1.00                     | 0.98              |
| 1:A:728:ARG:HD2   | 1:A:1134:LEU:HB2  | 1.45                     | 0.98              |
| 1:B:84:ASN:CA     | 1:B:87:GLU:HB2    | 1.93                     | 0.98              |
| 1:B:1452:TRP:HZ3  | 1:B:1527:MET:HB3  | 1.20                     | 0.98              |
| 1:C:84:ASN:HA     | 1:C:87:GLU:HB2    | 1.00                     | 0.98              |
| 1:C:956:PRO:HD2   | 1:C:959:TYR:CG    | 1.97                     | 0.98              |
| 1:D:1000:ARG:CZ   | 1:D:1007:TYR:OH   | 2.12                     | 0.98              |
| 1:D:4831:UNK:O    | 1:D:4835:UNK:N    | 1.95                     | 0.98              |
| 1:A:84:ASN:CA     | 1:A:87:GLU:HB2    | 1.93                     | 0.98              |
| 1:A:1000:ARG:HE   | 1:A:1016:ARG:HG2  | 1.27                     | 0.98              |
| 1:B:479:GLN:NE2   | 1:B:534:UNK:N     | 2.09                     | 0.98              |
| 1:C:84:ASN:HA     | 1:C:87:GLU:CB     | 1.92                     | 0.98              |
| 1:C:1004:GLY:HA2  | 1:C:1007:TYR:CD1  | 1.98                     | 0.98              |
| 1:C:1017:ARG:HH11 | 1:C:1017:ARG:CG   | 1.74                     | 0.98              |
| 1:A:1000:ARG:CZ   | 1:A:1007:TYR:OH   | 2.11                     | 0.98              |
| 1:A:1438:ARG:CA   | 1:A:1515:VAL:HG13 | 1.92                     | 0.98              |
| 1:B:752:VAL:HG21  | 1:B:754:SER:HB2   | 1.42                     | 0.98              |
| 1:C:1022:VAL:O    | 1:C:1022:VAL:HG23 | 1.63                     | 0.98              |
| 1:D:207:SER:OG    | 1:D:269:TRP:CZ3   | 2.16                     | 0.98              |
| 1:A:956:PRO:CG    | 1:A:959:TYR:CG    | 2.44                     | 0.98              |
| 1:B:207:SER:OG    | 1:B:269:TRP:CZ3   | 2.16                     | 0.98              |
| 1:B:657:THR:CG2   | 1:B:662:TRP:CE2   | 2.46                     | 0.98              |
| 1:B:1017:ARG:CG   | 1:B:1017:ARG:HH11 | 1.74                     | 0.98              |
| 1:B:956:PRO:HD2   | 1:B:959:TYR:CG    | 1.97                     | 0.97              |
| 1:B:3673:UNK:O    | 1:B:3680:UNK:N    | 1.97                     | 0.97              |
| 1:A:3673:UNK:O    | 1:A:3680:UNK:N    | 1.97                     | 0.97              |
| 1:A:4561:UNK:CB   | 1:A:4565:UNK:CB   | 2.42                     | 0.97              |
| 1:D:84:ASN:CA     | 1:D:87:GLU:HB2    | 1.93                     | 0.97              |
| 1:A:1450:VAL:O    | 1:A:1529:PHE:CZ   | 2.18                     | 0.97              |
| 1:B:1474:VAL:HG23 | 1:B:1540:PHE:HE2  | 1.27                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:21:VAL:HG13   | 1:C:205:ILE:CD1   | 1.95                     | 0.97              |
| 1:C:1000:ARG:CZ   | 1:C:1007:TYR:OH   | 2.11                     | 0.97              |
| 1:D:1450:VAL:O    | 1:D:1529:PHE:CZ   | 2.17                     | 0.97              |
| 1:A:657:THR:CG2   | 1:A:662:TRP:CE2   | 2.46                     | 0.97              |
| 1:B:1004:GLY:HA2  | 1:B:1007:TYR:CD1  | 1.98                     | 0.97              |
| 1:C:207:SER:OG    | 1:C:269:TRP:CZ3   | 2.17                     | 0.97              |
| 1:C:1000:ARG:HE   | 1:C:1016:ARG:HG2  | 1.27                     | 0.97              |
| 1:D:1474:VAL:HG23 | 1:D:1540:PHE:HE2  | 1.28                     | 0.97              |
| 1:A:956:PRO:HD2   | 1:A:959:TYR:CG    | 1.97                     | 0.97              |
| 1:C:4831:UNK:O    | 1:C:4835:UNK:N    | 1.96                     | 0.97              |
| 1:D:1000:ARG:HE   | 1:D:1016:ARG:HG2  | 1.27                     | 0.97              |
| 1:D:1004:GLY:HA2  | 1:D:1007:TYR:CD1  | 1.98                     | 0.97              |
| 1:A:1474:VAL:HG23 | 1:A:1540:PHE:HE2  | 1.28                     | 0.97              |
| 1:B:207:SER:HA    | 1:B:269:TRP:HZ3   | 1.27                     | 0.97              |
| 1:C:728:ARG:HD2   | 1:C:1134:LEU:HB2  | 1.45                     | 0.97              |
| 1:D:728:ARG:HD2   | 1:D:1134:LEU:HB2  | 1.45                     | 0.97              |
| 1:A:1004:GLY:HA2  | 1:A:1007:TYR:CD1  | 1.98                     | 0.97              |
| 1:A:21:VAL:HG13   | 1:A:205:ILE:CD1   | 1.95                     | 0.97              |
| 1:B:1018:ASN:O    | 1:B:1021:LEU:HD22 | 1.64                     | 0.97              |
| 1:D:752:VAL:CG1   | 1:D:769:GLU:CB    | 2.40                     | 0.96              |
| 1:B:4561:UNK:CB   | 1:B:4565:UNK:CB   | 2.42                     | 0.96              |
| 1:D:2296:UNK:CA   | 1:D:2352:UNK:CB   | 2.43                     | 0.96              |
| 1:D:4561:UNK:CB   | 1:D:4565:UNK:CB   | 2.42                     | 0.96              |
| 1:B:752:VAL:CG1   | 1:B:769:GLU:CB    | 2.40                     | 0.96              |
| 1:C:993:HIS:CA    | 1:C:996:TRP:CE3   | 2.42                     | 0.96              |
| 1:D:3673:UNK:O    | 1:D:3680:UNK:N    | 1.97                     | 0.96              |
| 1:A:1000:ARG:NH2  | 1:A:1016:ARG:HG2  | 1.81                     | 0.96              |
| 1:D:1022:VAL:O    | 1:D:1022:VAL:HG23 | 1.63                     | 0.96              |
| 1:C:1000:ARG:NH2  | 1:C:1016:ARG:HG2  | 1.81                     | 0.96              |
| 1:D:207:SER:HA    | 1:D:269:TRP:HZ3   | 1.27                     | 0.96              |
| 1:D:21:VAL:HG13   | 1:D:205:ILE:CD1   | 1.95                     | 0.96              |
| 1:D:752:VAL:HG21  | 1:D:754:SER:HB2   | 1.42                     | 0.96              |
| 1:D:1018:ASN:O    | 1:D:1021:LEU:HD22 | 1.64                     | 0.96              |
| 1:A:1022:VAL:O    | 1:A:1022:VAL:HG23 | 1.63                     | 0.96              |
| 1:B:1474:VAL:CG2  | 1:B:1540:PHE:HE2  | 1.79                     | 0.96              |
| 1:C:3673:UNK:O    | 1:C:3680:UNK:N    | 1.97                     | 0.96              |
| 1:C:4561:UNK:CB   | 1:C:4565:UNK:CB   | 2.42                     | 0.96              |
| 1:A:1018:ASN:O    | 1:A:1021:LEU:HD22 | 1.64                     | 0.95              |
| 1:A:1813:UNK:O    | 1:A:1817:UNK:O    | 1.84                     | 0.95              |
| 1:A:2296:UNK:CA   | 1:A:2352:UNK:CB   | 2.43                     | 0.95              |
| 1:C:956:PRO:HG3   | 1:C:959:TYR:CD1   | 1.94                     | 0.95              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:1450:VAL:O    | 1:B:1529:PHE:CZ  | 2.18                     | 0.95              |
| 1:C:1813:UNK:O    | 1:C:1817:UNK:O   | 1.84                     | 0.95              |
| 1:B:426:ARG:NH2   | 1:B:796:ARG:HH22 | 1.55                     | 0.95              |
| 1:C:84:ASN:CA     | 1:C:87:GLU:HB2   | 1.93                     | 0.95              |
| 1:D:1004:GLY:CA   | 1:D:1007:TYR:CZ  | 2.50                     | 0.95              |
| 1:D:1813:UNK:O    | 1:D:1817:UNK:O   | 1.84                     | 0.95              |
| 1:A:1434:TYR:CD1  | 1:A:1570:LYS:HD2 | 2.02                     | 0.95              |
| 1:B:1002:ALA:HA   | 1:B:1005:TRP:HD1 | 1.30                     | 0.95              |
| 1:C:1450:VAL:O    | 1:C:1529:PHE:CZ  | 2.18                     | 0.95              |
| 1:A:1474:VAL:CG2  | 1:A:1540:PHE:HE2 | 1.80                     | 0.95              |
| 1:B:1000:ARG:NH2  | 1:B:1016:ARG:HG2 | 1.81                     | 0.95              |
| 1:B:1813:UNK:O    | 1:B:1817:UNK:O   | 1.84                     | 0.95              |
| 1:D:207:SER:N     | 1:D:269:TRP:CE3  | 2.34                     | 0.95              |
| 1:D:956:PRO:HD3   | 1:D:959:TYR:HD2  | 1.19                     | 0.95              |
| 1:D:1434:TYR:CD1  | 1:D:1570:LYS:HD2 | 2.02                     | 0.95              |
| 1:A:1004:GLY:CA   | 1:A:1007:TYR:CZ  | 2.49                     | 0.95              |
| 1:B:21:VAL:HG13   | 1:B:205:ILE:CD1  | 1.95                     | 0.95              |
| 1:C:956:PRO:CG    | 1:C:959:TYR:CG   | 2.44                     | 0.95              |
| 1:A:317:ARG:NH2   | 1:A:322:LYS:CA   | 2.20                     | 0.95              |
| 1:A:956:PRO:CG    | 1:A:959:TYR:CD2  | 2.50                     | 0.95              |
| 1:C:956:PRO:HG2   | 1:C:959:TYR:CD1  | 2.02                     | 0.95              |
| 1:B:1000:ARG:HH21 | 1:B:1016:ARG:HG2 | 1.29                     | 0.95              |
| 1:B:2296:UNK:CA   | 1:B:2352:UNK:CB  | 2.43                     | 0.95              |
| 1:D:998:ARG:CD    | 1:D:999:ASP:N    | 2.30                     | 0.95              |
| 1:B:207:SER:N     | 1:B:269:TRP:CE3  | 2.34                     | 0.95              |
| 1:C:998:ARG:CD    | 1:C:999:ASP:N    | 2.30                     | 0.95              |
| 1:C:1017:ARG:N    | 1:C:1017:ARG:CD  | 2.30                     | 0.95              |
| 1:C:207:SER:N     | 1:C:269:TRP:CE3  | 2.34                     | 0.94              |
| 1:C:317:ARG:NH2   | 1:C:322:LYS:CA   | 2.20                     | 0.94              |
| 1:C:1017:ARG:HH11 | 1:C:1017:ARG:CB  | 1.80                     | 0.94              |
| 1:D:1000:ARG:NE   | 1:D:1016:ARG:HG2 | 1.81                     | 0.94              |
| 1:D:1016:ARG:NH1  | 1:D:1016:ARG:CB  | 2.30                     | 0.94              |
| 1:B:956:PRO:CG    | 1:B:959:TYR:CD2  | 2.50                     | 0.94              |
| 1:C:1000:ARG:NE   | 1:C:1016:ARG:HG2 | 1.81                     | 0.94              |
| 1:C:1474:VAL:CG2  | 1:C:1540:PHE:HE2 | 1.80                     | 0.94              |
| 1:D:1000:ARG:NH2  | 1:D:1016:ARG:HG2 | 1.81                     | 0.94              |
| 1:A:207:SER:N     | 1:A:269:TRP:CE3  | 2.34                     | 0.94              |
| 1:A:207:SER:HA    | 1:A:269:TRP:HZ3  | 1.27                     | 0.94              |
| 1:A:1000:ARG:NE   | 1:A:1016:ARG:HG2 | 1.81                     | 0.94              |
| 1:A:1454:THR:HB   | 1:A:1455:PRO:HD2 | 1.49                     | 0.94              |
| 1:B:1016:ARG:NH1  | 1:B:1016:ARG:CB  | 2.30                     | 0.94              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:1017:ARG:HH11 | 1:B:1017:ARG:CB  | 1.80                     | 0.94              |
| 1:B:1454:THR:HB   | 1:B:1455:PRO:HD2 | 1.49                     | 0.94              |
| 1:C:956:PRO:CG    | 1:C:959:TYR:CD2  | 2.50                     | 0.94              |
| 1:C:1002:ALA:HA   | 1:C:1005:TRP:HD1 | 1.30                     | 0.94              |
| 1:D:1474:VAL:CG2  | 1:D:1540:PHE:HE2 | 1.80                     | 0.94              |
| 1:A:1016:ARG:NH1  | 1:A:1016:ARG:CB  | 2.30                     | 0.94              |
| 1:B:1004:GLY:CA   | 1:B:1007:TYR:CZ  | 2.49                     | 0.94              |
| 1:C:2296:UNK:CA   | 1:C:2352:UNK:CB  | 2.43                     | 0.94              |
| 1:D:317:ARG:NH1   | 1:D:322:LYS:CA   | 2.29                     | 0.94              |
| 1:D:1452:TRP:HZ3  | 1:D:1527:MET:HB3 | 1.20                     | 0.94              |
| 1:A:1000:ARG:HH21 | 1:A:1016:ARG:HG2 | 1.29                     | 0.94              |
| 1:A:995:VAL:O     | 1:A:998:ARG:HG3  | 1.68                     | 0.94              |
| 1:B:1000:ARG:NE   | 1:B:1016:ARG:HG2 | 1.81                     | 0.94              |
| 1:C:1452:TRP:CH2  | 1:C:1527:MET:CB  | 2.42                     | 0.94              |
| 1:D:995:VAL:O     | 1:D:998:ARG:HG3  | 1.68                     | 0.94              |
| 1:A:1017:ARG:N    | 1:A:1017:ARG:CD  | 2.30                     | 0.94              |
| 1:A:3899:UNK:C    | 1:A:3910:UNK:H2  | 1.81                     | 0.94              |
| 1:B:1434:TYR:CD1  | 1:B:1570:LYS:HD2 | 2.02                     | 0.94              |
| 1:B:1452:TRP:CH2  | 1:B:1527:MET:CB  | 2.42                     | 0.94              |
| 1:B:3899:UNK:C    | 1:B:3910:UNK:H2  | 1.81                     | 0.94              |
| 1:C:752:VAL:CG1   | 1:C:769:GLU:CB   | 2.40                     | 0.94              |
| 1:D:855:PRO:HG3   | 1:D:994:ASN:C    | 1.93                     | 0.94              |
| 1:D:1433:TYR:O    | 1:D:1520:VAL:O   | 1.86                     | 0.94              |
| 1:A:317:ARG:NH1   | 1:A:322:LYS:CA   | 2.29                     | 0.94              |
| 1:A:855:PRO:HG3   | 1:A:994:ASN:C    | 1.93                     | 0.94              |
| 1:B:995:VAL:O     | 1:B:998:ARG:HG3  | 1.68                     | 0.94              |
| 1:B:998:ARG:HH22  | 1:B:1002:ALA:HB3 | 1.32                     | 0.94              |
| 1:C:995:VAL:O     | 1:C:998:ARG:HG3  | 1.68                     | 0.94              |
| 1:D:1017:ARG:HH11 | 1:D:1017:ARG:CB  | 1.80                     | 0.94              |
| 1:C:426:ARG:NH2   | 1:C:796:ARG:HH22 | 1.55                     | 0.93              |
| 1:C:1434:TYR:CZ   | 1:C:1570:LYS:HD2 | 2.03                     | 0.93              |
| 1:C:3899:UNK:C    | 1:C:3910:UNK:H2  | 1.81                     | 0.93              |
| 1:D:1434:TYR:CZ   | 1:D:1570:LYS:HD2 | 2.03                     | 0.93              |
| 1:D:3899:UNK:C    | 1:D:3910:UNK:H2  | 1.81                     | 0.93              |
| 1:A:1433:TYR:O    | 1:A:1520:VAL:O   | 1.86                     | 0.93              |
| 1:A:4583:UNK:O    | 1:D:4884:UNK:CB  | 2.06                     | 0.93              |
| 1:B:1017:ARG:N    | 1:B:1017:ARG:CD  | 2.30                     | 0.93              |
| 1:C:855:PRO:HG3   | 1:C:994:ASN:C    | 1.93                     | 0.93              |
| 1:C:1016:ARG:NH1  | 1:C:1016:ARG:CB  | 2.30                     | 0.93              |
| 1:C:2285:UNK:C    | 1:C:2286:UNK:N   | 2.32                     | 0.93              |
| 1:A:1000:ARG:HG2  | 1:A:1018:ASN:ND2 | 1.84                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1017:ARG:HH11 | 1:A:1017:ARG:CB   | 1.80                     | 0.93              |
| 1:B:998:ARG:CD    | 1:B:999:ASP:N     | 2.30                     | 0.93              |
| 1:D:1000:ARG:HG2  | 1:D:1018:ASN:ND2  | 1.83                     | 0.93              |
| 1:C:1434:TYR:CD1  | 1:C:1570:LYS:HD2  | 2.02                     | 0.93              |
| 1:A:752:VAL:CG1   | 1:A:769:GLU:CB    | 2.40                     | 0.93              |
| 1:C:998:ARG:HH22  | 1:C:1002:ALA:HB3  | 1.32                     | 0.93              |
| 1:D:4645:UNK:O    | 1:D:4649:UNK:N    | 2.02                     | 0.93              |
| 1:A:728:ARG:CB    | 1:A:1134:LEU:HD22 | 1.99                     | 0.93              |
| 1:B:956:PRO:HG2   | 1:B:959:TYR:CD1   | 2.02                     | 0.93              |
| 1:C:1000:ARG:HG2  | 1:C:1018:ASN:ND2  | 1.84                     | 0.93              |
| 1:C:4884:UNK:CB   | 1:D:4583:UNK:O    | 2.09                     | 0.93              |
| 1:A:4645:UNK:O    | 1:A:4649:UNK:N    | 2.02                     | 0.93              |
| 1:B:1434:TYR:CZ   | 1:B:1570:LYS:HD2  | 2.03                     | 0.93              |
| 1:D:998:ARG:HH22  | 1:D:1002:ALA:HB3  | 1.32                     | 0.93              |
| 1:D:1450:VAL:HG13 | 1:D:1518:CYS:SG   | 2.09                     | 0.93              |
| 1:A:998:ARG:CD    | 1:A:999:ASP:N     | 2.30                     | 0.93              |
| 1:A:2285:UNK:C    | 1:A:2286:UNK:N    | 2.32                     | 0.93              |
| 1:C:1000:ARG:HH21 | 1:C:1016:ARG:HG2  | 1.29                     | 0.93              |
| 1:C:1452:TRP:HZ3  | 1:C:1527:MET:HB3  | 1.20                     | 0.93              |
| 1:C:4645:UNK:O    | 1:C:4649:UNK:N    | 2.02                     | 0.93              |
| 1:D:956:PRO:CG    | 1:D:959:TYR:CD2   | 2.50                     | 0.93              |
| 1:A:1434:TYR:CZ   | 1:A:1570:LYS:HD2  | 2.03                     | 0.92              |
| 1:B:1000:ARG:HG2  | 1:B:1018:ASN:ND2  | 1.84                     | 0.92              |
| 1:D:1017:ARG:N    | 1:D:1017:ARG:CD   | 2.30                     | 0.92              |
| 1:A:954:LYS:HB3   | 1:A:971:ASP:OD2   | 1.70                     | 0.92              |
| 1:A:1020:ARG:HA   | 1:A:1020:ARG:HE   | 1.34                     | 0.92              |
| 1:B:1433:TYR:O    | 1:B:1520:VAL:O    | 1.86                     | 0.92              |
| 1:D:728:ARG:CB    | 1:D:1134:LEU:HD22 | 1.99                     | 0.92              |
| 1:C:1004:GLY:CA   | 1:C:1007:TYR:CZ   | 2.50                     | 0.92              |
| 1:B:317:ARG:NH2   | 1:B:322:LYS:CA    | 2.20                     | 0.92              |
| 1:B:1017:ARG:NH1  | 1:B:1017:ARG:HA   | 1.85                     | 0.92              |
| 1:B:1450:VAL:HG13 | 1:B:1518:CYS:SG   | 2.09                     | 0.92              |
| 1:B:2611:UNK:CB   | 1:B:2685:UNK:CB   | 2.48                     | 0.92              |
| 1:C:1433:TYR:O    | 1:C:1520:VAL:O    | 1.86                     | 0.92              |
| 1:D:956:PRO:HG2   | 1:D:959:TYR:CD1   | 2.02                     | 0.92              |
| 1:A:1450:VAL:HG13 | 1:A:1518:CYS:SG   | 2.09                     | 0.92              |
| 1:B:4645:UNK:O    | 1:B:4649:UNK:N    | 2.02                     | 0.92              |
| 1:D:75:VAL:HG13   | 1:D:76:ARG:H      | 1.35                     | 0.92              |
| 1:D:317:ARG:NH2   | 1:D:322:LYS:C     | 2.28                     | 0.92              |
| 1:A:317:ARG:NH2   | 1:A:322:LYS:C     | 2.28                     | 0.92              |
| 1:A:956:PRO:HG2   | 1:A:959:TYR:CD1   | 2.02                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:728:ARG:CB    | 1:B:1134:LEU:HD22 | 1.99                     | 0.92              |
| 1:B:728:ARG:NH1   | 1:B:1133:HIS:CG   | 2.16                     | 0.92              |
| 1:C:317:ARG:NH2   | 1:C:322:LYS:C     | 2.28                     | 0.92              |
| 1:C:1454:THR:HB   | 1:C:1455:PRO:HD2  | 1.49                     | 0.92              |
| 1:C:2611:UNK:CB   | 1:C:2685:UNK:CB   | 2.48                     | 0.92              |
| 1:D:954:LYS:HB3   | 1:D:971:ASP:OD2   | 1.70                     | 0.92              |
| 1:A:75:VAL:O      | 1:A:79:GLN:NE2    | 2.03                     | 0.92              |
| 1:A:998:ARG:HH22  | 1:A:1002:ALA:HB3  | 1.32                     | 0.92              |
| 1:B:855:PRO:HG3   | 1:B:994:ASN:C     | 1.93                     | 0.92              |
| 1:B:2285:UNK:C    | 1:B:2286:UNK:N    | 2.32                     | 0.92              |
| 1:C:1450:VAL:HG13 | 1:C:1518:CYS:SG   | 2.09                     | 0.92              |
| 1:D:1454:THR:HB   | 1:D:1455:PRO:HD2  | 1.48                     | 0.92              |
| 1:D:2285:UNK:C    | 1:D:2286:UNK:N    | 2.32                     | 0.92              |
| 1:A:80:GLU:OE1    | 1:B:3932:UNK:CA   | 2.18                     | 0.92              |
| 1:B:75:VAL:HG13   | 1:B:76:ARG:H      | 1.35                     | 0.92              |
| 1:B:207:SER:N     | 1:B:269:TRP:HZ3   | 1.60                     | 0.92              |
| 1:C:75:VAL:O      | 1:C:79:GLN:NE2    | 2.03                     | 0.92              |
| 1:C:954:LYS:HB3   | 1:C:971:ASP:OD2   | 1.70                     | 0.92              |
| 1:C:998:ARG:NH2   | 1:C:1002:ALA:CB   | 2.30                     | 0.92              |
| 1:C:1439:VAL:H    | 1:C:1515:VAL:CA   | 1.83                     | 0.92              |
| 1:B:956:PRO:CG    | 1:B:959:TYR:CG    | 2.44                     | 0.92              |
| 1:C:999:ASP:O     | 1:C:1003:GLN:HG2  | 1.70                     | 0.92              |
| 1:A:75:VAL:HG13   | 1:A:76:ARG:H      | 1.35                     | 0.91              |
| 1:A:657:THR:HG21  | 1:A:662:TRP:CE2   | 2.05                     | 0.91              |
| 1:A:1017:ARG:NH1  | 1:A:1017:ARG:HA   | 1.85                     | 0.91              |
| 1:B:317:ARG:NH2   | 1:B:322:LYS:C     | 2.28                     | 0.91              |
| 1:D:1000:ARG:HH21 | 1:D:1016:ARG:HG2  | 1.29                     | 0.91              |
| 1:D:2611:UNK:CB   | 1:D:2685:UNK:CB   | 2.48                     | 0.91              |
| 1:A:3932:UNK:CA   | 1:D:80:GLU:OE1    | 2.18                     | 0.91              |
| 1:A:4732:UNK:O    | 1:A:4736:UNK:N    | 2.04                     | 0.91              |
| 1:B:954:LYS:HB3   | 1:B:971:ASP:OD2   | 1.70                     | 0.91              |
| 1:B:998:ARG:NH2   | 1:B:1002:ALA:CB   | 2.30                     | 0.91              |
| 1:C:1437:VAL:HG21 | 1:C:1518:CYS:HB2  | 1.52                     | 0.91              |
| 1:B:317:ARG:NH1   | 1:B:322:LYS:CA    | 2.29                     | 0.91              |
| 1:B:1020:ARG:HA   | 1:B:1020:ARG:HE   | 1.34                     | 0.91              |
| 1:C:657:THR:HG1   | 1:C:662:TRP:CG    | 1.89                     | 0.91              |
| 1:B:4732:UNK:O    | 1:B:4736:UNK:N    | 2.04                     | 0.91              |
| 1:A:1437:VAL:HG21 | 1:A:1518:CYS:HB2  | 1.52                     | 0.91              |
| 1:B:80:GLU:OE1    | 1:C:3932:UNK:CA   | 2.18                     | 0.91              |
| 1:B:1437:VAL:HG21 | 1:B:1518:CYS:HB2  | 1.52                     | 0.91              |
| 1:C:728:ARG:CB    | 1:C:1134:LEU:HD22 | 1.99                     | 0.91              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:75:VAL:O      | 1:D:79:GLN:NE2   | 2.03                     | 0.91              |
| 1:D:999:ASP:O     | 1:D:1003:GLN:HG2 | 1.70                     | 0.91              |
| 1:A:2611:UNK:CB   | 1:A:2685:UNK:CB  | 2.48                     | 0.91              |
| 1:A:4854:UNK:O    | 1:A:4858:UNK:N   | 2.04                     | 0.91              |
| 1:C:75:VAL:HG13   | 1:C:76:ARG:H     | 1.34                     | 0.91              |
| 1:A:657:THR:HG1   | 1:A:662:TRP:CG   | 1.89                     | 0.91              |
| 1:A:728:ARG:NH1   | 1:A:1133:HIS:CG  | 2.16                     | 0.91              |
| 1:A:1439:VAL:H    | 1:A:1515:VAL:CA  | 1.83                     | 0.91              |
| 1:B:1474:VAL:CG2  | 1:B:1540:PHE:CE2 | 2.54                     | 0.91              |
| 1:C:4732:UNK:O    | 1:C:4736:UNK:N   | 2.04                     | 0.91              |
| 1:D:4732:UNK:O    | 1:D:4736:UNK:N   | 2.04                     | 0.91              |
| 1:A:999:ASP:O     | 1:A:1003:GLN:HG2 | 1.70                     | 0.90              |
| 1:A:1020:ARG:HH11 | 1:A:1024:TYR:HA  | 1.08                     | 0.90              |
| 1:C:956:PRO:HD3   | 1:C:959:TYR:HD2  | 1.19                     | 0.90              |
| 1:B:1002:ALA:CA   | 1:B:1005:TRP:CD1 | 2.54                     | 0.90              |
| 1:D:1002:ALA:CA   | 1:D:1005:TRP:CD1 | 2.54                     | 0.90              |
| 1:B:3900:UNK:CA   | 1:B:3910:UNK:CB  | 2.48                     | 0.90              |
| 1:A:1002:ALA:CA   | 1:A:1005:TRP:CD1 | 2.54                     | 0.90              |
| 1:A:1474:VAL:CG2  | 1:A:1540:PHE:CE2 | 2.54                     | 0.90              |
| 1:A:4884:UNK:CB   | 1:B:4583:UNK:O   | 2.07                     | 0.90              |
| 1:C:317:ARG:NH1   | 1:C:322:LYS:CA   | 2.29                     | 0.90              |
| 1:D:752:VAL:CG1   | 1:D:769:GLU:CD   | 2.44                     | 0.90              |
| 1:D:1450:VAL:C    | 1:D:1529:PHE:CZ  | 2.50                     | 0.90              |
| 1:A:1002:ALA:HA   | 1:A:1005:TRP:HD1 | 1.30                     | 0.90              |
| 1:B:75:VAL:O      | 1:B:79:GLN:NE2   | 2.03                     | 0.90              |
| 1:B:999:ASP:O     | 1:B:1003:GLN:HG2 | 1.70                     | 0.90              |
| 1:D:1017:ARG:NH1  | 1:D:1017:ARG:HA  | 1.85                     | 0.90              |
| 1:D:1437:VAL:HG21 | 1:D:1518:CYS:HB2 | 1.52                     | 0.90              |
| 1:D:1474:VAL:CG2  | 1:D:1540:PHE:CE2 | 2.54                     | 0.90              |
| 1:B:657:THR:HG1   | 1:B:662:TRP:CG   | 1.89                     | 0.90              |
| 1:B:998:ARG:C     | 1:B:998:ARG:NE   | 2.30                     | 0.90              |
| 1:C:1017:ARG:HA   | 1:C:1017:ARG:NH1 | 1.85                     | 0.90              |
| 1:D:1016:ARG:C    | 1:D:1017:ARG:NE  | 2.30                     | 0.90              |
| 1:B:4854:UNK:O    | 1:B:4858:UNK:N   | 2.04                     | 0.90              |
| 1:C:1002:ALA:CA   | 1:C:1005:TRP:CD1 | 2.54                     | 0.90              |
| 1:C:4854:UNK:O    | 1:C:4858:UNK:N   | 2.04                     | 0.90              |
| 1:D:4854:UNK:O    | 1:D:4858:UNK:N   | 2.04                     | 0.90              |
| 1:D:207:SER:N     | 1:D:269:TRP:HZ3  | 1.60                     | 0.90              |
| 1:D:1439:VAL:H    | 1:D:1515:VAL:CA  | 1.83                     | 0.90              |
| 1:A:1450:VAL:C    | 1:A:1529:PHE:CZ  | 2.50                     | 0.90              |
| 1:B:323:LEU:HD22  | 1:B:323:LEU:H    | 1.37                     | 0.90              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:1016:ARG:C    | 1:B:1017:ARG:NE  | 2.30                     | 0.90              |
| 1:B:998:ARG:C     | 1:B:998:ARG:CZ   | 2.46                     | 0.89              |
| 1:C:752:VAL:CG1   | 1:C:769:GLU:CD   | 2.44                     | 0.89              |
| 1:D:1002:ALA:HA   | 1:D:1005:TRP:HD1 | 1.30                     | 0.89              |
| 1:B:752:VAL:CG1   | 1:B:769:GLU:CD   | 2.44                     | 0.89              |
| 1:A:998:ARG:C     | 1:A:998:ARG:NE   | 2.30                     | 0.89              |
| 1:C:80:GLU:OE1    | 1:D:3932:UNK:CA  | 2.20                     | 0.89              |
| 1:C:1450:VAL:C    | 1:C:1529:PHE:CZ  | 2.50                     | 0.89              |
| 1:D:1020:ARG:HH11 | 1:D:1024:TYR:HA  | 1.08                     | 0.89              |
| 1:A:998:ARG:C     | 1:A:998:ARG:CZ   | 2.45                     | 0.89              |
| 1:B:3205:UNK:HA   | 1:B:3208:UNK:CB  | 2.03                     | 0.89              |
| 1:A:3895:UNK:O    | 1:A:3899:UNK:N   | 2.06                     | 0.89              |
| 1:B:3268:UNK:H    | 1:B:3271:UNK:CB  | 1.86                     | 0.89              |
| 1:C:728:ARG:NH1   | 1:C:1133:HIS:CG  | 2.16                     | 0.89              |
| 1:D:1450:VAL:CG1  | 1:D:1518:CYS:SG  | 2.61                     | 0.89              |
| 1:D:3894:UNK:O    | 1:D:3898:UNK:CB  | 2.21                     | 0.89              |
| 1:A:993:HIS:CA    | 1:A:996:TRP:CE3  | 2.42                     | 0.89              |
| 1:A:1016:ARG:C    | 1:A:1017:ARG:NE  | 2.30                     | 0.89              |
| 1:B:1439:VAL:H    | 1:B:1515:VAL:CA  | 1.83                     | 0.89              |
| 1:B:3895:UNK:O    | 1:B:3899:UNK:N   | 2.06                     | 0.89              |
| 1:C:479:GLN:NE2   | 1:C:534:UNK:H2   | 1.70                     | 0.89              |
| 1:C:998:ARG:C     | 1:C:998:ARG:CZ   | 2.46                     | 0.89              |
| 1:C:3567:UNK:O    | 1:C:3570:UNK:O   | 1.91                     | 0.89              |
| 1:B:4645:UNK:HA   | 1:B:4648:UNK:CB  | 2.02                     | 0.89              |
| 1:C:1016:ARG:C    | 1:C:1017:ARG:NE  | 2.30                     | 0.89              |
| 1:B:3894:UNK:O    | 1:B:3898:UNK:CB  | 2.21                     | 0.89              |
| 1:C:998:ARG:C     | 1:C:998:ARG:NE   | 2.30                     | 0.89              |
| 1:D:3205:UNK:HA   | 1:D:3208:UNK:CB  | 2.03                     | 0.89              |
| 1:A:752:VAL:CG1   | 1:A:769:GLU:CD   | 2.44                     | 0.89              |
| 1:B:1450:VAL:C    | 1:B:1529:PHE:CZ  | 2.50                     | 0.89              |
| 1:C:1450:VAL:CG1  | 1:C:1518:CYS:SG  | 2.61                     | 0.89              |
| 1:C:1474:VAL:CG2  | 1:C:1540:PHE:CE2 | 2.54                     | 0.89              |
| 1:A:3894:UNK:O    | 1:A:3898:UNK:CB  | 2.21                     | 0.89              |
| 1:B:998:ARG:HD3   | 1:B:999:ASP:CG   | 1.98                     | 0.88              |
| 1:C:3268:UNK:H    | 1:C:3271:UNK:CB  | 1.86                     | 0.88              |
| 1:D:998:ARG:HD3   | 1:D:999:ASP:CG   | 1.98                     | 0.88              |
| 1:D:3268:UNK:H    | 1:D:3271:UNK:CB  | 1.86                     | 0.88              |
| 1:D:4645:UNK:HA   | 1:D:4648:UNK:CB  | 2.03                     | 0.88              |
| 1:D:4712:UNK:O    | 1:D:4720:UNK:N   | 1.94                     | 0.88              |
| 1:A:998:ARG:HD3   | 1:A:999:ASP:CG   | 1.98                     | 0.88              |
| 1:A:1020:ARG:HH12 | 1:A:1024:TYR:HA  | 1.35                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1450:VAL:CG1  | 1:A:1518:CYS:SG   | 2.61                     | 0.88              |
| 1:B:3567:UNK:O    | 1:B:3570:UNK:O    | 1.91                     | 0.88              |
| 1:C:323:LEU:HD22  | 1:C:323:LEU:H     | 1.37                     | 0.88              |
| 1:D:998:ARG:C     | 1:D:998:ARG:NE    | 2.30                     | 0.88              |
| 1:D:3900:UNK:CA   | 1:D:3910:UNK:CB   | 2.48                     | 0.88              |
| 1:D:657:THR:HG1   | 1:D:662:TRP:CG    | 1.91                     | 0.88              |
| 1:C:3205:UNK:HA   | 1:C:3208:UNK:CB   | 2.03                     | 0.88              |
| 1:A:207:SER:N     | 1:A:269:TRP:HZ3   | 1.60                     | 0.88              |
| 1:A:479:GLN:NE2   | 1:A:534:UNK:H2    | 1.70                     | 0.88              |
| 1:A:3205:UNK:HA   | 1:A:3208:UNK:CB   | 2.03                     | 0.88              |
| 1:A:4730:UNK:O    | 1:A:4731:UNK:O    | 1.92                     | 0.88              |
| 1:A:1444:GLU:OE1  | 1:A:1478:ASP:CB   | 2.22                     | 0.88              |
| 1:A:4645:UNK:HA   | 1:A:4648:UNK:CB   | 2.03                     | 0.88              |
| 1:B:1450:VAL:CG1  | 1:B:1518:CYS:SG   | 2.61                     | 0.88              |
| 1:C:424:LYS:HZ1   | 1:C:505:GLU:HB2   | 1.37                     | 0.88              |
| 1:C:3894:UNK:O    | 1:C:3898:UNK:CB   | 2.21                     | 0.88              |
| 1:C:4645:UNK:HA   | 1:C:4648:UNK:CB   | 2.03                     | 0.88              |
| 1:D:1444:GLU:OE1  | 1:D:1478:ASP:CB   | 2.22                     | 0.88              |
| 1:C:727:ALA:O     | 1:C:1134:LEU:HD21 | 1.74                     | 0.88              |
| 1:C:998:ARG:HD3   | 1:C:999:ASP:CG    | 1.98                     | 0.88              |
| 1:C:4730:UNK:O    | 1:C:4731:UNK:O    | 1.92                     | 0.88              |
| 1:D:479:GLN:NE2   | 1:D:534:UNK:H2    | 1.70                     | 0.88              |
| 1:D:1000:ARG:CG   | 1:D:1018:ASN:ND2  | 2.37                     | 0.88              |
| 1:B:1444:GLU:OE1  | 1:B:1478:ASP:CB   | 2.22                     | 0.88              |
| 1:D:727:ALA:O     | 1:D:1134:LEU:HD21 | 1.74                     | 0.88              |
| 1:A:323:LEU:H     | 1:A:323:LEU:HD22  | 1.37                     | 0.88              |
| 1:B:1000:ARG:NE   | 1:B:1016:ARG:CD   | 2.37                     | 0.88              |
| 1:B:1020:ARG:NH1  | 1:B:1024:TYR:CA   | 2.31                     | 0.88              |
| 1:D:998:ARG:C     | 1:D:998:ARG:CZ    | 2.45                     | 0.88              |
| 1:D:1020:ARG:HH12 | 1:D:1024:TYR:HA   | 1.35                     | 0.88              |
| 1:C:4712:UNK:O    | 1:C:4720:UNK:N    | 1.94                     | 0.88              |
| 1:D:998:ARG:NH2   | 1:D:1002:ALA:CB   | 2.30                     | 0.88              |
| 1:A:3900:UNK:CA   | 1:A:3910:UNK:CB   | 2.48                     | 0.87              |
| 1:C:1000:ARG:NE   | 1:C:1016:ARG:CD   | 2.37                     | 0.87              |
| 1:D:86:VAL:HG22   | 1:D:87:GLU:OE1    | 1.74                     | 0.87              |
| 1:D:323:LEU:H     | 1:D:323:LEU:HD22  | 1.37                     | 0.87              |
| 1:D:1845:UNK:HA   | 1:D:1848:UNK:CB   | 2.04                     | 0.87              |
| 1:B:1007:TYR:OH   | 1:B:1015:ALA:O    | 1.92                     | 0.87              |
| 1:C:1020:ARG:HH11 | 1:C:1024:TYR:HA   | 1.08                     | 0.87              |
| 1:A:1000:ARG:NE   | 1:A:1016:ARG:CD   | 2.37                     | 0.87              |
| 1:A:1438:ARG:HA   | 1:A:1515:VAL:CG1  | 2.02                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1474:VAL:HG23 | 1:A:1540:PHE:CE2  | 2.10                     | 0.87              |
| 1:B:657:THR:HG21  | 1:B:662:TRP:CE2   | 2.05                     | 0.87              |
| 1:C:3400:UNK:O    | 1:C:3404:UNK:N    | 2.08                     | 0.87              |
| 1:A:3268:UNK:H    | 1:A:3271:UNK:CB   | 1.86                     | 0.87              |
| 1:B:86:VAL:HG22   | 1:B:87:GLU:OE1    | 1.74                     | 0.87              |
| 1:C:954:LYS:N     | 1:C:971:ASP:OD1   | 2.07                     | 0.87              |
| 1:C:1000:ARG:CG   | 1:C:1018:ASN:ND2  | 2.37                     | 0.87              |
| 1:D:657:THR:CG2   | 1:D:662:TRP:CH2   | 2.52                     | 0.87              |
| 1:D:3400:UNK:O    | 1:D:3404:UNK:N    | 2.08                     | 0.87              |
| 1:D:4730:UNK:O    | 1:D:4731:UNK:O    | 1.92                     | 0.87              |
| 1:A:1000:ARG:CZ   | 1:A:1016:ARG:HG2  | 2.05                     | 0.87              |
| 1:A:1459:GLN:HG2  | 1:A:1553:PHE:CD1  | 2.09                     | 0.87              |
| 1:B:1000:ARG:CG   | 1:B:1018:ASN:ND2  | 2.37                     | 0.87              |
| 1:C:83:ALA:O      | 1:C:86:VAL:HG13   | 1.75                     | 0.87              |
| 1:D:1465:ASP:CA   | 1:D:1553:PHE:CD2  | 2.57                     | 0.87              |
| 1:D:3895:UNK:O    | 1:D:3899:UNK:N    | 2.06                     | 0.87              |
| 1:A:998:ARG:NH2   | 1:A:1002:ALA:CB   | 2.30                     | 0.87              |
| 1:A:1845:UNK:HA   | 1:A:1848:UNK:CB   | 2.04                     | 0.87              |
| 1:B:727:ALA:O     | 1:B:1134:LEU:HD21 | 1.74                     | 0.87              |
| 1:B:1459:GLN:HG2  | 1:B:1553:PHE:CD1  | 2.09                     | 0.87              |
| 1:B:4730:UNK:O    | 1:B:4731:UNK:O    | 1.92                     | 0.87              |
| 1:C:1845:UNK:HA   | 1:C:1848:UNK:CB   | 2.05                     | 0.87              |
| 1:A:727:ALA:O     | 1:A:1134:LEU:HD21 | 1.74                     | 0.87              |
| 1:B:83:ALA:O      | 1:B:86:VAL:HG13   | 1.75                     | 0.87              |
| 1:C:1007:TYR:OH   | 1:C:1015:ALA:O    | 1.92                     | 0.87              |
| 1:C:1017:ARG:HD2  | 1:C:1017:ARG:H    | 1.39                     | 0.87              |
| 1:C:1444:GLU:OE1  | 1:C:1478:ASP:CB   | 2.22                     | 0.87              |
| 1:A:1000:ARG:CG   | 1:A:1018:ASN:ND2  | 2.37                     | 0.87              |
| 1:B:1017:ARG:HH11 | 1:B:1017:ARG:HG3  | 1.38                     | 0.87              |
| 1:B:1465:ASP:CA   | 1:B:1553:PHE:CD2  | 2.57                     | 0.87              |
| 1:B:1474:VAL:HG23 | 1:B:1540:PHE:CE2  | 2.10                     | 0.87              |
| 1:C:3895:UNK:O    | 1:C:3899:UNK:N    | 2.06                     | 0.87              |
| 1:D:83:ALA:O      | 1:D:86:VAL:HG13   | 1.75                     | 0.87              |
| 1:A:86:VAL:HG22   | 1:A:87:GLU:OE1    | 1.74                     | 0.87              |
| 1:B:956:PRO:HG3   | 1:B:959:TYR:CD1   | 1.94                     | 0.87              |
| 1:D:1474:VAL:HG23 | 1:D:1540:PHE:CE2  | 2.10                     | 0.87              |
| 1:B:479:GLN:NE2   | 1:B:534:UNK:H2    | 1.70                     | 0.86              |
| 1:B:993:HIS:CA    | 1:B:996:TRP:CE3   | 2.42                     | 0.86              |
| 1:C:86:VAL:HG22   | 1:C:87:GLU:OE1    | 1.74                     | 0.86              |
| 1:B:322:LYS:HB3   | 1:B:323:LEU:C     | 2.00                     | 0.86              |
| 1:B:4712:UNK:O    | 1:B:4720:UNK:N    | 1.94                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:855:PRO:HG3   | 1:C:994:ASN:O     | 1.76                     | 0.86              |
| 1:C:1459:GLN:HG2  | 1:C:1553:PHE:CD1  | 2.09                     | 0.86              |
| 1:D:3567:UNK:O    | 1:D:3570:UNK:O    | 1.91                     | 0.86              |
| 1:A:954:LYS:N     | 1:A:971:ASP:OD1   | 2.07                     | 0.86              |
| 1:A:1434:TYR:CE1  | 1:A:1570:LYS:HB2  | 2.11                     | 0.86              |
| 1:B:996:TRP:HZ2   | 1:B:1021:LEU:HD13 | 1.04                     | 0.86              |
| 1:D:1000:ARG:NE   | 1:D:1016:ARG:CD   | 2.37                     | 0.86              |
| 1:D:1000:ARG:CZ   | 1:D:1016:ARG:HG2  | 2.05                     | 0.86              |
| 1:D:1020:ARG:HA   | 1:D:1020:ARG:HE   | 1.34                     | 0.86              |
| 1:B:1434:TYR:CE1  | 1:B:1570:LYS:HB2  | 2.11                     | 0.86              |
| 1:B:1845:UNK:HA   | 1:B:1848:UNK:CB   | 2.04                     | 0.86              |
| 1:C:1017:ARG:HH11 | 1:C:1017:ARG:HG3  | 1.38                     | 0.86              |
| 1:D:322:LYS:HB3   | 1:D:323:LEU:C     | 2.00                     | 0.86              |
| 1:A:3567:UNK:O    | 1:A:3570:UNK:O    | 1.91                     | 0.86              |
| 1:D:1017:ARG:HH11 | 1:D:1017:ARG:HG3  | 1.38                     | 0.86              |
| 1:C:1465:ASP:CA   | 1:C:1553:PHE:CD2  | 2.57                     | 0.86              |
| 1:C:1474:VAL:HG23 | 1:C:1540:PHE:CE2  | 2.10                     | 0.86              |
| 1:C:3900:UNK:CA   | 1:C:3910:UNK:CB   | 2.48                     | 0.86              |
| 1:D:954:LYS:N     | 1:D:971:ASP:OD1   | 2.07                     | 0.86              |
| 1:D:1017:ARG:HD2  | 1:D:1017:ARG:H    | 1.39                     | 0.86              |
| 1:A:322:LYS:HB3   | 1:A:323:LEU:C     | 2.01                     | 0.86              |
| 1:A:728:ARG:CZ    | 1:A:1119:GLU:HA   | 2.06                     | 0.86              |
| 1:A:855:PRO:HG3   | 1:A:994:ASN:O     | 1.76                     | 0.86              |
| 1:A:1465:ASP:CA   | 1:A:1553:PHE:CD2  | 2.57                     | 0.86              |
| 1:B:1000:ARG:CZ   | 1:B:1016:ARG:HG2  | 2.05                     | 0.86              |
| 1:C:111:HIS:HD2   | 1:C:114:SER:H     | 1.23                     | 0.86              |
| 1:D:82:LEU:O      | 1:D:85:THR:OG1    | 1.94                     | 0.86              |
| 1:A:545:UNK:HA    | 1:A:548:UNK:CB    | 2.06                     | 0.86              |
| 1:A:657:THR:CG2   | 1:A:662:TRP:CH2   | 2.52                     | 0.86              |
| 1:B:1020:ARG:HH11 | 1:B:1024:TYR:HA   | 1.08                     | 0.86              |
| 1:D:728:ARG:NH1   | 1:D:1133:HIS:CG   | 2.16                     | 0.86              |
| 1:B:545:UNK:HA    | 1:B:548:UNK:CB    | 2.06                     | 0.86              |
| 1:D:1459:GLN:HG2  | 1:D:1553:PHE:CD1  | 2.09                     | 0.86              |
| 1:B:1016:ARG:C    | 1:B:1017:ARG:CZ   | 2.49                     | 0.86              |
| 1:B:3400:UNK:O    | 1:B:3404:UNK:N    | 2.08                     | 0.86              |
| 1:C:1000:ARG:CZ   | 1:C:1016:ARG:HG2  | 2.05                     | 0.86              |
| 1:A:4712:UNK:O    | 1:A:4720:UNK:N    | 1.94                     | 0.85              |
| 1:C:3804:UNK:H    | 1:C:3807:UNK:CB   | 1.89                     | 0.85              |
| 1:D:111:HIS:HD2   | 1:D:114:SER:H     | 1.23                     | 0.85              |
| 1:A:76:ARG:HA     | 1:A:79:GLN:CD     | 2.02                     | 0.85              |
| 1:B:728:ARG:CZ    | 1:B:1119:GLU:HA   | 2.06                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:855:PRO:HG3   | 1:B:994:ASN:O     | 1.76                     | 0.85              |
| 1:B:2299:UNK:CB   | 1:B:2352:UNK:CB   | 2.54                     | 0.85              |
| 1:D:728:ARG:CZ    | 1:D:1119:GLU:HA   | 2.06                     | 0.85              |
| 1:D:1020:ARG:NH1  | 1:D:1024:TYR:CA   | 2.31                     | 0.85              |
| 1:D:1434:TYR:CE1  | 1:D:1570:LYS:HB2  | 2.11                     | 0.85              |
| 1:A:1017:ARG:HH11 | 1:A:1017:ARG:HG3  | 1.38                     | 0.85              |
| 1:C:752:VAL:CG1   | 1:C:769:GLU:CG    | 2.49                     | 0.85              |
| 1:C:953:THR:C     | 1:C:959:TYR:CD2   | 2.54                     | 0.85              |
| 1:C:2299:UNK:CB   | 1:C:2352:UNK:CB   | 2.54                     | 0.85              |
| 1:D:3804:UNK:H    | 1:D:3807:UNK:CB   | 1.89                     | 0.85              |
| 1:A:83:ALA:O      | 1:A:86:VAL:HG13   | 1.75                     | 0.85              |
| 1:A:956:PRO:O     | 1:A:957:LYS:C     | 2.19                     | 0.85              |
| 1:A:996:TRP:HZ2   | 1:A:1021:LEU:HD13 | 1.04                     | 0.85              |
| 1:A:1000:ARG:HG2  | 1:A:1018:ASN:CG   | 2.01                     | 0.85              |
| 1:A:1016:ARG:C    | 1:A:1017:ARG:CZ   | 2.49                     | 0.85              |
| 1:A:3400:UNK:O    | 1:A:3404:UNK:N    | 2.08                     | 0.85              |
| 1:B:1438:ARG:HA   | 1:B:1515:VAL:CG1  | 2.02                     | 0.85              |
| 1:D:1000:ARG:HH21 | 1:D:1016:ARG:CG   | 1.73                     | 0.85              |
| 1:D:1001:VAL:C    | 1:D:1005:TRP:CE2  | 2.54                     | 0.85              |
| 1:D:1007:TYR:OH   | 1:D:1015:ALA:O    | 1.92                     | 0.85              |
| 1:C:728:ARG:CZ    | 1:C:1119:GLU:HA   | 2.06                     | 0.85              |
| 1:D:321:GLU:OE1   | 1:D:321:GLU:N     | 2.10                     | 0.85              |
| 1:D:953:THR:C     | 1:D:959:TYR:CD2   | 2.54                     | 0.85              |
| 1:A:1001:VAL:C    | 1:A:1005:TRP:CE2  | 2.54                     | 0.85              |
| 1:B:111:HIS:HD2   | 1:B:114:SER:H     | 1.23                     | 0.85              |
| 1:B:953:THR:C     | 1:B:959:TYR:CD2   | 2.54                     | 0.85              |
| 1:B:1003:GLN:O    | 1:B:1007:TYR:CD2  | 2.30                     | 0.85              |
| 1:C:322:LYS:HB3   | 1:C:323:LEU:C     | 2.00                     | 0.85              |
| 1:D:855:PRO:HG3   | 1:D:994:ASN:O     | 1.75                     | 0.85              |
| 1:D:1016:ARG:C    | 1:D:1017:ARG:CZ   | 2.49                     | 0.85              |
| 1:A:1003:GLN:O    | 1:A:1007:TYR:CD2  | 2.30                     | 0.85              |
| 1:A:3804:UNK:H    | 1:A:3807:UNK:CB   | 1.89                     | 0.85              |
| 1:B:82:LEU:O      | 1:B:85:THR:OG1    | 1.94                     | 0.85              |
| 1:B:956:PRO:O     | 1:B:957:LYS:C     | 2.19                     | 0.85              |
| 1:B:1007:TYR:CD1  | 1:B:1007:TYR:O    | 2.30                     | 0.85              |
| 1:C:1001:VAL:O    | 1:C:1005:TRP:CE2  | 2.30                     | 0.85              |
| 1:D:1001:VAL:O    | 1:D:1005:TRP:CE2  | 2.30                     | 0.85              |
| 1:D:1438:ARG:HA   | 1:D:1515:VAL:CG1  | 2.02                     | 0.85              |
| 1:A:953:THR:C     | 1:A:959:TYR:CD2   | 2.54                     | 0.85              |
| 1:A:1007:TYR:CD1  | 1:A:1007:TYR:O    | 2.30                     | 0.85              |
| 1:A:1444:GLU:HB2  | 1:A:1445:PRO:C    | 2.02                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:76:ARG:HA     | 1:B:79:GLN:CD     | 2.02                     | 0.85              |
| 1:C:545:UNK:HA    | 1:C:548:UNK:CB    | 2.06                     | 0.85              |
| 1:C:1434:TYR:CE1  | 1:C:1570:LYS:HB2  | 2.11                     | 0.85              |
| 1:A:1007:TYR:OH   | 1:A:1015:ALA:O    | 1.92                     | 0.85              |
| 1:B:321:GLU:OE1   | 1:B:321:GLU:N     | 2.10                     | 0.85              |
| 1:B:3986:UNK:HA   | 1:B:3989:UNK:CB   | 2.07                     | 0.85              |
| 1:C:76:ARG:HA     | 1:C:79:GLN:CD     | 2.02                     | 0.85              |
| 1:C:998:ARG:O     | 1:C:1001:VAL:HG12 | 1.77                     | 0.85              |
| 1:C:1000:ARG:HG2  | 1:C:1018:ASN:CG   | 2.01                     | 0.85              |
| 1:C:1001:VAL:C    | 1:C:1005:TRP:CE2  | 2.54                     | 0.85              |
| 1:D:1003:GLN:O    | 1:D:1007:TYR:CD2  | 2.30                     | 0.85              |
| 1:A:3986:UNK:HA   | 1:A:3989:UNK:CB   | 2.07                     | 0.84              |
| 1:B:207:SER:HA    | 1:B:269:TRP:CZ3   | 2.08                     | 0.84              |
| 1:B:1001:VAL:O    | 1:B:1005:TRP:CE2  | 2.30                     | 0.84              |
| 1:B:3804:UNK:H    | 1:B:3807:UNK:CB   | 1.89                     | 0.84              |
| 1:C:82:LEU:O      | 1:C:85:THR:OG1    | 1.94                     | 0.84              |
| 1:C:956:PRO:O     | 1:C:957:LYS:C     | 2.19                     | 0.84              |
| 1:C:1007:TYR:CD1  | 1:C:1007:TYR:O    | 2.30                     | 0.84              |
| 1:A:479:GLN:OE1   | 1:A:537:UNK:CB    | 2.26                     | 0.84              |
| 1:A:1001:VAL:O    | 1:A:1005:TRP:CE2  | 2.30                     | 0.84              |
| 1:C:1016:ARG:C    | 1:C:1017:ARG:CZ   | 2.49                     | 0.84              |
| 1:C:1020:ARG:HH12 | 1:C:1024:TYR:HA   | 1.35                     | 0.84              |
| 1:D:76:ARG:HA     | 1:D:79:GLN:CD     | 2.01                     | 0.84              |
| 1:D:1000:ARG:HG2  | 1:D:1018:ASN:CG   | 2.01                     | 0.84              |
| 1:A:1964:UNK:CB   | 1:A:2011:UNK:CB   | 2.56                     | 0.84              |
| 1:B:1007:TYR:O    | 1:B:1007:TYR:HD1  | 1.60                     | 0.84              |
| 1:B:1020:ARG:HH12 | 1:B:1024:TYR:HA   | 1.35                     | 0.84              |
| 1:D:956:PRO:O     | 1:D:957:LYS:C     | 2.19                     | 0.84              |
| 1:D:959:TYR:HB3   | 1:D:963:ASN:HD22  | 1.43                     | 0.84              |
| 1:D:993:HIS:O     | 1:D:996:TRP:CE3   | 2.30                     | 0.84              |
| 1:D:996:TRP:HZ2   | 1:D:1021:LEU:HD13 | 1.04                     | 0.84              |
| 1:B:657:THR:CG2   | 1:B:662:TRP:CH2   | 2.52                     | 0.84              |
| 1:B:993:HIS:O     | 1:B:996:TRP:CE3   | 2.30                     | 0.84              |
| 1:C:321:GLU:OE1   | 1:C:321:GLU:N     | 2.10                     | 0.84              |
| 1:C:959:TYR:HB3   | 1:C:963:ASN:HD22  | 1.43                     | 0.84              |
| 1:C:1020:ARG:HA   | 1:C:1020:ARG:HE   | 1.34                     | 0.84              |
| 1:D:1444:GLU:HB2  | 1:D:1445:PRO:C    | 2.02                     | 0.84              |
| 1:A:993:HIS:O     | 1:A:996:TRP:CE3   | 2.30                     | 0.84              |
| 1:B:954:LYS:N     | 1:B:971:ASP:OD1   | 2.07                     | 0.84              |
| 1:A:2299:UNK:CB   | 1:A:2352:UNK:CB   | 2.54                     | 0.84              |
| 1:B:1000:ARG:HG2  | 1:B:1018:ASN:CG   | 2.01                     | 0.84              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:1020:ARG:NH1 | 1:C:1024:TYR:CA   | 2.31                     | 0.84              |
| 1:D:323:LEU:HB2  | 1:D:324:ASP:C     | 2.03                     | 0.84              |
| 1:D:1001:VAL:O   | 1:D:1005:TRP:CD2  | 2.30                     | 0.84              |
| 1:D:1007:TYR:CD1 | 1:D:1007:TYR:O    | 2.30                     | 0.84              |
| 1:D:1964:UNK:CB  | 1:D:2011:UNK:CB   | 2.56                     | 0.84              |
| 1:D:2299:UNK:CB  | 1:D:2352:UNK:CB   | 2.54                     | 0.84              |
| 1:A:76:ARG:HA    | 1:A:79:GLN:OE1    | 1.78                     | 0.84              |
| 1:A:323:LEU:HB2  | 1:A:324:ASP:C     | 2.03                     | 0.84              |
| 1:B:479:GLN:OE1  | 1:B:537:UNK:CB    | 2.26                     | 0.84              |
| 1:B:1001:VAL:O   | 1:B:1005:TRP:CD2  | 2.30                     | 0.84              |
| 1:B:1001:VAL:C   | 1:B:1005:TRP:CE2  | 2.54                     | 0.84              |
| 1:C:479:GLN:OE1  | 1:C:537:UNK:CB    | 2.26                     | 0.84              |
| 1:C:1001:VAL:O   | 1:C:1005:TRP:CD2  | 2.30                     | 0.84              |
| 1:A:959:TYR:HB3  | 1:A:963:ASN:HD22  | 1.43                     | 0.84              |
| 1:A:998:ARG:O    | 1:A:1001:VAL:HG12 | 1.77                     | 0.84              |
| 1:B:76:ARG:HA    | 1:B:79:GLN:OE1    | 1.78                     | 0.84              |
| 1:C:1007:TYR:O   | 1:C:1007:TYR:HD1  | 1.60                     | 0.84              |
| 1:D:479:GLN:OE1  | 1:D:537:UNK:CB    | 2.26                     | 0.84              |
| 1:A:321:GLU:OE1  | 1:A:321:GLU:N     | 2.10                     | 0.84              |
| 1:A:993:HIS:CE1  | 1:A:1020:ARG:HA   | 2.12                     | 0.84              |
| 1:B:998:ARG:O    | 1:B:1001:VAL:HG12 | 1.77                     | 0.84              |
| 1:C:3986:UNK:HA  | 1:C:3989:UNK:CB   | 2.07                     | 0.84              |
| 1:D:3986:UNK:HA  | 1:D:3989:UNK:CB   | 2.07                     | 0.84              |
| 1:A:1001:VAL:O   | 1:A:1005:TRP:CD2  | 2.30                     | 0.84              |
| 1:B:324:ASP:HB2  | 1:B:325:THR:C     | 2.03                     | 0.84              |
| 1:B:1444:GLU:HB2 | 1:B:1445:PRO:C    | 2.02                     | 0.84              |
| 1:C:993:HIS:O    | 1:C:996:TRP:CE3   | 2.30                     | 0.84              |
| 1:D:545:UNK:HA   | 1:D:548:UNK:CB    | 2.06                     | 0.84              |
| 1:A:82:LEU:O     | 1:A:85:THR:OG1    | 1.94                     | 0.83              |
| 1:A:657:THR:CB   | 1:A:662:TRP:CD2   | 2.61                     | 0.83              |
| 1:B:323:LEU:HB2  | 1:B:324:ASP:C     | 2.03                     | 0.83              |
| 1:C:1964:UNK:CB  | 1:C:2011:UNK:CB   | 2.55                     | 0.83              |
| 1:B:1017:ARG:HD2 | 1:B:1017:ARG:H    | 1.39                     | 0.83              |
| 1:B:1001:VAL:C   | 1:B:1005:TRP:NE1  | 2.37                     | 0.83              |
| 1:B:1964:UNK:CB  | 1:B:2011:UNK:CB   | 2.56                     | 0.83              |
| 1:C:1003:GLN:O   | 1:C:1007:TYR:CD2  | 2.30                     | 0.83              |
| 1:A:1017:ARG:HD2 | 1:A:1017:ARG:H    | 1.39                     | 0.83              |
| 1:B:993:HIS:CE1  | 1:B:1020:ARG:HA   | 2.12                     | 0.83              |
| 1:D:76:ARG:HA    | 1:D:79:GLN:OE1    | 1.78                     | 0.83              |
| 1:A:728:ARG:CB   | 1:A:1134:LEU:HD23 | 2.07                     | 0.83              |
| 1:B:4116:UNK:O   | 1:B:4123:UNK:HA   | 1.78                     | 0.83              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:324:ASP:HB2  | 1:C:325:THR:C     | 2.03                     | 0.83              |
| 1:C:4116:UNK:O   | 1:C:4123:UNK:HA   | 1.78                     | 0.83              |
| 1:D:993:HIS:CE1  | 1:D:1020:ARG:HA   | 2.13                     | 0.83              |
| 1:C:1001:VAL:C   | 1:C:1005:TRP:NE1  | 2.37                     | 0.83              |
| 1:A:1001:VAL:C   | 1:A:1005:TRP:NE1  | 2.37                     | 0.83              |
| 1:B:1000:ARG:HD2 | 1:B:1000:ARG:O    | 1.79                     | 0.83              |
| 1:C:323:LEU:HB2  | 1:C:324:ASP:C     | 2.03                     | 0.83              |
| 1:A:752:VAL:CG1  | 1:A:769:GLU:CG    | 2.49                     | 0.83              |
| 1:A:1007:TYR:O   | 1:A:1007:TYR:HD1  | 1.60                     | 0.83              |
| 1:C:1000:ARG:O   | 1:C:1000:ARG:HD2  | 1.79                     | 0.83              |
| 1:C:1444:GLU:HB2 | 1:C:1445:PRO:C    | 2.02                     | 0.83              |
| 1:B:657:THR:CB   | 1:B:662:TRP:CD2   | 2.61                     | 0.83              |
| 1:D:998:ARG:O    | 1:D:1001:VAL:HG12 | 1.77                     | 0.83              |
| 1:C:207:SER:N    | 1:C:269:TRP:HZ3   | 1.60                     | 0.82              |
| 1:D:752:VAL:HG11 | 1:D:769:GLU:HG2   | 1.61                     | 0.82              |
| 1:D:1001:VAL:C   | 1:D:1005:TRP:NE1  | 2.37                     | 0.82              |
| 1:D:368:ARG:HG2  | 1:D:368:ARG:NH1   | 1.94                     | 0.82              |
| 1:D:993:HIS:CA   | 1:D:996:TRP:CE3   | 2.42                     | 0.82              |
| 1:D:4116:UNK:O   | 1:D:4123:UNK:HA   | 1.79                     | 0.82              |
| 1:A:324:ASP:HB2  | 1:A:325:THR:C     | 2.03                     | 0.82              |
| 1:A:4116:UNK:O   | 1:A:4123:UNK:HA   | 1.78                     | 0.82              |
| 1:B:4788:UNK:O   | 1:B:4792:UNK:N    | 2.13                     | 0.82              |
| 1:C:752:VAL:HG11 | 1:C:769:GLU:HG2   | 1.61                     | 0.82              |
| 1:D:4788:UNK:O   | 1:D:4792:UNK:N    | 2.13                     | 0.82              |
| 1:C:76:ARG:HA    | 1:C:79:GLN:OE1    | 1.78                     | 0.82              |
| 1:C:752:VAL:HB   | 1:C:753:PRO:C     | 2.04                     | 0.82              |
| 1:A:752:VAL:HB   | 1:A:753:PRO:C     | 2.04                     | 0.82              |
| 1:D:324:ASP:HB2  | 1:D:325:THR:C     | 2.03                     | 0.82              |
| 1:D:752:VAL:HB   | 1:D:753:PRO:C     | 2.04                     | 0.82              |
| 1:D:1017:ARG:NH1 | 1:D:1017:ARG:HG3  | 1.93                     | 0.82              |
| 1:A:111:HIS:HD2  | 1:A:114:SER:H     | 1.23                     | 0.82              |
| 1:B:954:LYS:CB   | 1:B:971:ASP:CG    | 2.53                     | 0.82              |
| 1:C:4788:UNK:O   | 1:C:4792:UNK:N    | 2.13                     | 0.82              |
| 1:D:1000:ARG:HD2 | 1:D:1000:ARG:O    | 1.79                     | 0.82              |
| 1:B:959:TYR:HB3  | 1:B:963:ASN:HD22  | 1.43                     | 0.82              |
| 1:B:752:VAL:HB   | 1:B:753:PRO:C     | 2.04                     | 0.82              |
| 1:C:1438:ARG:HA  | 1:C:1515:VAL:CG1  | 2.02                     | 0.82              |
| 1:A:990:GLU:O    | 1:A:993:HIS:CB    | 2.28                     | 0.81              |
| 1:A:1000:ARG:O   | 1:A:1000:ARG:HD2  | 1.79                     | 0.81              |
| 1:B:728:ARG:CB   | 1:B:1134:LEU:HD23 | 2.07                     | 0.81              |
| 1:C:954:LYS:CB   | 1:C:971:ASP:CG    | 2.53                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:954:LYS:CB    | 1:D:971:ASP:CG    | 2.53                     | 0.81              |
| 1:B:990:GLU:O     | 1:B:993:HIS:CB    | 2.28                     | 0.81              |
| 1:C:4818:UNK:H    | 1:C:4821:UNK:CB   | 1.93                     | 0.81              |
| 1:D:1453:VAL:O    | 1:D:1548:LEU:HA   | 1.81                     | 0.81              |
| 1:A:1453:VAL:O    | 1:A:1548:LEU:HA   | 1.81                     | 0.81              |
| 1:B:752:VAL:CG1   | 1:B:769:GLU:CG    | 2.49                     | 0.81              |
| 1:B:3265:UNK:O    | 1:B:3266:UNK:C    | 2.28                     | 0.81              |
| 1:C:1020:ARG:HH11 | 1:C:1024:TYR:CA   | 1.91                     | 0.81              |
| 1:D:4818:UNK:H    | 1:D:4821:UNK:CB   | 1.93                     | 0.81              |
| 1:B:1000:ARG:NE   | 1:B:1016:ARG:CG   | 2.44                     | 0.81              |
| 1:D:1007:TYR:O    | 1:D:1007:TYR:HD1  | 1.60                     | 0.81              |
| 1:D:1462:MET:HE1  | 1:D:1559:GLN:HG2  | 1.62                     | 0.81              |
| 1:A:77:ALA:HA     | 1:A:80:GLU:OE2    | 1.81                     | 0.81              |
| 1:A:4788:UNK:O    | 1:A:4792:UNK:N    | 2.12                     | 0.81              |
| 1:B:576:UNK:HA    | 1:B:579:UNK:CB    | 2.11                     | 0.81              |
| 1:B:1558:HIS:CD2  | 1:B:1559:GLN:H    | 1.99                     | 0.81              |
| 1:C:1558:HIS:CD2  | 1:C:1559:GLN:H    | 1.99                     | 0.81              |
| 1:D:990:GLU:O     | 1:D:993:HIS:CB    | 2.28                     | 0.81              |
| 1:D:1000:ARG:NE   | 1:D:1016:ARG:CG   | 2.44                     | 0.81              |
| 1:C:657:THR:CG2   | 1:C:662:TRP:CH2   | 2.52                     | 0.81              |
| 1:A:1000:ARG:CZ   | 1:A:1016:ARG:CG   | 2.59                     | 0.81              |
| 1:A:4818:UNK:H    | 1:A:4821:UNK:CB   | 1.93                     | 0.81              |
| 1:B:4818:UNK:H    | 1:B:4821:UNK:CB   | 1.93                     | 0.81              |
| 1:C:657:THR:CB    | 1:C:662:TRP:CD2   | 2.61                     | 0.81              |
| 1:C:3306:UNK:HA   | 1:C:3309:UNK:N    | 1.96                     | 0.81              |
| 1:D:131:LEU:HB3   | 1:D:178:ARG:HH12  | 1.46                     | 0.81              |
| 1:D:956:PRO:CD    | 1:D:959:TYR:CD1   | 2.58                     | 0.81              |
| 1:A:1000:ARG:NE   | 1:A:1016:ARG:CG   | 2.44                     | 0.81              |
| 1:C:1000:ARG:NE   | 1:C:1016:ARG:CG   | 2.44                     | 0.81              |
| 1:A:3265:UNK:O    | 1:A:3266:UNK:C    | 2.28                     | 0.81              |
| 1:B:1437:VAL:HG21 | 1:B:1518:CYS:CB   | 2.11                     | 0.81              |
| 1:B:1462:MET:HE1  | 1:B:1559:GLN:HG2  | 1.62                     | 0.81              |
| 1:B:2292:UNK:CB   | 1:B:2348:UNK:CB   | 2.59                     | 0.81              |
| 1:B:3306:UNK:HA   | 1:B:3309:UNK:N    | 1.96                     | 0.81              |
| 1:C:1462:MET:HE1  | 1:C:1559:GLN:HG2  | 1.62                     | 0.81              |
| 1:B:3316:UNK:CA   | 1:B:3322:UNK:CB   | 2.59                     | 0.80              |
| 1:D:728:ARG:CB    | 1:D:1134:LEU:HD23 | 2.07                     | 0.80              |
| 1:A:1437:VAL:HG21 | 1:A:1518:CYS:CB   | 2.11                     | 0.80              |
| 1:B:1020:ARG:HH11 | 1:B:1024:TYR:CA   | 1.91                     | 0.80              |
| 1:A:576:UNK:HA    | 1:A:579:UNK:CB    | 2.11                     | 0.80              |
| 1:A:1558:HIS:CD2  | 1:A:1559:GLN:H    | 1.99                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:956:PRO:HG2   | 1:B:959:TYR:CE1   | 2.15                     | 0.80              |
| 1:D:998:ARG:CD    | 1:D:999:ASP:OD1   | 2.30                     | 0.80              |
| 1:A:76:ARG:O      | 1:A:80:GLU:HG2    | 1.82                     | 0.80              |
| 1:A:954:LYS:CB    | 1:A:971:ASP:CG    | 2.53                     | 0.80              |
| 1:B:1851:UNK:HA   | 1:B:1854:UNK:CB   | 2.11                     | 0.80              |
| 1:C:4172:UNK:O    | 1:C:4175:UNK:N    | 2.15                     | 0.80              |
| 1:D:3265:UNK:O    | 1:D:3266:UNK:C    | 2.28                     | 0.80              |
| 1:A:1851:UNK:HA   | 1:A:1854:UNK:CB   | 2.11                     | 0.80              |
| 1:C:996:TRP:HZ2   | 1:C:1021:LEU:HD13 | 1.05                     | 0.80              |
| 1:C:1000:ARG:O    | 1:C:1000:ARG:CD   | 2.30                     | 0.80              |
| 1:D:1000:ARG:O    | 1:D:1000:ARG:CD   | 2.30                     | 0.80              |
| 1:D:1020:ARG:HH11 | 1:D:1024:TYR:CA   | 1.91                     | 0.80              |
| 1:D:1851:UNK:HA   | 1:D:1854:UNK:CB   | 2.11                     | 0.80              |
| 1:A:131:LEU:HB3   | 1:A:178:ARG:HH12  | 1.46                     | 0.80              |
| 1:B:77:ALA:HA     | 1:B:80:GLU:OE2    | 1.81                     | 0.80              |
| 1:B:1017:ARG:NH1  | 1:B:1017:ARG:HG3  | 1.93                     | 0.80              |
| 1:C:368:ARG:NH1   | 1:C:371:VAL:HB    | 1.97                     | 0.80              |
| 1:C:728:ARG:CB    | 1:C:1134:LEU:HD23 | 2.07                     | 0.80              |
| 1:D:1558:HIS:CD2  | 1:D:1559:GLN:H    | 1.99                     | 0.80              |
| 1:D:3316:UNK:CA   | 1:D:3322:UNK:CB   | 2.59                     | 0.80              |
| 1:A:998:ARG:CZ    | 1:A:998:ARG:O     | 2.30                     | 0.80              |
| 1:A:2292:UNK:CB   | 1:A:2348:UNK:CB   | 2.59                     | 0.80              |
| 1:B:1016:ARG:O    | 1:B:1017:ARG:CZ   | 2.30                     | 0.80              |
| 1:C:1851:UNK:HA   | 1:C:1854:UNK:CB   | 2.11                     | 0.80              |
| 1:C:3265:UNK:O    | 1:C:3266:UNK:C    | 2.28                     | 0.80              |
| 1:D:368:ARG:NH1   | 1:D:371:VAL:HB    | 1.97                     | 0.80              |
| 1:A:321:GLU:HB2   | 1:A:323:LEU:CD1   | 2.12                     | 0.80              |
| 1:B:752:VAL:HG11  | 1:B:769:GLU:HG2   | 1.61                     | 0.80              |
| 1:B:1021:LEU:O    | 1:B:1022:VAL:CG1  | 2.30                     | 0.80              |
| 1:C:77:ALA:HA     | 1:C:80:GLU:OE2    | 1.81                     | 0.80              |
| 1:C:990:GLU:O     | 1:C:993:HIS:CB    | 2.28                     | 0.80              |
| 1:C:1453:VAL:O    | 1:C:1548:LEU:HA   | 1.81                     | 0.80              |
| 1:D:1000:ARG:CZ   | 1:D:1016:ARG:CG   | 2.59                     | 0.80              |
| 1:D:2292:UNK:CB   | 1:D:2348:UNK:CB   | 2.59                     | 0.80              |
| 1:B:368:ARG:NH1   | 1:B:371:VAL:HB    | 1.97                     | 0.80              |
| 1:B:1018:ASN:O    | 1:B:1021:LEU:CD2  | 2.30                     | 0.80              |
| 1:B:4172:UNK:O    | 1:B:4175:UNK:N    | 2.15                     | 0.80              |
| 1:C:131:LEU:HB3   | 1:C:178:ARG:HH12  | 1.46                     | 0.80              |
| 1:C:206:CYS:C     | 1:C:269:TRP:CZ3   | 2.60                     | 0.80              |
| 1:C:998:ARG:CZ    | 1:C:998:ARG:O     | 2.30                     | 0.80              |
| 1:C:1437:VAL:HG21 | 1:C:1518:CYS:SG   | 2.22                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1437:VAL:HG21 | 1:C:1518:CYS:CB   | 2.11                     | 0.80              |
| 1:D:77:ALA:HA     | 1:D:80:GLU:OE2    | 1.81                     | 0.80              |
| 1:D:576:UNK:HA    | 1:D:579:UNK:CB    | 2.11                     | 0.80              |
| 1:D:956:PRO:HG3   | 1:D:959:TYR:CD1   | 1.94                     | 0.80              |
| 1:D:4172:UNK:O    | 1:D:4175:UNK:N    | 2.15                     | 0.80              |
| 1:A:207:SER:HA    | 1:A:269:TRP:CZ3   | 2.08                     | 0.80              |
| 1:A:368:ARG:NH1   | 1:A:371:VAL:HB    | 1.97                     | 0.80              |
| 1:B:1015:ALA:O    | 1:B:1016:ARG:CD   | 2.30                     | 0.80              |
| 1:D:1015:ALA:O    | 1:D:1016:ARG:CG   | 2.30                     | 0.80              |
| 1:A:206:CYS:C     | 1:A:269:TRP:CZ3   | 2.60                     | 0.79              |
| 1:A:1021:LEU:O    | 1:A:1022:VAL:CG2  | 2.30                     | 0.79              |
| 1:A:3316:UNK:CA   | 1:A:3322:UNK:CB   | 2.59                     | 0.79              |
| 1:A:4172:UNK:O    | 1:A:4175:UNK:N    | 2.15                     | 0.79              |
| 1:B:76:ARG:O      | 1:B:80:GLU:HG2    | 1.82                     | 0.79              |
| 1:B:1000:ARG:O    | 1:B:1000:ARG:CD   | 2.30                     | 0.79              |
| 1:C:993:HIS:CE1   | 1:C:1020:ARG:HA   | 2.12                     | 0.79              |
| 1:C:2292:UNK:CB   | 1:C:2348:UNK:CB   | 2.59                     | 0.79              |
| 1:C:3316:UNK:CA   | 1:C:3322:UNK:CB   | 2.59                     | 0.79              |
| 1:D:222:LEU:HD23  | 1:D:390:LEU:HD22  | 1.64                     | 0.79              |
| 1:D:657:THR:CB    | 1:D:662:TRP:CD2   | 2.61                     | 0.79              |
| 1:D:1018:ASN:CG   | 1:D:1021:LEU:HD21 | 2.07                     | 0.79              |
| 1:D:1021:LEU:O    | 1:D:1022:VAL:CG2  | 2.30                     | 0.79              |
| 1:D:1476:MET:CE   | 1:D:1516:ILE:CD1  | 2.60                     | 0.79              |
| 1:A:1021:LEU:O    | 1:A:1022:VAL:CG1  | 2.30                     | 0.79              |
| 1:A:1439:VAL:CG2  | 1:A:1516:ILE:HG22 | 2.13                     | 0.79              |
| 1:A:3306:UNK:HA   | 1:A:3309:UNK:N    | 1.96                     | 0.79              |
| 1:C:1020:ARG:NE   | 1:C:1020:ARG:CA   | 2.45                     | 0.79              |
| 1:C:1474:VAL:HB   | 1:C:1529:PHE:CE2  | 2.18                     | 0.79              |
| 1:D:207:SER:HA    | 1:D:269:TRP:CZ3   | 2.08                     | 0.79              |
| 1:D:998:ARG:HD3   | 1:D:999:ASP:H     | 1.47                     | 0.79              |
| 1:D:1437:VAL:HG21 | 1:D:1518:CYS:CB   | 2.11                     | 0.79              |
| 1:D:1452:TRP:HB3  | 1:D:1548:LEU:HB3  | 1.64                     | 0.79              |
| 1:A:1007:TYR:HE1  | 1:A:1015:ALA:CA   | 1.95                     | 0.79              |
| 1:B:321:GLU:HB2   | 1:B:323:LEU:CD1   | 2.13                     | 0.79              |
| 1:C:76:ARG:O      | 1:C:80:GLU:HG2    | 1.82                     | 0.79              |
| 1:C:1016:ARG:O    | 1:C:1017:ARG:CZ   | 2.30                     | 0.79              |
| 1:C:1018:ASN:CG   | 1:C:1021:LEU:HD21 | 2.07                     | 0.79              |
| 1:D:206:CYS:C     | 1:D:269:TRP:CZ3   | 2.60                     | 0.79              |
| 1:D:321:GLU:HB2   | 1:D:323:LEU:CD1   | 2.12                     | 0.79              |
| 1:D:1017:ARG:NH1  | 1:D:1017:ARG:CA   | 2.46                     | 0.79              |
| 1:D:1474:VAL:HG22 | 1:D:1540:PHE:CE2  | 2.18                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:572:UNK:O     | 1:A:575:UNK:CB    | 2.31                     | 0.79              |
| 1:A:998:ARG:CD    | 1:A:999:ASP:OD1   | 2.30                     | 0.79              |
| 1:A:1474:VAL:HB   | 1:A:1529:PHE:CE2  | 2.18                     | 0.79              |
| 1:B:256:ALA:HB3   | 1:B:481:GLU:OE2   | 1.83                     | 0.79              |
| 1:B:998:ARG:CD    | 1:B:999:ASP:OD1   | 2.30                     | 0.79              |
| 1:C:576:UNK:HA    | 1:C:579:UNK:CB    | 2.11                     | 0.79              |
| 1:C:1474:VAL:HG22 | 1:C:1540:PHE:CE2  | 2.18                     | 0.79              |
| 1:C:1477:GLY:O    | 1:C:1510:SER:O    | 2.01                     | 0.79              |
| 1:D:1021:LEU:O    | 1:D:1022:VAL:CG1  | 2.30                     | 0.79              |
| 1:A:222:LEU:HD23  | 1:A:390:LEU:HD22  | 1.64                     | 0.79              |
| 1:A:1018:ASN:CG   | 1:A:1021:LEU:HD21 | 2.07                     | 0.79              |
| 1:A:1437:VAL:HG21 | 1:A:1518:CYS:SG   | 2.22                     | 0.79              |
| 1:A:1462:MET:HE1  | 1:A:1559:GLN:HG2  | 1.62                     | 0.79              |
| 1:B:1018:ASN:CG   | 1:B:1021:LEU:HD21 | 2.07                     | 0.79              |
| 1:C:572:UNK:O     | 1:C:575:UNK:CB    | 2.31                     | 0.79              |
| 1:C:1015:ALA:O    | 1:C:1016:ARG:CG   | 2.30                     | 0.79              |
| 1:C:1021:LEU:O    | 1:C:1022:VAL:CG2  | 2.30                     | 0.79              |
| 1:A:1020:ARG:HH11 | 1:A:1024:TYR:CA   | 1.91                     | 0.79              |
| 1:C:1000:ARG:CZ   | 1:C:1016:ARG:CG   | 2.59                     | 0.79              |
| 1:C:1018:ASN:O    | 1:C:1021:LEU:CD2  | 2.30                     | 0.79              |
| 1:D:3306:UNK:HA   | 1:D:3309:UNK:N    | 1.96                     | 0.79              |
| 1:A:1015:ALA:O    | 1:A:1016:ARG:CD   | 2.30                     | 0.79              |
| 1:B:1007:TYR:HE1  | 1:B:1015:ALA:CA   | 1.95                     | 0.79              |
| 1:B:1015:ALA:O    | 1:B:1016:ARG:CG   | 2.30                     | 0.79              |
| 1:C:321:GLU:HB2   | 1:C:323:LEU:CD1   | 2.12                     | 0.79              |
| 1:C:998:ARG:CD    | 1:C:999:ASP:OD1   | 2.30                     | 0.79              |
| 1:C:1000:ARG:HE   | 1:C:1016:ARG:CG   | 1.96                     | 0.79              |
| 1:D:572:UNK:O     | 1:D:575:UNK:CB    | 2.31                     | 0.79              |
| 1:D:1016:ARG:O    | 1:D:1017:ARG:CZ   | 2.30                     | 0.79              |
| 1:D:1437:VAL:HG21 | 1:D:1518:CYS:SG   | 2.23                     | 0.79              |
| 1:A:256:ALA:HB3   | 1:A:481:GLU:OE2   | 1.83                     | 0.79              |
| 1:A:1016:ARG:O    | 1:A:1017:ARG:CZ   | 2.30                     | 0.79              |
| 1:A:1432:THR:OG1  | 1:A:1523:ALA:CB   | 2.30                     | 0.79              |
| 1:B:1453:VAL:O    | 1:B:1548:LEU:HA   | 1.81                     | 0.79              |
| 1:B:1474:VAL:HG22 | 1:B:1540:PHE:CE2  | 2.17                     | 0.79              |
| 1:C:1015:ALA:O    | 1:C:1016:ARG:CD   | 2.30                     | 0.79              |
| 1:C:1018:ASN:HB2  | 1:C:1021:LEU:HD22 | 1.64                     | 0.79              |
| 1:D:1439:VAL:CG2  | 1:D:1516:ILE:HG22 | 2.13                     | 0.79              |
| 1:A:1474:VAL:HG22 | 1:A:1540:PHE:CE2  | 2.17                     | 0.79              |
| 1:A:1476:MET:CE   | 1:A:1516:ILE:CD1  | 2.60                     | 0.79              |
| 1:A:3317:UNK:N    | 1:A:3322:UNK:CB   | 2.46                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1000:ARG:CZ   | 1:B:1016:ARG:CD   | 2.61                     | 0.79              |
| 1:B:1432:THR:OG1  | 1:B:1523:ALA:CB   | 2.30                     | 0.79              |
| 1:B:1437:VAL:HG21 | 1:B:1518:CYS:SG   | 2.22                     | 0.79              |
| 1:B:1476:MET:CE   | 1:B:1516:ILE:CD1  | 2.60                     | 0.79              |
| 1:C:207:SER:HA    | 1:C:269:TRP:CZ3   | 2.08                     | 0.79              |
| 1:C:256:ALA:HB3   | 1:C:481:GLU:OE2   | 1.83                     | 0.79              |
| 1:C:953:THR:CG2   | 1:C:971:ASP:OD1   | 2.31                     | 0.79              |
| 1:C:1017:ARG:NH1  | 1:C:1017:ARG:HG3  | 1.93                     | 0.79              |
| 1:D:76:ARG:O      | 1:D:80:GLU:HG2    | 1.82                     | 0.79              |
| 1:D:1007:TYR:HE1  | 1:D:1015:ALA:CA   | 1.95                     | 0.79              |
| 1:D:1018:ASN:HB2  | 1:D:1021:LEU:HD22 | 1.64                     | 0.79              |
| 1:D:1474:VAL:HB   | 1:D:1529:PHE:CE2  | 2.17                     | 0.79              |
| 1:A:953:THR:CG2   | 1:A:971:ASP:OD1   | 2.31                     | 0.79              |
| 1:A:1000:ARG:O    | 1:A:1000:ARG:CD   | 2.30                     | 0.79              |
| 1:A:1015:ALA:O    | 1:A:1016:ARG:CG   | 2.30                     | 0.79              |
| 1:A:1452:TRP:HB3  | 1:A:1548:LEU:HB3  | 1.64                     | 0.79              |
| 1:B:998:ARG:CZ    | 1:B:998:ARG:O     | 2.30                     | 0.79              |
| 1:B:206:CYS:C     | 1:B:269:TRP:CZ3   | 2.60                     | 0.78              |
| 1:C:1021:LEU:O    | 1:C:1022:VAL:CG1  | 2.30                     | 0.78              |
| 1:C:1452:TRP:HB3  | 1:C:1548:LEU:HB3  | 1.64                     | 0.78              |
| 1:C:1476:MET:CE   | 1:C:1516:ILE:CD1  | 2.60                     | 0.78              |
| 1:D:1000:ARG:CZ   | 1:D:1016:ARG:CD   | 2.61                     | 0.78              |
| 1:A:1018:ASN:O    | 1:A:1021:LEU:CD2  | 2.30                     | 0.78              |
| 1:B:362:PRO:HD3   | 1:B:374:LYS:HG2   | 1.65                     | 0.78              |
| 1:B:368:ARG:HG2   | 1:B:368:ARG:NH1   | 1.94                     | 0.78              |
| 1:B:1439:VAL:CG2  | 1:B:1516:ILE:HG22 | 2.13                     | 0.78              |
| 1:B:1452:TRP:HB3  | 1:B:1548:LEU:HB3  | 1.64                     | 0.78              |
| 1:B:1474:VAL:HB   | 1:B:1529:PHE:CE2  | 2.18                     | 0.78              |
| 1:B:2292:UNK:CA   | 1:B:2348:UNK:CB   | 2.61                     | 0.78              |
| 1:C:317:ARG:CZ    | 1:C:322:LYS:C     | 2.56                     | 0.78              |
| 1:C:445:LEU:HD23  | 1:C:521:LEU:HB2   | 1.65                     | 0.78              |
| 1:D:998:ARG:CZ    | 1:D:998:ARG:O     | 2.30                     | 0.78              |
| 1:D:1015:ALA:O    | 1:D:1016:ARG:CD   | 2.30                     | 0.78              |
| 1:D:2292:UNK:CA   | 1:D:2348:UNK:CB   | 2.61                     | 0.78              |
| 1:A:82:LEU:HD11   | 1:A:144:GLU:OE2   | 1.84                     | 0.78              |
| 1:A:657:THR:CG2   | 1:A:662:TRP:CZ2   | 2.66                     | 0.78              |
| 1:B:321:GLU:HB2   | 1:B:323:LEU:HD13  | 1.65                     | 0.78              |
| 1:C:1000:ARG:CZ   | 1:C:1016:ARG:CD   | 2.61                     | 0.78              |
| 1:D:82:LEU:HD11   | 1:D:144:GLU:OE2   | 1.84                     | 0.78              |
| 1:D:256:ALA:HB3   | 1:D:481:GLU:OE2   | 1.83                     | 0.78              |
| 1:D:4710:UNK:O    | 1:D:4719:UNK:CB   | 2.31                     | 0.78              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:362:PRO:HD3  | 1:A:374:LYS:HG2   | 1.65                     | 0.78              |
| 1:A:1437:VAL:CG2 | 1:A:1518:CYS:HB2  | 2.14                     | 0.78              |
| 1:A:1477:GLY:O   | 1:A:1510:SER:O    | 2.00                     | 0.78              |
| 1:B:131:LEU:HB3  | 1:B:178:ARG:HH12  | 1.46                     | 0.78              |
| 1:B:445:LEU:HD23 | 1:B:521:LEU:HB2   | 1.65                     | 0.78              |
| 1:B:1000:ARG:HE  | 1:B:1016:ARG:CG   | 1.96                     | 0.78              |
| 1:B:3317:UNK:N   | 1:B:3322:UNK:CB   | 2.46                     | 0.78              |
| 1:C:1017:ARG:NH1 | 1:C:1017:ARG:CA   | 2.46                     | 0.78              |
| 1:C:3317:UNK:N   | 1:C:3322:UNK:CB   | 2.46                     | 0.78              |
| 1:A:998:ARG:HD3  | 1:A:999:ASP:H     | 1.48                     | 0.78              |
| 1:A:1437:VAL:C   | 1:A:1516:ILE:O    | 2.27                     | 0.78              |
| 1:A:2292:UNK:CA  | 1:A:2348:UNK:CB   | 2.61                     | 0.78              |
| 1:B:572:UNK:O    | 1:B:575:UNK:CB    | 2.31                     | 0.78              |
| 1:A:445:LEU:HD23 | 1:A:521:LEU:HB2   | 1.65                     | 0.78              |
| 1:B:1017:ARG:NH1 | 1:B:1017:ARG:CA   | 2.46                     | 0.78              |
| 1:B:1018:ASN:HB2 | 1:B:1021:LEU:HD22 | 1.64                     | 0.78              |
| 1:B:1021:LEU:O   | 1:B:1022:VAL:CG2  | 2.30                     | 0.78              |
| 1:B:1437:VAL:C   | 1:B:1516:ILE:O    | 2.27                     | 0.78              |
| 1:C:1007:TYR:HE1 | 1:C:1015:ALA:CA   | 1.95                     | 0.78              |
| 1:C:1439:VAL:CG2 | 1:C:1516:ILE:HG22 | 2.13                     | 0.78              |
| 1:D:1432:THR:OG1 | 1:D:1523:ALA:CB   | 2.30                     | 0.78              |
| 1:A:1017:ARG:NH1 | 1:A:1017:ARG:CA   | 2.46                     | 0.78              |
| 1:B:424:LYS:NZ   | 1:B:505:GLU:HB2   | 1.99                     | 0.78              |
| 1:B:657:THR:CG2  | 1:B:662:TRP:CZ2   | 2.66                     | 0.78              |
| 1:B:1000:ARG:CZ  | 1:B:1016:ARG:CG   | 2.59                     | 0.78              |
| 1:D:953:THR:CG2  | 1:D:971:ASP:OD1   | 2.31                     | 0.78              |
| 1:A:321:GLU:HB2  | 1:A:323:LEU:HD13  | 1.65                     | 0.78              |
| 1:A:1000:ARG:CZ  | 1:A:1016:ARG:CD   | 2.61                     | 0.78              |
| 1:B:317:ARG:CZ   | 1:B:322:LYS:C     | 2.56                     | 0.78              |
| 1:C:207:SER:CB   | 1:C:269:TRP:HZ3   | 1.97                     | 0.78              |
| 1:D:77:ALA:HA    | 1:D:80:GLU:CG     | 2.14                     | 0.78              |
| 1:D:1000:ARG:HE  | 1:D:1016:ARG:CG   | 1.96                     | 0.78              |
| 1:D:1018:ASN:O   | 1:D:1021:LEU:CD2  | 2.30                     | 0.78              |
| 1:B:953:THR:CG2  | 1:B:971:ASP:OD1   | 2.31                     | 0.78              |
| 1:B:1477:GLY:O   | 1:B:1510:SER:O    | 2.00                     | 0.78              |
| 1:D:1434:TYR:CD1 | 1:D:1570:LYS:HB2  | 2.19                     | 0.78              |
| 1:D:1437:VAL:C   | 1:D:1516:ILE:O    | 2.27                     | 0.78              |
| 1:B:77:ALA:HA    | 1:B:80:GLU:CD     | 2.10                     | 0.78              |
| 1:C:77:ALA:HA    | 1:C:80:GLU:CG     | 2.14                     | 0.78              |
| 1:C:1437:VAL:O   | 1:C:1516:ILE:C    | 2.27                     | 0.78              |
| 1:D:445:LEU:HD23 | 1:D:521:LEU:HB2   | 1.65                     | 0.78              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:77:ALA:HA    | 1:A:80:GLU:CD     | 2.09                     | 0.77              |
| 1:A:4710:UNK:O   | 1:A:4719:UNK:CB   | 2.31                     | 0.77              |
| 1:B:1437:VAL:CG2 | 1:B:1518:CYS:HB2  | 2.14                     | 0.77              |
| 1:C:222:LEU:HD23 | 1:C:390:LEU:HD22  | 1.64                     | 0.77              |
| 1:C:2292:UNK:CA  | 1:C:2348:UNK:CB   | 2.61                     | 0.77              |
| 1:C:4710:UNK:O   | 1:C:4719:UNK:CB   | 2.32                     | 0.77              |
| 1:D:207:SER:CB   | 1:D:269:TRP:HZ3   | 1.97                     | 0.77              |
| 1:D:1437:VAL:CG2 | 1:D:1518:CYS:HB2  | 2.14                     | 0.77              |
| 1:D:1477:GLY:O   | 1:D:1510:SER:O    | 2.00                     | 0.77              |
| 1:A:77:ALA:HA    | 1:A:80:GLU:CG     | 2.14                     | 0.77              |
| 1:A:1000:ARG:HE  | 1:A:1016:ARG:CG   | 1.96                     | 0.77              |
| 1:A:1434:TYR:CD1 | 1:A:1570:LYS:HB2  | 2.18                     | 0.77              |
| 1:B:222:LEU:HD23 | 1:B:390:LEU:HD22  | 1.64                     | 0.77              |
| 1:B:1001:VAL:CG1 | 1:B:1005:TRP:HE1  | 1.87                     | 0.77              |
| 1:C:77:ALA:HA    | 1:C:80:GLU:CD     | 2.10                     | 0.77              |
| 1:C:82:LEU:HD11  | 1:C:144:GLU:OE2   | 1.84                     | 0.77              |
| 1:C:657:THR:CG2  | 1:C:662:TRP:CZ2   | 2.66                     | 0.77              |
| 1:C:1434:TYR:CD1 | 1:C:1570:LYS:HB2  | 2.18                     | 0.77              |
| 1:D:317:ARG:CZ   | 1:D:322:LYS:C     | 2.56                     | 0.77              |
| 1:D:424:LYS:NZ   | 1:D:505:GLU:HB2   | 1.99                     | 0.77              |
| 1:D:1437:VAL:O   | 1:D:1516:ILE:C    | 2.27                     | 0.77              |
| 1:B:855:PRO:HA   | 1:B:994:ASN:ND2   | 1.85                     | 0.77              |
| 1:B:4710:UNK:O   | 1:B:4719:UNK:CB   | 2.32                     | 0.77              |
| 1:C:424:LYS:NZ   | 1:C:505:GLU:HB2   | 1.99                     | 0.77              |
| 1:C:1022:VAL:O   | 1:C:1023:PRO:C    | 2.27                     | 0.77              |
| 1:A:1020:ARG:NH1 | 1:A:1024:TYR:CA   | 2.31                     | 0.77              |
| 1:C:1018:ASN:CB  | 1:C:1021:LEU:CD2  | 2.30                     | 0.77              |
| 1:C:1437:VAL:CG2 | 1:C:1518:CYS:HB2  | 2.14                     | 0.77              |
| 1:D:657:THR:CG2  | 1:D:662:TRP:CZ2   | 2.67                     | 0.77              |
| 1:D:3317:UNK:N   | 1:D:3322:UNK:CB   | 2.46                     | 0.77              |
| 1:A:1022:VAL:O   | 1:A:1023:PRO:C    | 2.27                     | 0.77              |
| 1:B:1434:TYR:CD1 | 1:B:1570:LYS:HB2  | 2.18                     | 0.77              |
| 1:B:1471:ALA:O   | 1:B:1472:VAL:HG23 | 1.85                     | 0.77              |
| 1:A:317:ARG:CZ   | 1:A:322:LYS:C     | 2.56                     | 0.77              |
| 1:B:77:ALA:HA    | 1:B:80:GLU:CG     | 2.14                     | 0.77              |
| 1:B:82:LEU:HD11  | 1:B:144:GLU:OE2   | 1.84                     | 0.77              |
| 1:C:321:GLU:HB2  | 1:C:323:LEU:HD13  | 1.65                     | 0.77              |
| 1:C:855:PRO:HA   | 1:C:994:ASN:ND2   | 1.85                     | 0.77              |
| 1:D:1471:ALA:O   | 1:D:1472:VAL:HG23 | 1.84                     | 0.77              |
| 1:B:998:ARG:HD3  | 1:B:999:ASP:H     | 1.47                     | 0.77              |
| 1:C:1437:VAL:C   | 1:C:1516:ILE:O    | 2.27                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:69:LEU:HD22   | 1:D:107:ILE:HD11  | 1.67                     | 0.77              |
| 1:D:1022:VAL:O    | 1:D:1022:VAL:CG2  | 2.33                     | 0.77              |
| 1:A:329:ARG:HG3   | 1:A:329:ARG:NH1   | 1.97                     | 0.77              |
| 1:B:1021:LEU:HD13 | 1:B:1021:LEU:N    | 1.98                     | 0.77              |
| 1:B:4644:UNK:O    | 1:B:4648:UNK:N    | 2.18                     | 0.77              |
| 1:C:999:ASP:O     | 1:C:1003:GLN:CG   | 2.33                     | 0.77              |
| 1:C:3306:UNK:HA   | 1:C:3309:UNK:CB   | 2.15                     | 0.77              |
| 1:D:321:GLU:HB2   | 1:D:323:LEU:HD13  | 1.65                     | 0.77              |
| 1:D:999:ASP:O     | 1:D:1003:GLN:CG   | 2.33                     | 0.77              |
| 1:D:1021:LEU:HD13 | 1:D:1021:LEU:N    | 1.98                     | 0.77              |
| 1:B:207:SER:CB    | 1:B:269:TRP:HZ3   | 1.97                     | 0.77              |
| 1:B:424:LYS:HZ1   | 1:B:505:GLU:HB2   | 1.48                     | 0.77              |
| 1:C:4644:UNK:O    | 1:C:4648:UNK:N    | 2.18                     | 0.77              |
| 1:A:4644:UNK:O    | 1:A:4648:UNK:N    | 2.18                     | 0.76              |
| 1:A:4847:UNK:O    | 1:A:4851:UNK:N    | 2.19                     | 0.76              |
| 1:D:4644:UNK:O    | 1:D:4648:UNK:N    | 2.18                     | 0.76              |
| 1:C:1022:VAL:O    | 1:C:1022:VAL:CG2  | 2.33                     | 0.76              |
| 1:D:362:PRO:HD3   | 1:D:374:LYS:HG2   | 1.65                     | 0.76              |
| 1:D:1001:VAL:CG1  | 1:D:1005:TRP:HE1  | 1.87                     | 0.76              |
| 1:A:207:SER:CB    | 1:A:269:TRP:HZ3   | 1.97                     | 0.76              |
| 1:A:1021:LEU:HD13 | 1:A:1021:LEU:N    | 1.98                     | 0.76              |
| 1:B:752:VAL:HB    | 1:B:754:SER:N     | 2.00                     | 0.76              |
| 1:C:752:VAL:HB    | 1:C:754:SER:N     | 2.00                     | 0.76              |
| 1:D:424:LYS:HZ1   | 1:D:505:GLU:HB2   | 1.50                     | 0.76              |
| 1:D:1022:VAL:O    | 1:D:1023:PRO:C    | 2.27                     | 0.76              |
| 1:B:999:ASP:O     | 1:B:1003:GLN:CG   | 2.33                     | 0.76              |
| 1:B:4847:UNK:O    | 1:B:4851:UNK:N    | 2.19                     | 0.76              |
| 1:D:728:ARG:CD    | 1:D:1134:LEU:HB2  | 2.16                     | 0.76              |
| 1:A:752:VAL:HG11  | 1:A:769:GLU:HG2   | 1.61                     | 0.76              |
| 1:A:1437:VAL:O    | 1:A:1516:ILE:C    | 2.27                     | 0.76              |
| 1:C:69:LEU:HD22   | 1:C:107:ILE:HD11  | 1.67                     | 0.76              |
| 1:C:362:PRO:HD3   | 1:C:374:LYS:HG2   | 1.65                     | 0.76              |
| 1:A:1001:VAL:CG1  | 1:A:1005:TRP:HE1  | 1.87                     | 0.76              |
| 1:A:1017:ARG:NH1  | 1:A:1017:ARG:HG3  | 1.93                     | 0.76              |
| 1:A:1471:ALA:O    | 1:A:1472:VAL:HG23 | 1.84                     | 0.76              |
| 1:C:12:GLN:OE1    | 1:C:165:VAL:N     | 2.19                     | 0.76              |
| 1:C:727:ALA:O     | 1:C:1134:LEU:CD2  | 2.33                     | 0.76              |
| 1:C:728:ARG:CD    | 1:C:1134:LEU:HB2  | 2.16                     | 0.76              |
| 1:C:998:ARG:HD3   | 1:C:999:ASP:H     | 1.48                     | 0.76              |
| 1:C:1471:ALA:O    | 1:C:1472:VAL:HG23 | 1.85                     | 0.76              |
| 1:A:424:LYS:HZ1   | 1:A:505:GLU:HB2   | 1.48                     | 0.76              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1022:VAL:O   | 1:A:1022:VAL:CG2  | 2.33                     | 0.76              |
| 1:B:1437:VAL:O   | 1:B:1516:ILE:C    | 2.27                     | 0.76              |
| 1:A:999:ASP:O    | 1:A:1003:GLN:CG   | 2.33                     | 0.76              |
| 1:A:1018:ASN:CB  | 1:A:1021:LEU:CD2  | 2.30                     | 0.76              |
| 1:B:12:GLN:OE1   | 1:B:165:VAL:N     | 2.19                     | 0.76              |
| 1:B:3306:UNK:HA  | 1:B:3309:UNK:CB   | 2.15                     | 0.76              |
| 1:D:77:ALA:HA    | 1:D:80:GLU:CD     | 2.10                     | 0.76              |
| 1:B:1022:VAL:O   | 1:B:1023:PRO:C    | 2.27                     | 0.76              |
| 1:D:4847:UNK:O   | 1:D:4851:UNK:N    | 2.19                     | 0.76              |
| 1:A:368:ARG:HG2  | 1:A:368:ARG:NH1   | 1.94                     | 0.76              |
| 1:A:727:ALA:O    | 1:A:1134:LEU:CD2  | 2.33                     | 0.76              |
| 1:D:3306:UNK:HA  | 1:D:3309:UNK:CB   | 2.15                     | 0.76              |
| 1:B:727:ALA:O    | 1:B:1134:LEU:CD2  | 2.33                     | 0.75              |
| 1:B:1022:VAL:O   | 1:B:1022:VAL:CG2  | 2.33                     | 0.75              |
| 1:C:79:GLN:HG2   | 1:C:80:GLU:N      | 2.01                     | 0.75              |
| 1:D:12:GLN:OE1   | 1:D:165:VAL:N     | 2.19                     | 0.75              |
| 1:D:1020:ARG:NE  | 1:D:1020:ARG:CA   | 2.45                     | 0.75              |
| 1:B:69:LEU:HD22  | 1:B:107:ILE:HD11  | 1.67                     | 0.75              |
| 1:C:1018:ASN:C   | 1:C:1021:LEU:HD22 | 2.12                     | 0.75              |
| 1:C:1494:MET:HB3 | 1:C:1540:PHE:CE1  | 2.22                     | 0.75              |
| 1:A:80:GLU:CD    | 1:B:3932:UNK:CB   | 2.59                     | 0.75              |
| 1:A:322:LYS:N    | 1:A:323:LEU:HA    | 2.02                     | 0.75              |
| 1:B:322:LYS:HE2  | 1:B:324:ASP:OD1   | 1.87                     | 0.75              |
| 1:C:4847:UNK:O   | 1:C:4851:UNK:N    | 2.19                     | 0.75              |
| 1:D:1018:ASN:C   | 1:D:1021:LEU:HD22 | 2.12                     | 0.75              |
| 1:A:69:LEU:HD22  | 1:A:107:ILE:HD11  | 1.66                     | 0.75              |
| 1:A:424:LYS:NZ   | 1:A:505:GLU:HB2   | 1.99                     | 0.75              |
| 1:A:1018:ASN:C   | 1:A:1021:LEU:HD22 | 2.12                     | 0.75              |
| 1:D:322:LYS:N    | 1:D:323:LEU:HA    | 2.02                     | 0.75              |
| 1:D:727:ALA:O    | 1:D:1134:LEU:CD2  | 2.33                     | 0.75              |
| 1:A:12:GLN:OE1   | 1:A:165:VAL:N     | 2.19                     | 0.75              |
| 1:A:75:VAL:N     | 1:A:78:LEU:HG     | 2.00                     | 0.75              |
| 1:B:323:LEU:HD23 | 1:B:324:ASP:O     | 1.87                     | 0.75              |
| 1:C:322:LYS:HE2  | 1:C:324:ASP:OD1   | 1.87                     | 0.75              |
| 1:C:1003:GLN:C   | 1:C:1007:TYR:CE2  | 2.65                     | 0.75              |
| 1:D:752:VAL:HB   | 1:D:754:SER:N     | 2.00                     | 0.75              |
| 1:B:75:VAL:HG13  | 1:B:76:ARG:N      | 2.02                     | 0.75              |
| 1:D:1422:ASP:HB3 | 1:D:1549:PHE:CE1  | 2.21                     | 0.75              |
| 1:A:752:VAL:HB   | 1:A:754:SER:N     | 2.00                     | 0.75              |
| 1:A:999:ASP:O    | 1:A:1003:GLN:CD   | 2.30                     | 0.75              |
| 1:C:82:LEU:O     | 1:C:82:LEU:HD23   | 1.87                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:728:ARG:CD    | 1:A:1134:LEU:HB2  | 2.16                     | 0.75              |
| 1:A:1494:MET:HB3  | 1:A:1540:PHE:CE1  | 2.22                     | 0.75              |
| 1:B:1003:GLN:C    | 1:B:1007:TYR:CE2  | 2.65                     | 0.75              |
| 1:B:1018:ASN:HB2  | 1:B:1021:LEU:HD21 | 0.75                     | 0.75              |
| 1:C:75:VAL:HG13   | 1:C:76:ARG:N      | 2.02                     | 0.75              |
| 1:A:855:PRO:HA    | 1:A:994:ASN:ND2   | 1.85                     | 0.74              |
| 1:B:728:ARG:CD    | 1:B:1134:LEU:HB2  | 2.16                     | 0.74              |
| 1:B:1494:MET:HB3  | 1:B:1540:PHE:CE1  | 2.21                     | 0.74              |
| 1:D:1494:MET:HB3  | 1:D:1540:PHE:CE1  | 2.22                     | 0.74              |
| 1:A:323:LEU:HD23  | 1:A:324:ASP:O     | 1.87                     | 0.74              |
| 1:A:996:TRP:HZ2   | 1:A:1021:LEU:CD1  | 1.90                     | 0.74              |
| 1:B:1422:ASP:HB3  | 1:B:1549:PHE:CE1  | 2.21                     | 0.74              |
| 1:C:1018:ASN:HB2  | 1:C:1021:LEU:HD21 | 0.75                     | 0.74              |
| 1:D:1003:GLN:C    | 1:D:1007:TYR:CE2  | 2.65                     | 0.74              |
| 1:A:1422:ASP:HB3  | 1:A:1549:PHE:CE1  | 2.22                     | 0.74              |
| 1:A:3306:UNK:HA   | 1:A:3309:UNK:CB   | 2.15                     | 0.74              |
| 1:D:82:LEU:O      | 1:D:82:LEU:HD23   | 1.87                     | 0.74              |
| 1:D:1444:GLU:HB2  | 1:D:1445:PRO:O    | 1.88                     | 0.74              |
| 1:A:1020:ARG:NE   | 1:A:1020:ARG:CA   | 2.45                     | 0.74              |
| 1:B:1555:LEU:HB3  | 1:B:1556:PRO:HD3  | 1.70                     | 0.74              |
| 1:A:752:VAL:N     | 1:A:753:PRO:HA    | 2.03                     | 0.74              |
| 1:A:956:PRO:HG3   | 1:A:959:TYR:CD1   | 1.94                     | 0.74              |
| 1:A:1003:GLN:C    | 1:A:1007:TYR:CE2  | 2.65                     | 0.74              |
| 1:A:1018:ASN:HB2  | 1:A:1021:LEU:HD21 | 0.75                     | 0.74              |
| 1:A:1432:THR:HG1  | 1:A:1523:ALA:HB2  | 1.50                     | 0.74              |
| 1:B:1018:ASN:C    | 1:B:1021:LEU:HD22 | 2.12                     | 0.74              |
| 1:B:1462:MET:C    | 1:B:1555:LEU:HD22 | 2.13                     | 0.74              |
| 1:B:4055:UNK:H    | 1:B:4058:UNK:CB   | 2.01                     | 0.74              |
| 1:C:1021:LEU:HD13 | 1:C:1021:LEU:N    | 1.98                     | 0.74              |
| 1:C:4573:UNK:CB   | 1:C:4809:UNK:CB   | 2.65                     | 0.74              |
| 1:D:999:ASP:O     | 1:D:1003:GLN:CD   | 2.30                     | 0.74              |
| 1:A:322:LYS:HE2   | 1:A:324:ASP:OD1   | 1.87                     | 0.74              |
| 1:B:322:LYS:N     | 1:B:323:LEU:HA    | 2.02                     | 0.74              |
| 1:C:323:LEU:HD23  | 1:C:324:ASP:O     | 1.87                     | 0.74              |
| 1:C:1462:MET:C    | 1:C:1555:LEU:HD22 | 2.13                     | 0.74              |
| 1:D:322:LYS:HE2   | 1:D:324:ASP:OD1   | 1.87                     | 0.74              |
| 1:D:487:VAL:HG13  | 1:D:522:LEU:HD12  | 1.69                     | 0.74              |
| 1:B:999:ASP:O     | 1:B:1003:GLN:CD   | 2.30                     | 0.74              |
| 1:C:1422:ASP:HB3  | 1:C:1549:PHE:CE1  | 2.21                     | 0.74              |
| 1:C:1432:THR:OG1  | 1:C:1523:ALA:CB   | 2.30                     | 0.74              |
| 1:D:75:VAL:HG13   | 1:D:76:ARG:N      | 2.02                     | 0.74              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:323:LEU:HD23 | 1:D:324:ASP:O     | 1.87                     | 0.74              |
| 1:D:1462:MET:C   | 1:D:1555:LEU:HD22 | 2.13                     | 0.74              |
| 1:D:1555:LEU:HB3 | 1:D:1556:PRO:HD3  | 1.70                     | 0.74              |
| 1:A:75:VAL:HG13  | 1:A:76:ARG:N      | 2.02                     | 0.74              |
| 1:C:487:VAL:HG13 | 1:C:522:LEU:HD12  | 1.69                     | 0.74              |
| 1:B:1020:ARG:NE  | 1:B:1020:ARG:CA   | 2.45                     | 0.74              |
| 1:D:75:VAL:N     | 1:D:78:LEU:HG     | 2.00                     | 0.74              |
| 1:D:1018:ASN:HB2 | 1:D:1021:LEU:HD21 | 0.75                     | 0.74              |
| 1:A:79:GLN:HG2   | 1:A:80:GLU:N      | 2.01                     | 0.74              |
| 1:A:82:LEU:O     | 1:A:82:LEU:HD23   | 1.87                     | 0.74              |
| 1:A:1462:MET:C   | 1:A:1555:LEU:HD22 | 2.13                     | 0.74              |
| 1:A:1555:LEU:HB3 | 1:A:1556:PRO:HD3  | 1.70                     | 0.74              |
| 1:A:4573:UNK:CB  | 1:A:4809:UNK:CB   | 2.65                     | 0.74              |
| 1:A:4703:UNK:HA  | 1:A:4706:UNK:CB   | 2.18                     | 0.74              |
| 1:B:80:GLU:CD    | 1:C:3932:UNK:CB   | 2.60                     | 0.74              |
| 1:C:999:ASP:O    | 1:C:1003:GLN:CD   | 2.30                     | 0.74              |
| 1:B:1444:GLU:HB2 | 1:B:1445:PRO:O    | 1.88                     | 0.73              |
| 1:C:1555:LEU:HB3 | 1:C:1556:PRO:HD3  | 1.70                     | 0.73              |
| 1:C:4055:UNK:H   | 1:C:4058:UNK:CB   | 2.01                     | 0.73              |
| 1:B:82:LEU:O     | 1:B:82:LEU:HD23   | 1.87                     | 0.73              |
| 1:B:752:VAL:N    | 1:B:753:PRO:HA    | 2.03                     | 0.73              |
| 1:B:1453:VAL:O   | 1:B:1549:PHE:N    | 2.21                     | 0.73              |
| 1:C:323:LEU:N    | 1:C:324:ASP:HA    | 2.03                     | 0.73              |
| 1:C:1453:VAL:O   | 1:C:1549:PHE:N    | 2.21                     | 0.73              |
| 1:D:4573:UNK:CB  | 1:D:4809:UNK:CB   | 2.65                     | 0.73              |
| 1:A:4055:UNK:H   | 1:A:4058:UNK:CB   | 2.01                     | 0.73              |
| 1:B:1007:TYR:HE1 | 1:B:1015:ALA:HA   | 1.53                     | 0.73              |
| 1:D:752:VAL:N    | 1:D:753:PRO:HA    | 2.03                     | 0.73              |
| 1:D:4055:UNK:H   | 1:D:4058:UNK:CB   | 2.01                     | 0.73              |
| 1:D:4703:UNK:HA  | 1:D:4706:UNK:CB   | 2.18                     | 0.73              |
| 1:A:1000:ARG:CD  | 1:A:1000:ARG:C    | 2.60                     | 0.73              |
| 1:D:752:VAL:CG1  | 1:D:769:GLU:CG    | 2.49                     | 0.73              |
| 1:A:323:LEU:N    | 1:A:324:ASP:HA    | 2.03                     | 0.73              |
| 1:B:79:GLN:HG2   | 1:B:80:GLU:N      | 2.01                     | 0.73              |
| 1:B:4573:UNK:CB  | 1:B:4809:UNK:CB   | 2.66                     | 0.73              |
| 1:C:752:VAL:N    | 1:C:753:PRO:HA    | 2.03                     | 0.73              |
| 1:C:1000:ARG:CD  | 1:C:1000:ARG:C    | 2.60                     | 0.73              |
| 1:C:4797:UNK:O   | 1:C:4801:UNK:CB   | 2.37                     | 0.73              |
| 1:D:205:ILE:O    | 1:D:269:TRP:CA    | 2.34                     | 0.73              |
| 1:D:1000:ARG:CD  | 1:D:1000:ARG:C    | 2.60                     | 0.73              |
| 1:A:1007:TYR:HE1 | 1:A:1015:ALA:HA   | 1.54                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1444:GLU:OE1  | 1:A:1478:ASP:CA   | 2.37                     | 0.73              |
| 1:B:4797:UNK:O    | 1:B:4801:UNK:CB   | 2.37                     | 0.73              |
| 1:B:323:LEU:N     | 1:B:324:ASP:HA    | 2.03                     | 0.73              |
| 1:B:1000:ARG:CD   | 1:B:1000:ARG:C    | 2.60                     | 0.73              |
| 1:D:323:LEU:HD22  | 1:D:323:LEU:N     | 2.03                     | 0.73              |
| 1:A:4797:UNK:O    | 1:A:4801:UNK:CB   | 2.37                     | 0.73              |
| 1:C:222:LEU:HA    | 1:C:390:LEU:HD23  | 1.71                     | 0.73              |
| 1:D:79:GLN:HG2    | 1:D:80:GLU:N      | 2.01                     | 0.73              |
| 1:D:1018:ASN:CB   | 1:D:1021:LEU:CD2  | 2.30                     | 0.73              |
| 1:D:1453:VAL:O    | 1:D:1549:PHE:N    | 2.21                     | 0.73              |
| 1:A:487:VAL:HG13  | 1:A:522:LEU:HD12  | 1.69                     | 0.73              |
| 1:A:1444:GLU:HB2  | 1:A:1445:PRO:O    | 1.88                     | 0.73              |
| 1:C:1466:LEU:H    | 1:C:1553:PHE:CB   | 2.02                     | 0.73              |
| 1:D:323:LEU:N     | 1:D:324:ASP:HA    | 2.03                     | 0.73              |
| 1:B:323:LEU:HD22  | 1:B:323:LEU:N     | 2.03                     | 0.73              |
| 1:B:1444:GLU:OE1  | 1:B:1478:ASP:CA   | 2.37                     | 0.73              |
| 1:B:4703:UNK:HA   | 1:B:4706:UNK:CB   | 2.18                     | 0.73              |
| 1:D:1432:THR:HG1  | 1:D:1523:ALA:HB2  | 1.51                     | 0.73              |
| 1:D:1444:GLU:OE1  | 1:D:1478:ASP:CA   | 2.37                     | 0.73              |
| 1:A:1018:ASN:HB2  | 1:A:1021:LEU:HD22 | 1.64                     | 0.72              |
| 1:B:1466:LEU:H    | 1:B:1553:PHE:CB   | 2.02                     | 0.72              |
| 1:A:21:VAL:CG1    | 1:A:205:ILE:HD11  | 2.04                     | 0.72              |
| 1:A:222:LEU:HA    | 1:A:390:LEU:HD23  | 1.71                     | 0.72              |
| 1:A:323:LEU:HD22  | 1:A:323:LEU:N     | 2.03                     | 0.72              |
| 1:C:205:ILE:O     | 1:C:269:TRP:CA    | 2.34                     | 0.72              |
| 1:C:993:HIS:C     | 1:C:996:TRP:CE3   | 2.67                     | 0.72              |
| 1:C:1444:GLU:HB2  | 1:C:1445:PRO:O    | 1.88                     | 0.72              |
| 1:A:1017:ARG:HH11 | 1:A:1017:ARG:CA   | 2.03                     | 0.72              |
| 1:A:3932:UNK:CB   | 1:D:80:GLU:CD     | 2.61                     | 0.72              |
| 1:B:205:ILE:O     | 1:B:269:TRP:CA    | 2.34                     | 0.72              |
| 1:C:996:TRP:HZ2   | 1:C:1021:LEU:CD1  | 1.90                     | 0.72              |
| 1:D:956:PRO:HG2   | 1:D:959:TYR:CE1   | 2.15                     | 0.72              |
| 1:B:222:LEU:HA    | 1:B:390:LEU:HD23  | 1.71                     | 0.72              |
| 1:B:364:PRO:C     | 1:B:369:LEU:HD12  | 2.14                     | 0.72              |
| 1:B:487:VAL:HG13  | 1:B:522:LEU:HD12  | 1.69                     | 0.72              |
| 1:C:207:SER:CB    | 1:C:269:TRP:CZ3   | 2.73                     | 0.72              |
| 1:C:322:LYS:N     | 1:C:323:LEU:HA    | 2.02                     | 0.72              |
| 1:D:996:TRP:CZ2   | 1:D:1020:ARG:N    | 2.49                     | 0.72              |
| 1:C:323:LEU:HD22  | 1:C:323:LEU:N     | 2.03                     | 0.72              |
| 1:C:4703:UNK:HA   | 1:C:4706:UNK:CB   | 2.18                     | 0.72              |
| 1:D:4797:UNK:O    | 1:D:4801:UNK:CB   | 2.37                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1471:ALA:O    | 1:B:1472:VAL:CG2  | 2.38                     | 0.72              |
| 1:C:1471:ALA:O    | 1:C:1472:VAL:CG2  | 2.38                     | 0.72              |
| 1:D:222:LEU:HA    | 1:D:390:LEU:HD23  | 1.71                     | 0.72              |
| 1:D:1017:ARG:HH11 | 1:D:1017:ARG:CA   | 2.02                     | 0.72              |
| 1:A:3894:UNK:O    | 1:A:3898:UNK:N    | 2.23                     | 0.72              |
| 1:B:21:VAL:CG1    | 1:B:205:ILE:HD11  | 2.04                     | 0.72              |
| 1:A:993:HIS:C     | 1:A:996:TRP:CE3   | 2.67                     | 0.72              |
| 1:B:996:TRP:CZ2   | 1:B:1020:ARG:N    | 2.49                     | 0.72              |
| 1:B:1017:ARG:HH11 | 1:B:1017:ARG:CA   | 2.02                     | 0.72              |
| 1:C:80:GLU:CD     | 1:D:3932:UNK:CB   | 2.61                     | 0.72              |
| 1:C:1007:TYR:HE1  | 1:C:1015:ALA:HA   | 1.53                     | 0.72              |
| 1:D:364:PRO:C     | 1:D:369:LEU:HD12  | 2.14                     | 0.72              |
| 1:D:752:VAL:CG1   | 1:D:769:GLU:OE1   | 2.38                     | 0.72              |
| 1:D:1477:GLY:C    | 1:D:1509:ILE:CG2  | 2.63                     | 0.72              |
| 1:A:2327:UNK:H    | 1:A:2330:UNK:CB   | 2.03                     | 0.72              |
| 1:B:3894:UNK:O    | 1:B:3898:UNK:N    | 2.23                     | 0.72              |
| 1:C:1444:GLU:OE1  | 1:C:1478:ASP:CA   | 2.37                     | 0.72              |
| 1:C:1477:GLY:C    | 1:C:1509:ILE:CG2  | 2.63                     | 0.72              |
| 1:D:956:PRO:C     | 1:D:958:THR:N     | 2.48                     | 0.72              |
| 1:D:993:HIS:C     | 1:D:996:TRP:CE3   | 2.67                     | 0.72              |
| 1:D:1471:ALA:O    | 1:D:1472:VAL:CG2  | 2.38                     | 0.72              |
| 1:A:752:VAL:CG1   | 1:A:769:GLU:OE1   | 2.38                     | 0.71              |
| 1:A:956:PRO:C     | 1:A:958:THR:N     | 2.48                     | 0.71              |
| 1:B:1021:LEU:C    | 1:B:1022:VAL:HG13 | 2.15                     | 0.71              |
| 1:D:1466:LEU:H    | 1:D:1553:PHE:CB   | 2.02                     | 0.71              |
| 1:A:1435:TYR:HE2  | 1:A:1520:VAL:HB   | 1.55                     | 0.71              |
| 1:A:1471:ALA:O    | 1:A:1472:VAL:CG2  | 2.38                     | 0.71              |
| 1:B:1439:VAL:CB   | 1:B:1514:LEU:O    | 2.16                     | 0.71              |
| 1:B:1477:GLY:C    | 1:B:1509:ILE:CG2  | 2.63                     | 0.71              |
| 1:D:2327:UNK:H    | 1:D:2330:UNK:CB   | 2.03                     | 0.71              |
| 1:A:364:PRO:C     | 1:A:369:LEU:HD12  | 2.14                     | 0.71              |
| 1:A:1021:LEU:C    | 1:A:1022:VAL:HG13 | 2.15                     | 0.71              |
| 1:A:1466:LEU:H    | 1:A:1553:PHE:CB   | 2.02                     | 0.71              |
| 1:D:657:THR:HG1   | 1:D:662:TRP:CD1   | 2.08                     | 0.71              |
| 1:C:364:PRO:C     | 1:C:369:LEU:HD12  | 2.14                     | 0.71              |
| 1:C:1435:TYR:HE2  | 1:C:1520:VAL:HB   | 1.55                     | 0.71              |
| 1:D:991:ASN:O     | 1:D:995:VAL:HG23  | 1.90                     | 0.71              |
| 1:A:1477:GLY:C    | 1:A:1509:ILE:CG2  | 2.63                     | 0.71              |
| 1:B:1452:TRP:CH2  | 1:B:1527:MET:CG   | 2.73                     | 0.71              |
| 1:C:3894:UNK:O    | 1:C:3898:UNK:N    | 2.23                     | 0.71              |
| 1:C:1017:ARG:HH11 | 1:C:1017:ARG:CA   | 2.03                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:1021:LEU:C   | 1:C:1022:VAL:HG13 | 2.15                     | 0.71              |
| 1:D:1007:TYR:HE1 | 1:D:1015:ALA:HA   | 1.54                     | 0.71              |
| 1:B:1435:TYR:HE2 | 1:B:1520:VAL:HB   | 1.55                     | 0.71              |
| 1:B:2327:UNK:H   | 1:B:2330:UNK:CB   | 2.03                     | 0.71              |
| 1:B:4710:UNK:C   | 1:B:4719:UNK:CB   | 2.66                     | 0.71              |
| 1:C:1429:ASN:HB2 | 1:C:1547:LYS:HB2  | 1.73                     | 0.71              |
| 1:C:991:ASN:O    | 1:C:995:VAL:HG23  | 1.90                     | 0.71              |
| 1:D:207:SER:CB   | 1:D:269:TRP:CZ3   | 2.73                     | 0.71              |
| 1:D:1435:TYR:HE2 | 1:D:1520:VAL:HB   | 1.55                     | 0.71              |
| 1:A:1453:VAL:O   | 1:A:1549:PHE:N    | 2.21                     | 0.71              |
| 1:B:993:HIS:C    | 1:B:996:TRP:CE3   | 2.67                     | 0.71              |
| 1:B:1016:ARG:CB  | 1:B:1016:ARG:HH11 | 2.02                     | 0.71              |
| 1:C:368:ARG:HG2  | 1:C:368:ARG:NH1   | 1.94                     | 0.71              |
| 1:C:1452:TRP:CH2 | 1:C:1527:MET:CG   | 2.73                     | 0.71              |
| 1:C:1462:MET:CE  | 1:C:1559:GLN:HG2  | 2.21                     | 0.71              |
| 1:B:1001:VAL:O   | 1:B:1005:TRP:CG   | 2.44                     | 0.71              |
| 1:C:1007:TYR:CE1 | 1:C:1015:ALA:HB1  | 2.26                     | 0.71              |
| 1:C:2327:UNK:H   | 1:C:2330:UNK:CB   | 2.03                     | 0.71              |
| 1:D:4561:UNK:O   | 1:D:4564:UNK:N    | 2.24                     | 0.71              |
| 1:B:1007:TYR:CE1 | 1:B:1015:ALA:HB1  | 2.26                     | 0.70              |
| 1:C:956:PRO:C    | 1:C:958:THR:N     | 2.48                     | 0.70              |
| 1:A:1429:ASN:HB2 | 1:A:1547:LYS:HB2  | 1.73                     | 0.70              |
| 1:B:752:VAL:CG1  | 1:B:769:GLU:OE1   | 2.38                     | 0.70              |
| 1:B:991:ASN:O    | 1:B:995:VAL:HG23  | 1.90                     | 0.70              |
| 1:C:752:VAL:CG1  | 1:C:769:GLU:OE1   | 2.38                     | 0.70              |
| 1:D:1007:TYR:CE1 | 1:D:1015:ALA:HB1  | 2.26                     | 0.70              |
| 1:A:998:ARG:HD2  | 1:A:999:ASP:OD1   | 1.92                     | 0.70              |
| 1:B:4561:UNK:O   | 1:B:4564:UNK:N    | 2.24                     | 0.70              |
| 1:C:1439:VAL:CB  | 1:C:1514:LEU:O    | 2.16                     | 0.70              |
| 1:D:998:ARG:HD2  | 1:D:999:ASP:OD1   | 1.91                     | 0.70              |
| 1:A:1001:VAL:O   | 1:A:1005:TRP:CG   | 2.44                     | 0.70              |
| 1:B:1429:ASN:HB2 | 1:B:1547:LYS:HB2  | 1.73                     | 0.70              |
| 1:C:21:VAL:CG1   | 1:C:205:ILE:HD11  | 2.04                     | 0.70              |
| 1:D:1462:MET:CE  | 1:D:1559:GLN:HG2  | 2.21                     | 0.70              |
| 1:A:991:ASN:O    | 1:A:995:VAL:HG23  | 1.90                     | 0.70              |
| 1:C:75:VAL:N     | 1:C:78:LEU:HG     | 2.00                     | 0.70              |
| 1:D:323:LEU:HB2  | 1:D:325:THR:N     | 2.07                     | 0.70              |
| 1:D:1439:VAL:CB  | 1:D:1514:LEU:O    | 2.16                     | 0.70              |
| 1:D:3894:UNK:O   | 1:D:3898:UNK:N    | 2.23                     | 0.70              |
| 1:A:1007:TYR:CE1 | 1:A:1015:ALA:HB1  | 2.26                     | 0.70              |
| 1:B:1462:MET:CE  | 1:B:1559:GLN:HG2  | 2.21                     | 0.70              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1016:ARG:CB  | 1:A:1016:ARG:HH11 | 2.02                     | 0.70              |
| 1:B:1004:GLY:HA3 | 1:B:1015:ALA:HB2  | 1.71                     | 0.70              |
| 1:C:323:LEU:H    | 1:C:323:LEU:CD2   | 2.04                     | 0.70              |
| 1:A:323:LEU:H    | 1:A:323:LEU:CD2   | 2.04                     | 0.70              |
| 1:A:1462:MET:CE  | 1:A:1559:GLN:HG2  | 2.21                     | 0.70              |
| 1:C:3134:UNK:O   | 1:C:3138:UNK:N    | 2.25                     | 0.70              |
| 1:D:1429:ASN:HB2 | 1:D:1547:LYS:HB2  | 1.73                     | 0.70              |
| 1:B:2073:UNK:CB  | 1:B:2094:UNK:CA   | 2.69                     | 0.70              |
| 1:C:126:SER:HB3  | 1:C:130:LYS:HD2   | 1.74                     | 0.70              |
| 1:C:1016:ARG:CB  | 1:C:1016:ARG:HH11 | 2.03                     | 0.70              |
| 1:D:1021:LEU:C   | 1:D:1022:VAL:HG13 | 2.15                     | 0.70              |
| 1:A:2073:UNK:CB  | 1:A:2094:UNK:CA   | 2.69                     | 0.70              |
| 1:B:1494:MET:HA  | 1:B:1540:PHE:CZ   | 2.27                     | 0.70              |
| 1:D:1001:VAL:O   | 1:D:1005:TRP:CG   | 2.44                     | 0.70              |
| 1:A:323:LEU:HB2  | 1:A:325:THR:N     | 2.07                     | 0.69              |
| 1:B:323:LEU:H    | 1:B:323:LEU:CD2   | 2.04                     | 0.69              |
| 1:B:728:ARG:HG3  | 1:B:1119:GLU:OE2  | 1.92                     | 0.69              |
| 1:C:1001:VAL:O   | 1:C:1005:TRP:CG   | 2.44                     | 0.69              |
| 1:C:4561:UNK:O   | 1:C:4564:UNK:N    | 2.24                     | 0.69              |
| 1:A:728:ARG:HG3  | 1:A:1119:GLU:OE2  | 1.92                     | 0.69              |
| 1:A:1466:LEU:H   | 1:A:1553:PHE:HB3  | 1.57                     | 0.69              |
| 1:B:323:LEU:HB2  | 1:B:325:THR:N     | 2.07                     | 0.69              |
| 1:C:1434:TYR:CD1 | 1:C:1570:LYS:CG   | 2.76                     | 0.69              |
| 1:C:2073:UNK:CB  | 1:C:2094:UNK:CA   | 2.69                     | 0.69              |
| 1:A:1434:TYR:CD1 | 1:A:1570:LYS:CG   | 2.75                     | 0.69              |
| 1:A:3932:UNK:HA  | 1:D:80:GLU:OE1    | 1.92                     | 0.69              |
| 1:B:956:PRO:C    | 1:B:958:THR:N     | 2.48                     | 0.69              |
| 1:D:332:GLU:OE1  | 1:D:332:GLU:HA    | 1.92                     | 0.69              |
| 1:D:1016:ARG:CB  | 1:D:1016:ARG:HH11 | 2.02                     | 0.69              |
| 1:A:207:SER:CB   | 1:A:269:TRP:CZ3   | 2.73                     | 0.69              |
| 1:C:1439:VAL:CA  | 1:C:1515:VAL:HA   | 2.18                     | 0.69              |
| 1:C:1494:MET:HA  | 1:C:1540:PHE:CZ   | 2.27                     | 0.69              |
| 1:B:207:SER:CB   | 1:B:269:TRP:CZ3   | 2.73                     | 0.69              |
| 1:B:1003:GLN:OE1 | 1:B:1003:GLN:CA   | 2.41                     | 0.69              |
| 1:B:1466:LEU:H   | 1:B:1553:PHE:HB3  | 1.57                     | 0.69              |
| 1:C:1452:TRP:HB3 | 1:C:1548:LEU:CB   | 2.23                     | 0.69              |
| 1:D:324:ASP:N    | 1:D:325:THR:HA    | 2.07                     | 0.69              |
| 1:D:1434:TYR:CD1 | 1:D:1570:LYS:CG   | 2.76                     | 0.69              |
| 1:D:3134:UNK:O   | 1:D:3138:UNK:N    | 2.25                     | 0.69              |
| 1:A:205:ILE:O    | 1:A:269:TRP:CA    | 2.34                     | 0.69              |
| 1:A:332:GLU:OE1  | 1:A:332:GLU:HA    | 1.92                     | 0.69              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:1020:ARG:O    | 1:B:1020:ARG:HD3 | 1.93                     | 0.69              |
| 1:B:1434:TYR:CD1  | 1:B:1570:LYS:CG  | 2.75                     | 0.69              |
| 1:B:1452:TRP:HB3  | 1:B:1548:LEU:CB  | 2.23                     | 0.69              |
| 1:B:3134:UNK:O    | 1:B:3138:UNK:N   | 2.25                     | 0.69              |
| 1:A:275:ARG:HH22  | 1:A:336:PRO:HD2  | 1.58                     | 0.69              |
| 1:A:324:ASP:N     | 1:A:325:THR:HA   | 2.07                     | 0.69              |
| 1:A:1452:TRP:CH2  | 1:A:1527:MET:CG  | 2.73                     | 0.69              |
| 1:A:3134:UNK:O    | 1:A:3138:UNK:N   | 2.25                     | 0.69              |
| 1:B:998:ARG:HD2   | 1:B:999:ASP:OD1  | 1.91                     | 0.69              |
| 1:C:1000:ARG:NE   | 1:C:1007:TYR:OH  | 2.26                     | 0.69              |
| 1:D:953:THR:HG22  | 1:D:971:ASP:OD1  | 1.92                     | 0.69              |
| 1:D:1494:MET:HA   | 1:D:1540:PHE:CZ  | 2.27                     | 0.69              |
| 1:A:80:GLU:OE1    | 1:B:3932:UNK:HA  | 1.93                     | 0.69              |
| 1:A:996:TRP:CZ2   | 1:A:1020:ARG:N   | 2.49                     | 0.69              |
| 1:A:1020:ARG:O    | 1:A:1020:ARG:HD3 | 1.93                     | 0.69              |
| 1:A:1439:VAL:CB   | 1:A:1514:LEU:O   | 2.16                     | 0.69              |
| 1:A:4117:UNK:CB   | 1:A:4121:UNK:HA  | 2.23                     | 0.69              |
| 1:B:657:THR:HG22  | 1:B:662:TRP:CZ2  | 2.28                     | 0.69              |
| 1:B:1439:VAL:CA   | 1:B:1515:VAL:HA  | 2.18                     | 0.69              |
| 1:C:323:LEU:HB2   | 1:C:325:THR:N    | 2.07                     | 0.69              |
| 1:C:324:ASP:N     | 1:C:325:THR:HA   | 2.07                     | 0.69              |
| 1:C:998:ARG:HD2   | 1:C:999:ASP:OD1  | 1.92                     | 0.69              |
| 1:D:2073:UNK:CB   | 1:D:2094:UNK:CA  | 2.69                     | 0.69              |
| 1:A:126:SER:HB3   | 1:A:130:LYS:HD2  | 1.74                     | 0.69              |
| 1:A:1472:VAL:HG11 | 1:A:1527:MET:SD  | 2.33                     | 0.69              |
| 1:A:1494:MET:HA   | 1:A:1540:PHE:CZ  | 2.27                     | 0.69              |
| 1:B:1434:TYR:CD1  | 1:B:1570:LYS:CD  | 2.71                     | 0.69              |
| 1:C:206:CYS:C     | 1:C:269:TRP:CE3  | 2.70                     | 0.69              |
| 1:A:953:THR:HG22  | 1:A:971:ASP:OD1  | 1.92                     | 0.69              |
| 1:B:953:THR:HG22  | 1:B:971:ASP:OD1  | 1.92                     | 0.69              |
| 1:C:1001:VAL:CG1  | 1:C:1005:TRP:NE1 | 2.50                     | 0.69              |
| 1:C:1466:LEU:H    | 1:C:1553:PHE:HB3 | 1.57                     | 0.69              |
| 1:D:87:GLU:OE1    | 1:D:87:GLU:N     | 2.26                     | 0.69              |
| 1:D:126:SER:HB3   | 1:D:130:LYS:HD2  | 1.74                     | 0.69              |
| 1:D:206:CYS:C     | 1:D:269:TRP:CE3  | 2.71                     | 0.69              |
| 1:D:1452:TRP:HB3  | 1:D:1548:LEU:CB  | 2.23                     | 0.69              |
| 1:D:4117:UNK:CB   | 1:D:4121:UNK:HA  | 2.23                     | 0.69              |
| 1:A:1452:TRP:HB3  | 1:A:1548:LEU:CB  | 2.23                     | 0.68              |
| 1:A:4561:UNK:O    | 1:A:4564:UNK:N   | 2.24                     | 0.68              |
| 1:B:953:THR:HG23  | 1:B:971:ASP:OD1  | 1.92                     | 0.68              |
| 1:B:1018:ASN:CB   | 1:B:1021:LEU:CD2 | 2.30                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1472:VAL:HG11 | 1:C:1527:MET:SD   | 2.33                     | 0.68              |
| 1:D:1452:TRP:CH2  | 1:D:1527:MET:CG   | 2.73                     | 0.68              |
| 1:B:206:CYS:C     | 1:B:269:TRP:CE3   | 2.70                     | 0.68              |
| 1:B:275:ARG:HH22  | 1:B:336:PRO:HD2   | 1.57                     | 0.68              |
| 1:B:324:ASP:N     | 1:B:325:THR:HA    | 2.07                     | 0.68              |
| 1:C:953:THR:HG23  | 1:C:971:ASP:OD1   | 1.93                     | 0.68              |
| 1:A:206:CYS:C     | 1:A:269:TRP:CE3   | 2.70                     | 0.68              |
| 1:C:87:GLU:OE1    | 1:C:87:GLU:N      | 2.26                     | 0.68              |
| 1:C:996:TRP:CZ2   | 1:C:1020:ARG:N    | 2.49                     | 0.68              |
| 1:C:1476:MET:CE   | 1:C:1516:ILE:HD11 | 2.17                     | 0.68              |
| 1:D:323:LEU:H     | 1:D:323:LEU:CD2   | 2.04                     | 0.68              |
| 1:B:4117:UNK:CB   | 1:B:4121:UNK:HA   | 2.23                     | 0.68              |
| 1:C:469:ARG:HA    | 1:C:472:ARG:NH1   | 2.09                     | 0.68              |
| 1:C:998:ARG:HD3   | 1:C:999:ASP:OD1   | 1.93                     | 0.68              |
| 1:C:4117:UNK:CB   | 1:C:4121:UNK:HA   | 2.23                     | 0.68              |
| 1:D:956:PRO:HD2   | 1:D:959:TYR:CB    | 2.24                     | 0.68              |
| 1:D:988:LEU:HB3   | 1:D:1039:LEU:HD22 | 1.76                     | 0.68              |
| 1:D:1558:HIS:CD2  | 1:D:1559:GLN:N    | 2.62                     | 0.68              |
| 1:A:956:PRO:HD2   | 1:A:959:TYR:CB    | 2.24                     | 0.68              |
| 1:B:1472:VAL:HG11 | 1:B:1527:MET:SD   | 2.33                     | 0.68              |
| 1:C:332:GLU:OE1   | 1:C:332:GLU:HA    | 1.92                     | 0.68              |
| 1:D:469:ARG:HA    | 1:D:472:ARG:NH1   | 2.09                     | 0.68              |
| 1:D:953:THR:HG23  | 1:D:971:ASP:OD1   | 1.92                     | 0.68              |
| 1:D:1472:VAL:HG11 | 1:D:1527:MET:SD   | 2.33                     | 0.68              |
| 1:A:362:PRO:HG2   | 1:A:364:PRO:HB3   | 1.75                     | 0.68              |
| 1:B:80:GLU:OE1    | 1:C:3932:UNK:HA   | 1.92                     | 0.68              |
| 1:B:82:LEU:CD1    | 1:B:144:GLU:OE2   | 2.42                     | 0.68              |
| 1:B:126:SER:HB3   | 1:B:130:LYS:HD2   | 1.74                     | 0.68              |
| 1:C:953:THR:HG22  | 1:C:971:ASP:OD1   | 1.92                     | 0.68              |
| 1:D:362:PRO:HG2   | 1:D:364:PRO:HB3   | 1.75                     | 0.68              |
| 1:D:728:ARG:HG3   | 1:D:1119:GLU:OE2  | 1.92                     | 0.68              |
| 1:D:1459:GLN:HG2  | 1:D:1553:PHE:HD1  | 1.58                     | 0.68              |
| 1:A:988:LEU:HB3   | 1:A:1039:LEU:HD22 | 1.76                     | 0.68              |
| 1:B:988:LEU:HB3   | 1:B:1039:LEU:HD22 | 1.76                     | 0.68              |
| 1:C:728:ARG:HG3   | 1:C:1119:GLU:OE2  | 1.92                     | 0.68              |
| 1:D:4710:UNK:C    | 1:D:4719:UNK:CB   | 2.66                     | 0.68              |
| 1:A:87:GLU:OE1    | 1:A:87:GLU:N      | 2.26                     | 0.68              |
| 1:A:131:LEU:HB3   | 1:A:178:ARG:NH1   | 2.09                     | 0.68              |
| 1:A:657:THR:HB    | 1:A:662:TRP:NE1   | 2.09                     | 0.68              |
| 1:D:1466:LEU:H    | 1:D:1553:PHE:HB3  | 1.57                     | 0.68              |
| 1:A:1003:GLN:CA   | 1:A:1003:GLN:OE1  | 2.41                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:368:ARG:HH12 | 1:B:371:VAL:HB    | 1.57                     | 0.68              |
| 1:C:275:ARG:HH22 | 1:C:336:PRO:HD2   | 1.58                     | 0.68              |
| 1:C:956:PRO:HD2  | 1:C:959:TYR:CB    | 2.24                     | 0.68              |
| 1:C:1020:ARG:O   | 1:C:1020:ARG:HD3  | 1.93                     | 0.68              |
| 1:C:1558:HIS:CD2 | 1:C:1559:GLN:N    | 2.61                     | 0.68              |
| 1:D:275:ARG:HH22 | 1:D:336:PRO:HD2   | 1.57                     | 0.68              |
| 1:D:1003:GLN:OE1 | 1:D:1003:GLN:CA   | 2.41                     | 0.68              |
| 1:A:151:HIS:HB2  | 1:A:170:ILE:HG22  | 1.76                     | 0.68              |
| 1:A:368:ARG:HH12 | 1:A:371:VAL:HB    | 1.57                     | 0.68              |
| 1:C:1434:TYR:CD1 | 1:C:1570:LYS:CD   | 2.71                     | 0.68              |
| 1:A:953:THR:HG23 | 1:A:971:ASP:OD1   | 1.93                     | 0.67              |
| 1:A:1558:HIS:CD2 | 1:A:1559:GLN:N    | 2.62                     | 0.67              |
| 1:B:131:LEU:HB3  | 1:B:178:ARG:NH1   | 2.09                     | 0.67              |
| 1:B:329:ARG:HG3  | 1:B:329:ARG:NH1   | 1.97                     | 0.67              |
| 1:B:332:GLU:OE1  | 1:B:332:GLU:HA    | 1.92                     | 0.67              |
| 1:B:362:PRO:HG2  | 1:B:364:PRO:HB3   | 1.75                     | 0.67              |
| 1:B:953:THR:O    | 1:B:959:TYR:CE2   | 2.44                     | 0.67              |
| 1:A:1429:ASN:HB2 | 1:A:1547:LYS:HD2  | 1.76                     | 0.67              |
| 1:B:469:ARG:HA   | 1:B:472:ARG:NH1   | 2.09                     | 0.67              |
| 1:C:988:LEU:HB3  | 1:C:1039:LEU:HD22 | 1.76                     | 0.67              |
| 1:A:82:LEU:CD1   | 1:A:144:GLU:OE2   | 2.42                     | 0.67              |
| 1:A:1004:GLY:HA3 | 1:A:1015:ALA:HB2  | 1.71                     | 0.67              |
| 1:B:87:GLU:OE1   | 1:B:87:GLU:N      | 2.26                     | 0.67              |
| 1:B:2299:UNK:CB  | 1:B:2352:UNK:C    | 2.73                     | 0.67              |
| 1:B:76:ARG:O     | 1:B:79:GLN:HG2    | 1.95                     | 0.67              |
| 1:B:956:PRO:HD2  | 1:B:959:TYR:CB    | 2.24                     | 0.67              |
| 1:B:1558:HIS:CD2 | 1:B:1559:GLN:N    | 2.62                     | 0.67              |
| 1:D:131:LEU:HB3  | 1:D:178:ARG:NH1   | 2.09                     | 0.67              |
| 1:D:368:ARG:HH12 | 1:D:371:VAL:HB    | 1.57                     | 0.67              |
| 1:D:1434:TYR:CD1 | 1:D:1570:LYS:CD   | 2.71                     | 0.67              |
| 1:A:4710:UNK:C   | 1:A:4719:UNK:CB   | 2.66                     | 0.67              |
| 1:C:76:ARG:O     | 1:C:79:GLN:HG2    | 1.95                     | 0.67              |
| 1:C:1004:GLY:HA3 | 1:C:1015:ALA:HB2  | 1.71                     | 0.67              |
| 1:D:1000:ARG:NE  | 1:D:1007:TYR:OH   | 2.26                     | 0.67              |
| 1:D:1453:VAL:O   | 1:D:1548:LEU:CA   | 2.43                     | 0.67              |
| 1:A:1000:ARG:NE  | 1:A:1007:TYR:OH   | 2.26                     | 0.67              |
| 1:C:80:GLU:OE1   | 1:D:3932:UNK:HA   | 1.94                     | 0.67              |
| 1:C:368:ARG:HH12 | 1:C:371:VAL:HB    | 1.57                     | 0.67              |
| 1:C:953:THR:O    | 1:C:959:TYR:CE2   | 2.44                     | 0.67              |
| 1:D:1000:ARG:HG3 | 1:D:1018:ASN:ND2  | 2.10                     | 0.67              |
| 1:D:1020:ARG:O   | 1:D:1020:ARG:HD3  | 1.93                     | 0.67              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:19:GLU:HG2    | 1:B:205:ILE:HG13 | 1.77                     | 0.67              |
| 1:B:75:VAL:N      | 1:B:78:LEU:HG    | 2.00                     | 0.67              |
| 1:C:82:LEU:CD1    | 1:C:144:GLU:OE2  | 2.42                     | 0.67              |
| 1:C:131:LEU:HB3   | 1:C:178:ARG:NH1  | 2.09                     | 0.67              |
| 1:C:329:ARG:HG3   | 1:C:329:ARG:NH1  | 1.97                     | 0.67              |
| 1:C:362:PRO:HG2   | 1:C:364:PRO:HB3  | 1.75                     | 0.67              |
| 1:D:19:GLU:HG2    | 1:D:205:ILE:HG13 | 1.77                     | 0.67              |
| 1:D:1001:VAL:O    | 1:D:1005:TRP:CD1 | 2.48                     | 0.67              |
| 1:D:1466:LEU:CD2  | 1:D:1551:ALA:O   | 2.41                     | 0.67              |
| 1:A:469:ARG:HA    | 1:A:472:ARG:NH1  | 2.09                     | 0.67              |
| 1:B:1001:VAL:HG13 | 1:B:1005:TRP:CE2 | 2.30                     | 0.67              |
| 1:C:19:GLU:HG2    | 1:C:205:ILE:HG13 | 1.77                     | 0.67              |
| 1:C:2299:UNK:CB   | 1:C:2352:UNK:C   | 2.73                     | 0.67              |
| 1:D:210:GLU:HG3   | 1:D:337:PRO:HG3  | 1.76                     | 0.67              |
| 1:A:19:GLU:HG2    | 1:A:205:ILE:HG13 | 1.77                     | 0.67              |
| 1:B:752:VAL:CG2   | 1:B:754:SER:CB   | 2.71                     | 0.67              |
| 1:B:1001:VAL:O    | 1:B:1005:TRP:CD1 | 2.48                     | 0.67              |
| 1:C:1000:ARG:HG3  | 1:C:1018:ASN:ND2 | 2.10                     | 0.67              |
| 1:C:1003:GLN:CA   | 1:C:1003:GLN:OE1 | 2.41                     | 0.67              |
| 1:A:1001:VAL:HG13 | 1:A:1005:TRP:CE2 | 2.30                     | 0.67              |
| 1:A:1453:VAL:O    | 1:A:1548:LEU:CA  | 2.43                     | 0.67              |
| 1:D:76:ARG:O      | 1:D:79:GLN:HG2   | 1.95                     | 0.67              |
| 1:D:151:HIS:HB2   | 1:D:170:ILE:HG22 | 1.76                     | 0.67              |
| 1:D:657:THR:HB    | 1:D:662:TRP:NE1  | 2.09                     | 0.67              |
| 1:C:657:THR:HB    | 1:C:662:TRP:NE1  | 2.09                     | 0.66              |
| 1:D:82:LEU:CD1    | 1:D:144:GLU:OE2  | 2.42                     | 0.66              |
| 1:D:1439:VAL:CA   | 1:D:1515:VAL:HA  | 2.18                     | 0.66              |
| 1:A:210:GLU:HG3   | 1:A:337:PRO:HG3  | 1.76                     | 0.66              |
| 1:A:996:TRP:HE1   | 1:A:1018:ASN:HB3 | 1.61                     | 0.66              |
| 1:A:998:ARG:NE    | 1:A:999:ASP:N    | 2.43                     | 0.66              |
| 1:A:1001:VAL:O    | 1:A:1005:TRP:CD1 | 2.48                     | 0.66              |
| 1:A:2299:UNK:CB   | 1:A:2352:UNK:C   | 2.73                     | 0.66              |
| 1:B:956:PRO:CD    | 1:B:959:TYR:CB   | 2.73                     | 0.66              |
| 1:B:956:PRO:C     | 1:B:958:THR:H    | 2.02                     | 0.66              |
| 1:C:657:THR:HG1   | 1:C:662:TRP:CD1  | 2.14                     | 0.66              |
| 1:C:752:VAL:CG2   | 1:C:754:SER:CB   | 2.71                     | 0.66              |
| 1:C:851:PHE:CE2   | 1:C:1021:LEU:HA  | 2.31                     | 0.66              |
| 1:C:956:PRO:HG2   | 1:C:959:TYR:CE1  | 2.15                     | 0.66              |
| 1:D:855:PRO:HA    | 1:D:994:ASN:ND2  | 1.85                     | 0.66              |
| 1:D:956:PRO:C     | 1:D:958:THR:H    | 2.03                     | 0.66              |
| 1:D:959:TYR:HB3   | 1:D:963:ASN:ND2  | 2.11                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:2299:UNK:CB   | 1:D:2352:UNK:C    | 2.73                     | 0.66              |
| 1:A:426:ARG:CZ    | 1:A:796:ARG:HH22  | 2.08                     | 0.66              |
| 1:A:954:LYS:C     | 1:A:959:TYR:HD2   | 2.04                     | 0.66              |
| 1:A:1459:GLN:HG2  | 1:A:1553:PHE:HD1  | 1.58                     | 0.66              |
| 1:B:954:LYS:C     | 1:B:959:TYR:HD2   | 2.04                     | 0.66              |
| 1:B:956:PRO:HD2   | 1:B:959:TYR:H     | 1.60                     | 0.66              |
| 1:C:956:PRO:C     | 1:C:958:THR:H     | 2.03                     | 0.66              |
| 1:D:21:VAL:CG1    | 1:D:205:ILE:HD11  | 2.04                     | 0.66              |
| 1:D:954:LYS:C     | 1:D:959:TYR:HD2   | 2.04                     | 0.66              |
| 1:A:959:TYR:HB3   | 1:A:963:ASN:ND2   | 2.11                     | 0.66              |
| 1:B:657:THR:HB    | 1:B:662:TRP:NE1   | 2.09                     | 0.66              |
| 1:B:996:TRP:CH2   | 1:B:1021:LEU:HD13 | 2.25                     | 0.66              |
| 1:C:426:ARG:CZ    | 1:C:796:ARG:HH22  | 2.08                     | 0.66              |
| 1:C:1459:GLN:HG2  | 1:C:1553:PHE:HD1  | 1.58                     | 0.66              |
| 1:A:76:ARG:O      | 1:A:79:GLN:HG2    | 1.95                     | 0.66              |
| 1:B:151:HIS:HB2   | 1:B:170:ILE:HG22  | 1.76                     | 0.66              |
| 1:B:1000:ARG:HG3  | 1:B:1018:ASN:ND2  | 2.10                     | 0.66              |
| 1:D:953:THR:O     | 1:D:959:TYR:CE2   | 2.44                     | 0.66              |
| 1:D:998:ARG:HD3   | 1:D:999:ASP:OD1   | 1.93                     | 0.66              |
| 1:D:1439:VAL:CG1  | 1:D:1514:LEU:O    | 2.43                     | 0.66              |
| 1:A:1439:VAL:CA   | 1:A:1515:VAL:HA   | 2.18                     | 0.66              |
| 1:A:1658:UNK:O    | 1:A:1665:UNK:CB   | 2.44                     | 0.66              |
| 1:D:657:THR:HG22  | 1:D:662:TRP:CZ2   | 2.29                     | 0.66              |
| 1:A:657:THR:HG1   | 1:A:662:TRP:CD1   | 2.14                     | 0.66              |
| 1:B:1439:VAL:HG12 | 1:B:1514:LEU:O    | 1.96                     | 0.66              |
| 1:C:210:GLU:HG3   | 1:C:337:PRO:HG3   | 1.76                     | 0.66              |
| 1:C:954:LYS:C     | 1:C:959:TYR:HD2   | 2.04                     | 0.66              |
| 1:C:1001:VAL:O    | 1:C:1005:TRP:CD1  | 2.48                     | 0.66              |
| 1:C:1429:ASN:HB2  | 1:C:1547:LYS:HD2  | 1.76                     | 0.66              |
| 1:C:1439:VAL:HG12 | 1:C:1514:LEU:O    | 1.96                     | 0.66              |
| 1:C:1439:VAL:CG1  | 1:C:1514:LEU:O    | 2.43                     | 0.66              |
| 1:D:1429:ASN:HB2  | 1:D:1547:LYS:HD2  | 1.76                     | 0.66              |
| 1:A:1439:VAL:CG1  | 1:A:1514:LEU:O    | 2.43                     | 0.66              |
| 1:B:1016:ARG:CZ   | 1:B:1016:ARG:CB   | 2.61                     | 0.66              |
| 1:B:1429:ASN:HB2  | 1:B:1547:LYS:HD2  | 1.76                     | 0.66              |
| 1:C:1453:VAL:O    | 1:C:1548:LEU:CA   | 2.43                     | 0.66              |
| 1:C:4710:UNK:C    | 1:C:4719:UNK:CB   | 2.66                     | 0.66              |
| 1:D:426:ARG:CZ    | 1:D:796:ARG:HH22  | 2.08                     | 0.66              |
| 1:A:1000:ARG:HG3  | 1:A:1018:ASN:ND2  | 2.10                     | 0.66              |
| 1:B:996:TRP:HZ2   | 1:B:1021:LEU:CD1  | 1.90                     | 0.66              |
| 1:B:1439:VAL:CG1  | 1:B:1514:LEU:O    | 2.43                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:84:ASN:HD22  | 1:D:84:ASN:N      | 1.94                     | 0.66              |
| 1:D:1444:GLU:N   | 1:D:1445:PRO:HA   | 2.11                     | 0.66              |
| 1:A:1434:TYR:CD1 | 1:A:1570:LYS:CD   | 2.71                     | 0.66              |
| 1:B:948:ASP:HB3  | 1:B:959:TYR:HE1   | 1.61                     | 0.66              |
| 1:B:1444:GLU:N   | 1:B:1445:PRO:HA   | 2.10                     | 0.66              |
| 1:D:1658:UNK:O   | 1:D:1665:UNK:CB   | 2.44                     | 0.66              |
| 1:A:956:PRO:HD2  | 1:A:959:TYR:H     | 1.60                     | 0.65              |
| 1:A:956:PRO:HG2  | 1:A:959:TYR:CE1   | 2.15                     | 0.65              |
| 1:B:1658:UNK:O   | 1:B:1665:UNK:CB   | 2.44                     | 0.65              |
| 1:C:84:ASN:HD22  | 1:C:84:ASN:N      | 1.94                     | 0.65              |
| 1:A:851:PHE:CE2  | 1:A:1021:LEU:HA   | 2.31                     | 0.65              |
| 1:A:948:ASP:HB3  | 1:A:959:TYR:HE1   | 1.62                     | 0.65              |
| 1:B:84:ASN:HD22  | 1:B:84:ASN:N      | 1.94                     | 0.65              |
| 1:B:317:ARG:HH12 | 1:B:322:LYS:HA    | 1.58                     | 0.65              |
| 1:B:996:TRP:HE1  | 1:B:1018:ASN:HB3  | 1.60                     | 0.65              |
| 1:D:996:TRP:HE1  | 1:D:1018:ASN:HB3  | 1.60                     | 0.65              |
| 1:A:1003:GLN:OE1 | 1:A:1003:GLN:N    | 2.30                     | 0.65              |
| 1:B:1000:ARG:NE  | 1:B:1007:TYR:OH   | 2.26                     | 0.65              |
| 1:B:1453:VAL:O   | 1:B:1548:LEU:CA   | 2.43                     | 0.65              |
| 1:C:151:HIS:HB2  | 1:C:170:ILE:HG22  | 1.76                     | 0.65              |
| 1:C:959:TYR:HB3  | 1:C:963:ASN:ND2   | 2.11                     | 0.65              |
| 1:D:948:ASP:HB3  | 1:D:959:TYR:HE1   | 1.62                     | 0.65              |
| 1:A:84:ASN:HD22  | 1:A:84:ASN:N      | 1.94                     | 0.65              |
| 1:A:1422:ASP:HB3 | 1:A:1549:PHE:HE1  | 1.61                     | 0.65              |
| 1:B:426:ARG:CZ   | 1:B:796:ARG:HH22  | 2.08                     | 0.65              |
| 1:B:999:ASP:O    | 1:B:1003:GLN:NE2  | 2.30                     | 0.65              |
| 1:B:1003:GLN:OE1 | 1:B:1003:GLN:N    | 2.30                     | 0.65              |
| 1:C:948:ASP:HB3  | 1:C:959:TYR:HE1   | 1.61                     | 0.65              |
| 1:A:956:PRO:C    | 1:A:958:THR:H     | 2.03                     | 0.65              |
| 1:B:424:LYS:HB3  | 1:B:506:TYR:HD1   | 1.61                     | 0.65              |
| 1:B:851:PHE:CE2  | 1:B:1021:LEU:HA   | 2.31                     | 0.65              |
| 1:C:424:LYS:HB3  | 1:C:506:TYR:HD1   | 1.61                     | 0.65              |
| 1:C:752:VAL:CB   | 1:C:754:SER:HB2   | 2.27                     | 0.65              |
| 1:C:994:ASN:OD1  | 1:C:995:VAL:N     | 2.30                     | 0.65              |
| 1:A:994:ASN:OD1  | 1:A:995:VAL:N     | 2.30                     | 0.65              |
| 1:A:1476:MET:CE  | 1:A:1516:ILE:HD11 | 2.17                     | 0.65              |
| 1:B:210:GLU:HG3  | 1:B:337:PRO:HG3   | 1.76                     | 0.65              |
| 1:B:1000:ARG:NH1 | 1:B:1007:TYR:OH   | 2.30                     | 0.65              |
| 1:C:657:THR:HG21 | 1:C:662:TRP:CE2   | 2.05                     | 0.65              |
| 1:C:1444:GLU:N   | 1:C:1445:PRO:HA   | 2.10                     | 0.65              |
| 1:C:1466:LEU:CD2 | 1:C:1551:ALA:O    | 2.41                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:996:TRP:HZ2  | 1:D:1021:LEU:CD1  | 1.90                     | 0.65              |
| 1:B:728:ARG:HD2  | 1:B:1134:LEU:HD22 | 1.79                     | 0.65              |
| 1:A:415:ILE:HB   | 1:A:493:ARG:NH1   | 2.12                     | 0.65              |
| 1:A:953:THR:O    | 1:A:959:TYR:CE2   | 2.44                     | 0.65              |
| 1:B:1001:VAL:CG1 | 1:B:1005:TRP:NE1  | 2.50                     | 0.65              |
| 1:B:1018:ASN:N   | 1:B:1018:ASN:OD1  | 2.30                     | 0.65              |
| 1:C:1018:ASN:OD1 | 1:C:1018:ASN:N    | 2.30                     | 0.65              |
| 1:C:4086:UNK:O   | 1:C:4124:UNK:HA   | 1.97                     | 0.65              |
| 1:D:752:VAL:CB   | 1:D:754:SER:HB2   | 2.27                     | 0.65              |
| 1:B:994:ASN:OD1  | 1:B:995:VAL:N     | 2.30                     | 0.65              |
| 1:C:728:ARG:HD2  | 1:C:1134:LEU:HD22 | 1.79                     | 0.65              |
| 1:C:948:ASP:OD2  | 1:C:959:TYR:HE1   | 1.79                     | 0.65              |
| 1:C:1015:ALA:O   | 1:C:1016:ARG:NE   | 2.30                     | 0.65              |
| 1:D:567:UNK:O    | 1:D:570:UNK:N     | 2.30                     | 0.65              |
| 1:D:851:PHE:CE2  | 1:D:1021:LEU:HA   | 2.31                     | 0.65              |
| 1:B:948:ASP:HB3  | 1:B:959:TYR:CE1   | 2.32                     | 0.65              |
| 1:B:1015:ALA:O   | 1:B:1016:ARG:NE   | 2.30                     | 0.65              |
| 1:C:567:UNK:O    | 1:C:570:UNK:N     | 2.30                     | 0.65              |
| 1:C:948:ASP:HB3  | 1:C:959:TYR:CE1   | 2.32                     | 0.65              |
| 1:C:1658:UNK:O   | 1:C:1665:UNK:CB   | 2.44                     | 0.65              |
| 1:D:948:ASP:OD2  | 1:D:959:TYR:HE1   | 1.79                     | 0.65              |
| 1:D:1003:GLN:OE1 | 1:D:1003:GLN:N    | 2.30                     | 0.65              |
| 1:A:424:LYS:HB3  | 1:A:506:TYR:HD1   | 1.61                     | 0.64              |
| 1:A:657:THR:HB   | 1:A:662:TRP:CZ2   | 2.31                     | 0.64              |
| 1:A:998:ARG:HD3  | 1:A:999:ASP:OD1   | 1.93                     | 0.64              |
| 1:A:1444:GLU:N   | 1:A:1445:PRO:HA   | 2.11                     | 0.64              |
| 1:A:4086:UNK:O   | 1:A:4124:UNK:HA   | 1.96                     | 0.64              |
| 1:C:208:CYS:O    | 1:C:334:MET:HG3   | 1.97                     | 0.64              |
| 1:C:324:ASP:HB2  | 1:C:326:ALA:N     | 2.12                     | 0.64              |
| 1:C:956:PRO:HD2  | 1:C:959:TYR:H     | 1.61                     | 0.64              |
| 1:C:999:ASP:O    | 1:C:1003:GLN:NE2  | 2.30                     | 0.64              |
| 1:A:998:ARG:CD   | 1:A:998:ARG:C     | 2.70                     | 0.64              |
| 1:B:415:ILE:HB   | 1:B:493:ARG:NH1   | 2.12                     | 0.64              |
| 1:B:752:VAL:HG11 | 1:B:769:GLU:OE1   | 1.97                     | 0.64              |
| 1:B:1459:GLN:HG2 | 1:B:1553:PHE:HD1  | 1.57                     | 0.64              |
| 1:C:415:ILE:HB   | 1:C:493:ARG:NH1   | 2.12                     | 0.64              |
| 1:C:1003:GLN:OE1 | 1:C:1003:GLN:N    | 2.30                     | 0.64              |
| 1:D:415:ILE:HB   | 1:D:493:ARG:NH1   | 2.12                     | 0.64              |
| 1:D:657:THR:HB   | 1:D:662:TRP:CZ2   | 2.32                     | 0.64              |
| 1:D:1001:VAL:CG1 | 1:D:1005:TRP:NE1  | 2.50                     | 0.64              |
| 1:A:752:VAL:CB   | 1:A:754:SER:HB2   | 2.27                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:368:ARG:NH2  | 1:B:369:LEU:HD13 | 2.13                     | 0.64              |
| 1:B:1466:LEU:CD2 | 1:B:1551:ALA:O   | 2.41                     | 0.64              |
| 1:D:4086:UNK:O   | 1:D:4124:UNK:HA  | 1.96                     | 0.64              |
| 1:A:1018:ASN:N   | 1:A:1018:ASN:OD1 | 2.30                     | 0.64              |
| 1:B:170:ILE:HG12 | 1:B:197:GLN:HE21 | 1.63                     | 0.64              |
| 1:B:4086:UNK:O   | 1:B:4124:UNK:HA  | 1.96                     | 0.64              |
| 1:C:998:ARG:NE   | 1:C:999:ASP:N    | 2.43                     | 0.64              |
| 1:D:1422:ASP:HB3 | 1:D:1549:PHE:HE1 | 1.61                     | 0.64              |
| 1:A:657:THR:HG22 | 1:A:662:TRP:CZ2  | 2.28                     | 0.64              |
| 1:A:999:ASP:O    | 1:A:1003:GLN:NE2 | 2.30                     | 0.64              |
| 1:B:324:ASP:HB2  | 1:B:326:ALA:N    | 2.12                     | 0.64              |
| 1:B:657:THR:HB   | 1:B:662:TRP:CZ2  | 2.32                     | 0.64              |
| 1:B:948:ASP:OD2  | 1:B:959:TYR:HE1  | 1.79                     | 0.64              |
| 1:B:959:TYR:HB3  | 1:B:963:ASN:ND2  | 2.11                     | 0.64              |
| 1:B:1478:ASP:O   | 1:B:1509:ILE:CG2 | 2.46                     | 0.64              |
| 1:C:995:VAL:O    | 1:C:998:ARG:CG   | 2.44                     | 0.64              |
| 1:C:1000:ARG:CD  | 1:C:1016:ARG:HD2 | 2.28                     | 0.64              |
| 1:D:994:ASN:OD1  | 1:D:995:VAL:N    | 2.30                     | 0.64              |
| 1:D:3398:UNK:O   | 1:D:3400:UNK:N   | 2.31                     | 0.64              |
| 1:A:1434:TYR:CE1 | 1:A:1570:LYS:CB  | 2.80                     | 0.64              |
| 1:B:1000:ARG:CD  | 1:B:1016:ARG:HD2 | 2.28                     | 0.64              |
| 1:B:1474:VAL:HB  | 1:B:1529:PHE:HE2 | 1.63                     | 0.64              |
| 1:B:1558:HIS:CG  | 1:B:1559:GLN:H   | 2.14                     | 0.64              |
| 1:C:222:LEU:HA   | 1:C:390:LEU:CD2  | 2.28                     | 0.64              |
| 1:C:368:ARG:NH2  | 1:C:369:LEU:HD13 | 2.13                     | 0.64              |
| 1:C:1558:HIS:CG  | 1:C:1559:GLN:H   | 2.13                     | 0.64              |
| 1:D:208:CYS:O    | 1:D:334:MET:HG3  | 1.97                     | 0.64              |
| 1:D:324:ASP:HB2  | 1:D:326:ALA:N    | 2.12                     | 0.64              |
| 1:D:999:ASP:O    | 1:D:1003:GLN:NE2 | 2.30                     | 0.64              |
| 1:A:948:ASP:OD2  | 1:A:959:TYR:HE1  | 1.79                     | 0.64              |
| 1:A:1000:ARG:NH1 | 1:A:1007:TYR:OH  | 2.30                     | 0.64              |
| 1:A:1474:VAL:HB  | 1:A:1529:PHE:HE2 | 1.63                     | 0.64              |
| 1:A:1478:ASP:O   | 1:A:1509:ILE:CG2 | 2.46                     | 0.64              |
| 1:B:222:LEU:HA   | 1:B:390:LEU:CD2  | 2.28                     | 0.64              |
| 1:B:752:VAL:CB   | 1:B:754:SER:HB2  | 2.27                     | 0.64              |
| 1:C:3398:UNK:O   | 1:C:3400:UNK:N   | 2.31                     | 0.64              |
| 1:D:222:LEU:HA   | 1:D:390:LEU:CD2  | 2.28                     | 0.64              |
| 1:D:956:PRO:HD2  | 1:D:959:TYR:H    | 1.61                     | 0.64              |
| 1:D:1018:ASN:N   | 1:D:1018:ASN:OD1 | 2.30                     | 0.64              |
| 1:A:1001:VAL:CG1 | 1:A:1005:TRP:NE1 | 2.50                     | 0.64              |
| 1:A:1015:ALA:O   | 1:A:1016:ARG:NE  | 2.30                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:208:CYS:O     | 1:B:334:MET:HG3   | 1.97                     | 0.64              |
| 1:B:424:LYS:HB3   | 1:B:506:TYR:CD1   | 2.33                     | 0.64              |
| 1:B:1434:TYR:CE1  | 1:B:1570:LYS:CB   | 2.80                     | 0.64              |
| 1:C:350:HIS:HD2   | 1:C:353:SER:H     | 1.46                     | 0.64              |
| 1:C:993:HIS:C     | 1:C:996:TRP:HE3   | 2.06                     | 0.64              |
| 1:C:996:TRP:HE1   | 1:C:1018:ASN:HB3  | 1.60                     | 0.64              |
| 1:C:1474:VAL:HB   | 1:C:1529:PHE:HE2  | 1.63                     | 0.64              |
| 1:C:1478:ASP:O    | 1:C:1509:ILE:CG2  | 2.46                     | 0.64              |
| 1:D:998:ARG:NE    | 1:D:999:ASP:N     | 2.43                     | 0.64              |
| 1:A:567:UNK:O     | 1:A:570:UNK:N     | 2.30                     | 0.64              |
| 1:A:948:ASP:HB3   | 1:A:959:TYR:CE1   | 2.32                     | 0.64              |
| 1:B:76:ARG:HD3    | 1:C:3929:UNK:O    | 1.98                     | 0.64              |
| 1:C:1000:ARG:NH1  | 1:C:1007:TYR:OH   | 2.30                     | 0.64              |
| 1:C:4703:UNK:CA   | 1:C:4706:UNK:CB   | 2.72                     | 0.64              |
| 1:D:368:ARG:NH2   | 1:D:369:LEU:HD13  | 2.13                     | 0.64              |
| 1:D:424:LYS:HB3   | 1:D:506:TYR:HD1   | 1.61                     | 0.64              |
| 1:D:1085:SER:HA   | 1:D:1155:LEU:HG   | 1.80                     | 0.64              |
| 1:D:1439:VAL:HG12 | 1:D:1514:LEU:O    | 1.96                     | 0.64              |
| 1:D:1558:HIS:CG   | 1:D:1559:GLN:H    | 2.13                     | 0.64              |
| 1:A:956:PRO:CD    | 1:A:959:TYR:CB    | 2.73                     | 0.64              |
| 1:A:1439:VAL:HG12 | 1:A:1514:LEU:O    | 1.96                     | 0.64              |
| 1:A:3398:UNK:O    | 1:A:3400:UNK:N    | 2.31                     | 0.64              |
| 1:B:350:HIS:HD2   | 1:B:353:SER:H     | 1.46                     | 0.64              |
| 1:B:998:ARG:CD    | 1:B:998:ARG:C     | 2.70                     | 0.64              |
| 1:C:170:ILE:HG12  | 1:C:197:GLN:HE21  | 1.63                     | 0.64              |
| 1:C:424:LYS:HB3   | 1:C:506:TYR:CD1   | 2.33                     | 0.64              |
| 1:C:1001:VAL:HG13 | 1:C:1005:TRP:CE2  | 2.30                     | 0.64              |
| 1:D:170:ILE:HG12  | 1:D:197:GLN:HE21  | 1.63                     | 0.64              |
| 1:D:948:ASP:HB3   | 1:D:959:TYR:CE1   | 2.32                     | 0.64              |
| 1:D:992:GLY:O     | 1:D:996:TRP:HB3   | 1.98                     | 0.64              |
| 1:D:1478:ASP:O    | 1:D:1509:ILE:CG2  | 2.46                     | 0.64              |
| 1:D:2285:UNK:C    | 1:D:2286:UNK:H    | 2.11                     | 0.64              |
| 1:A:324:ASP:HB2   | 1:A:326:ALA:N     | 2.12                     | 0.63              |
| 1:A:368:ARG:NH2   | 1:A:369:LEU:HD13  | 2.13                     | 0.63              |
| 1:A:2285:UNK:C    | 1:A:2286:UNK:H    | 2.11                     | 0.63              |
| 1:B:567:UNK:O     | 1:B:570:UNK:N     | 2.30                     | 0.63              |
| 1:B:992:GLY:O     | 1:B:996:TRP:HB3   | 1.98                     | 0.63              |
| 1:B:1434:TYR:HE1  | 1:B:1570:LYS:HB2  | 1.62                     | 0.63              |
| 1:B:1471:ALA:C    | 1:B:1472:VAL:HG23 | 2.24                     | 0.63              |
| 1:D:255:HIS:CD2   | 1:D:480:GLU:HG2   | 2.34                     | 0.63              |
| 1:A:424:LYS:HB3   | 1:A:506:TYR:CD1   | 2.33                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:1004:GLY:O   | 1:B:1008:SER:C    | 2.41                     | 0.63              |
| 1:B:3398:UNK:O   | 1:B:3400:UNK:N    | 2.31                     | 0.63              |
| 1:D:728:ARG:HD2  | 1:D:1134:LEU:HD22 | 1.79                     | 0.63              |
| 1:A:76:ARG:HD3   | 1:B:3929:UNK:O    | 1.98                     | 0.63              |
| 1:D:426:ARG:HH21 | 1:D:796:ARG:HH12  | 0.68                     | 0.63              |
| 1:D:998:ARG:CD   | 1:D:998:ARG:C     | 2.70                     | 0.63              |
| 1:D:1000:ARG:NH1 | 1:D:1007:TYR:OH   | 2.30                     | 0.63              |
| 1:D:1004:GLY:O   | 1:D:1008:SER:C    | 2.41                     | 0.63              |
| 1:D:1015:ALA:O   | 1:D:1016:ARG:NE   | 2.30                     | 0.63              |
| 1:A:728:ARG:HD2  | 1:A:1134:LEU:HD22 | 1.79                     | 0.63              |
| 1:A:992:GLY:O    | 1:A:996:TRP:HB3   | 1.98                     | 0.63              |
| 1:C:255:HIS:CD2  | 1:C:480:GLU:HG2   | 2.34                     | 0.63              |
| 1:C:992:GLY:O    | 1:C:996:TRP:HB3   | 1.98                     | 0.63              |
| 1:C:1001:VAL:CG1 | 1:C:1005:TRP:HE1  | 1.87                     | 0.63              |
| 1:D:1004:GLY:HA3 | 1:D:1015:ALA:HB2  | 1.71                     | 0.63              |
| 1:D:1474:VAL:HB  | 1:D:1529:PHE:HE2  | 1.62                     | 0.63              |
| 1:D:1492:CYS:SG  | 1:D:1539:PHE:CE1  | 2.92                     | 0.63              |
| 1:A:170:ILE:HG12 | 1:A:197:GLN:HE21  | 1.63                     | 0.63              |
| 1:A:208:CYS:O    | 1:A:334:MET:HG3   | 1.97                     | 0.63              |
| 1:B:2285:UNK:C   | 1:B:2286:UNK:H    | 2.11                     | 0.63              |
| 1:C:1434:TYR:CE1 | 1:C:1570:LYS:CB   | 2.80                     | 0.63              |
| 1:C:2285:UNK:C   | 1:C:2286:UNK:H    | 2.11                     | 0.63              |
| 1:D:657:THR:HG21 | 1:D:662:TRP:CE2   | 2.05                     | 0.63              |
| 1:D:1000:ARG:CD  | 1:D:1016:ARG:HD2  | 2.28                     | 0.63              |
| 1:D:1434:TYR:CE1 | 1:D:1570:LYS:CB   | 2.80                     | 0.63              |
| 1:A:222:LEU:HA   | 1:A:390:LEU:CD2   | 2.28                     | 0.63              |
| 1:A:426:ARG:HH21 | 1:A:796:ARG:HH12  | 0.68                     | 0.63              |
| 1:B:472:ARG:HA   | 1:B:475:GLN:HE21  | 1.64                     | 0.63              |
| 1:B:1007:TYR:CD2 | 1:B:1016:ARG:NH2  | 2.67                     | 0.63              |
| 1:C:1004:GLY:O   | 1:C:1008:SER:C    | 2.41                     | 0.63              |
| 1:A:255:HIS:CD2  | 1:A:480:GLU:HG2   | 2.34                     | 0.63              |
| 1:A:1492:CYS:SG  | 1:A:1539:PHE:CE1  | 2.92                     | 0.63              |
| 1:A:3929:UNK:O   | 1:D:76:ARG:HD3    | 1.98                     | 0.63              |
| 1:B:1085:SER:HA  | 1:B:1155:LEU:HG   | 1.80                     | 0.63              |
| 1:C:472:ARG:HA   | 1:C:475:GLN:HE21  | 1.64                     | 0.63              |
| 1:C:998:ARG:CD   | 1:C:998:ARG:C     | 2.70                     | 0.63              |
| 1:A:472:ARG:HA   | 1:A:475:GLN:HE21  | 1.64                     | 0.63              |
| 1:C:1085:SER:HA  | 1:C:1155:LEU:HG   | 1.80                     | 0.63              |
| 1:C:1471:ALA:C   | 1:C:1472:VAL:HG23 | 2.24                     | 0.63              |
| 1:D:4703:UNK:CA  | 1:D:4706:UNK:CB   | 2.72                     | 0.63              |
| 1:D:4792:UNK:O   | 1:D:4796:UNK:N    | 2.32                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:954:LYS:HG2  | 1:A:955:LEU:HG    | 1.81                     | 0.63              |
| 1:A:1000:ARG:CD  | 1:A:1016:ARG:HD2  | 2.28                     | 0.63              |
| 1:A:1004:GLY:O   | 1:A:1008:SER:C    | 2.41                     | 0.63              |
| 1:A:1434:TYR:HE1 | 1:A:1570:LYS:HB2  | 1.62                     | 0.63              |
| 1:B:319:SER:C    | 1:B:321:GLU:OE1   | 2.42                     | 0.63              |
| 1:B:954:LYS:HG2  | 1:B:955:LEU:HG    | 1.81                     | 0.63              |
| 1:C:657:THR:HB   | 1:C:662:TRP:CZ2   | 2.31                     | 0.63              |
| 1:D:954:LYS:HG2  | 1:D:955:LEU:HG    | 1.81                     | 0.63              |
| 1:D:956:PRO:CD   | 1:D:959:TYR:CB    | 2.73                     | 0.63              |
| 1:A:4666:UNK:O   | 1:A:4670:UNK:N    | 2.32                     | 0.62              |
| 1:B:998:ARG:HD3  | 1:B:999:ASP:OD1   | 1.93                     | 0.62              |
| 1:B:1422:ASP:HB3 | 1:B:1549:PHE:HE1  | 1.61                     | 0.62              |
| 1:B:1492:CYS:SG  | 1:B:1539:PHE:CE1  | 2.92                     | 0.62              |
| 1:B:4703:UNK:CA  | 1:B:4706:UNK:CB   | 2.72                     | 0.62              |
| 1:C:1492:CYS:SG  | 1:C:1539:PHE:CE1  | 2.92                     | 0.62              |
| 1:A:350:HIS:HD2  | 1:A:353:SER:H     | 1.46                     | 0.62              |
| 1:A:2428:UNK:CB  | 1:A:2498:UNK:N    | 2.62                     | 0.62              |
| 1:B:255:HIS:CD2  | 1:B:480:GLU:HG2   | 2.34                     | 0.62              |
| 1:B:1021:LEU:O   | 1:B:1022:VAL:CB   | 2.47                     | 0.62              |
| 1:C:76:ARG:HD3   | 1:D:3929:UNK:O    | 2.00                     | 0.62              |
| 1:C:319:SER:C    | 1:C:321:GLU:OE1   | 2.42                     | 0.62              |
| 1:C:1021:LEU:O   | 1:C:1022:VAL:CB   | 2.47                     | 0.62              |
| 1:C:2428:UNK:CB  | 1:C:2498:UNK:N    | 2.62                     | 0.62              |
| 1:D:319:SER:C    | 1:D:321:GLU:OE1   | 2.42                     | 0.62              |
| 1:D:752:VAL:HG11 | 1:D:769:GLU:OE1   | 1.96                     | 0.62              |
| 1:A:1471:ALA:C   | 1:A:1472:VAL:HG23 | 2.24                     | 0.62              |
| 1:B:4666:UNK:O   | 1:B:4670:UNK:N    | 2.32                     | 0.62              |
| 1:C:363:ASP:HB2  | 1:C:369:LEU:HD11  | 1.82                     | 0.62              |
| 1:C:4792:UNK:O   | 1:C:4796:UNK:N    | 2.32                     | 0.62              |
| 1:A:1007:TYR:CD2 | 1:A:1016:ARG:NH2  | 2.67                     | 0.62              |
| 1:A:4792:UNK:O   | 1:A:4796:UNK:N    | 2.32                     | 0.62              |
| 1:B:363:ASP:HB2  | 1:B:369:LEU:HD11  | 1.82                     | 0.62              |
| 1:C:1007:TYR:CD2 | 1:C:1016:ARG:NH2  | 2.67                     | 0.62              |
| 1:D:752:VAL:CG2  | 1:D:754:SER:CB    | 2.71                     | 0.62              |
| 1:C:284:HIS:HD2  | 1:C:287:THR:H     | 1.47                     | 0.62              |
| 1:C:3317:UNK:CB  | 1:C:3323:UNK:CB   | 2.78                     | 0.62              |
| 1:D:2428:UNK:CB  | 1:D:2498:UNK:N    | 2.62                     | 0.62              |
| 1:A:3317:UNK:CB  | 1:A:3323:UNK:CB   | 2.78                     | 0.62              |
| 1:B:284:HIS:HD2  | 1:B:287:THR:H     | 1.47                     | 0.62              |
| 1:B:855:PRO:CA   | 1:B:994:ASN:CB    | 2.73                     | 0.62              |
| 1:B:982:THR:HA   | 1:B:985:VAL:HB    | 1.82                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:4666:UNK:O   | 1:D:4670:UNK:N   | 2.32                     | 0.62              |
| 1:A:329:ARG:HH11 | 1:A:329:ARG:CG   | 2.04                     | 0.62              |
| 1:C:954:LYS:HG2  | 1:C:955:LEU:HG   | 1.81                     | 0.62              |
| 1:D:472:ARG:HA   | 1:D:475:GLN:HE21 | 1.64                     | 0.62              |
| 1:D:1132:TRP:HE3 | 1:D:1135:GLY:HA2 | 1.65                     | 0.62              |
| 1:A:1085:SER:HA  | 1:A:1155:LEU:HG  | 1.80                     | 0.62              |
| 1:A:4703:UNK:CA  | 1:A:4706:UNK:CB  | 2.72                     | 0.62              |
| 1:B:995:VAL:O    | 1:B:998:ARG:CG   | 2.44                     | 0.62              |
| 1:C:317:ARG:HH12 | 1:C:322:LYS:HA   | 1.58                     | 0.62              |
| 1:C:4666:UNK:O   | 1:C:4670:UNK:N   | 2.32                     | 0.62              |
| 1:A:467:LYS:NZ   | 1:A:467:LYS:HB3  | 2.15                     | 0.62              |
| 1:A:1466:LEU:CD2 | 1:A:1551:ALA:O   | 2.41                     | 0.62              |
| 1:D:855:PRO:CA   | 1:D:994:ASN:CB   | 2.73                     | 0.62              |
| 1:D:982:THR:HA   | 1:D:985:VAL:HB   | 1.82                     | 0.62              |
| 1:D:1007:TYR:CD2 | 1:D:1016:ARG:NH2 | 2.67                     | 0.62              |
| 1:D:1434:TYR:HE1 | 1:D:1570:LYS:HB2 | 1.62                     | 0.62              |
| 1:D:3317:UNK:CB  | 1:D:3323:UNK:CB  | 2.78                     | 0.62              |
| 1:A:284:HIS:HD2  | 1:A:287:THR:H    | 1.47                     | 0.62              |
| 1:A:1462:MET:O   | 1:A:1553:PHE:HZ  | 1.83                     | 0.62              |
| 1:C:859:VAL:HG13 | 1:C:860:GLN:HG3  | 1.80                     | 0.62              |
| 1:C:1422:ASP:HB3 | 1:C:1549:PHE:HE1 | 1.61                     | 0.62              |
| 1:D:317:ARG:NE   | 1:D:322:LYS:O    | 2.33                     | 0.62              |
| 1:D:350:HIS:HD2  | 1:D:353:SER:H    | 1.46                     | 0.62              |
| 1:D:467:LYS:NZ   | 1:D:467:LYS:HB3  | 2.15                     | 0.62              |
| 1:A:859:VAL:HG13 | 1:A:860:GLN:HG3  | 1.80                     | 0.61              |
| 1:B:729:PRO:O    | 1:B:730:VAL:HG23 | 2.00                     | 0.61              |
| 1:B:859:VAL:HG13 | 1:B:860:GLN:HG3  | 1.80                     | 0.61              |
| 1:B:2428:UNK:CB  | 1:B:2498:UNK:N   | 2.62                     | 0.61              |
| 1:B:3317:UNK:CB  | 1:B:3323:UNK:CB  | 2.78                     | 0.61              |
| 1:C:92:SER:OG    | 1:C:94:GLN:NE2   | 2.25                     | 0.61              |
| 1:C:322:LYS:HG2  | 1:C:324:ASP:OD1  | 2.00                     | 0.61              |
| 1:D:329:ARG:HG3  | 1:D:329:ARG:NH1  | 1.97                     | 0.61              |
| 1:A:319:SER:C    | 1:A:321:GLU:OE1  | 2.42                     | 0.61              |
| 1:A:363:ASP:HB2  | 1:A:369:LEU:HD11 | 1.82                     | 0.61              |
| 1:A:995:VAL:O    | 1:A:998:ARG:CG   | 2.44                     | 0.61              |
| 1:A:1132:TRP:HE3 | 1:A:1135:GLY:HA2 | 1.65                     | 0.61              |
| 1:B:4792:UNK:O   | 1:B:4796:UNK:N   | 2.32                     | 0.61              |
| 1:C:1132:TRP:HE3 | 1:C:1135:GLY:HA2 | 1.65                     | 0.61              |
| 1:C:4113:UNK:HA  | 1:C:4116:UNK:N   | 2.15                     | 0.61              |
| 1:D:328:LYS:HZ2  | 1:D:329:ARG:N    | 1.98                     | 0.61              |
| 1:A:77:ALA:HA    | 1:A:80:GLU:HG2   | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:79:GLN:HG2    | 1:D:80:GLU:H      | 1.65                     | 0.61              |
| 1:D:993:HIS:C     | 1:D:996:TRP:HE3   | 2.06                     | 0.61              |
| 1:A:1437:VAL:H    | 1:A:1517:GLY:HA2  | 1.66                     | 0.61              |
| 1:B:1132:TRP:HE3  | 1:B:1135:GLY:HA2  | 1.65                     | 0.61              |
| 1:B:1473:THR:O    | 1:B:1540:PHE:CZ   | 2.54                     | 0.61              |
| 1:B:4684:UNK:HA   | 1:B:4687:UNK:CB   | 2.30                     | 0.61              |
| 1:D:4113:UNK:HA   | 1:D:4116:UNK:N    | 2.15                     | 0.61              |
| 1:A:4113:UNK:HA   | 1:A:4116:UNK:N    | 2.15                     | 0.61              |
| 1:A:4172:UNK:O    | 1:A:4173:UNK:C    | 2.48                     | 0.61              |
| 1:B:322:LYS:HG2   | 1:B:324:ASP:OD1   | 2.00                     | 0.61              |
| 1:B:1557:THR:O    | 1:B:1558:HIS:C    | 2.43                     | 0.61              |
| 1:C:12:GLN:NE2    | 1:C:165:VAL:O     | 2.34                     | 0.61              |
| 1:C:1462:MET:O    | 1:C:1553:PHE:HZ   | 1.83                     | 0.61              |
| 1:D:284:HIS:HD2   | 1:D:287:THR:H     | 1.47                     | 0.61              |
| 1:D:424:LYS:HB3   | 1:D:506:TYR:CD1   | 2.33                     | 0.61              |
| 1:D:859:VAL:HG13  | 1:D:860:GLN:HG3   | 1.80                     | 0.61              |
| 1:B:77:ALA:HA     | 1:B:80:GLU:HG2    | 1.82                     | 0.61              |
| 1:B:317:ARG:NE    | 1:B:322:LYS:O     | 2.33                     | 0.61              |
| 1:B:4113:UNK:HA   | 1:B:4116:UNK:N    | 2.15                     | 0.61              |
| 1:C:317:ARG:NE    | 1:C:322:LYS:O     | 2.33                     | 0.61              |
| 1:C:953:THR:HB    | 1:C:959:TYR:CZ    | 2.36                     | 0.61              |
| 1:C:1473:THR:O    | 1:C:1540:PHE:CZ   | 2.54                     | 0.61              |
| 1:C:1495:VAL:H    | 1:C:1540:PHE:HZ   | 1.48                     | 0.61              |
| 1:A:996:TRP:CH2   | 1:A:1021:LEU:HD13 | 2.25                     | 0.61              |
| 1:A:1474:VAL:HG21 | 1:A:1539:PHE:CG   | 2.35                     | 0.61              |
| 1:B:92:SER:OG     | 1:B:94:GLN:NE2    | 2.25                     | 0.61              |
| 1:C:328:LYS:HZ2   | 1:C:329:ARG:N     | 1.98                     | 0.61              |
| 1:C:855:PRO:CA    | 1:C:994:ASN:CB    | 2.73                     | 0.61              |
| 1:D:77:ALA:HA     | 1:D:80:GLU:HG2    | 1.82                     | 0.61              |
| 1:D:366:ALA:N     | 1:D:369:LEU:HG    | 2.16                     | 0.61              |
| 1:D:424:LYS:HZ1   | 1:D:506:TYR:H     | 1.49                     | 0.61              |
| 1:D:995:VAL:O     | 1:D:998:ARG:CG    | 2.44                     | 0.61              |
| 1:D:1021:LEU:O    | 1:D:1022:VAL:CB   | 2.47                     | 0.61              |
| 1:A:1021:LEU:O    | 1:A:1022:VAL:CB   | 2.47                     | 0.61              |
| 1:B:328:LYS:HZ2   | 1:B:329:ARG:N     | 1.98                     | 0.61              |
| 1:D:111:HIS:CD2   | 1:D:114:SER:H     | 2.13                     | 0.61              |
| 1:D:363:ASP:HB2   | 1:D:369:LEU:HD11  | 1.82                     | 0.61              |
| 1:D:953:THR:HB    | 1:D:959:TYR:CZ    | 2.36                     | 0.61              |
| 1:D:1471:ALA:C    | 1:D:1472:VAL:HG23 | 2.24                     | 0.61              |
| 1:A:12:GLN:NE2    | 1:A:165:VAL:O     | 2.34                     | 0.61              |
| 1:B:4172:UNK:O    | 1:B:4173:UNK:C    | 2.48                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:77:ALA:HA     | 1:C:80:GLU:HG2    | 1.82                     | 0.61              |
| 1:C:729:PRO:O     | 1:C:730:VAL:HG23  | 2.01                     | 0.61              |
| 1:D:1000:ARG:HG3  | 1:D:1018:ASN:HD21 | 1.66                     | 0.61              |
| 1:D:1476:MET:CE   | 1:D:1516:ILE:HD11 | 2.17                     | 0.61              |
| 1:A:111:HIS:CD2   | 1:A:114:SER:H     | 2.13                     | 0.61              |
| 1:A:317:ARG:CZ    | 1:A:322:LYS:O     | 2.49                     | 0.61              |
| 1:A:317:ARG:NE    | 1:A:322:LYS:O     | 2.33                     | 0.61              |
| 1:A:1473:THR:O    | 1:A:1540:PHE:CZ   | 2.54                     | 0.61              |
| 1:B:467:LYS:NZ    | 1:B:467:LYS:HB3   | 2.15                     | 0.61              |
| 1:B:1462:MET:O    | 1:B:1553:PHE:HZ   | 1.83                     | 0.61              |
| 1:C:998:ARG:HD3   | 1:C:999:ASP:CA    | 2.31                     | 0.61              |
| 1:C:4684:UNK:HA   | 1:C:4687:UNK:CB   | 2.30                     | 0.61              |
| 1:D:1474:VAL:HG21 | 1:D:1539:PHE:CG   | 2.35                     | 0.61              |
| 1:A:322:LYS:HG2   | 1:A:324:ASP:OD1   | 2.00                     | 0.60              |
| 1:A:2428:UNK:CB   | 1:A:2498:UNK:H2   | 2.14                     | 0.60              |
| 1:A:4684:UNK:HA   | 1:A:4687:UNK:CB   | 2.30                     | 0.60              |
| 1:B:12:GLN:NE2    | 1:B:165:VAL:O     | 2.34                     | 0.60              |
| 1:B:317:ARG:CZ    | 1:B:322:LYS:O     | 2.49                     | 0.60              |
| 1:B:2428:UNK:CB   | 1:B:2498:UNK:H2   | 2.14                     | 0.60              |
| 1:C:317:ARG:CZ    | 1:C:322:LYS:O     | 2.49                     | 0.60              |
| 1:C:1434:TYR:HE1  | 1:C:1570:LYS:HB2  | 1.62                     | 0.60              |
| 1:D:322:LYS:HG2   | 1:D:324:ASP:OD1   | 2.00                     | 0.60              |
| 1:D:355:LEU:HB2   | 1:D:378:LEU:HD23  | 1.84                     | 0.60              |
| 1:D:1441:ALA:CB   | 1:D:1513:ASP:CA   | 2.73                     | 0.60              |
| 1:D:1473:THR:O    | 1:D:1540:PHE:CZ   | 2.54                     | 0.60              |
| 1:A:729:PRO:O     | 1:A:730:VAL:HG23  | 2.01                     | 0.60              |
| 1:A:752:VAL:HG11  | 1:A:769:GLU:OE1   | 1.96                     | 0.60              |
| 1:B:1474:VAL:HG21 | 1:B:1539:PHE:CG   | 2.35                     | 0.60              |
| 1:C:982:THR:HA    | 1:C:985:VAL:HB    | 1.82                     | 0.60              |
| 1:D:1462:MET:O    | 1:D:1553:PHE:HZ   | 1.83                     | 0.60              |
| 1:D:4684:UNK:HA   | 1:D:4687:UNK:CB   | 2.31                     | 0.60              |
| 1:B:255:HIS:CG    | 1:B:480:GLU:HG2   | 2.37                     | 0.60              |
| 1:C:366:ALA:N     | 1:C:369:LEU:HG    | 2.16                     | 0.60              |
| 1:D:855:PRO:N     | 1:D:994:ASN:HB2   | 2.16                     | 0.60              |
| 1:D:1557:THR:O    | 1:D:1558:HIS:C    | 2.43                     | 0.60              |
| 1:A:953:THR:HB    | 1:A:959:TYR:CZ    | 2.36                     | 0.60              |
| 1:A:4797:UNK:O    | 1:A:4801:UNK:C    | 2.50                     | 0.60              |
| 1:B:320:LYS:O     | 1:B:356:TRP:HZ2   | 1.85                     | 0.60              |
| 1:B:998:ARG:HD3   | 1:B:999:ASP:CA    | 2.31                     | 0.60              |
| 1:C:855:PRO:N     | 1:C:994:ASN:HB2   | 2.16                     | 0.60              |
| 1:C:1474:VAL:HG21 | 1:C:1539:PHE:CG   | 2.35                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:467:LYS:HB3  | 1:C:467:LYS:NZ    | 2.15                     | 0.60              |
| 1:D:12:GLN:NE2   | 1:D:165:VAL:O     | 2.34                     | 0.60              |
| 1:D:461:HIS:HA   | 1:D:462:GLU:C     | 2.26                     | 0.60              |
| 1:D:1465:ASP:CB  | 1:D:1553:PHE:CD2  | 2.85                     | 0.60              |
| 1:D:3137:UNK:CB  | 1:D:3191:UNK:CB   | 2.80                     | 0.60              |
| 1:A:982:THR:HA   | 1:A:985:VAL:HB    | 1.82                     | 0.60              |
| 1:A:3137:UNK:CB  | 1:A:3191:UNK:CB   | 2.80                     | 0.60              |
| 1:B:366:ALA:N    | 1:B:369:LEU:HG    | 2.16                     | 0.60              |
| 1:B:1495:VAL:H   | 1:B:1540:PHE:HZ   | 1.48                     | 0.60              |
| 1:A:328:LYS:HZ2  | 1:A:329:ARG:N     | 1.98                     | 0.60              |
| 1:A:1495:VAL:H   | 1:A:1540:PHE:HZ   | 1.48                     | 0.60              |
| 1:B:461:HIS:HA   | 1:B:462:GLU:C     | 2.26                     | 0.60              |
| 1:B:1435:TYR:CE2 | 1:B:1520:VAL:HB   | 2.37                     | 0.60              |
| 1:C:255:HIS:CG   | 1:C:480:GLU:HG2   | 2.37                     | 0.60              |
| 1:C:4172:UNK:O   | 1:C:4173:UNK:C    | 2.48                     | 0.60              |
| 1:D:317:ARG:HH12 | 1:D:322:LYS:HA    | 1.58                     | 0.60              |
| 1:D:1495:VAL:H   | 1:D:1540:PHE:HZ   | 1.48                     | 0.60              |
| 1:A:355:LEU:HB2  | 1:A:378:LEU:HD23  | 1.84                     | 0.60              |
| 1:C:4797:UNK:O   | 1:C:4801:UNK:C    | 2.50                     | 0.60              |
| 1:D:729:PRO:O    | 1:D:730:VAL:HG23  | 2.00                     | 0.60              |
| 1:A:752:VAL:CG2  | 1:A:754:SER:CB    | 2.71                     | 0.60              |
| 1:A:752:VAL:HG13 | 1:A:769:GLU:OE1   | 2.01                     | 0.60              |
| 1:B:1000:ARG:HG3 | 1:B:1018:ASN:HD21 | 1.66                     | 0.60              |
| 1:B:1436:SER:HB3 | 1:B:1567:GLY:HA3  | 1.84                     | 0.60              |
| 1:B:1465:ASP:HA  | 1:B:1553:PHE:CB   | 2.31                     | 0.60              |
| 1:C:773:LEU:HA   | 1:C:777:PHE:CZ    | 2.37                     | 0.60              |
| 1:C:1000:ARG:HG3 | 1:C:1018:ASN:HD21 | 1.67                     | 0.60              |
| 1:C:1465:ASP:CB  | 1:C:1553:PHE:CD2  | 2.85                     | 0.60              |
| 1:C:1557:THR:O   | 1:C:1558:HIS:C    | 2.43                     | 0.60              |
| 1:C:4855:UNK:O   | 1:C:4859:UNK:CB   | 2.50                     | 0.60              |
| 1:D:728:ARG:HD2  | 1:D:1134:LEU:CB   | 2.29                     | 0.60              |
| 1:D:2428:UNK:CB  | 1:D:2498:UNK:H2   | 2.14                     | 0.60              |
| 1:A:255:HIS:CG   | 1:A:480:GLU:HG2   | 2.37                     | 0.60              |
| 1:A:366:ALA:N    | 1:A:369:LEU:HG    | 2.16                     | 0.60              |
| 1:A:948:ASP:OD2  | 1:A:959:TYR:CE1   | 2.55                     | 0.60              |
| 1:A:993:HIS:C    | 1:A:996:TRP:HE3   | 2.06                     | 0.60              |
| 1:A:1435:TYR:CE2 | 1:A:1520:VAL:HB   | 2.37                     | 0.60              |
| 1:A:3400:UNK:O   | 1:A:3404:UNK:CB   | 2.50                     | 0.60              |
| 1:A:4855:UNK:O   | 1:A:4859:UNK:CB   | 2.50                     | 0.60              |
| 1:B:953:THR:HB   | 1:B:959:TYR:CZ    | 2.36                     | 0.60              |
| 1:B:1465:ASP:CB  | 1:B:1553:PHE:CD2  | 2.84                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:355:LEU:HB2   | 1:C:378:LEU:HD23  | 1.83                     | 0.60              |
| 1:C:752:VAL:HG13  | 1:C:769:GLU:OE1   | 2.01                     | 0.60              |
| 1:D:320:LYS:O     | 1:D:356:TRP:HZ2   | 1.85                     | 0.60              |
| 1:D:752:VAL:HG13  | 1:D:769:GLU:OE1   | 2.01                     | 0.60              |
| 1:A:1465:ASP:CB   | 1:A:1553:PHE:CD2  | 2.85                     | 0.59              |
| 1:B:752:VAL:HG13  | 1:B:769:GLU:OE1   | 2.01                     | 0.59              |
| 1:B:1437:VAL:H    | 1:B:1517:GLY:HA2  | 1.66                     | 0.59              |
| 1:B:1474:VAL:HG21 | 1:B:1539:PHE:CB   | 2.32                     | 0.59              |
| 1:D:996:TRP:C     | 1:D:996:TRP:CD1   | 2.80                     | 0.59              |
| 1:D:1437:VAL:H    | 1:D:1517:GLY:HA2  | 1.65                     | 0.59              |
| 1:B:12:GLN:HE22   | 1:B:164:ARG:HB3   | 1.67                     | 0.59              |
| 1:C:79:GLN:HG2    | 1:C:80:GLU:H      | 1.65                     | 0.59              |
| 1:C:996:TRP:CD1   | 1:C:996:TRP:C     | 2.80                     | 0.59              |
| 1:C:996:TRP:CH2   | 1:C:1021:LEU:HD13 | 2.25                     | 0.59              |
| 1:C:2428:UNK:CB   | 1:C:2498:UNK:H2   | 2.14                     | 0.59              |
| 1:D:948:ASP:OD2   | 1:D:959:TYR:CE1   | 2.55                     | 0.59              |
| 1:A:424:LYS:HZ1   | 1:A:506:TYR:H     | 1.50                     | 0.59              |
| 1:A:1474:VAL:HG21 | 1:A:1539:PHE:CB   | 2.33                     | 0.59              |
| 1:B:948:ASP:OD2   | 1:B:959:TYR:CE1   | 2.55                     | 0.59              |
| 1:B:3400:UNK:O    | 1:B:3404:UNK:CB   | 2.50                     | 0.59              |
| 1:B:4797:UNK:O    | 1:B:4801:UNK:C    | 2.50                     | 0.59              |
| 1:C:320:LYS:O     | 1:C:356:TRP:HZ2   | 1.85                     | 0.59              |
| 1:D:4100:UNK:O    | 1:D:4101:UNK:C    | 2.51                     | 0.59              |
| 1:D:4855:UNK:O    | 1:D:4859:UNK:CB   | 2.50                     | 0.59              |
| 1:A:12:GLN:HE22   | 1:A:164:ARG:HB3   | 1.67                     | 0.59              |
| 1:A:461:HIS:HA    | 1:A:462:GLU:C     | 2.26                     | 0.59              |
| 1:A:855:PRO:N     | 1:A:994:ASN:HB2   | 2.16                     | 0.59              |
| 1:A:1016:ARG:CZ   | 1:A:1016:ARG:CB   | 2.61                     | 0.59              |
| 1:B:773:LEU:HA    | 1:B:777:PHE:CZ    | 2.37                     | 0.59              |
| 1:B:855:PRO:N     | 1:B:994:ASN:HB2   | 2.16                     | 0.59              |
| 1:B:1434:TYR:CD1  | 1:B:1570:LYS:CB   | 2.85                     | 0.59              |
| 1:C:1004:GLY:N    | 1:C:1007:TYR:CZ   | 2.70                     | 0.59              |
| 1:D:773:LEU:HA    | 1:D:777:PHE:CZ    | 2.37                     | 0.59              |
| 1:A:9:ASP:OD1     | 1:A:11:VAL:N      | 2.35                     | 0.59              |
| 1:A:1557:THR:O    | 1:A:1558:HIS:C    | 2.43                     | 0.59              |
| 1:A:4100:UNK:O    | 1:A:4101:UNK:C    | 2.51                     | 0.59              |
| 1:B:1452:TRP:CG   | 1:B:1527:MET:CE   | 2.85                     | 0.59              |
| 1:C:461:HIS:HA    | 1:C:462:GLU:C     | 2.26                     | 0.59              |
| 1:C:1435:TYR:CE2  | 1:C:1520:VAL:HB   | 2.37                     | 0.59              |
| 1:D:998:ARG:HD3   | 1:D:999:ASP:CA    | 2.31                     | 0.59              |
| 1:D:1465:ASP:HA   | 1:D:1553:PHE:CB   | 2.31                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:728:ARG:CG    | 1:A:1134:LEU:HD22 | 2.33                     | 0.59              |
| 1:A:4667:UNK:O    | 1:A:4671:UNK:N    | 2.36                     | 0.59              |
| 1:B:4855:UNK:O    | 1:B:4859:UNK:CB   | 2.50                     | 0.59              |
| 1:C:1022:VAL:CG2  | 1:C:1027:LEU:CD2  | 2.81                     | 0.59              |
| 1:C:4667:UNK:O    | 1:C:4671:UNK:N    | 2.36                     | 0.59              |
| 1:D:4172:UNK:O    | 1:D:4173:UNK:C    | 2.48                     | 0.59              |
| 1:D:4797:UNK:O    | 1:D:4801:UNK:C    | 2.50                     | 0.59              |
| 1:A:1004:GLY:N    | 1:A:1007:TYR:CZ   | 2.70                     | 0.59              |
| 1:A:1436:SER:HB3  | 1:A:1567:GLY:HA3  | 1.84                     | 0.59              |
| 1:B:111:HIS:CD2   | 1:B:114:SER:H     | 2.13                     | 0.59              |
| 1:B:355:LEU:HB2   | 1:B:378:LEU:HD23  | 1.84                     | 0.59              |
| 1:B:993:HIS:C     | 1:B:996:TRP:HE3   | 2.06                     | 0.59              |
| 1:B:1004:GLY:N    | 1:B:1007:TYR:CZ   | 2.70                     | 0.59              |
| 1:C:1434:TYR:CD1  | 1:C:1570:LYS:CB   | 2.85                     | 0.59              |
| 1:C:1436:SER:HB3  | 1:C:1567:GLY:HA3  | 1.84                     | 0.59              |
| 1:C:1437:VAL:H    | 1:C:1517:GLY:HA2  | 1.65                     | 0.59              |
| 1:C:3137:UNK:CB   | 1:C:3191:UNK:CB   | 2.80                     | 0.59              |
| 1:D:1494:MET:HA   | 1:D:1540:PHE:HZ   | 1.66                     | 0.59              |
| 1:D:3400:UNK:O    | 1:D:3404:UNK:CB   | 2.50                     | 0.59              |
| 1:A:996:TRP:C     | 1:A:996:TRP:CD1   | 2.80                     | 0.59              |
| 1:A:998:ARG:HD3   | 1:A:999:ASP:CA    | 2.31                     | 0.59              |
| 1:B:996:TRP:CD1   | 1:B:996:TRP:C     | 2.80                     | 0.59              |
| 1:B:2003:UNK:H    | 1:B:2006:UNK:CB   | 2.16                     | 0.59              |
| 1:C:3400:UNK:O    | 1:C:3404:UNK:CB   | 2.50                     | 0.59              |
| 1:D:368:ARG:HH11  | 1:D:368:ARG:CG    | 2.04                     | 0.59              |
| 1:D:578:UNK:HA    | 1:D:581:UNK:CB    | 2.33                     | 0.59              |
| 1:D:1016:ARG:CZ   | 1:D:1016:ARG:CB   | 2.61                     | 0.59              |
| 1:D:1435:TYR:CE2  | 1:D:1520:VAL:HB   | 2.37                     | 0.59              |
| 1:A:320:LYS:O     | 1:A:356:TRP:HZ2   | 1.85                     | 0.59              |
| 1:A:3697:UNK:HA   | 1:A:3701:UNK:CB   | 2.33                     | 0.59              |
| 1:B:753:PRO:CG    | 1:B:773:LEU:HD12  | 2.07                     | 0.59              |
| 1:C:111:HIS:CD2   | 1:C:114:SER:H     | 2.13                     | 0.59              |
| 1:C:956:PRO:CD    | 1:C:959:TYR:CB    | 2.73                     | 0.59              |
| 1:C:1474:VAL:HG21 | 1:C:1539:PHE:CB   | 2.33                     | 0.59              |
| 1:C:2003:UNK:H    | 1:C:2006:UNK:CB   | 2.16                     | 0.59              |
| 1:D:1022:VAL:CG2  | 1:D:1027:LEU:CD2  | 2.81                     | 0.59              |
| 1:D:4667:UNK:O    | 1:D:4671:UNK:N    | 2.36                     | 0.59              |
| 1:A:79:GLN:HG2    | 1:A:80:GLU:H      | 1.66                     | 0.59              |
| 1:A:727:ALA:HB1   | 1:A:1119:GLU:OE2  | 2.03                     | 0.59              |
| 1:A:773:LEU:HA    | 1:A:777:PHE:CZ    | 2.37                     | 0.59              |
| 1:A:953:THR:C     | 1:A:959:TYR:CE2   | 2.81                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1434:TYR:CD1  | 1:A:1570:LYS:CB   | 2.85                     | 0.59              |
| 1:A:1471:ALA:HB1  | 1:A:1548:LEU:HD23 | 1.85                     | 0.59              |
| 1:B:1018:ASN:C    | 1:B:1021:LEU:CD2  | 2.76                     | 0.59              |
| 1:B:4684:UNK:O    | 1:B:4687:UNK:N    | 2.36                     | 0.59              |
| 1:C:728:ARG:CG    | 1:C:1134:LEU:HD22 | 2.33                     | 0.59              |
| 1:C:948:ASP:OD2   | 1:C:959:TYR:CE1   | 2.55                     | 0.59              |
| 1:C:1018:ASN:C    | 1:C:1021:LEU:CD2  | 2.76                     | 0.59              |
| 1:D:682:LEU:HD11  | 1:D:787:VAL:HG11  | 1.85                     | 0.59              |
| 1:D:727:ALA:HB1   | 1:D:1119:GLU:OE2  | 2.03                     | 0.59              |
| 1:D:1436:SER:HB3  | 1:D:1567:GLY:HA3  | 1.84                     | 0.59              |
| 1:A:1022:VAL:CG2  | 1:A:1027:LEU:CD2  | 2.81                     | 0.58              |
| 1:B:79:GLN:HG2    | 1:B:80:GLU:H      | 1.65                     | 0.58              |
| 1:B:682:LEU:HD11  | 1:B:787:VAL:HG11  | 1.85                     | 0.58              |
| 1:B:4667:UNK:O    | 1:B:4671:UNK:N    | 2.36                     | 0.58              |
| 1:C:1471:ALA:HB1  | 1:C:1548:LEU:HD23 | 1.85                     | 0.58              |
| 1:D:317:ARG:CZ    | 1:D:322:LYS:O     | 2.49                     | 0.58              |
| 1:D:1474:VAL:HG21 | 1:D:1539:PHE:CB   | 2.33                     | 0.58              |
| 1:A:682:LEU:HD11  | 1:A:787:VAL:HG11  | 1.85                     | 0.58              |
| 1:A:2003:UNK:H    | 1:A:2006:UNK:CB   | 2.16                     | 0.58              |
| 1:B:9:ASP:OD1     | 1:B:11:VAL:N      | 2.35                     | 0.58              |
| 1:B:953:THR:C     | 1:B:959:TYR:CE2   | 2.81                     | 0.58              |
| 1:C:682:LEU:HD11  | 1:C:787:VAL:HG11  | 1.85                     | 0.58              |
| 1:D:12:GLN:HE22   | 1:D:164:ARG:HB3   | 1.67                     | 0.58              |
| 1:D:1004:GLY:N    | 1:D:1007:TYR:CZ   | 2.70                     | 0.58              |
| 1:D:1452:TRP:CG   | 1:D:1527:MET:CE   | 2.85                     | 0.58              |
| 1:A:995:VAL:C     | 1:A:998:ARG:HG3   | 2.29                     | 0.58              |
| 1:A:1000:ARG:HG3  | 1:A:1018:ASN:HD21 | 1.66                     | 0.58              |
| 1:A:1452:TRP:CG   | 1:A:1527:MET:CE   | 2.86                     | 0.58              |
| 1:A:1465:ASP:HA   | 1:A:1553:PHE:CB   | 2.31                     | 0.58              |
| 1:A:4684:UNK:O    | 1:A:4687:UNK:N    | 2.36                     | 0.58              |
| 1:B:728:ARG:CG    | 1:B:1134:LEU:HD22 | 2.33                     | 0.58              |
| 1:B:1022:VAL:CG2  | 1:B:1027:LEU:CD2  | 2.81                     | 0.58              |
| 1:B:1494:MET:HA   | 1:B:1540:PHE:HZ   | 1.67                     | 0.58              |
| 1:B:3137:UNK:CB   | 1:B:3191:UNK:CB   | 2.80                     | 0.58              |
| 1:B:3697:UNK:HA   | 1:B:3701:UNK:CB   | 2.33                     | 0.58              |
| 1:C:12:GLN:HE22   | 1:C:164:ARG:HB3   | 1.67                     | 0.58              |
| 1:C:75:VAL:CG1    | 1:C:76:ARG:H      | 2.13                     | 0.58              |
| 1:C:578:UNK:HA    | 1:C:581:UNK:CB    | 2.33                     | 0.58              |
| 1:C:879:HIS:CE1   | 1:C:906:CYS:SG    | 2.97                     | 0.58              |
| 1:C:4100:UNK:O    | 1:C:4101:UNK:C    | 2.51                     | 0.58              |
| 1:B:77:ALA:CA     | 1:B:80:GLU:HG2    | 2.34                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:426:ARG:HH21  | 1:B:796:ARG:HH12  | 0.68                     | 0.58              |
| 1:B:727:ALA:HB1   | 1:B:1119:GLU:OE2  | 2.03                     | 0.58              |
| 1:B:1471:ALA:HB1  | 1:B:1548:LEU:HD23 | 1.85                     | 0.58              |
| 1:B:1476:MET:CE   | 1:B:1516:ILE:HD11 | 2.17                     | 0.58              |
| 1:C:727:ALA:HB1   | 1:C:1119:GLU:OE2  | 2.03                     | 0.58              |
| 1:A:578:UNK:HA    | 1:A:581:UNK:CB    | 2.33                     | 0.58              |
| 1:A:1466:LEU:HD13 | 1:A:1551:ALA:HB3  | 1.86                     | 0.58              |
| 1:A:3133:UNK:CB   | 1:A:3173:UNK:CB   | 2.82                     | 0.58              |
| 1:A:3986:UNK:HA   | 1:A:3989:UNK:N    | 2.18                     | 0.58              |
| 1:B:1003:GLN:O    | 1:B:1007:TYR:CE2  | 2.57                     | 0.58              |
| 1:B:1478:ASP:C    | 1:B:1509:ILE:HG22 | 2.29                     | 0.58              |
| 1:C:1452:TRP:CG   | 1:C:1527:MET:CE   | 2.85                     | 0.58              |
| 1:C:1478:ASP:C    | 1:C:1509:ILE:HG22 | 2.29                     | 0.58              |
| 1:D:255:HIS:CG    | 1:D:480:GLU:HG2   | 2.37                     | 0.58              |
| 1:D:728:ARG:CG    | 1:D:1134:LEU:HD22 | 2.33                     | 0.58              |
| 1:D:1471:ALA:HB1  | 1:D:1548:LEU:HD23 | 1.85                     | 0.58              |
| 1:B:578:UNK:HA    | 1:B:581:UNK:CB    | 2.33                     | 0.58              |
| 1:B:1466:LEU:HD13 | 1:B:1551:ALA:HB3  | 1.86                     | 0.58              |
| 1:C:728:ARG:HH11  | 1:C:1134:LEU:N    | 2.02                     | 0.58              |
| 1:C:1494:MET:HA   | 1:C:1540:PHE:HZ   | 1.67                     | 0.58              |
| 1:D:953:THR:C     | 1:D:959:TYR:CE2   | 2.81                     | 0.58              |
| 1:D:1434:TYR:CD1  | 1:D:1570:LYS:CB   | 2.85                     | 0.58              |
| 1:D:2003:UNK:H    | 1:D:2006:UNK:CB   | 2.16                     | 0.58              |
| 1:D:3986:UNK:HA   | 1:D:3989:UNK:N    | 2.18                     | 0.58              |
| 1:A:879:HIS:CE1   | 1:A:906:CYS:SG    | 2.97                     | 0.58              |
| 1:A:1000:ARG:O    | 1:A:1000:ARG:HD3  | 2.03                     | 0.58              |
| 1:A:1003:GLN:O    | 1:A:1007:TYR:CE2  | 2.57                     | 0.58              |
| 1:A:1478:ASP:C    | 1:A:1509:ILE:HG22 | 2.29                     | 0.58              |
| 1:B:3133:UNK:CB   | 1:B:3173:UNK:CB   | 2.82                     | 0.58              |
| 1:C:77:ALA:CA     | 1:C:80:GLU:HG2    | 2.34                     | 0.58              |
| 1:D:728:ARG:HH11  | 1:D:1134:LEU:N    | 2.02                     | 0.58              |
| 1:A:1018:ASN:C    | 1:A:1021:LEU:CD2  | 2.76                     | 0.58              |
| 1:B:879:HIS:CE1   | 1:B:906:CYS:SG    | 2.97                     | 0.58              |
| 1:B:3986:UNK:HA   | 1:B:3989:UNK:N    | 2.19                     | 0.58              |
| 1:B:4100:UNK:O    | 1:B:4101:UNK:C    | 2.51                     | 0.58              |
| 1:C:1444:GLU:OE1  | 1:C:1478:ASP:HA   | 2.04                     | 0.58              |
| 1:D:367:LEU:C     | 1:D:369:LEU:HD23  | 2.29                     | 0.58              |
| 1:A:75:VAL:CG1    | 1:A:76:ARG:H      | 2.14                     | 0.58              |
| 1:A:1494:MET:HA   | 1:A:1540:PHE:HZ   | 1.67                     | 0.58              |
| 1:B:955:LEU:N     | 1:B:959:TYR:HD2   | 2.02                     | 0.58              |
| 1:B:995:VAL:C     | 1:B:998:ARG:HG3   | 2.29                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:953:THR:C     | 1:C:959:TYR:CE2   | 2.81                     | 0.58              |
| 1:D:320:LYS:O     | 1:D:356:TRP:CZ2   | 2.57                     | 0.58              |
| 1:D:322:LYS:HB2   | 1:D:322:LYS:NZ    | 2.19                     | 0.58              |
| 1:D:879:HIS:CE1   | 1:D:906:CYS:SG    | 2.96                     | 0.58              |
| 1:D:1478:ASP:C    | 1:D:1509:ILE:HG22 | 2.29                     | 0.58              |
| 1:A:320:LYS:O     | 1:A:356:TRP:CZ2   | 2.57                     | 0.58              |
| 1:A:322:LYS:HB2   | 1:A:322:LYS:NZ    | 2.19                     | 0.58              |
| 1:A:955:LEU:N     | 1:A:959:TYR:HD2   | 2.02                     | 0.58              |
| 1:A:3821:UNK:O    | 1:A:3826:UNK:CB   | 2.52                     | 0.58              |
| 1:B:1454:THR:CB   | 1:B:1455:PRO:HD2  | 2.30                     | 0.58              |
| 1:C:1473:THR:O    | 1:C:1540:PHE:HZ   | 1.87                     | 0.58              |
| 1:D:995:VAL:C     | 1:D:998:ARG:HG3   | 2.29                     | 0.58              |
| 1:D:996:TRP:CH2   | 1:D:1021:LEU:HD13 | 2.25                     | 0.58              |
| 1:B:367:LEU:C     | 1:B:369:LEU:HD23  | 2.29                     | 0.57              |
| 1:B:1001:VAL:CG1  | 1:B:1002:ALA:N    | 2.67                     | 0.57              |
| 1:C:1450:VAL:HG11 | 1:C:1518:CYS:SG   | 2.44                     | 0.57              |
| 1:C:1466:LEU:HD13 | 1:C:1551:ALA:HB3  | 1.86                     | 0.57              |
| 1:C:3697:UNK:HA   | 1:C:3701:UNK:CB   | 2.33                     | 0.57              |
| 1:C:3986:UNK:HA   | 1:C:3989:UNK:N    | 2.19                     | 0.57              |
| 1:D:1450:VAL:HG11 | 1:D:1518:CYS:SG   | 2.44                     | 0.57              |
| 1:A:77:ALA:CA     | 1:A:80:GLU:HG2    | 2.34                     | 0.57              |
| 1:C:9:ASP:OD1     | 1:C:11:VAL:N      | 2.35                     | 0.57              |
| 1:C:1001:VAL:CG1  | 1:C:1002:ALA:N    | 2.67                     | 0.57              |
| 1:D:4684:UNK:O    | 1:D:4687:UNK:N    | 2.36                     | 0.57              |
| 1:A:855:PRO:CA    | 1:A:994:ASN:HB2   | 2.34                     | 0.57              |
| 1:A:1454:THR:HB   | 1:A:1455:PRO:CD   | 2.29                     | 0.57              |
| 1:B:424:LYS:HZ1   | 1:B:506:TYR:H     | 1.50                     | 0.57              |
| 1:B:855:PRO:CA    | 1:B:994:ASN:HB2   | 2.34                     | 0.57              |
| 1:B:3821:UNK:O    | 1:B:3826:UNK:CB   | 2.52                     | 0.57              |
| 1:C:75:VAL:HA     | 1:C:78:LEU:HD12   | 1.86                     | 0.57              |
| 1:C:1004:GLY:CA   | 1:C:1015:ALA:CB   | 2.60                     | 0.57              |
| 1:C:3133:UNK:CB   | 1:C:3173:UNK:CB   | 2.81                     | 0.57              |
| 1:C:3821:UNK:O    | 1:C:3826:UNK:CB   | 2.52                     | 0.57              |
| 1:C:4113:UNK:CA   | 1:C:4116:UNK:CB   | 2.76                     | 0.57              |
| 1:D:92:SER:OG     | 1:D:94:GLN:NE2    | 2.25                     | 0.57              |
| 1:D:1466:LEU:HD13 | 1:D:1551:ALA:HB3  | 1.86                     | 0.57              |
| 1:D:3133:UNK:CB   | 1:D:3173:UNK:CB   | 2.82                     | 0.57              |
| 1:B:320:LYS:O     | 1:B:356:TRP:CZ2   | 2.57                     | 0.57              |
| 1:B:322:LYS:HB2   | 1:B:322:LYS:NZ    | 2.19                     | 0.57              |
| 1:C:322:LYS:NZ    | 1:C:322:LYS:HB2   | 2.19                     | 0.57              |
| 1:D:1003:GLN:CD   | 1:D:1003:GLN:N    | 2.62                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:152:PRO:HB3  | 1:A:157:ARG:HB2   | 1.87                     | 0.57              |
| 1:A:728:ARG:HH11 | 1:A:1134:LEU:N    | 2.02                     | 0.57              |
| 1:A:1001:VAL:CG1 | 1:A:1002:ALA:N    | 2.67                     | 0.57              |
| 1:C:152:PRO:HB3  | 1:C:157:ARG:HB2   | 1.87                     | 0.57              |
| 1:C:566:UNK:CB   | 1:C:570:UNK:CB    | 2.83                     | 0.57              |
| 1:C:1003:GLN:O   | 1:C:1007:TYR:CE2  | 2.57                     | 0.57              |
| 1:C:1003:GLN:CD  | 1:C:1003:GLN:N    | 2.62                     | 0.57              |
| 1:D:4113:UNK:CA  | 1:D:4116:UNK:CB   | 2.76                     | 0.57              |
| 1:A:566:UNK:CB   | 1:A:570:UNK:CB    | 2.83                     | 0.57              |
| 1:B:566:UNK:CB   | 1:B:570:UNK:CB    | 2.83                     | 0.57              |
| 1:D:75:VAL:CG1   | 1:D:76:ARG:H      | 2.14                     | 0.57              |
| 1:D:566:UNK:CB   | 1:D:570:UNK:CB    | 2.83                     | 0.57              |
| 1:D:1018:ASN:C   | 1:D:1021:LEU:CD2  | 2.76                     | 0.57              |
| 1:D:3697:UNK:HA  | 1:D:3701:UNK:CB   | 2.33                     | 0.57              |
| 1:A:367:LEU:C    | 1:A:369:LEU:HD23  | 2.29                     | 0.57              |
| 1:D:321:GLU:HB2  | 1:D:323:LEU:HD12  | 1.87                     | 0.57              |
| 1:D:1003:GLN:O   | 1:D:1007:TYR:CE2  | 2.57                     | 0.57              |
| 1:D:3821:UNK:O   | 1:D:3826:UNK:CB   | 2.52                     | 0.57              |
| 1:A:3931:UNK:N   | 1:D:76:ARG:NH1    | 2.46                     | 0.57              |
| 1:B:4113:UNK:CA  | 1:B:4116:UNK:CB   | 2.76                     | 0.57              |
| 1:C:367:LEU:C    | 1:C:369:LEU:HD23  | 2.29                     | 0.57              |
| 1:C:1132:TRP:CE3 | 1:C:1135:GLY:HA2  | 2.40                     | 0.57              |
| 1:D:77:ALA:CA    | 1:D:80:GLU:HG2    | 2.34                     | 0.57              |
| 1:A:1558:HIS:CG  | 1:A:1559:GLN:N    | 2.73                     | 0.57              |
| 1:B:152:PRO:HB3  | 1:B:157:ARG:HB2   | 1.87                     | 0.57              |
| 1:B:657:THR:HG1  | 1:B:662:TRP:CD1   | 2.23                     | 0.57              |
| 1:B:728:ARG:HD2  | 1:B:1134:LEU:CB   | 2.29                     | 0.57              |
| 1:B:728:ARG:HH11 | 1:B:1134:LEU:N    | 2.02                     | 0.57              |
| 1:B:753:PRO:CG   | 1:B:773:LEU:HD13  | 2.12                     | 0.57              |
| 1:B:1003:GLN:OE1 | 1:B:1003:GLN:HA   | 2.05                     | 0.57              |
| 1:C:426:ARG:HH21 | 1:C:796:ARG:HH12  | 0.68                     | 0.57              |
| 1:D:1444:GLU:OE1 | 1:D:1478:ASP:HA   | 2.04                     | 0.57              |
| 1:A:1558:HIS:CG  | 1:A:1559:GLN:H    | 2.14                     | 0.57              |
| 1:B:725:HIS:O    | 1:B:726:VAL:O     | 2.23                     | 0.57              |
| 1:B:1444:GLU:OE1 | 1:B:1478:ASP:HA   | 2.04                     | 0.57              |
| 1:C:955:LEU:N    | 1:C:959:TYR:HD2   | 2.02                     | 0.57              |
| 1:C:4703:UNK:C   | 1:C:4707:UNK:CB   | 2.75                     | 0.57              |
| 1:D:75:VAL:HA    | 1:D:78:LEU:HD12   | 1.87                     | 0.57              |
| 1:D:1000:ARG:CG  | 1:D:1018:ASN:HD21 | 2.16                     | 0.57              |
| 1:D:1001:VAL:CG1 | 1:D:1002:ALA:N    | 2.67                     | 0.57              |
| 1:D:1452:TRP:CH2 | 1:D:1527:MET:HG2  | 2.40                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1496:TRP:HB2  | 1:D:1540:PHE:CD1  | 2.40                     | 0.57              |
| 1:B:75:VAL:HA     | 1:B:78:LEU:HD12   | 1.86                     | 0.56              |
| 1:B:1132:TRP:CE3  | 1:B:1135:GLY:HA2  | 2.40                     | 0.56              |
| 1:C:320:LYS:O     | 1:C:356:TRP:CZ2   | 2.57                     | 0.56              |
| 1:C:995:VAL:C     | 1:C:998:ARG:HG3   | 2.29                     | 0.56              |
| 1:C:4684:UNK:O    | 1:C:4687:UNK:N    | 2.36                     | 0.56              |
| 1:D:329:ARG:HH11  | 1:D:329:ARG:CG    | 2.04                     | 0.56              |
| 1:B:1442:GLY:H    | 1:B:1514:LEU:HB2  | 1.70                     | 0.56              |
| 1:C:672:VAL:HB    | 1:C:673:PRO:HD2   | 1.87                     | 0.56              |
| 1:C:913:LEU:HD22  | 1:C:917:GLU:OE1   | 2.06                     | 0.56              |
| 1:C:1452:TRP:CH2  | 1:C:1527:MET:HG2  | 2.40                     | 0.56              |
| 1:D:82:LEU:HD23   | 1:D:82:LEU:C      | 2.30                     | 0.56              |
| 1:D:725:HIS:O     | 1:D:726:VAL:O     | 2.23                     | 0.56              |
| 1:D:1132:TRP:CE3  | 1:D:1135:GLY:HA2  | 2.40                     | 0.56              |
| 1:A:75:VAL:HA     | 1:A:78:LEU:HD12   | 1.86                     | 0.56              |
| 1:A:92:SER:OG     | 1:A:94:GLN:NE2    | 2.25                     | 0.56              |
| 1:A:913:LEU:HD22  | 1:A:917:GLU:OE1   | 2.06                     | 0.56              |
| 1:A:1132:TRP:CE3  | 1:A:1135:GLY:HA2  | 2.39                     | 0.56              |
| 1:A:1450:VAL:HG11 | 1:A:1518:CYS:SG   | 2.44                     | 0.56              |
| 1:B:913:LEU:HD22  | 1:B:917:GLU:OE1   | 2.05                     | 0.56              |
| 1:B:1454:THR:HB   | 1:B:1455:PRO:CD   | 2.29                     | 0.56              |
| 1:B:3133:UNK:O    | 1:B:3137:UNK:N    | 2.39                     | 0.56              |
| 1:C:1496:TRP:HB2  | 1:C:1540:PHE:CD1  | 2.40                     | 0.56              |
| 1:D:152:PRO:HB3   | 1:D:157:ARG:HB2   | 1.87                     | 0.56              |
| 1:D:913:LEU:HD22  | 1:D:917:GLU:OE1   | 2.06                     | 0.56              |
| 1:D:955:LEU:N     | 1:D:959:TYR:HD2   | 2.02                     | 0.56              |
| 1:D:1000:ARG:O    | 1:D:1000:ARG:HD3  | 2.04                     | 0.56              |
| 1:D:1558:HIS:CG   | 1:D:1559:GLN:N    | 2.73                     | 0.56              |
| 1:A:3133:UNK:O    | 1:A:3137:UNK:N    | 2.39                     | 0.56              |
| 1:A:4818:UNK:O    | 1:A:4821:UNK:N    | 2.39                     | 0.56              |
| 1:B:1000:ARG:O    | 1:B:1000:ARG:HD3  | 2.04                     | 0.56              |
| 1:B:1450:VAL:HG11 | 1:B:1518:CYS:SG   | 2.45                     | 0.56              |
| 1:C:1465:ASP:HA   | 1:C:1553:PHE:CB   | 2.31                     | 0.56              |
| 1:D:1452:TRP:C    | 1:D:1548:LEU:HD23 | 2.30                     | 0.56              |
| 1:D:1492:CYS:HG   | 1:D:1539:PHE:HE1  | 1.54                     | 0.56              |
| 1:D:3133:UNK:O    | 1:D:3137:UNK:N    | 2.39                     | 0.56              |
| 1:D:4818:UNK:O    | 1:D:4821:UNK:N    | 2.39                     | 0.56              |
| 1:A:725:HIS:O     | 1:A:726:VAL:O     | 2.23                     | 0.56              |
| 1:A:855:PRO:CA    | 1:A:994:ASN:CB    | 2.73                     | 0.56              |
| 1:A:1452:TRP:HZ2  | 1:A:1519:LEU:C    | 2.14                     | 0.56              |
| 1:B:82:LEU:HD23   | 1:B:82:LEU:C      | 2.30                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1452:TRP:HZ2  | 1:B:1519:LEU:C    | 2.14                     | 0.56              |
| 1:B:1452:TRP:C    | 1:B:1548:LEU:HD23 | 2.30                     | 0.56              |
| 1:B:1496:TRP:HB2  | 1:B:1540:PHE:CD1  | 2.40                     | 0.56              |
| 1:B:4818:UNK:O    | 1:B:4821:UNK:N    | 2.39                     | 0.56              |
| 1:C:1452:TRP:HZ2  | 1:C:1519:LEU:C    | 2.14                     | 0.56              |
| 1:D:1433:TYR:CD1  | 1:D:1569:GLN:HB2  | 2.41                     | 0.56              |
| 1:D:1442:GLY:H    | 1:D:1514:LEU:HB2  | 1.70                     | 0.56              |
| 1:D:1452:TRP:HZ2  | 1:D:1519:LEU:C    | 2.14                     | 0.56              |
| 1:D:1465:ASP:HB3  | 1:D:1468:LYS:HG3  | 1.88                     | 0.56              |
| 1:A:1442:GLY:H    | 1:A:1514:LEU:HB2  | 1.70                     | 0.56              |
| 1:A:1473:THR:O    | 1:A:1540:PHE:HZ   | 1.87                     | 0.56              |
| 1:B:1433:TYR:CD1  | 1:B:1569:GLN:HB2  | 2.41                     | 0.56              |
| 1:C:721:LEU:HD21  | 1:C:737:LEU:HA    | 1.88                     | 0.56              |
| 1:C:725:HIS:O     | 1:C:726:VAL:O     | 2.23                     | 0.56              |
| 1:C:855:PRO:CA    | 1:C:994:ASN:HB2   | 2.35                     | 0.56              |
| 1:C:4848:UNK:HA   | 1:C:4851:UNK:CB   | 2.36                     | 0.56              |
| 1:D:9:ASP:OD1     | 1:D:11:VAL:N      | 2.35                     | 0.56              |
| 1:D:721:LEU:HD21  | 1:D:737:LEU:HA    | 1.88                     | 0.56              |
| 1:A:1003:GLN:CD   | 1:A:1003:GLN:N    | 2.62                     | 0.56              |
| 1:B:721:LEU:HD21  | 1:B:737:LEU:HA    | 1.88                     | 0.56              |
| 1:C:429:GLY:N     | 1:C:505:GLU:HG2   | 2.21                     | 0.56              |
| 1:C:1439:VAL:HG21 | 1:C:1516:ILE:HG22 | 1.87                     | 0.56              |
| 1:C:3400:UNK:CB   | 1:C:3403:UNK:CB   | 2.84                     | 0.56              |
| 1:D:672:VAL:HB    | 1:D:673:PRO:HD2   | 1.87                     | 0.56              |
| 1:D:1439:VAL:HG23 | 1:D:1516:ILE:HG22 | 1.88                     | 0.56              |
| 1:A:1496:TRP:HB2  | 1:A:1540:PHE:CD1  | 2.40                     | 0.56              |
| 1:C:4818:UNK:O    | 1:C:4821:UNK:N    | 2.39                     | 0.56              |
| 1:D:429:GLY:N     | 1:D:505:GLU:HG2   | 2.21                     | 0.56              |
| 1:D:773:LEU:HD23  | 1:D:777:PHE:CZ    | 2.41                     | 0.56              |
| 1:D:1003:GLN:OE1  | 1:D:1003:GLN:HA   | 2.05                     | 0.56              |
| 1:D:4848:UNK:HA   | 1:D:4851:UNK:CB   | 2.36                     | 0.56              |
| 1:A:1441:ALA:CB   | 1:A:1513:ASP:CA   | 2.73                     | 0.56              |
| 1:A:4848:UNK:HA   | 1:A:4851:UNK:CB   | 2.36                     | 0.56              |
| 1:B:1473:THR:O    | 1:B:1540:PHE:HZ   | 1.87                     | 0.56              |
| 1:B:1558:HIS:CG   | 1:B:1559:GLN:N    | 2.73                     | 0.56              |
| 1:C:82:LEU:HD23   | 1:C:82:LEU:C      | 2.30                     | 0.56              |
| 1:D:784:SER:O     | 1:D:785:ALA:HB3   | 2.06                     | 0.56              |
| 1:D:948:ASP:O     | 1:D:958:THR:OG1   | 2.20                     | 0.56              |
| 1:D:1473:THR:O    | 1:D:1540:PHE:HZ   | 1.88                     | 0.56              |
| 1:A:321:GLU:CB    | 1:A:323:LEU:HD13  | 2.36                     | 0.55              |
| 1:A:429:GLY:N     | 1:A:505:GLU:HG2   | 2.21                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:773:LEU:HD23  | 1:A:777:PHE:CZ    | 2.41                     | 0.55              |
| 1:A:1017:ARG:N    | 1:A:1017:ARG:NE   | 2.53                     | 0.55              |
| 1:A:1433:TYR:CD1  | 1:A:1569:GLN:HB2  | 2.41                     | 0.55              |
| 1:A:1444:GLU:OE1  | 1:A:1478:ASP:HA   | 2.04                     | 0.55              |
| 1:A:1452:TRP:C    | 1:A:1548:LEU:HD23 | 2.30                     | 0.55              |
| 1:C:1000:ARG:O    | 1:C:1000:ARG:HD3  | 2.04                     | 0.55              |
| 1:A:948:ASP:O     | 1:A:958:THR:OG1   | 2.20                     | 0.55              |
| 1:A:3400:UNK:CB   | 1:A:3403:UNK:CB   | 2.84                     | 0.55              |
| 1:C:321:GLU:HB2   | 1:C:323:LEU:HD12  | 1.87                     | 0.55              |
| 1:C:1433:TYR:CD1  | 1:C:1569:GLN:HB2  | 2.41                     | 0.55              |
| 1:C:1444:GLU:CD   | 1:C:1478:ASP:HA   | 2.31                     | 0.55              |
| 1:C:3306:UNK:CA   | 1:C:3309:UNK:CB   | 2.84                     | 0.55              |
| 1:D:1494:MET:HG2  | 1:D:1539:PHE:HB3  | 1.88                     | 0.55              |
| 1:D:4144:UNK:C    | 1:D:4145:UNK:CA   | 2.85                     | 0.55              |
| 1:A:82:LEU:HD23   | 1:A:82:LEU:C      | 2.30                     | 0.55              |
| 1:A:1003:GLN:OE1  | 1:A:1003:GLN:HA   | 2.05                     | 0.55              |
| 1:A:1021:LEU:HD13 | 1:A:1021:LEU:H    | 1.72                     | 0.55              |
| 1:A:4103:UNK:O    | 1:A:4104:UNK:O    | 2.25                     | 0.55              |
| 1:C:508:GLY:H     | 1:C:511:ALA:HB3   | 1.72                     | 0.55              |
| 1:C:1442:GLY:H    | 1:C:1514:LEU:HB2  | 1.70                     | 0.55              |
| 1:C:3133:UNK:O    | 1:C:3137:UNK:N    | 2.38                     | 0.55              |
| 1:D:508:GLY:H     | 1:D:511:ALA:HB3   | 1.72                     | 0.55              |
| 1:D:855:PRO:CA    | 1:D:994:ASN:HB2   | 2.35                     | 0.55              |
| 1:C:773:LEU:HD23  | 1:C:777:PHE:CZ    | 2.41                     | 0.55              |
| 1:C:1465:ASP:HB3  | 1:C:1468:LYS:HG3  | 1.88                     | 0.55              |
| 1:A:753:PRO:CG    | 1:A:773:LEU:HD12  | 2.07                     | 0.55              |
| 1:A:2428:UNK:HA   | 1:A:2498:UNK:N    | 2.22                     | 0.55              |
| 1:A:4144:UNK:C    | 1:A:4145:UNK:CA   | 2.85                     | 0.55              |
| 1:B:1021:LEU:HD13 | 1:B:1021:LEU:H    | 1.72                     | 0.55              |
| 1:B:4103:UNK:O    | 1:B:4104:UNK:O    | 2.25                     | 0.55              |
| 1:B:4848:UNK:HA   | 1:B:4851:UNK:CB   | 2.36                     | 0.55              |
| 1:C:76:ARG:NH1    | 1:D:3931:UNK:N    | 2.48                     | 0.55              |
| 1:C:1452:TRP:C    | 1:C:1548:LEU:HD23 | 2.30                     | 0.55              |
| 1:D:1000:ARG:HD2  | 1:D:1000:ARG:C    | 2.29                     | 0.55              |
| 1:D:3400:UNK:CB   | 1:D:3403:UNK:CB   | 2.84                     | 0.55              |
| 1:D:4103:UNK:O    | 1:D:4104:UNK:O    | 2.25                     | 0.55              |
| 1:A:1452:TRP:CH2  | 1:A:1527:MET:HG2  | 2.40                     | 0.55              |
| 1:A:3306:UNK:CA   | 1:A:3309:UNK:CB   | 2.84                     | 0.55              |
| 1:B:321:GLU:HB2   | 1:B:323:LEU:HD12  | 1.87                     | 0.55              |
| 1:C:1435:TYR:HB2  | 1:C:1518:CYS:O    | 2.07                     | 0.55              |
| 1:C:4703:UNK:HA   | 1:C:4706:UNK:C    | 2.32                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:429:GLY:N     | 1:B:505:GLU:HG2   | 2.21                     | 0.55              |
| 1:B:3306:UNK:CA   | 1:B:3309:UNK:CB   | 2.84                     | 0.55              |
| 1:C:2428:UNK:HA   | 1:C:2498:UNK:N    | 2.22                     | 0.55              |
| 1:C:4103:UNK:O    | 1:C:4104:UNK:O    | 2.25                     | 0.55              |
| 1:D:993:HIS:HD1   | 1:D:1035:ASN:ND2  | 2.05                     | 0.55              |
| 1:A:672:VAL:HB    | 1:A:673:PRO:HD2   | 1.87                     | 0.55              |
| 1:A:1494:MET:HG2  | 1:A:1539:PHE:HB3  | 1.88                     | 0.55              |
| 1:A:4675:UNK:O    | 1:A:4678:UNK:N    | 2.40                     | 0.55              |
| 1:B:948:ASP:O     | 1:B:958:THR:OG1   | 2.20                     | 0.55              |
| 1:B:1018:ASN:CA   | 1:B:1021:LEU:CD2  | 2.85                     | 0.55              |
| 1:B:1439:VAL:HG21 | 1:B:1516:ILE:HG22 | 1.87                     | 0.55              |
| 1:D:3306:UNK:CA   | 1:D:3309:UNK:CB   | 2.84                     | 0.55              |
| 1:B:1439:VAL:HG23 | 1:B:1516:ILE:HG22 | 1.89                     | 0.55              |
| 1:B:1444:GLU:CD   | 1:B:1478:ASP:HA   | 2.32                     | 0.55              |
| 1:B:1452:TRP:CH2  | 1:B:1527:MET:HG2  | 2.40                     | 0.55              |
| 1:B:4144:UNK:C    | 1:B:4145:UNK:CA   | 2.85                     | 0.55              |
| 1:C:1454:THR:HB   | 1:C:1455:PRO:CD   | 2.29                     | 0.55              |
| 1:C:3398:UNK:C    | 1:C:3400:UNK:C    | 2.85                     | 0.55              |
| 1:D:1021:LEU:CD1  | 1:D:1021:LEU:N    | 2.70                     | 0.55              |
| 1:D:1021:LEU:C    | 1:D:1022:VAL:HG22 | 2.32                     | 0.55              |
| 1:A:321:GLU:CG    | 1:A:323:LEU:CD1   | 2.85                     | 0.55              |
| 1:A:1465:ASP:HB3  | 1:A:1468:LYS:HG3  | 1.88                     | 0.55              |
| 1:B:249:GLY:H     | 1:B:372:LEU:HD11  | 1.72                     | 0.55              |
| 1:B:508:GLY:H     | 1:B:511:ALA:HB3   | 1.72                     | 0.55              |
| 1:B:773:LEU:HD23  | 1:B:777:PHE:CZ    | 2.41                     | 0.55              |
| 1:B:1003:GLN:CD   | 1:B:1003:GLN:N    | 2.62                     | 0.55              |
| 1:B:3400:UNK:CB   | 1:B:3403:UNK:CB   | 2.84                     | 0.55              |
| 1:C:1018:ASN:CA   | 1:C:1021:LEU:CD2  | 2.85                     | 0.55              |
| 1:C:4144:UNK:C    | 1:C:4145:UNK:CA   | 2.85                     | 0.55              |
| 1:C:4675:UNK:O    | 1:C:4678:UNK:N    | 2.40                     | 0.55              |
| 1:D:1435:TYR:HB2  | 1:D:1518:CYS:O    | 2.07                     | 0.55              |
| 1:D:1444:GLU:CD   | 1:D:1478:ASP:HA   | 2.32                     | 0.55              |
| 1:A:508:GLY:H     | 1:A:511:ALA:HB3   | 1.72                     | 0.54              |
| 1:A:1018:ASN:CA   | 1:A:1021:LEU:CD2  | 2.85                     | 0.54              |
| 1:B:672:VAL:HB    | 1:B:673:PRO:HD2   | 1.87                     | 0.54              |
| 1:B:1021:LEU:C    | 1:B:1022:VAL:HG22 | 2.32                     | 0.54              |
| 1:B:2195:UNK:CB   | 1:B:2198:UNK:CB   | 2.85                     | 0.54              |
| 1:D:321:GLU:CB    | 1:D:323:LEU:CD1   | 2.85                     | 0.54              |
| 1:D:1439:VAL:HG21 | 1:D:1516:ILE:HG22 | 1.87                     | 0.54              |
| 1:D:2428:UNK:HA   | 1:D:2498:UNK:N    | 2.22                     | 0.54              |
| 1:D:4703:UNK:HA   | 1:D:4706:UNK:C    | 2.32                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:76:ARG:NH1    | 1:B:3931:UNK:N    | 2.47                     | 0.54              |
| 1:A:721:LEU:HD21  | 1:A:737:LEU:HA    | 1.88                     | 0.54              |
| 1:A:1450:VAL:HG13 | 1:A:1518:CYS:HG   | 1.72                     | 0.54              |
| 1:A:1494:MET:CA   | 1:A:1540:PHE:CZ   | 2.90                     | 0.54              |
| 1:B:321:GLU:CG    | 1:B:323:LEU:CD1   | 2.85                     | 0.54              |
| 1:B:441:VAL:O     | 1:B:445:LEU:HD13  | 2.07                     | 0.54              |
| 1:B:1452:TRP:CG   | 1:B:1527:MET:HE2  | 2.42                     | 0.54              |
| 1:B:2428:UNK:HA   | 1:B:2498:UNK:N    | 2.22                     | 0.54              |
| 1:C:441:VAL:O     | 1:C:445:LEU:HD13  | 2.07                     | 0.54              |
| 1:C:784:SER:O     | 1:C:785:ALA:HB3   | 2.06                     | 0.54              |
| 1:C:1021:LEU:HD13 | 1:C:1021:LEU:H    | 1.72                     | 0.54              |
| 1:C:4224:UNK:C    | 1:C:4232:UNK:C    | 2.85                     | 0.54              |
| 1:A:317:ARG:HH12  | 1:A:322:LYS:HA    | 1.58                     | 0.54              |
| 1:A:728:ARG:NH1   | 1:A:1134:LEU:N    | 2.56                     | 0.54              |
| 1:B:914:PRO:HD2   | 1:B:917:GLU:OE1   | 2.07                     | 0.54              |
| 1:B:1494:MET:HG2  | 1:B:1539:PHE:HB3  | 1.88                     | 0.54              |
| 1:C:4144:UNK:C    | 1:C:4145:UNK:CB   | 2.85                     | 0.54              |
| 1:D:256:ALA:HA    | 1:D:259:LEU:HD13  | 1.89                     | 0.54              |
| 1:D:1018:ASN:CA   | 1:D:1021:LEU:CD2  | 2.85                     | 0.54              |
| 1:D:1454:THR:HB   | 1:D:1455:PRO:CD   | 2.29                     | 0.54              |
| 1:D:4675:UNK:O    | 1:D:4678:UNK:N    | 2.40                     | 0.54              |
| 1:A:1435:TYR:HB2  | 1:A:1518:CYS:O    | 2.07                     | 0.54              |
| 1:A:1444:GLU:CD   | 1:A:1478:ASP:HA   | 2.32                     | 0.54              |
| 1:A:2195:UNK:CB   | 1:A:2198:UNK:CB   | 2.85                     | 0.54              |
| 1:A:4144:UNK:C    | 1:A:4145:UNK:CB   | 2.85                     | 0.54              |
| 1:B:75:VAL:CG1    | 1:B:76:ARG:H      | 2.14                     | 0.54              |
| 1:B:993:HIS:HD1   | 1:B:1035:ASN:ND2  | 2.05                     | 0.54              |
| 1:B:1435:TYR:HB2  | 1:B:1518:CYS:O    | 2.07                     | 0.54              |
| 1:B:3398:UNK:C    | 1:B:3400:UNK:C    | 2.85                     | 0.54              |
| 1:C:1452:TRP:CG   | 1:C:1527:MET:HE2  | 2.42                     | 0.54              |
| 1:C:1558:HIS:CG   | 1:C:1559:GLN:N    | 2.73                     | 0.54              |
| 1:C:2195:UNK:CB   | 1:C:2198:UNK:CB   | 2.85                     | 0.54              |
| 1:D:1022:VAL:CG2  | 1:D:1027:LEU:HD23 | 2.38                     | 0.54              |
| 1:D:2195:UNK:CB   | 1:D:2198:UNK:CB   | 2.85                     | 0.54              |
| 1:D:3398:UNK:C    | 1:D:3400:UNK:C    | 2.85                     | 0.54              |
| 1:D:4117:UNK:CB   | 1:D:4121:UNK:CA   | 2.85                     | 0.54              |
| 1:B:728:ARG:NH1   | 1:B:1134:LEU:N    | 2.56                     | 0.54              |
| 1:B:1465:ASP:HB3  | 1:B:1468:LYS:HG3  | 1.88                     | 0.54              |
| 1:C:657:THR:HG22  | 1:C:662:TRP:CZ2   | 2.28                     | 0.54              |
| 1:A:146:CYS:HG    | 1:A:147:TRP:CD1   | 2.26                     | 0.54              |
| 1:A:225:GLY:O     | 1:A:227:MET:N     | 2.40                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:256:ALA:HA    | 1:A:259:LEU:HD13  | 1.89                     | 0.54              |
| 1:A:1000:ARG:CG   | 1:A:1018:ASN:HD21 | 2.16                     | 0.54              |
| 1:B:784:SER:O     | 1:B:785:ALA:HB3   | 2.06                     | 0.54              |
| 1:B:1017:ARG:N    | 1:B:1017:ARG:NE   | 2.53                     | 0.54              |
| 1:B:1494:MET:CA   | 1:B:1540:PHE:CZ   | 2.90                     | 0.54              |
| 1:C:4117:UNK:CB   | 1:C:4121:UNK:CA   | 2.85                     | 0.54              |
| 1:D:321:GLU:CG    | 1:D:323:LEU:CD1   | 2.85                     | 0.54              |
| 1:D:2428:UNK:CA   | 1:D:2498:UNK:H2   | 2.21                     | 0.54              |
| 1:D:4224:UNK:C    | 1:D:4232:UNK:C    | 2.85                     | 0.54              |
| 1:A:914:PRO:HD2   | 1:A:917:GLU:OE1   | 2.07                     | 0.54              |
| 1:A:993:HIS:HD1   | 1:A:1035:ASN:ND2  | 2.05                     | 0.54              |
| 1:B:321:GLU:CB    | 1:B:323:LEU:HD13  | 2.36                     | 0.54              |
| 1:B:1492:CYS:HG   | 1:B:1539:PHE:HE1  | 1.53                     | 0.54              |
| 1:B:4144:UNK:C    | 1:B:4145:UNK:CB   | 2.85                     | 0.54              |
| 1:D:1021:LEU:HD13 | 1:D:1021:LEU:H    | 1.72                     | 0.54              |
| 1:A:80:GLU:OE1    | 1:B:3932:UNK:C    | 2.55                     | 0.54              |
| 1:A:441:VAL:O     | 1:A:445:LEU:HD13  | 2.07                     | 0.54              |
| 1:A:784:SER:O     | 1:A:785:ALA:HB3   | 2.06                     | 0.54              |
| 1:A:3398:UNK:C    | 1:A:3400:UNK:C    | 2.85                     | 0.54              |
| 1:A:4732:UNK:O    | 1:A:4735:UNK:N    | 2.41                     | 0.54              |
| 1:B:1022:VAL:CG2  | 1:B:1027:LEU:HD23 | 2.38                     | 0.54              |
| 1:B:2428:UNK:CA   | 1:B:2498:UNK:H2   | 2.21                     | 0.54              |
| 1:B:4117:UNK:CB   | 1:B:4121:UNK:CA   | 2.85                     | 0.54              |
| 1:B:4675:UNK:O    | 1:B:4678:UNK:N    | 2.40                     | 0.54              |
| 1:D:441:VAL:O     | 1:D:445:LEU:HD13  | 2.07                     | 0.54              |
| 1:D:1433:TYR:HD1  | 1:D:1569:GLN:HB2  | 1.73                     | 0.54              |
| 1:D:1494:MET:CA   | 1:D:1540:PHE:CZ   | 2.90                     | 0.54              |
| 1:A:1452:TRP:CG   | 1:A:1527:MET:HE2  | 2.42                     | 0.54              |
| 1:A:4113:UNK:CA   | 1:A:4116:UNK:CB   | 2.76                     | 0.54              |
| 1:B:4703:UNK:HA   | 1:B:4706:UNK:C    | 2.32                     | 0.54              |
| 1:C:659:TYR:C     | 1:C:750:LEU:HD21  | 2.33                     | 0.54              |
| 1:C:728:ARG:NH1   | 1:C:1134:LEU:N    | 2.56                     | 0.54              |
| 1:C:993:HIS:HD1   | 1:C:1035:ASN:ND2  | 2.05                     | 0.54              |
| 1:C:1003:GLN:OE1  | 1:C:1003:GLN:HA   | 2.05                     | 0.54              |
| 1:C:2428:UNK:CA   | 1:C:2498:UNK:H2   | 2.21                     | 0.54              |
| 1:D:1442:GLY:N    | 1:D:1514:LEU:HB2  | 2.18                     | 0.54              |
| 1:D:1851:UNK:CA   | 1:D:1854:UNK:CB   | 2.85                     | 0.54              |
| 1:D:4144:UNK:C    | 1:D:4145:UNK:CB   | 2.85                     | 0.54              |
| 1:A:9:ASP:OD1     | 1:A:11:VAL:HB     | 2.08                     | 0.54              |
| 1:A:249:GLY:H     | 1:A:372:LEU:HD11  | 1.72                     | 0.54              |
| 1:A:1466:LEU:H    | 1:A:1553:PHE:HB2  | 1.73                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:652:ARG:HD2  | 1:B:778:PHE:HB2   | 1.90                     | 0.54              |
| 1:B:1000:ARG:HD2 | 1:B:1000:ARG:C    | 2.29                     | 0.54              |
| 1:C:752:VAL:HG11 | 1:C:769:GLU:OE1   | 1.96                     | 0.54              |
| 1:C:914:PRO:HD2  | 1:C:917:GLU:OE1   | 2.08                     | 0.54              |
| 1:C:1022:VAL:CG2 | 1:C:1027:LEU:HD23 | 2.38                     | 0.54              |
| 1:C:4172:UNK:C   | 1:C:4174:UNK:N    | 2.71                     | 0.54              |
| 1:D:728:ARG:NH1  | 1:D:1134:LEU:N    | 2.56                     | 0.54              |
| 1:D:728:ARG:CD   | 1:D:1134:LEU:HD22 | 2.38                     | 0.54              |
| 1:D:1496:TRP:HZ2 | 1:D:1543:GLU:HG3  | 1.73                     | 0.54              |
| 1:A:229:GLU:OE2  | 1:A:374:LYS:HE2   | 2.08                     | 0.53              |
| 1:A:1007:TYR:CE1 | 1:A:1015:ALA:CA   | 2.86                     | 0.53              |
| 1:B:400:ALA:O    | 1:B:404:ILE:HG12  | 2.09                     | 0.53              |
| 1:B:4224:UNK:C   | 1:B:4232:UNK:C    | 2.85                     | 0.53              |
| 1:C:1017:ARG:N   | 1:C:1017:ARG:NE   | 2.53                     | 0.53              |
| 1:D:4220:UNK:O   | 1:D:4224:UNK:N    | 2.42                     | 0.53              |
| 1:A:998:ARG:NH2  | 1:A:998:ARG:O     | 2.41                     | 0.53              |
| 1:A:1433:TYR:HD1 | 1:A:1569:GLN:HB2  | 1.73                     | 0.53              |
| 1:A:1496:TRP:HZ2 | 1:A:1543:GLU:HG3  | 1.73                     | 0.53              |
| 1:A:4224:UNK:C   | 1:A:4232:UNK:C    | 2.85                     | 0.53              |
| 1:B:4220:UNK:O   | 1:B:4224:UNK:N    | 2.42                     | 0.53              |
| 1:C:321:GLU:CG   | 1:C:323:LEU:CD1   | 2.85                     | 0.53              |
| 1:C:341:TYR:HA   | 1:C:390:LEU:O     | 2.08                     | 0.53              |
| 1:C:1494:MET:HG2 | 1:C:1539:PHE:HB3  | 1.88                     | 0.53              |
| 1:C:1494:MET:CA  | 1:C:1540:PHE:CZ   | 2.90                     | 0.53              |
| 1:C:1496:TRP:HZ2 | 1:C:1543:GLU:HG3  | 1.73                     | 0.53              |
| 1:C:1851:UNK:CA  | 1:C:1854:UNK:CB   | 2.85                     | 0.53              |
| 1:D:9:ASP:OD1    | 1:D:11:VAL:HB     | 2.09                     | 0.53              |
| 1:D:321:GLU:CB   | 1:D:323:LEU:HD13  | 2.36                     | 0.53              |
| 1:D:340:LYS:HB2  | 1:D:343:GLU:HB2   | 1.90                     | 0.53              |
| 1:D:400:ALA:O    | 1:D:404:ILE:HG12  | 2.09                     | 0.53              |
| 1:A:340:LYS:HB2  | 1:A:343:GLU:HB2   | 1.91                     | 0.53              |
| 1:A:1000:ARG:HD2 | 1:A:1000:ARG:C    | 2.29                     | 0.53              |
| 1:A:1021:LEU:C   | 1:A:1022:VAL:HG22 | 2.32                     | 0.53              |
| 1:A:2428:UNK:CA  | 1:A:2498:UNK:H2   | 2.21                     | 0.53              |
| 1:B:225:GLY:O    | 1:B:227:MET:N     | 2.40                     | 0.53              |
| 1:B:340:LYS:HB2  | 1:B:343:GLU:HB2   | 1.90                     | 0.53              |
| 1:B:4732:UNK:O   | 1:B:4735:UNK:N    | 2.41                     | 0.53              |
| 1:C:131:LEU:O    | 1:C:178:ARG:NH1   | 2.42                     | 0.53              |
| 1:C:225:GLY:O    | 1:C:227:MET:N     | 2.40                     | 0.53              |
| 1:C:350:HIS:HB2  | 1:C:378:LEU:HD21  | 1.90                     | 0.53              |
| 1:C:429:GLY:O    | 1:C:431:PRO:HD3   | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:728:ARG:CD    | 1:C:1134:LEU:HD22 | 2.38                     | 0.53              |
| 1:C:4732:UNK:O    | 1:C:4735:UNK:N    | 2.41                     | 0.53              |
| 1:D:998:ARG:NH2   | 1:D:998:ARG:O     | 2.41                     | 0.53              |
| 1:D:3205:UNK:CA   | 1:D:3208:UNK:CB   | 2.84                     | 0.53              |
| 1:D:4732:UNK:O    | 1:D:4735:UNK:N    | 2.41                     | 0.53              |
| 1:A:728:ARG:CD    | 1:A:1134:LEU:HD22 | 2.39                     | 0.53              |
| 1:A:3932:UNK:C    | 1:D:80:GLU:OE1    | 2.56                     | 0.53              |
| 1:B:256:ALA:HA    | 1:B:259:LEU:HD13  | 1.89                     | 0.53              |
| 1:B:429:GLY:O     | 1:B:431:PRO:HD3   | 2.09                     | 0.53              |
| 1:B:1496:TRP:HZ2  | 1:B:1543:GLU:HG3  | 1.73                     | 0.53              |
| 1:C:249:GLY:H     | 1:C:372:LEU:HD11  | 1.72                     | 0.53              |
| 1:C:321:GLU:CB    | 1:C:323:LEU:HD13  | 2.36                     | 0.53              |
| 1:C:652:ARG:HD2   | 1:C:778:PHE:HB2   | 1.90                     | 0.53              |
| 1:D:249:GLY:H     | 1:D:372:LEU:HD11  | 1.72                     | 0.53              |
| 1:D:659:TYR:C     | 1:D:750:LEU:HD21  | 2.33                     | 0.53              |
| 1:D:914:PRO:HD2   | 1:D:917:GLU:OE1   | 2.07                     | 0.53              |
| 1:D:1466:LEU:H    | 1:D:1553:PHE:HB2  | 1.74                     | 0.53              |
| 1:A:321:GLU:CB    | 1:A:323:LEU:CD1   | 2.85                     | 0.53              |
| 1:A:400:ALA:O     | 1:A:404:ILE:HG12  | 2.09                     | 0.53              |
| 1:A:429:GLY:O     | 1:A:431:PRO:HD3   | 2.09                     | 0.53              |
| 1:A:4703:UNK:C    | 1:A:4707:UNK:CB   | 2.75                     | 0.53              |
| 1:B:73:LEU:O      | 1:B:106:ALA:N     | 2.40                     | 0.53              |
| 1:B:131:LEU:O     | 1:B:178:ARG:NH1   | 2.41                     | 0.53              |
| 1:B:1433:TYR:HD1  | 1:B:1569:GLN:HB2  | 1.73                     | 0.53              |
| 1:B:1441:ALA:CB   | 1:B:1513:ASP:CA   | 2.73                     | 0.53              |
| 1:C:1000:ARG:HD2  | 1:C:1000:ARG:C    | 2.29                     | 0.53              |
| 1:A:455:PRO:O     | 1:A:456:SER:OG    | 2.27                     | 0.53              |
| 1:A:4220:UNK:O    | 1:A:4224:UNK:N    | 2.41                     | 0.53              |
| 1:B:229:GLU:OE2   | 1:B:374:LYS:HE2   | 2.08                     | 0.53              |
| 1:B:321:GLU:CB    | 1:B:323:LEU:CD1   | 2.85                     | 0.53              |
| 1:B:1000:ARG:CG   | 1:B:1018:ASN:HD21 | 2.16                     | 0.53              |
| 1:B:1466:LEU:H    | 1:B:1553:PHE:HB2  | 1.73                     | 0.53              |
| 1:C:9:ASP:OD1     | 1:C:11:VAL:HB     | 2.08                     | 0.53              |
| 1:C:256:ALA:HA    | 1:C:259:LEU:HD13  | 1.89                     | 0.53              |
| 1:C:657:THR:CB    | 1:C:662:TRP:CZ2   | 2.91                     | 0.53              |
| 1:A:322:LYS:HB3   | 1:A:324:ASP:N     | 2.23                     | 0.53              |
| 1:A:659:TYR:C     | 1:A:750:LEU:HD21  | 2.33                     | 0.53              |
| 1:A:1022:VAL:CG2  | 1:A:1027:LEU:HD23 | 2.38                     | 0.53              |
| 1:A:1439:VAL:HG21 | 1:A:1516:ILE:HG22 | 1.87                     | 0.53              |
| 1:A:1478:ASP:N    | 1:A:1509:ILE:CG2  | 2.72                     | 0.53              |
| 1:C:78:LEU:HD13   | 1:C:106:ALA:H     | 1.74                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:3673:UNK:C   | 1:C:3680:UNK:H2   | 2.22                     | 0.53              |
| 1:C:3842:UNK:O   | 1:C:3845:UNK:N    | 2.42                     | 0.53              |
| 1:C:4220:UNK:O   | 1:C:4224:UNK:N    | 2.42                     | 0.53              |
| 1:D:78:LEU:HD13  | 1:D:106:ALA:H     | 1.74                     | 0.53              |
| 1:D:266:ARG:NE   | 1:D:332:GLU:OE2   | 2.41                     | 0.53              |
| 1:D:341:TYR:HA   | 1:D:390:LEU:O     | 2.09                     | 0.53              |
| 1:D:429:GLY:O    | 1:D:431:PRO:HD3   | 2.09                     | 0.53              |
| 1:D:1452:TRP:CG  | 1:D:1527:MET:HE2  | 2.42                     | 0.53              |
| 1:D:1478:ASP:N   | 1:D:1509:ILE:CG2  | 2.72                     | 0.53              |
| 1:A:131:LEU:O    | 1:A:178:ARG:NH1   | 2.42                     | 0.53              |
| 1:A:1477:GLY:CA  | 1:A:1509:ILE:HG23 | 2.39                     | 0.53              |
| 1:C:323:LEU:N    | 1:C:324:ASP:CA    | 2.72                     | 0.53              |
| 1:C:340:LYS:HB2  | 1:C:343:GLU:HB2   | 1.90                     | 0.53              |
| 1:C:400:ALA:O    | 1:C:404:ILE:HG12  | 2.09                     | 0.53              |
| 1:C:728:ARG:HD2  | 1:C:1134:LEU:CB   | 2.28                     | 0.53              |
| 1:C:1492:CYS:HG  | 1:C:1539:PHE:HE1  | 1.56                     | 0.53              |
| 1:D:74:SER:HA    | 1:D:105:HIS:CD2   | 2.44                     | 0.53              |
| 1:D:146:CYS:HG   | 1:D:147:TRP:CD1   | 2.26                     | 0.53              |
| 1:D:322:LYS:HB3  | 1:D:324:ASP:N     | 2.23                     | 0.53              |
| 1:D:652:ARG:HD2  | 1:D:778:PHE:HB2   | 1.90                     | 0.53              |
| 1:D:3673:UNK:C   | 1:D:3680:UNK:H2   | 2.22                     | 0.53              |
| 1:B:80:GLU:OE1   | 1:C:3932:UNK:C    | 2.57                     | 0.53              |
| 1:B:324:ASP:N    | 1:B:325:THR:CA    | 2.72                     | 0.53              |
| 1:B:1478:ASP:N   | 1:B:1509:ILE:CG2  | 2.72                     | 0.53              |
| 1:B:1851:UNK:CA  | 1:B:1854:UNK:CB   | 2.85                     | 0.53              |
| 1:C:1007:TYR:CZ  | 1:C:1015:ALA:HB1  | 2.44                     | 0.53              |
| 1:C:1442:GLY:N   | 1:C:1514:LEU:HB2  | 2.18                     | 0.53              |
| 1:A:350:HIS:HB2  | 1:A:378:LEU:HD21  | 1.90                     | 0.53              |
| 1:A:545:UNK:CA   | 1:A:548:UNK:CB    | 2.85                     | 0.53              |
| 1:A:728:ARG:HD2  | 1:A:1134:LEU:CB   | 2.28                     | 0.53              |
| 1:B:659:TYR:C    | 1:B:750:LEU:HD21  | 2.33                     | 0.53              |
| 1:C:324:ASP:N    | 1:C:325:THR:CA    | 2.72                     | 0.53              |
| 1:C:998:ARG:NH2  | 1:C:998:ARG:O     | 2.41                     | 0.53              |
| 1:C:1016:ARG:C   | 1:C:1017:ARG:CD   | 2.80                     | 0.53              |
| 1:C:1478:ASP:N   | 1:C:1509:ILE:CG2  | 2.72                     | 0.53              |
| 1:D:229:GLU:OE2  | 1:D:374:LYS:HE2   | 2.09                     | 0.53              |
| 1:D:322:LYS:HB2  | 1:D:322:LYS:HZ2   | 1.73                     | 0.53              |
| 1:D:455:PRO:O    | 1:D:456:SER:OG    | 2.27                     | 0.53              |
| 1:D:1007:TYR:CE1 | 1:D:1015:ALA:CB   | 2.92                     | 0.53              |
| 1:A:74:SER:HA    | 1:A:105:HIS:CD2   | 2.44                     | 0.52              |
| 1:A:321:GLU:HB2  | 1:A:323:LEU:HD12  | 1.86                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:341:TYR:HA    | 1:A:390:LEU:O     | 2.08                     | 0.52              |
| 1:A:994:ASN:C     | 1:A:994:ASN:OD1   | 2.51                     | 0.52              |
| 1:A:1453:VAL:HA   | 1:A:1471:ALA:CB   | 2.39                     | 0.52              |
| 1:A:1478:ASP:N    | 1:A:1509:ILE:HG21 | 2.24                     | 0.52              |
| 1:A:4117:UNK:CB   | 1:A:4121:UNK:CA   | 2.85                     | 0.52              |
| 1:B:146:CYS:HG    | 1:B:147:TRP:CD1   | 2.26                     | 0.52              |
| 1:B:998:ARG:NH2   | 1:B:998:ARG:O     | 2.41                     | 0.52              |
| 1:C:229:GLU:OE2   | 1:C:374:LYS:HE2   | 2.08                     | 0.52              |
| 1:D:131:LEU:O     | 1:D:178:ARG:NH1   | 2.41                     | 0.52              |
| 1:D:323:LEU:N     | 1:D:324:ASP:CA    | 2.72                     | 0.52              |
| 1:D:465:GLN:OE1   | 1:D:465:GLN:N     | 2.42                     | 0.52              |
| 1:D:728:ARG:NH2   | 1:D:1119:GLU:O    | 2.42                     | 0.52              |
| 1:D:1022:VAL:CG2  | 1:D:1027:LEU:HD21 | 2.39                     | 0.52              |
| 1:D:1454:THR:CB   | 1:D:1455:PRO:HD2  | 2.30                     | 0.52              |
| 1:A:4703:UNK:HA   | 1:A:4706:UNK:C    | 2.32                     | 0.52              |
| 1:B:322:LYS:HB2   | 1:B:322:LYS:HZ2   | 1.74                     | 0.52              |
| 1:B:994:ASN:C     | 1:B:994:ASN:OD1   | 2.51                     | 0.52              |
| 1:C:322:LYS:HB3   | 1:C:324:ASP:N     | 2.23                     | 0.52              |
| 1:C:322:LYS:N     | 1:C:323:LEU:CA    | 2.73                     | 0.52              |
| 1:C:1007:TYR:CE1  | 1:C:1015:ALA:CB   | 2.92                     | 0.52              |
| 1:C:1453:VAL:HA   | 1:C:1471:ALA:CB   | 2.40                     | 0.52              |
| 1:A:998:ARG:CD    | 1:A:999:ASP:CG    | 2.76                     | 0.52              |
| 1:A:1439:VAL:HG23 | 1:A:1516:ILE:HG22 | 1.88                     | 0.52              |
| 1:A:1450:VAL:HG21 | 1:A:1516:ILE:HD13 | 1.91                     | 0.52              |
| 1:B:350:HIS:HB2   | 1:B:378:LEU:HD21  | 1.90                     | 0.52              |
| 1:B:455:PRO:O     | 1:B:456:SER:OG    | 2.27                     | 0.52              |
| 1:B:1004:GLY:CA   | 1:B:1015:ALA:CB   | 2.60                     | 0.52              |
| 1:B:3842:UNK:O    | 1:B:3845:UNK:N    | 2.42                     | 0.52              |
| 1:C:321:GLU:CB    | 1:C:323:LEU:CD1   | 2.85                     | 0.52              |
| 1:C:994:ASN:C     | 1:C:994:ASN:OD1   | 2.51                     | 0.52              |
| 1:C:1433:TYR:HD1  | 1:C:1569:GLN:HB2  | 1.74                     | 0.52              |
| 1:D:994:ASN:C     | 1:D:994:ASN:OD1   | 2.51                     | 0.52              |
| 1:D:3842:UNK:O    | 1:D:3845:UNK:N    | 2.42                     | 0.52              |
| 1:A:1007:TYR:CZ   | 1:A:1015:ALA:HB1  | 2.44                     | 0.52              |
| 1:B:78:LEU:HD13   | 1:B:106:ALA:H     | 1.74                     | 0.52              |
| 1:B:266:ARG:NE    | 1:B:332:GLU:OE2   | 2.41                     | 0.52              |
| 1:B:323:LEU:N     | 1:B:324:ASP:CA    | 2.72                     | 0.52              |
| 1:B:3673:UNK:C    | 1:B:3680:UNK:H2   | 2.22                     | 0.52              |
| 1:C:1478:ASP:N    | 1:C:1509:ILE:HG21 | 2.25                     | 0.52              |
| 1:D:1452:TRP:CZ2  | 1:D:1519:LEU:O    | 2.63                     | 0.52              |
| 1:A:445:LEU:HD21  | 1:A:522:LEU:HD22  | 1.92                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:941:MET:HG2  | 1:A:1051:TYR:CZ   | 2.45                     | 0.52              |
| 1:B:728:ARG:CD   | 1:B:1134:LEU:HD22 | 2.38                     | 0.52              |
| 1:B:1081:TYR:O   | 1:B:1082:THR:C    | 2.53                     | 0.52              |
| 1:B:1477:GLY:CA  | 1:B:1509:ILE:HG23 | 2.39                     | 0.52              |
| 1:C:74:SER:HA    | 1:C:105:HIS:CD2   | 2.44                     | 0.52              |
| 1:C:80:GLU:OE1   | 1:D:3932:UNK:C    | 2.58                     | 0.52              |
| 1:C:146:CYS:HG   | 1:C:147:TRP:CD1   | 2.26                     | 0.52              |
| 1:C:728:ARG:NH2  | 1:C:1119:GLU:O    | 2.42                     | 0.52              |
| 1:D:429:GLY:H    | 1:D:505:GLU:HG2   | 1.75                     | 0.52              |
| 1:A:78:LEU:HD13  | 1:A:106:ALA:H     | 1.74                     | 0.52              |
| 1:A:652:ARG:HD2  | 1:A:778:PHE:HB2   | 1.90                     | 0.52              |
| 1:A:728:ARG:NH2  | 1:A:1119:GLU:O    | 2.42                     | 0.52              |
| 1:A:752:VAL:N    | 1:A:753:PRO:CA    | 2.73                     | 0.52              |
| 1:A:1851:UNK:CA  | 1:A:1854:UNK:CB   | 2.85                     | 0.52              |
| 1:A:3986:UNK:CA  | 1:A:3989:UNK:CB   | 2.85                     | 0.52              |
| 1:B:9:ASP:OD1    | 1:B:11:VAL:HB     | 2.09                     | 0.52              |
| 1:B:545:UNK:CA   | 1:B:548:UNK:CB    | 2.85                     | 0.52              |
| 1:B:1478:ASP:N   | 1:B:1509:ILE:HG21 | 2.25                     | 0.52              |
| 1:B:4796:UNK:O   | 1:B:4801:UNK:O    | 2.28                     | 0.52              |
| 1:C:948:ASP:O    | 1:C:958:THR:OG1   | 2.20                     | 0.52              |
| 1:C:1434:TYR:CE1 | 1:C:1570:LYS:CG   | 2.93                     | 0.52              |
| 1:D:350:HIS:HB2  | 1:D:378:LEU:HD21  | 1.90                     | 0.52              |
| 1:D:445:LEU:HD21 | 1:D:522:LEU:HD22  | 1.92                     | 0.52              |
| 1:D:1453:VAL:HA  | 1:D:1471:ALA:CB   | 2.39                     | 0.52              |
| 1:D:1471:ALA:HB1 | 1:D:1548:LEU:CD2  | 2.40                     | 0.52              |
| 1:D:4796:UNK:O   | 1:D:4801:UNK:O    | 2.27                     | 0.52              |
| 1:A:1001:VAL:O   | 1:A:1005:TRP:NE1  | 2.40                     | 0.52              |
| 1:B:341:TYR:HA   | 1:B:390:LEU:O     | 2.09                     | 0.52              |
| 1:B:1001:VAL:C   | 1:B:1005:TRP:CD1  | 2.88                     | 0.52              |
| 1:B:1007:TYR:CE1 | 1:B:1015:ALA:CB   | 2.92                     | 0.52              |
| 1:C:266:ARG:NE   | 1:C:332:GLU:OE2   | 2.41                     | 0.52              |
| 1:C:368:ARG:NH2  | 1:C:371:VAL:O     | 2.43                     | 0.52              |
| 1:C:1001:VAL:C   | 1:C:1005:TRP:CD1  | 2.88                     | 0.52              |
| 1:D:753:PRO:CG   | 1:D:773:LEU:HD13  | 2.12                     | 0.52              |
| 1:D:998:ARG:CD   | 1:D:999:ASP:CG    | 2.75                     | 0.52              |
| 1:D:4232:UNK:CB  | 1:D:4234:UNK:N    | 2.73                     | 0.52              |
| 1:A:1452:TRP:CZ2 | 1:A:1519:LEU:O    | 2.63                     | 0.52              |
| 1:A:1477:GLY:HA3 | 1:A:1509:ILE:HG23 | 1.91                     | 0.52              |
| 1:B:657:THR:CB   | 1:B:662:TRP:CZ2   | 2.91                     | 0.52              |
| 1:B:1453:VAL:HA  | 1:B:1471:ALA:CB   | 2.39                     | 0.52              |
| 1:B:2073:UNK:CB  | 1:B:2094:UNK:N    | 2.73                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:4232:UNK:CB   | 1:B:4234:UNK:N    | 2.73                     | 0.52              |
| 1:C:429:GLY:H     | 1:C:505:GLU:HG2   | 1.75                     | 0.52              |
| 1:C:455:PRO:O     | 1:C:456:SER:OG    | 2.27                     | 0.52              |
| 1:C:2073:UNK:CB   | 1:C:2094:UNK:N    | 2.73                     | 0.52              |
| 1:D:322:LYS:NZ    | 1:D:322:LYS:CB    | 2.73                     | 0.52              |
| 1:D:752:VAL:HB    | 1:D:754:SER:HB2   | 1.91                     | 0.52              |
| 1:D:1007:TYR:CZ   | 1:D:1015:ALA:HB1  | 2.44                     | 0.52              |
| 1:D:1081:TYR:O    | 1:D:1082:THR:C    | 2.53                     | 0.52              |
| 1:D:2073:UNK:CB   | 1:D:2094:UNK:N    | 2.73                     | 0.52              |
| 1:D:2428:UNK:CB   | 1:D:2498:UNK:CA   | 2.87                     | 0.52              |
| 1:A:465:GLN:OE1   | 1:A:465:GLN:N     | 2.42                     | 0.52              |
| 1:A:1022:VAL:CG2  | 1:A:1027:LEU:HD21 | 2.39                     | 0.52              |
| 1:B:728:ARG:NH2   | 1:B:1119:GLU:O    | 2.42                     | 0.52              |
| 1:B:1007:TYR:CZ   | 1:B:1015:ALA:HB1  | 2.44                     | 0.52              |
| 1:B:1471:ALA:HB1  | 1:B:1548:LEU:CD2  | 2.40                     | 0.52              |
| 1:B:1477:GLY:HA3  | 1:B:1509:ILE:HG23 | 1.91                     | 0.52              |
| 1:C:322:LYS:NZ    | 1:C:322:LYS:CB    | 2.73                     | 0.52              |
| 1:C:3673:UNK:C    | 1:C:3680:UNK:N    | 2.72                     | 0.52              |
| 1:C:4232:UNK:CB   | 1:C:4234:UNK:N    | 2.73                     | 0.52              |
| 1:A:81:MET:SD     | 1:A:81:MET:C      | 2.93                     | 0.52              |
| 1:A:3842:UNK:O    | 1:A:3845:UNK:N    | 2.42                     | 0.52              |
| 1:B:1022:VAL:CG2  | 1:B:1027:LEU:HD21 | 2.39                     | 0.52              |
| 1:C:81:MET:C      | 1:C:81:MET:SD     | 2.93                     | 0.52              |
| 1:C:1022:VAL:C    | 1:C:1023:PRO:O    | 2.50                     | 0.52              |
| 1:C:1450:VAL:HG21 | 1:C:1516:ILE:HD13 | 1.91                     | 0.52              |
| 1:C:2428:UNK:CB   | 1:C:2498:UNK:CA   | 2.87                     | 0.52              |
| 1:C:4796:UNK:O    | 1:C:4801:UNK:O    | 2.27                     | 0.52              |
| 1:D:752:VAL:N     | 1:D:753:PRO:CA    | 2.73                     | 0.52              |
| 1:D:941:MET:HG2   | 1:D:1051:TYR:CZ   | 2.45                     | 0.52              |
| 1:A:275:ARG:CG    | 1:A:278:GLN:HB2   | 2.40                     | 0.51              |
| 1:A:429:GLY:H     | 1:A:505:GLU:HG2   | 1.75                     | 0.51              |
| 1:A:1478:ASP:C    | 1:A:1509:ILE:CG2  | 2.83                     | 0.51              |
| 1:A:2822:THR:OG1  | 1:A:2938:THR:OG1  | 2.28                     | 0.51              |
| 1:A:3673:UNK:C    | 1:A:3680:UNK:N    | 2.72                     | 0.51              |
| 1:A:4232:UNK:CB   | 1:A:4234:UNK:N    | 2.73                     | 0.51              |
| 1:A:4796:UNK:O    | 1:A:4801:UNK:O    | 2.28                     | 0.51              |
| 1:B:322:LYS:NZ    | 1:B:322:LYS:CB    | 2.73                     | 0.51              |
| 1:B:1452:TRP:CZ2  | 1:B:1519:LEU:O    | 2.63                     | 0.51              |
| 1:C:206:CYS:HB3   | 1:C:271:GLY:C     | 2.35                     | 0.51              |
| 1:C:1439:VAL:HG23 | 1:C:1516:ILE:HG22 | 1.88                     | 0.51              |
| 1:C:1452:TRP:CZ2  | 1:C:1519:LEU:O    | 2.63                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:1471:ALA:HB1 | 1:C:1548:LEU:CD2  | 2.40                     | 0.51              |
| 1:D:81:MET:SD    | 1:D:81:MET:C      | 2.93                     | 0.51              |
| 1:D:225:GLY:O    | 1:D:227:MET:N     | 2.40                     | 0.51              |
| 1:D:275:ARG:CG   | 1:D:278:GLN:HB2   | 2.40                     | 0.51              |
| 1:D:1477:GLY:CA  | 1:D:1509:ILE:HG23 | 2.39                     | 0.51              |
| 1:D:1478:ASP:C   | 1:D:1509:ILE:CG2  | 2.83                     | 0.51              |
| 1:A:69:LEU:HD13  | 1:A:101:LEU:HD11  | 1.92                     | 0.51              |
| 1:B:322:LYS:HB3  | 1:B:324:ASP:N     | 2.23                     | 0.51              |
| 1:B:729:PRO:O    | 1:B:730:VAL:CG2   | 2.58                     | 0.51              |
| 1:B:941:MET:HG2  | 1:B:1051:TYR:CZ   | 2.45                     | 0.51              |
| 1:B:4172:UNK:C   | 1:B:4174:UNK:N    | 2.71                     | 0.51              |
| 1:C:1478:ASP:C   | 1:C:1509:ILE:CG2  | 2.83                     | 0.51              |
| 1:A:324:ASP:N    | 1:A:325:THR:CA    | 2.72                     | 0.51              |
| 1:A:1471:ALA:HB1 | 1:A:1548:LEU:CD2  | 2.40                     | 0.51              |
| 1:B:299:LEU:HB2  | 1:B:378:LEU:HD12  | 1.93                     | 0.51              |
| 1:B:727:ALA:HB1  | 1:B:1119:GLU:CD   | 2.35                     | 0.51              |
| 1:C:727:ALA:HB1  | 1:C:1119:GLU:CD   | 2.35                     | 0.51              |
| 1:D:206:CYS:HB3  | 1:D:271:GLY:C     | 2.35                     | 0.51              |
| 1:D:1001:VAL:C   | 1:D:1005:TRP:CD1  | 2.88                     | 0.51              |
| 1:A:323:LEU:N    | 1:A:324:ASP:CA    | 2.72                     | 0.51              |
| 1:A:1016:ARG:C   | 1:A:1017:ARG:CD   | 2.80                     | 0.51              |
| 1:A:1081:TYR:O   | 1:A:1082:THR:C    | 2.53                     | 0.51              |
| 1:A:2073:UNK:CB  | 1:A:2094:UNK:N    | 2.73                     | 0.51              |
| 1:B:275:ARG:CG   | 1:B:278:GLN:HB2   | 2.41                     | 0.51              |
| 1:B:445:LEU:HD21 | 1:B:522:LEU:HD22  | 1.92                     | 0.51              |
| 1:B:752:VAL:HB   | 1:B:754:SER:HB2   | 1.91                     | 0.51              |
| 1:B:752:VAL:N    | 1:B:753:PRO:CA    | 2.73                     | 0.51              |
| 1:B:1478:ASP:O   | 1:B:1509:ILE:HG21 | 2.11                     | 0.51              |
| 1:C:941:MET:HG2  | 1:C:1051:TYR:CZ   | 2.45                     | 0.51              |
| 1:C:1081:TYR:O   | 1:C:1082:THR:C    | 2.53                     | 0.51              |
| 1:C:4124:UNK:O   | 1:C:4125:UNK:C    | 2.57                     | 0.51              |
| 1:D:1478:ASP:O   | 1:D:1509:ILE:HG21 | 2.11                     | 0.51              |
| 1:D:4124:UNK:O   | 1:D:4125:UNK:C    | 2.57                     | 0.51              |
| 1:A:266:ARG:NE   | 1:A:332:GLU:OE2   | 2.42                     | 0.51              |
| 1:A:1001:VAL:C   | 1:A:1005:TRP:CD1  | 2.88                     | 0.51              |
| 1:A:1492:CYS:HG  | 1:A:1539:PHE:HE1  | 1.59                     | 0.51              |
| 1:B:322:LYS:N    | 1:B:323:LEU:CA    | 2.73                     | 0.51              |
| 1:B:429:GLY:H    | 1:B:505:GLU:HG2   | 1.75                     | 0.51              |
| 1:C:591:UNK:O    | 1:C:592:UNK:C     | 2.59                     | 0.51              |
| 1:D:368:ARG:NH2  | 1:D:371:VAL:O     | 2.43                     | 0.51              |
| 1:D:1477:GLY:HA3 | 1:D:1509:ILE:HG23 | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:81:MET:SD     | 1:B:81:MET:C      | 2.93                     | 0.51              |
| 1:C:321:GLU:HG2   | 1:C:323:LEU:CD1   | 2.41                     | 0.51              |
| 1:A:266:ARG:O     | 1:A:270:SER:OG    | 2.26                     | 0.51              |
| 1:A:368:ARG:NH2   | 1:A:371:VAL:O     | 2.43                     | 0.51              |
| 1:A:436:LEU:O     | 1:A:438:ILE:N     | 2.44                     | 0.51              |
| 1:A:729:PRO:O     | 1:A:730:VAL:CG2   | 2.58                     | 0.51              |
| 1:A:4172:UNK:C    | 1:A:4174:UNK:N    | 2.71                     | 0.51              |
| 1:B:1434:TYR:CE1  | 1:B:1570:LYS:CG   | 2.93                     | 0.51              |
| 1:C:69:LEU:HD13   | 1:C:101:LEU:HD11  | 1.92                     | 0.51              |
| 1:C:299:LEU:HB2   | 1:C:378:LEU:HD12  | 1.93                     | 0.51              |
| 1:C:729:PRO:O     | 1:C:730:VAL:CG2   | 2.58                     | 0.51              |
| 1:C:1022:VAL:CG2  | 1:C:1027:LEU:HD21 | 2.39                     | 0.51              |
| 1:C:1477:GLY:CA   | 1:C:1509:ILE:HG23 | 2.39                     | 0.51              |
| 1:C:1478:ASP:O    | 1:C:1509:ILE:HG21 | 2.11                     | 0.51              |
| 1:C:2822:THR:OG1  | 1:C:2938:THR:OG1  | 2.28                     | 0.51              |
| 1:D:321:GLU:HG2   | 1:D:323:LEU:CD1   | 2.41                     | 0.51              |
| 1:D:1016:ARG:C    | 1:D:1017:ARG:CD   | 2.80                     | 0.51              |
| 1:D:1450:VAL:HG21 | 1:D:1516:ILE:HD13 | 1.91                     | 0.51              |
| 1:D:1478:ASP:N    | 1:D:1509:ILE:HG21 | 2.25                     | 0.51              |
| 1:D:4063:UNK:O    | 1:D:4066:UNK:CB   | 2.59                     | 0.51              |
| 1:A:322:LYS:NZ    | 1:A:322:LYS:CB    | 2.73                     | 0.51              |
| 1:B:321:GLU:HG2   | 1:B:323:LEU:CD1   | 2.41                     | 0.51              |
| 1:B:3673:UNK:C    | 1:B:3680:UNK:N    | 2.72                     | 0.51              |
| 1:B:4062:UNK:O    | 1:B:4066:UNK:N    | 2.44                     | 0.51              |
| 1:C:445:LEU:HD21  | 1:C:522:LEU:HD22  | 1.92                     | 0.51              |
| 1:C:752:VAL:HB    | 1:C:754:SER:HB2   | 1.91                     | 0.51              |
| 1:C:752:VAL:N     | 1:C:753:PRO:CA    | 2.73                     | 0.51              |
| 1:C:4063:UNK:O    | 1:C:4066:UNK:CB   | 2.59                     | 0.51              |
| 1:A:1021:LEU:CD1  | 1:A:1021:LEU:N    | 2.70                     | 0.51              |
| 1:B:1478:ASP:C    | 1:B:1509:ILE:CG2  | 2.83                     | 0.51              |
| 1:B:4703:UNK:C    | 1:B:4707:UNK:CB   | 2.75                     | 0.51              |
| 1:C:73:LEU:O      | 1:C:106:ALA:N     | 2.40                     | 0.51              |
| 1:C:436:LEU:O     | 1:C:438:ILE:N     | 2.44                     | 0.51              |
| 1:C:465:GLN:OE1   | 1:C:465:GLN:N     | 2.41                     | 0.51              |
| 1:D:299:LEU:HB2   | 1:D:378:LEU:HD12  | 1.93                     | 0.51              |
| 1:D:324:ASP:N     | 1:D:325:THR:CA    | 2.72                     | 0.51              |
| 1:A:752:VAL:HB    | 1:A:754:SER:HB2   | 1.92                     | 0.51              |
| 1:A:1007:TYR:CE1  | 1:A:1015:ALA:CB   | 2.92                     | 0.51              |
| 1:A:1101:ARG:NH1  | 1:A:1114:GLU:HB3  | 2.26                     | 0.51              |
| 1:A:3673:UNK:C    | 1:A:3680:UNK:H2   | 2.22                     | 0.51              |
| 1:B:74:SER:HA     | 1:B:105:HIS:CD2   | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:591:UNK:O     | 1:B:592:UNK:C     | 2.59                     | 0.51              |
| 1:B:1450:VAL:HG21 | 1:B:1516:ILE:HD13 | 1.91                     | 0.51              |
| 1:B:4063:UNK:O    | 1:B:4066:UNK:CB   | 2.59                     | 0.51              |
| 1:D:729:PRO:O     | 1:D:730:VAL:CG2   | 2.58                     | 0.51              |
| 1:A:1434:TYR:CE1  | 1:A:1570:LYS:CG   | 2.93                     | 0.50              |
| 1:A:1442:GLY:N    | 1:A:1514:LEU:HB2  | 2.18                     | 0.50              |
| 1:A:4063:UNK:O    | 1:A:4066:UNK:CB   | 2.59                     | 0.50              |
| 1:B:69:LEU:HD13   | 1:B:101:LEU:HD11  | 1.92                     | 0.50              |
| 1:B:1007:TYR:CE1  | 1:B:1015:ALA:CA   | 2.86                     | 0.50              |
| 1:C:993:HIS:CD2   | 1:C:1024:TYR:HB2  | 2.46                     | 0.50              |
| 1:C:1101:ARG:NH1  | 1:C:1114:GLU:HB3  | 2.26                     | 0.50              |
| 1:C:1477:GLY:HA3  | 1:C:1509:ILE:HG23 | 1.91                     | 0.50              |
| 1:D:76:ARG:HA     | 1:D:79:GLN:NE2    | 2.27                     | 0.50              |
| 1:A:321:GLU:HG2   | 1:A:323:LEU:CD1   | 2.41                     | 0.50              |
| 1:A:686:TRP:HD1   | 1:A:777:PHE:CD2   | 2.30                     | 0.50              |
| 1:A:995:VAL:O     | 1:A:998:ARG:HD3   | 2.12                     | 0.50              |
| 1:B:953:THR:HB    | 1:B:959:TYR:CE2   | 2.47                     | 0.50              |
| 1:B:3268:UNK:N    | 1:B:3271:UNK:CB   | 2.67                     | 0.50              |
| 1:C:1422:ASP:HB3  | 1:C:1549:PHE:CZ   | 2.46                     | 0.50              |
| 1:C:4062:UNK:O    | 1:C:4066:UNK:N    | 2.44                     | 0.50              |
| 1:D:1101:ARG:NH1  | 1:D:1114:GLU:HB3  | 2.27                     | 0.50              |
| 1:A:73:LEU:O      | 1:A:106:ALA:N     | 2.40                     | 0.50              |
| 1:A:727:ALA:HB1   | 1:A:1119:GLU:CD   | 2.35                     | 0.50              |
| 1:A:4062:UNK:O    | 1:A:4066:UNK:N    | 2.44                     | 0.50              |
| 1:B:686:TRP:HD1   | 1:B:777:PHE:CD2   | 2.30                     | 0.50              |
| 1:B:4124:UNK:O    | 1:B:4125:UNK:C    | 2.57                     | 0.50              |
| 1:C:275:ARG:CG    | 1:C:278:GLN:HB2   | 2.41                     | 0.50              |
| 1:C:1437:VAL:CG2  | 1:C:1518:CYS:CB   | 2.84                     | 0.50              |
| 1:D:953:THR:HB    | 1:D:959:TYR:CE2   | 2.47                     | 0.50              |
| 1:D:1422:ASP:HB3  | 1:D:1549:PHE:CZ   | 2.46                     | 0.50              |
| 1:D:3983:UNK:HA   | 1:D:3986:UNK:CB   | 2.42                     | 0.50              |
| 1:D:4062:UNK:O    | 1:D:4066:UNK:N    | 2.44                     | 0.50              |
| 1:B:76:ARG:NH1    | 1:C:3931:UNK:N    | 2.46                     | 0.50              |
| 1:B:4972:UNK:O    | 1:B:4975:UNK:N    | 2.45                     | 0.50              |
| 1:C:1007:TYR:CE1  | 1:C:1015:ALA:CA   | 2.86                     | 0.50              |
| 1:C:4117:UNK:CB   | 1:C:4121:UNK:N    | 2.75                     | 0.50              |
| 1:D:69:LEU:HD13   | 1:D:101:LEU:HD11  | 1.92                     | 0.50              |
| 1:D:659:TYR:C     | 1:D:750:LEU:CD2   | 2.71                     | 0.50              |
| 1:A:322:LYS:N     | 1:A:323:LEU:CA    | 2.73                     | 0.50              |
| 1:A:4117:UNK:CB   | 1:A:4121:UNK:N    | 2.75                     | 0.50              |
| 1:B:206:CYS:HB3   | 1:B:271:GLY:C     | 2.35                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:1101:ARG:NH1 | 1:B:1114:GLU:HB3  | 2.27                     | 0.50              |
| 1:B:1136:SER:O   | 1:B:1137:GLU:HB2  | 2.12                     | 0.50              |
| 1:C:329:ARG:HH11 | 1:C:329:ARG:CG    | 2.04                     | 0.50              |
| 1:C:753:PRO:CG   | 1:C:773:LEU:HD13  | 2.12                     | 0.50              |
| 1:C:1021:LEU:C   | 1:C:1022:VAL:HG22 | 2.32                     | 0.50              |
| 1:D:436:LEU:O    | 1:D:438:ILE:N     | 2.44                     | 0.50              |
| 1:D:1437:VAL:HB  | 1:D:1516:ILE:O    | 2.12                     | 0.50              |
| 1:A:1422:ASP:HB3 | 1:A:1549:PHE:CZ   | 2.46                     | 0.50              |
| 1:A:3268:UNK:N   | 1:A:3271:UNK:CB   | 2.67                     | 0.50              |
| 1:B:368:ARG:NH2  | 1:B:371:VAL:O     | 2.43                     | 0.50              |
| 1:B:3986:UNK:CA  | 1:B:3989:UNK:CB   | 2.86                     | 0.50              |
| 1:C:4911:UNK:O   | 1:C:4915:UNK:CB   | 2.60                     | 0.50              |
| 1:D:995:VAL:O    | 1:D:998:ARG:HD3   | 2.11                     | 0.50              |
| 1:A:206:CYS:HB3  | 1:A:271:GLY:C     | 2.35                     | 0.50              |
| 1:A:2778:GLY:HA3 | 1:A:2787:THR:HB   | 1.93                     | 0.50              |
| 1:B:995:VAL:O    | 1:B:999:ASP:OD2   | 2.30                     | 0.50              |
| 1:B:1004:GLY:O   | 1:B:1008:SER:O    | 2.30                     | 0.50              |
| 1:C:3983:UNK:HA  | 1:C:3986:UNK:CB   | 2.42                     | 0.50              |
| 1:D:727:ALA:HB1  | 1:D:1119:GLU:CD   | 2.35                     | 0.50              |
| 1:D:4703:UNK:C   | 1:D:4707:UNK:CB   | 2.75                     | 0.50              |
| 1:A:76:ARG:HA    | 1:A:79:GLN:NE2    | 2.27                     | 0.50              |
| 1:A:953:THR:HB   | 1:A:959:TYR:CE2   | 2.47                     | 0.50              |
| 1:A:1437:VAL:CG2 | 1:A:1518:CYS:CB   | 2.84                     | 0.50              |
| 1:B:1422:ASP:HB3 | 1:B:1549:PHE:CZ   | 2.46                     | 0.50              |
| 1:B:4887:UNK:N   | 1:C:4585:UNK:CB   | 2.75                     | 0.50              |
| 1:C:727:ALA:O    | 1:C:728:ARG:HB2   | 2.12                     | 0.50              |
| 1:C:953:THR:HB   | 1:C:959:TYR:CE2   | 2.47                     | 0.50              |
| 1:C:1437:VAL:HB  | 1:C:1516:ILE:O    | 2.12                     | 0.50              |
| 1:D:4117:UNK:CB  | 1:D:4121:UNK:N    | 2.75                     | 0.50              |
| 1:D:4972:UNK:O   | 1:D:4975:UNK:N    | 2.45                     | 0.50              |
| 1:A:299:LEU:HB2  | 1:A:378:LEU:HD12  | 1.93                     | 0.50              |
| 1:A:4684:UNK:O   | 1:A:4688:UNK:N    | 2.45                     | 0.50              |
| 1:B:28:VAL:HG22  | 1:B:29:LEU:HD22   | 1.94                     | 0.50              |
| 1:B:101:LEU:HB3  | 1:B:150:MET:HE1   | 1.94                     | 0.50              |
| 1:B:4117:UNK:CB  | 1:B:4121:UNK:N    | 2.75                     | 0.50              |
| 1:C:222:LEU:HD22 | 1:C:390:LEU:HD21  | 1.89                     | 0.50              |
| 1:C:995:VAL:O    | 1:C:999:ASP:OD2   | 2.30                     | 0.50              |
| 1:C:1021:LEU:CD1 | 1:C:1021:LEU:N    | 2.70                     | 0.50              |
| 1:C:1452:TRP:O   | 1:C:1548:LEU:HD23 | 2.12                     | 0.50              |
| 1:C:1494:MET:CB  | 1:C:1540:PHE:CE1  | 2.94                     | 0.50              |
| 1:C:1495:VAL:N   | 1:C:1540:PHE:CZ   | 2.80                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:686:TRP:HD1   | 1:D:777:PHE:CD2   | 2.30                     | 0.50              |
| 1:D:956:PRO:HD2   | 1:D:959:TYR:N     | 2.27                     | 0.50              |
| 1:D:1016:ARG:O    | 1:D:1017:ARG:NH2  | 2.45                     | 0.50              |
| 1:D:3986:UNK:CA   | 1:D:3989:UNK:CB   | 2.86                     | 0.50              |
| 1:D:4172:UNK:C    | 1:D:4174:UNK:N    | 2.71                     | 0.50              |
| 1:A:82:LEU:C      | 1:A:82:LEU:CD2    | 2.85                     | 0.49              |
| 1:A:1437:VAL:HB   | 1:A:1516:ILE:O    | 2.12                     | 0.49              |
| 1:A:4972:UNK:O    | 1:A:4975:UNK:N    | 2.45                     | 0.49              |
| 1:B:196:MET:HA    | 1:B:196:MET:HE3   | 1.94                     | 0.49              |
| 1:B:1437:VAL:HB   | 1:B:1516:ILE:O    | 2.12                     | 0.49              |
| 1:B:2778:GLY:HA3  | 1:B:2787:THR:HB   | 1.93                     | 0.49              |
| 1:C:956:PRO:HD2   | 1:C:959:TYR:N     | 2.27                     | 0.49              |
| 1:C:1000:ARG:CG   | 1:C:1018:ASN:HD21 | 2.16                     | 0.49              |
| 1:C:1441:ALA:CB   | 1:C:1513:ASP:CA   | 2.73                     | 0.49              |
| 1:C:1466:LEU:H    | 1:C:1553:PHE:HB2  | 1.74                     | 0.49              |
| 1:C:2778:GLY:HA3  | 1:C:2787:THR:HB   | 1.94                     | 0.49              |
| 1:D:729:PRO:C     | 1:D:730:VAL:HG23  | 2.37                     | 0.49              |
| 1:D:4684:UNK:O    | 1:D:4688:UNK:N    | 2.45                     | 0.49              |
| 1:A:591:UNK:O     | 1:A:592:UNK:C     | 2.59                     | 0.49              |
| 1:A:993:HIS:CD2   | 1:A:1024:TYR:HB2  | 2.47                     | 0.49              |
| 1:A:1136:SER:O    | 1:A:1137:GLU:HB2  | 2.12                     | 0.49              |
| 1:A:2428:UNK:CB   | 1:A:2498:UNK:CA   | 2.87                     | 0.49              |
| 1:B:465:GLN:OE1   | 1:B:465:GLN:N     | 2.41                     | 0.49              |
| 1:B:993:HIS:CD2   | 1:B:1024:TYR:HB2  | 2.47                     | 0.49              |
| 1:B:1436:SER:O    | 1:B:1565:GLU:O    | 2.31                     | 0.49              |
| 1:C:76:ARG:HA     | 1:C:79:GLN:NE2    | 2.27                     | 0.49              |
| 1:C:4684:UNK:O    | 1:C:4688:UNK:N    | 2.45                     | 0.49              |
| 1:D:196:MET:HE3   | 1:D:196:MET:HA    | 1.94                     | 0.49              |
| 1:D:322:LYS:N     | 1:D:323:LEU:CA    | 2.73                     | 0.49              |
| 1:D:545:UNK:HA    | 1:D:548:UNK:N     | 2.28                     | 0.49              |
| 1:D:753:PRO:HD2   | 1:D:770:ALA:HA    | 1.95                     | 0.49              |
| 1:D:1007:TYR:CE1  | 1:D:1015:ALA:CA   | 2.86                     | 0.49              |
| 1:D:4911:UNK:O    | 1:D:4915:UNK:CB   | 2.60                     | 0.49              |
| 1:A:689:THR:HG22  | 1:A:778:PHE:CE2   | 2.47                     | 0.49              |
| 1:A:1046:LEU:HD13 | 1:A:1053:ILE:HG13 | 1.94                     | 0.49              |
| 1:B:73:LEU:O      | 1:B:78:LEU:CD1    | 2.61                     | 0.49              |
| 1:B:206:CYS:HB3   | 1:B:271:GLY:CA    | 2.43                     | 0.49              |
| 1:B:1495:VAL:N    | 1:B:1540:PHE:CZ   | 2.80                     | 0.49              |
| 1:B:4684:UNK:O    | 1:B:4688:UNK:N    | 2.45                     | 0.49              |
| 1:B:4911:UNK:O    | 1:B:4915:UNK:CB   | 2.60                     | 0.49              |
| 1:C:84:ASN:ND2    | 1:C:84:ASN:N      | 2.60                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:4972:UNK:O    | 1:C:4975:UNK:N    | 2.45                     | 0.49              |
| 1:D:206:CYS:HB3   | 1:D:271:GLY:CA    | 2.43                     | 0.49              |
| 1:D:319:SER:HA    | 1:D:347:PHE:CD1   | 2.48                     | 0.49              |
| 1:D:1027:LEU:HD22 | 1:D:1031:THR:HG21 | 1.95                     | 0.49              |
| 1:D:1046:LEU:HD13 | 1:D:1053:ILE:HG13 | 1.94                     | 0.49              |
| 1:D:1136:SER:O    | 1:D:1137:GLU:HB2  | 2.12                     | 0.49              |
| 1:A:1027:LEU:HD22 | 1:A:1031:THR:HG21 | 1.95                     | 0.49              |
| 1:A:1478:ASP:O    | 1:A:1509:ILE:HG21 | 2.11                     | 0.49              |
| 1:A:4911:UNK:O    | 1:A:4915:UNK:CB   | 2.60                     | 0.49              |
| 1:B:319:SER:HA    | 1:B:347:PHE:CD1   | 2.48                     | 0.49              |
| 1:B:436:LEU:O     | 1:B:438:ILE:N     | 2.44                     | 0.49              |
| 1:B:727:ALA:O     | 1:B:728:ARG:HB2   | 2.12                     | 0.49              |
| 1:B:1016:ARG:O    | 1:B:1017:ARG:NH2  | 2.45                     | 0.49              |
| 1:C:729:PRO:C     | 1:C:730:VAL:HG23  | 2.37                     | 0.49              |
| 1:C:1436:SER:O    | 1:C:1565:GLU:O    | 2.31                     | 0.49              |
| 1:D:1452:TRP:O    | 1:D:1548:LEU:HD23 | 2.12                     | 0.49              |
| 1:D:3673:UNK:C    | 1:D:3680:UNK:N    | 2.72                     | 0.49              |
| 1:A:101:LEU:HB3   | 1:A:150:MET:HE1   | 1.94                     | 0.49              |
| 1:A:319:SER:HA    | 1:A:347:PHE:CD1   | 2.48                     | 0.49              |
| 1:A:995:VAL:O     | 1:A:999:ASP:OD2   | 2.30                     | 0.49              |
| 1:B:1022:VAL:C    | 1:B:1023:PRO:O    | 2.50                     | 0.49              |
| 1:B:2428:UNK:CB   | 1:B:2498:UNK:CA   | 2.87                     | 0.49              |
| 1:C:101:LEU:HB3   | 1:C:150:MET:HE1   | 1.94                     | 0.49              |
| 1:C:196:MET:HA    | 1:C:196:MET:HE3   | 1.95                     | 0.49              |
| 1:C:1016:ARG:O    | 1:C:1017:ARG:NH2  | 2.45                     | 0.49              |
| 1:D:79:GLN:CG     | 1:D:80:GLU:N      | 2.75                     | 0.49              |
| 1:D:1436:SER:O    | 1:D:1565:GLU:O    | 2.31                     | 0.49              |
| 1:A:753:PRO:HD2   | 1:A:770:ALA:HA    | 1.95                     | 0.49              |
| 1:A:1436:SER:O    | 1:A:1565:GLU:O    | 2.31                     | 0.49              |
| 1:A:1452:TRP:O    | 1:A:1548:LEU:HD23 | 2.12                     | 0.49              |
| 1:B:995:VAL:O     | 1:B:998:ARG:HD3   | 2.12                     | 0.49              |
| 1:B:1007:TYR:O    | 1:B:1008:SER:OG   | 2.30                     | 0.49              |
| 1:C:206:CYS:HB3   | 1:C:271:GLY:CA    | 2.43                     | 0.49              |
| 1:C:319:SER:HA    | 1:C:347:PHE:CD1   | 2.48                     | 0.49              |
| 1:C:686:TRP:HD1   | 1:C:777:PHE:CD2   | 2.30                     | 0.49              |
| 1:C:1136:SER:O    | 1:C:1137:GLU:HB2  | 2.12                     | 0.49              |
| 1:D:2822:THR:OG1  | 1:D:2938:THR:OG1  | 2.29                     | 0.49              |
| 1:A:1016:ARG:O    | 1:A:1017:ARG:NH2  | 2.45                     | 0.49              |
| 1:A:1444:GLU:OE2  | 1:A:1478:ASP:HA   | 2.13                     | 0.49              |
| 1:A:4124:UNK:O    | 1:A:4125:UNK:C    | 2.57                     | 0.49              |
| 1:B:545:UNK:HA    | 1:B:548:UNK:N     | 2.27                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1007:TYR:C    | 1:B:1008:SER:OG   | 2.56                     | 0.49              |
| 1:B:1016:ARG:C    | 1:B:1017:ARG:CD   | 2.80                     | 0.49              |
| 1:B:1437:VAL:CG2  | 1:B:1518:CYS:CB   | 2.84                     | 0.49              |
| 1:B:1452:TRP:O    | 1:B:1548:LEU:HD23 | 2.12                     | 0.49              |
| 1:C:4887:UNK:N    | 1:D:4585:UNK:CB   | 2.74                     | 0.49              |
| 1:A:73:LEU:O      | 1:A:78:LEU:CD1    | 2.61                     | 0.49              |
| 1:B:689:THR:HG22  | 1:B:778:PHE:CE2   | 2.47                     | 0.49              |
| 1:C:995:VAL:O     | 1:C:998:ARG:HD3   | 2.12                     | 0.49              |
| 1:C:1462:MET:O    | 1:C:1553:PHE:CZ   | 2.66                     | 0.49              |
| 1:D:73:LEU:O      | 1:D:78:LEU:CD1    | 2.61                     | 0.49              |
| 1:D:993:HIS:CD2   | 1:D:1024:TYR:HB2  | 2.47                     | 0.49              |
| 1:A:1004:GLY:O    | 1:A:1008:SER:O    | 2.30                     | 0.49              |
| 1:A:1431:THR:HG23 | 1:A:1571:ASN:HA   | 1.95                     | 0.49              |
| 1:A:1495:VAL:N    | 1:A:1540:PHE:CZ   | 2.80                     | 0.49              |
| 1:A:3983:UNK:HA   | 1:A:3986:UNK:CB   | 2.42                     | 0.49              |
| 1:A:4887:UNK:N    | 1:B:4585:UNK:CB   | 2.74                     | 0.49              |
| 1:B:76:ARG:HA     | 1:B:79:GLN:NE2    | 2.27                     | 0.49              |
| 1:B:955:LEU:N     | 1:B:959:TYR:CD2   | 2.81                     | 0.49              |
| 1:C:82:LEU:C      | 1:C:82:LEU:CD2    | 2.85                     | 0.49              |
| 1:C:329:ARG:NE    | 1:C:329:ARG:HA    | 2.28                     | 0.49              |
| 1:D:689:THR:HG22  | 1:D:778:PHE:CE2   | 2.48                     | 0.49              |
| 1:D:995:VAL:O     | 1:D:999:ASP:OD2   | 2.30                     | 0.49              |
| 1:D:1431:THR:HG23 | 1:D:1571:ASN:HA   | 1.95                     | 0.49              |
| 1:A:196:MET:HE3   | 1:A:196:MET:HA    | 1.94                     | 0.49              |
| 1:A:249:GLY:N     | 1:A:372:LEU:HD11  | 2.28                     | 0.49              |
| 1:A:1022:VAL:C    | 1:A:1023:PRO:O    | 2.50                     | 0.49              |
| 1:A:4585:UNK:CB   | 1:D:4887:UNK:N    | 2.75                     | 0.49              |
| 1:B:249:GLY:N     | 1:B:372:LEU:HD11  | 2.28                     | 0.49              |
| 1:B:1442:GLY:N    | 1:B:1514:LEU:HB2  | 2.18                     | 0.49              |
| 1:D:82:LEU:C      | 1:D:82:LEU:CD2    | 2.85                     | 0.49              |
| 1:D:753:PRO:CB    | 1:D:773:LEU:CD1   | 2.88                     | 0.49              |
| 1:D:1434:TYR:CE1  | 1:D:1570:LYS:CG   | 2.93                     | 0.49              |
| 1:A:753:PRO:CG    | 1:A:773:LEU:HD13  | 2.12                     | 0.48              |
| 1:A:858:THR:HB    | 1:A:930:LYS:HB3   | 1.95                     | 0.48              |
| 1:A:3317:UNK:CB   | 1:A:3323:UNK:CA   | 2.91                     | 0.48              |
| 1:A:4645:UNK:CA   | 1:A:4648:UNK:CB   | 2.86                     | 0.48              |
| 1:B:1027:LEU:HD22 | 1:B:1031:THR:HG21 | 1.95                     | 0.48              |
| 1:B:1431:THR:HG23 | 1:B:1571:ASN:HA   | 1.95                     | 0.48              |
| 1:B:3983:UNK:HA   | 1:B:3986:UNK:CB   | 2.42                     | 0.48              |
| 1:C:28:VAL:HG22   | 1:C:29:LEU:HD22   | 1.94                     | 0.48              |
| 1:C:266:ARG:O     | 1:C:270:SER:OG    | 2.26                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:753:PRO:HD2   | 1:C:770:ALA:HA    | 1.95                     | 0.48              |
| 1:C:1444:GLU:OE2  | 1:C:1478:ASP:HA   | 2.13                     | 0.48              |
| 1:D:127:MET:HB3   | 1:D:130:LYS:HG3   | 1.95                     | 0.48              |
| 1:A:127:MET:HB3   | 1:A:130:LYS:HG3   | 1.95                     | 0.48              |
| 1:A:545:UNK:HA    | 1:A:548:UNK:N     | 2.27                     | 0.48              |
| 1:B:349:GLN:HB2   | 1:B:356:TRP:CZ3   | 2.48                     | 0.48              |
| 1:B:729:PRO:C     | 1:B:730:VAL:HG23  | 2.37                     | 0.48              |
| 1:B:2822:THR:OG1  | 1:B:2938:THR:OG1  | 2.29                     | 0.48              |
| 1:C:73:LEU:O      | 1:C:78:LEU:CD1    | 2.60                     | 0.48              |
| 1:C:328:LYS:NZ    | 1:C:329:ARG:O     | 2.46                     | 0.48              |
| 1:C:545:UNK:HA    | 1:C:548:UNK:N     | 2.27                     | 0.48              |
| 1:C:858:THR:HB    | 1:C:930:LYS:HB3   | 1.95                     | 0.48              |
| 1:C:1027:LEU:HD22 | 1:C:1031:THR:HG21 | 1.95                     | 0.48              |
| 1:C:1431:THR:HG23 | 1:C:1571:ASN:HA   | 1.95                     | 0.48              |
| 1:D:328:LYS:NZ    | 1:D:329:ARG:O     | 2.46                     | 0.48              |
| 1:D:727:ALA:O     | 1:D:728:ARG:HB2   | 2.12                     | 0.48              |
| 1:D:1004:GLY:O    | 1:D:1008:SER:O    | 2.30                     | 0.48              |
| 1:D:1429:ASN:HB2  | 1:D:1547:LYS:CB   | 2.43                     | 0.48              |
| 1:A:729:PRO:C     | 1:A:730:VAL:HG23  | 2.37                     | 0.48              |
| 1:A:1007:TYR:C    | 1:A:1008:SER:OG   | 2.56                     | 0.48              |
| 1:B:139:GLU:CD    | 1:B:139:GLU:H     | 2.21                     | 0.48              |
| 1:B:329:ARG:NE    | 1:B:329:ARG:HA    | 2.28                     | 0.48              |
| 1:C:881:LEU:HD13  | 1:C:968:ALA:HB2   | 1.96                     | 0.48              |
| 1:C:955:LEU:N     | 1:C:959:TYR:CD2   | 2.81                     | 0.48              |
| 1:D:73:LEU:O      | 1:D:106:ALA:N     | 2.40                     | 0.48              |
| 1:D:1429:ASN:CB   | 1:D:1547:LYS:HB2  | 2.42                     | 0.48              |
| 1:D:4645:UNK:CA   | 1:D:4648:UNK:CB   | 2.86                     | 0.48              |
| 1:A:206:CYS:HB3   | 1:A:271:GLY:CA    | 2.43                     | 0.48              |
| 1:A:955:LEU:N     | 1:A:959:TYR:CD2   | 2.81                     | 0.48              |
| 1:B:424:LYS:HZ1   | 1:B:506:TYR:N     | 2.11                     | 0.48              |
| 1:B:752:VAL:HB    | 1:B:754:SER:CA    | 2.43                     | 0.48              |
| 1:B:1431:THR:CG2  | 1:B:1571:ASN:HA   | 2.43                     | 0.48              |
| 1:B:1434:TYR:CD1  | 1:B:1570:LYS:HG3  | 2.48                     | 0.48              |
| 1:C:349:GLN:HB2   | 1:C:356:TRP:CZ3   | 2.48                     | 0.48              |
| 1:C:689:THR:HG22  | 1:C:778:PHE:CE2   | 2.47                     | 0.48              |
| 1:C:1016:ARG:CA   | 1:C:1017:ARG:NE   | 2.77                     | 0.48              |
| 1:C:1046:LEU:HD13 | 1:C:1053:ILE:HG13 | 1.94                     | 0.48              |
| 1:D:1494:MET:CB   | 1:D:1540:PHE:CE1  | 2.94                     | 0.48              |
| 1:D:2778:GLY:HA3  | 1:D:2787:THR:HB   | 1.93                     | 0.48              |
| 1:A:978:THR:HB    | 1:A:979:PRO:HD2   | 1.95                     | 0.48              |
| 1:A:1558:HIS:CD2  | 1:A:1559:GLN:HB2  | 2.49                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:82:LEU:C      | 1:B:82:LEU:CD2    | 2.85                     | 0.48              |
| 1:B:1558:HIS:CD2  | 1:B:1559:GLN:HB2  | 2.49                     | 0.48              |
| 1:C:424:LYS:HZ1   | 1:C:506:TYR:H     | 1.60                     | 0.48              |
| 1:D:421:PHE:HE2   | 1:D:436:LEU:HD21  | 1.79                     | 0.48              |
| 1:D:1016:ARG:CA   | 1:D:1017:ARG:NE   | 2.77                     | 0.48              |
| 1:A:349:GLN:HB2   | 1:A:356:TRP:CZ3   | 2.48                     | 0.48              |
| 1:A:977:LEU:HB3   | 1:A:981:GLN:HB2   | 1.96                     | 0.48              |
| 1:A:993:HIS:CE1   | 1:A:1020:ARG:CA   | 2.91                     | 0.48              |
| 1:A:4561:UNK:C    | 1:A:4564:UNK:N    | 2.77                     | 0.48              |
| 1:A:4855:UNK:O    | 1:A:4859:UNK:CA   | 2.61                     | 0.48              |
| 1:B:328:LYS:HB2   | 1:B:328:LYS:NZ    | 2.29                     | 0.48              |
| 1:B:462:GLU:O     | 1:B:465:GLN:HB3   | 2.14                     | 0.48              |
| 1:B:977:LEU:HB3   | 1:B:981:GLN:HB2   | 1.96                     | 0.48              |
| 1:B:978:THR:HB    | 1:B:979:PRO:HD2   | 1.96                     | 0.48              |
| 1:B:1046:LEU:HD13 | 1:B:1053:ILE:HG13 | 1.94                     | 0.48              |
| 1:C:249:GLY:N     | 1:C:372:LEU:HD11  | 2.28                     | 0.48              |
| 1:C:978:THR:HB    | 1:C:979:PRO:HD2   | 1.95                     | 0.48              |
| 1:C:1004:GLY:O    | 1:C:1008:SER:O    | 2.30                     | 0.48              |
| 1:C:1558:HIS:CD2  | 1:C:1559:GLN:HB2  | 2.49                     | 0.48              |
| 1:D:1444:GLU:OE2  | 1:D:1478:ASP:HA   | 2.13                     | 0.48              |
| 1:D:1477:GLY:C    | 1:D:1509:ILE:HG22 | 2.39                     | 0.48              |
| 1:A:462:GLU:O     | 1:A:465:GLN:HB3   | 2.14                     | 0.48              |
| 1:A:752:VAL:HB    | 1:A:754:SER:CA    | 2.43                     | 0.48              |
| 1:A:1429:ASN:HB2  | 1:A:1547:LYS:CB   | 2.43                     | 0.48              |
| 1:B:753:PRO:HD2   | 1:B:770:ALA:HA    | 1.95                     | 0.48              |
| 1:B:1438:ARG:CB   | 1:B:1515:VAL:HG13 | 2.44                     | 0.48              |
| 1:C:127:MET:HB3   | 1:C:130:LYS:HG3   | 1.96                     | 0.48              |
| 1:C:1431:THR:CG2  | 1:C:1571:ASN:HA   | 2.43                     | 0.48              |
| 1:D:28:VAL:HG22   | 1:D:29:LEU:HD22   | 1.94                     | 0.48              |
| 1:D:75:VAL:CG1    | 1:D:76:ARG:N      | 2.73                     | 0.48              |
| 1:D:977:LEU:HB3   | 1:D:981:GLN:HB2   | 1.96                     | 0.48              |
| 1:D:1431:THR:CG2  | 1:D:1571:ASN:HA   | 2.43                     | 0.48              |
| 1:A:28:VAL:HG22   | 1:A:29:LEU:HD22   | 1.94                     | 0.48              |
| 1:B:127:MET:HB3   | 1:B:130:LYS:HG3   | 1.95                     | 0.48              |
| 1:B:1444:GLU:OE2  | 1:B:1478:ASP:HA   | 2.13                     | 0.48              |
| 1:D:249:GLY:N     | 1:D:372:LEU:HD11  | 2.28                     | 0.48              |
| 1:D:329:ARG:HA    | 1:D:329:ARG:NE    | 2.28                     | 0.48              |
| 1:D:1434:TYR:CD1  | 1:D:1570:LYS:HG3  | 2.48                     | 0.48              |
| 1:A:1016:ARG:CA   | 1:A:1017:ARG:NE   | 2.77                     | 0.48              |
| 1:B:328:LYS:NZ    | 1:B:329:ARG:O     | 2.46                     | 0.48              |
| 1:C:328:LYS:NZ    | 1:C:328:LYS:HB2   | 2.29                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:753:PRO:CG   | 1:C:773:LEU:HD12  | 2.07                     | 0.48              |
| 1:D:101:LEU:HB3  | 1:D:150:MET:HE1   | 1.94                     | 0.48              |
| 1:D:328:LYS:NZ   | 1:D:328:LYS:HB2   | 2.29                     | 0.48              |
| 1:D:1558:HIS:CD2 | 1:D:1559:GLN:HB2  | 2.49                     | 0.48              |
| 1:D:2768:PHE:O   | 1:D:2772:GLN:HG2  | 2.14                     | 0.48              |
| 1:A:995:VAL:O    | 1:A:998:ARG:CD    | 2.62                     | 0.48              |
| 1:A:1454:THR:CB  | 1:A:1455:PRO:HD2  | 2.30                     | 0.48              |
| 1:B:995:VAL:O    | 1:B:998:ARG:CD    | 2.62                     | 0.48              |
| 1:B:4561:UNK:C   | 1:B:4564:UNK:N    | 2.77                     | 0.48              |
| 1:C:462:GLU:O    | 1:C:465:GLN:HB3   | 2.14                     | 0.48              |
| 1:C:1001:VAL:O   | 1:C:1005:TRP:NE1  | 2.40                     | 0.48              |
| 1:D:1495:VAL:N   | 1:D:1540:PHE:CZ   | 2.80                     | 0.48              |
| 1:A:79:GLN:CG    | 1:A:80:GLU:N      | 2.75                     | 0.47              |
| 1:B:881:LEU:HD13 | 1:B:968:ALA:HB2   | 1.95                     | 0.47              |
| 1:B:2768:PHE:O   | 1:B:2772:GLN:HG2  | 2.14                     | 0.47              |
| 1:C:139:GLU:H    | 1:C:139:GLU:CD    | 2.22                     | 0.47              |
| 1:C:752:VAL:HB   | 1:C:754:SER:CA    | 2.43                     | 0.47              |
| 1:C:977:LEU:HB3  | 1:C:981:GLN:HB2   | 1.96                     | 0.47              |
| 1:C:1438:ARG:CB  | 1:C:1515:VAL:HG13 | 2.44                     | 0.47              |
| 1:D:545:UNK:CA   | 1:D:548:UNK:CB    | 2.85                     | 0.47              |
| 1:D:855:PRO:HA   | 1:D:994:ASN:CB    | 2.20                     | 0.47              |
| 1:D:870:ILE:HG12 | 1:D:1051:TYR:CZ   | 2.49                     | 0.47              |
| 1:D:1438:ARG:CB  | 1:D:1515:VAL:HG13 | 2.44                     | 0.47              |
| 1:D:1462:MET:O   | 1:D:1553:PHE:CZ   | 2.66                     | 0.47              |
| 1:D:1496:TRP:CZ2 | 1:D:1543:GLU:HG3  | 2.49                     | 0.47              |
| 1:D:4561:UNK:C   | 1:D:4564:UNK:N    | 2.77                     | 0.47              |
| 1:A:328:LYS:NZ   | 1:A:329:ARG:O     | 2.46                     | 0.47              |
| 1:A:982:THR:O    | 1:A:986:ASP:N     | 2.47                     | 0.47              |
| 1:A:1474:VAL:CG2 | 1:A:1539:PHE:CB   | 2.92                     | 0.47              |
| 1:A:2768:PHE:O   | 1:A:2772:GLN:HG2  | 2.14                     | 0.47              |
| 1:B:79:GLN:CG    | 1:B:80:GLU:N      | 2.75                     | 0.47              |
| 1:B:266:ARG:O    | 1:B:270:SER:OG    | 2.26                     | 0.47              |
| 1:B:652:ARG:HG2  | 1:B:780:VAL:HB    | 1.96                     | 0.47              |
| 1:C:1429:ASN:HB2 | 1:C:1547:LYS:CB   | 2.43                     | 0.47              |
| 1:C:3317:UNK:CB  | 1:C:3323:UNK:CA   | 2.91                     | 0.47              |
| 1:C:4792:UNK:O   | 1:C:4795:UNK:N    | 2.47                     | 0.47              |
| 1:D:424:LYS:HZ1  | 1:D:506:TYR:N     | 2.10                     | 0.47              |
| 1:D:752:VAL:HB   | 1:D:754:SER:CA    | 2.43                     | 0.47              |
| 1:D:1000:ARG:C   | 1:D:1000:ARG:HD3  | 2.39                     | 0.47              |
| 1:D:1474:VAL:CG2 | 1:D:1539:PHE:CB   | 2.92                     | 0.47              |
| 1:A:1431:THR:CG2 | 1:A:1571:ASN:HA   | 2.43                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4222:UNK:O    | 1:A:4232:UNK:O    | 2.33                     | 0.47              |
| 1:B:680:THR:HG21  | 1:B:785:ALA:HB2   | 1.96                     | 0.47              |
| 1:B:1496:TRP:CZ2  | 1:B:1543:GLU:HG3  | 2.49                     | 0.47              |
| 1:C:107:ILE:HG22  | 1:C:148:TRP:O     | 2.15                     | 0.47              |
| 1:C:982:THR:O     | 1:C:986:ASP:N     | 2.47                     | 0.47              |
| 1:D:349:GLN:HB2   | 1:D:356:TRP:CZ3   | 2.48                     | 0.47              |
| 1:D:1004:GLY:O    | 1:D:1007:TYR:C    | 2.57                     | 0.47              |
| 1:D:2296:UNK:C    | 1:D:2352:UNK:CB   | 2.93                     | 0.47              |
| 1:D:3317:UNK:CB   | 1:D:3323:UNK:CA   | 2.91                     | 0.47              |
| 1:A:328:LYS:NZ    | 1:A:328:LYS:HB2   | 2.29                     | 0.47              |
| 1:A:329:ARG:HA    | 1:A:329:ARG:NE    | 2.28                     | 0.47              |
| 1:A:1812:UNK:O    | 1:A:1816:UNK:N    | 2.48                     | 0.47              |
| 1:A:2296:UNK:C    | 1:A:2352:UNK:CB   | 2.93                     | 0.47              |
| 1:A:4792:UNK:O    | 1:A:4795:UNK:N    | 2.47                     | 0.47              |
| 1:B:1477:GLY:C    | 1:B:1509:ILE:HG22 | 2.39                     | 0.47              |
| 1:B:1812:UNK:O    | 1:B:1816:UNK:N    | 2.48                     | 0.47              |
| 1:B:2428:UNK:CA   | 1:B:2498:UNK:N    | 2.78                     | 0.47              |
| 1:C:474:ARG:O     | 1:C:478:PHE:HD1   | 1.97                     | 0.47              |
| 1:C:1004:GLY:O    | 1:C:1007:TYR:C    | 2.57                     | 0.47              |
| 1:C:1189:LEU:HD12 | 1:C:1190:PRO:HD2  | 1.96                     | 0.47              |
| 1:C:1429:ASN:CB   | 1:C:1547:LYS:HB2  | 2.42                     | 0.47              |
| 1:C:4561:UNK:C    | 1:C:4564:UNK:N    | 2.77                     | 0.47              |
| 1:D:107:ILE:HG22  | 1:D:148:TRP:O     | 2.15                     | 0.47              |
| 1:D:462:GLU:O     | 1:D:465:GLN:HB3   | 2.14                     | 0.47              |
| 1:D:1812:UNK:O    | 1:D:1816:UNK:N    | 2.47                     | 0.47              |
| 1:A:1004:GLY:O    | 1:A:1007:TYR:C    | 2.58                     | 0.47              |
| 1:A:1462:MET:O    | 1:A:1553:PHE:CZ   | 2.66                     | 0.47              |
| 1:B:858:THR:HB    | 1:B:930:LYS:HB3   | 1.95                     | 0.47              |
| 1:B:1004:GLY:O    | 1:B:1007:TYR:C    | 2.57                     | 0.47              |
| 1:B:1016:ARG:CA   | 1:B:1017:ARG:NE   | 2.77                     | 0.47              |
| 1:B:4792:UNK:O    | 1:B:4795:UNK:N    | 2.47                     | 0.47              |
| 1:C:2768:PHE:O    | 1:C:2772:GLN:HG2  | 2.14                     | 0.47              |
| 1:D:474:ARG:O     | 1:D:478:PHE:HD1   | 1.98                     | 0.47              |
| 1:A:222:LEU:HD22  | 1:A:390:LEU:HD21  | 1.89                     | 0.47              |
| 1:A:419:ASP:OD2   | 1:A:493:ARG:NH1   | 2.48                     | 0.47              |
| 1:A:727:ALA:O     | 1:A:728:ARG:HB2   | 2.12                     | 0.47              |
| 1:A:870:ILE:HG12  | 1:A:1051:TYR:CZ   | 2.49                     | 0.47              |
| 1:A:881:LEU:HD13  | 1:A:968:ALA:HB2   | 1.95                     | 0.47              |
| 1:A:1477:GLY:C    | 1:A:1509:ILE:HG22 | 2.39                     | 0.47              |
| 1:A:1813:UNK:O    | 1:A:1817:UNK:N    | 2.42                     | 0.47              |
| 1:A:2428:UNK:CA   | 1:A:2498:UNK:N    | 2.78                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:1189:LEU:HD12 | 1:B:1190:PRO:HD2 | 1.96                     | 0.47              |
| 1:C:206:CYS:HA    | 1:C:269:TRP:CE3  | 2.50                     | 0.47              |
| 1:C:1812:UNK:O    | 1:C:1816:UNK:N   | 2.47                     | 0.47              |
| 1:C:2428:UNK:CA   | 1:C:2498:UNK:N   | 2.78                     | 0.47              |
| 1:D:995:VAL:O     | 1:D:998:ARG:CD   | 2.62                     | 0.47              |
| 1:D:1017:ARG:N    | 1:D:1017:ARG:NE  | 2.53                     | 0.47              |
| 1:A:170:ILE:HD11  | 1:A:197:GLN:HB3  | 1.97                     | 0.47              |
| 1:A:368:ARG:NH1   | 1:A:368:ARG:CG   | 2.71                     | 0.47              |
| 1:A:418:LEU:HA    | 1:A:421:PHE:CZ   | 2.50                     | 0.47              |
| 1:A:421:PHE:HE2   | 1:A:436:LEU:HD21 | 1.79                     | 0.47              |
| 1:A:1429:ASN:CB   | 1:A:1547:LYS:HB2 | 2.42                     | 0.47              |
| 1:A:1496:TRP:CZ2  | 1:A:1543:GLU:HG3 | 2.49                     | 0.47              |
| 1:A:3205:UNK:CA   | 1:A:3208:UNK:CB  | 2.84                     | 0.47              |
| 1:A:4905:UNK:N    | 1:A:4906:UNK:CA  | 2.78                     | 0.47              |
| 1:B:89:GLY:N      | 1:B:90:VAL:HA    | 2.30                     | 0.47              |
| 1:B:107:ILE:HG22  | 1:B:148:TRP:O    | 2.14                     | 0.47              |
| 1:B:170:ILE:HD11  | 1:B:197:GLN:HB3  | 1.97                     | 0.47              |
| 1:B:1462:MET:O    | 1:B:1553:PHE:CZ  | 2.66                     | 0.47              |
| 1:B:1474:VAL:CG2  | 1:B:1539:PHE:CB  | 2.92                     | 0.47              |
| 1:B:1494:MET:CB   | 1:B:1540:PHE:CE1 | 2.94                     | 0.47              |
| 1:C:322:LYS:HB2   | 1:C:322:LYS:HZ2  | 1.78                     | 0.47              |
| 1:C:421:PHE:HE2   | 1:C:436:LEU:HD21 | 1.79                     | 0.47              |
| 1:C:870:ILE:HG12  | 1:C:1051:TYR:CZ  | 2.49                     | 0.47              |
| 1:C:995:VAL:O     | 1:C:998:ARG:CD   | 2.62                     | 0.47              |
| 1:C:1000:ARG:C    | 1:C:1000:ARG:HD3 | 2.39                     | 0.47              |
| 1:C:1465:ASP:H    | 1:C:1468:LYS:HD2 | 1.80                     | 0.47              |
| 1:C:3986:UNK:CA   | 1:C:3989:UNK:CB  | 2.86                     | 0.47              |
| 1:C:4222:UNK:O    | 1:C:4232:UNK:O   | 2.33                     | 0.47              |
| 1:D:207:SER:N     | 1:D:269:TRP:HE3  | 2.07                     | 0.47              |
| 1:D:419:ASP:OD2   | 1:D:493:ARG:NH1  | 2.48                     | 0.47              |
| 1:D:652:ARG:HG2   | 1:D:780:VAL:HB   | 1.96                     | 0.47              |
| 1:D:881:LEU:HD13  | 1:D:968:ALA:HB2  | 1.96                     | 0.47              |
| 1:D:982:THR:O     | 1:D:986:ASP:N    | 2.47                     | 0.47              |
| 1:D:1465:ASP:H    | 1:D:1468:LYS:HD2 | 1.80                     | 0.47              |
| 1:D:4222:UNK:O    | 1:D:4232:UNK:O   | 2.33                     | 0.47              |
| 1:D:4792:UNK:O    | 1:D:4795:UNK:N   | 2.47                     | 0.47              |
| 1:B:424:LYS:HG2   | 1:B:506:TYR:CE1  | 2.50                     | 0.47              |
| 1:B:728:ARG:HH11  | 1:B:1133:HIS:C   | 2.23                     | 0.47              |
| 1:B:1021:LEU:CD1  | 1:B:1021:LEU:N   | 2.70                     | 0.47              |
| 1:C:419:ASP:OD2   | 1:C:493:ARG:NH1  | 2.48                     | 0.47              |
| 1:D:266:ARG:O     | 1:D:270:SER:OG   | 2.26                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:418:LEU:HA    | 1:D:421:PHE:CZ   | 2.50                     | 0.47              |
| 1:D:948:ASP:CB    | 1:D:959:TYR:HE1  | 2.26                     | 0.47              |
| 1:D:4855:UNK:O    | 1:D:4859:UNK:CA  | 2.61                     | 0.47              |
| 1:A:474:ARG:O     | 1:A:478:PHE:HD1  | 1.98                     | 0.47              |
| 1:A:652:ARG:HG2   | 1:A:780:VAL:HB   | 1.96                     | 0.47              |
| 1:A:948:ASP:CB    | 1:A:959:TYR:HE1  | 2.26                     | 0.47              |
| 1:A:1109:LEU:HD13 | 1:A:1120:LEU:HB2 | 1.97                     | 0.47              |
| 1:B:421:PHE:HE2   | 1:B:436:LEU:HD21 | 1.79                     | 0.47              |
| 1:B:1001:VAL:HG13 | 1:B:1002:ALA:N   | 2.30                     | 0.47              |
| 1:C:728:ARG:HH11  | 1:C:1133:HIS:C   | 2.23                     | 0.47              |
| 1:D:591:UNK:O     | 1:D:592:UNK:C    | 2.59                     | 0.47              |
| 1:D:858:THR:HB    | 1:D:930:LYS:HB3  | 1.95                     | 0.47              |
| 1:A:424:LYS:HZ1   | 1:A:506:TYR:N    | 2.11                     | 0.47              |
| 1:A:1441:ALA:HB1  | 1:A:1513:ASP:HA  | 1.97                     | 0.47              |
| 1:B:206:CYS:HA    | 1:B:269:TRP:CE3  | 2.50                     | 0.47              |
| 1:B:870:ILE:HG12  | 1:B:1051:TYR:CZ  | 2.49                     | 0.47              |
| 1:B:998:ARG:CD    | 1:B:999:ASP:CG   | 2.76                     | 0.47              |
| 1:B:1465:ASP:H    | 1:B:1468:LYS:HD2 | 1.80                     | 0.47              |
| 1:B:1471:ALA:C    | 1:B:1472:VAL:CG2 | 2.87                     | 0.47              |
| 1:C:424:LYS:HG2   | 1:C:506:TYR:CE1  | 2.50                     | 0.47              |
| 1:C:545:UNK:CA    | 1:C:548:UNK:CB   | 2.85                     | 0.47              |
| 1:C:652:ARG:HG2   | 1:C:780:VAL:HB   | 1.96                     | 0.47              |
| 1:C:1001:VAL:HG13 | 1:C:1002:ALA:N   | 2.30                     | 0.47              |
| 1:C:1437:VAL:CB   | 1:C:1516:ILE:O   | 2.63                     | 0.47              |
| 1:C:1454:THR:CB   | 1:C:1455:PRO:HD2 | 2.31                     | 0.47              |
| 1:C:1474:VAL:CG2  | 1:C:1539:PHE:CB  | 2.92                     | 0.47              |
| 1:C:1496:TRP:CZ2  | 1:C:1543:GLU:HG3 | 2.49                     | 0.47              |
| 1:C:4905:UNK:N    | 1:C:4906:UNK:CA  | 2.78                     | 0.47              |
| 1:D:728:ARG:HH11  | 1:D:1133:HIS:C   | 2.23                     | 0.47              |
| 1:A:424:LYS:NZ    | 1:A:506:TYR:CD1  | 2.83                     | 0.46              |
| 1:A:1434:TYR:CD1  | 1:A:1570:LYS:HG3 | 2.48                     | 0.46              |
| 1:B:275:ARG:HG2   | 1:B:278:GLN:HB2  | 1.98                     | 0.46              |
| 1:B:418:LEU:HA    | 1:B:421:PHE:CZ   | 2.50                     | 0.46              |
| 1:B:456:SER:OG    | 1:B:460:GLN:OE1  | 2.31                     | 0.46              |
| 1:B:728:ARG:CD    | 1:B:1133:HIS:CD2 | 2.96                     | 0.46              |
| 1:B:1441:ALA:HB1  | 1:B:1513:ASP:HA  | 1.97                     | 0.46              |
| 1:B:4905:UNK:N    | 1:B:4906:UNK:CA  | 2.78                     | 0.46              |
| 1:C:1452:TRP:HZ2  | 1:C:1519:LEU:O   | 1.98                     | 0.46              |
| 1:C:4788:UNK:HA   | 1:C:4791:UNK:CB  | 2.45                     | 0.46              |
| 1:D:978:THR:HB    | 1:D:979:PRO:HD2  | 1.96                     | 0.46              |
| 1:D:1555:LEU:HB3  | 1:D:1556:PRO:CD  | 2.44                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:206:CYS:HA    | 1:A:269:TRP:CE3   | 2.50                     | 0.46              |
| 1:A:424:LYS:HG2   | 1:A:506:TYR:CE1   | 2.50                     | 0.46              |
| 1:A:988:LEU:HD23  | 1:A:1039:LEU:HB2  | 1.97                     | 0.46              |
| 1:A:1438:ARG:CB   | 1:A:1515:VAL:HG13 | 2.44                     | 0.46              |
| 1:A:1494:MET:CB   | 1:A:1540:PHE:CE1  | 2.94                     | 0.46              |
| 1:B:728:ARG:HA    | 1:B:729:PRO:HA    | 1.63                     | 0.46              |
| 1:B:1453:VAL:HG22 | 1:B:1549:PHE:O    | 2.16                     | 0.46              |
| 1:B:4645:UNK:CA   | 1:B:4648:UNK:CB   | 2.86                     | 0.46              |
| 1:B:4788:UNK:HA   | 1:B:4791:UNK:CB   | 2.45                     | 0.46              |
| 1:B:4855:UNK:O    | 1:B:4859:UNK:CA   | 2.62                     | 0.46              |
| 1:C:275:ARG:HG2   | 1:C:278:GLN:HB2   | 1.97                     | 0.46              |
| 1:C:291:LEU:HD11  | 1:C:299:LEU:HD11  | 1.97                     | 0.46              |
| 1:C:688:LEU:HA    | 1:C:776:LEU:O     | 2.15                     | 0.46              |
| 1:C:1453:VAL:HG22 | 1:C:1549:PHE:O    | 2.16                     | 0.46              |
| 1:C:1471:ALA:C    | 1:C:1472:VAL:CG2  | 2.87                     | 0.46              |
| 1:D:170:ILE:HD11  | 1:D:197:GLN:HB3   | 1.97                     | 0.46              |
| 1:D:426:ARG:HG2   | 1:D:502:HIS:HB2   | 1.97                     | 0.46              |
| 1:D:855:PRO:CG    | 1:D:994:ASN:O     | 2.57                     | 0.46              |
| 1:D:1189:LEU:HD12 | 1:D:1190:PRO:HD2  | 1.96                     | 0.46              |
| 1:D:4788:UNK:HA   | 1:D:4791:UNK:CB   | 2.45                     | 0.46              |
| 1:A:89:GLY:N      | 1:A:90:VAL:HA     | 2.30                     | 0.46              |
| 1:A:275:ARG:HG2   | 1:A:278:GLN:HB2   | 1.98                     | 0.46              |
| 1:A:680:THR:HG21  | 1:A:785:ALA:HB2   | 1.96                     | 0.46              |
| 1:A:1465:ASP:H    | 1:A:1468:LYS:HD2  | 1.80                     | 0.46              |
| 1:B:688:LEU:HA    | 1:B:776:LEU:O     | 2.15                     | 0.46              |
| 1:B:948:ASP:CB    | 1:B:959:TYR:HE1   | 2.26                     | 0.46              |
| 1:B:2821:TRP:CD1  | 1:B:2939:ARG:HB3  | 2.51                     | 0.46              |
| 1:C:728:ARG:NH1   | 1:C:1133:HIS:C    | 2.74                     | 0.46              |
| 1:C:988:LEU:HD23  | 1:C:1039:LEU:HB2  | 1.97                     | 0.46              |
| 1:C:4895:UNK:O    | 1:C:4898:UNK:CB   | 2.64                     | 0.46              |
| 1:D:424:LYS:HG2   | 1:D:506:TYR:CE1   | 2.50                     | 0.46              |
| 1:D:680:THR:HG21  | 1:D:785:ALA:HB2   | 1.96                     | 0.46              |
| 1:D:1452:TRP:HB2  | 1:D:1527:MET:HE1  | 1.98                     | 0.46              |
| 1:A:2073:UNK:C    | 1:A:2094:UNK:CB   | 2.94                     | 0.46              |
| 1:A:2821:TRP:CD1  | 1:A:2939:ARG:HB3  | 2.51                     | 0.46              |
| 1:B:887:ILE:HA    | 1:B:891:TRP:O     | 2.16                     | 0.46              |
| 1:B:956:PRO:HD2   | 1:B:959:TYR:N     | 2.27                     | 0.46              |
| 1:B:1109:LEU:HD13 | 1:B:1120:LEU:HB2  | 1.97                     | 0.46              |
| 1:B:2073:UNK:C    | 1:B:2094:UNK:CB   | 2.94                     | 0.46              |
| 1:C:89:GLY:N      | 1:C:90:VAL:HA     | 2.30                     | 0.46              |
| 1:D:222:LEU:HD22  | 1:D:390:LEU:HD21  | 1.89                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:275:ARG:HG2   | 1:D:278:GLN:HB2   | 1.97                     | 0.46              |
| 1:D:291:LEU:HD11  | 1:D:299:LEU:HD11  | 1.97                     | 0.46              |
| 1:D:955:LEU:N     | 1:D:959:TYR:CD2   | 2.81                     | 0.46              |
| 1:D:1007:TYR:C    | 1:D:1008:SER:OG   | 2.56                     | 0.46              |
| 1:D:1452:TRP:HZ2  | 1:D:1519:LEU:O    | 1.99                     | 0.46              |
| 1:D:1453:VAL:HG22 | 1:D:1549:PHE:O    | 2.16                     | 0.46              |
| 1:D:1495:VAL:O    | 1:D:1495:VAL:HG12 | 2.16                     | 0.46              |
| 1:D:3306:UNK:HA   | 1:D:3309:UNK:CA   | 2.46                     | 0.46              |
| 1:A:107:ILE:HG22  | 1:A:148:TRP:O     | 2.15                     | 0.46              |
| 1:A:427:GLY:O     | 1:A:505:GLU:HG3   | 2.16                     | 0.46              |
| 1:A:728:ARG:HA    | 1:A:729:PRO:HA    | 1.63                     | 0.46              |
| 1:A:1189:LEU:HD12 | 1:A:1190:PRO:HD2  | 1.96                     | 0.46              |
| 1:B:222:LEU:HD22  | 1:B:390:LEU:HD21  | 1.89                     | 0.46              |
| 1:B:329:ARG:NH1   | 1:B:329:ARG:CG    | 2.71                     | 0.46              |
| 1:B:954:LYS:HZ2   | 1:B:955:LEU:HD11  | 1.81                     | 0.46              |
| 1:B:982:THR:O     | 1:B:986:ASP:N     | 2.47                     | 0.46              |
| 1:B:4222:UNK:O    | 1:B:4232:UNK:O    | 2.33                     | 0.46              |
| 1:B:4895:UNK:O    | 1:B:4898:UNK:CB   | 2.64                     | 0.46              |
| 1:C:887:ILE:HA    | 1:C:891:TRP:O     | 2.16                     | 0.46              |
| 1:C:1555:LEU:HB3  | 1:C:1556:PRO:CD   | 2.44                     | 0.46              |
| 1:D:89:GLY:N      | 1:D:90:VAL:HA     | 2.30                     | 0.46              |
| 1:D:728:ARG:NH1   | 1:D:1133:HIS:C    | 2.74                     | 0.46              |
| 1:A:456:SER:OG    | 1:A:460:GLN:OE1   | 2.31                     | 0.46              |
| 1:A:457:GLU:C     | 1:A:460:GLN:HB2   | 2.41                     | 0.46              |
| 1:A:728:ARG:HH11  | 1:A:1133:HIS:C    | 2.23                     | 0.46              |
| 1:A:1007:TYR:C    | 1:A:1008:SER:HG   | 2.23                     | 0.46              |
| 1:A:1452:TRP:HB2  | 1:A:1527:MET:HE1  | 1.98                     | 0.46              |
| 1:A:4561:UNK:C    | 1:A:4565:UNK:CB   | 2.94                     | 0.46              |
| 1:B:74:SER:HB2    | 1:B:75:VAL:H      | 1.42                     | 0.46              |
| 1:B:419:ASP:OD2   | 1:B:493:ARG:NH1   | 2.48                     | 0.46              |
| 1:B:469:ARG:HA    | 1:B:472:ARG:HH11  | 1.80                     | 0.46              |
| 1:B:753:PRO:CB    | 1:B:773:LEU:CD1   | 2.88                     | 0.46              |
| 1:B:855:PRO:HG3   | 1:B:994:ASN:CB    | 2.46                     | 0.46              |
| 1:B:855:PRO:CG    | 1:B:994:ASN:O     | 2.57                     | 0.46              |
| 1:B:1437:VAL:CB   | 1:B:1516:ILE:O    | 2.63                     | 0.46              |
| 1:B:2296:UNK:C    | 1:B:2352:UNK:CB   | 2.93                     | 0.46              |
| 1:C:170:ILE:HD11  | 1:C:197:GLN:HB3   | 1.97                     | 0.46              |
| 1:C:1007:TYR:CE1  | 1:C:1015:ALA:C    | 2.94                     | 0.46              |
| 1:C:1813:UNK:O    | 1:C:1817:UNK:N    | 2.42                     | 0.46              |
| 1:C:3304:UNK:C    | 1:C:3306:UNK:N    | 2.77                     | 0.46              |
| 1:C:3306:UNK:HA   | 1:C:3309:UNK:CA   | 2.46                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:879:HIS:HE1   | 1:D:906:CYS:SG   | 2.39                     | 0.46              |
| 1:D:1437:VAL:CB   | 1:D:1516:ILE:O   | 2.63                     | 0.46              |
| 1:D:1558:HIS:HD2  | 1:D:1559:GLN:HB2 | 1.81                     | 0.46              |
| 1:D:2428:UNK:CA   | 1:D:2498:UNK:N   | 2.78                     | 0.46              |
| 1:A:688:LEU:HA    | 1:A:776:LEU:O    | 2.15                     | 0.46              |
| 1:A:879:HIS:HE1   | 1:A:906:CYS:SG   | 2.39                     | 0.46              |
| 1:A:906:CYS:SG    | 1:A:907:LEU:N    | 2.89                     | 0.46              |
| 1:A:1007:TYR:CE1  | 1:A:1015:ALA:C   | 2.94                     | 0.46              |
| 1:A:1429:ASN:HB2  | 1:A:1547:LYS:CD  | 2.45                     | 0.46              |
| 1:A:1453:VAL:HG22 | 1:A:1549:PHE:O   | 2.16                     | 0.46              |
| 1:A:4788:UNK:HA   | 1:A:4791:UNK:CB  | 2.45                     | 0.46              |
| 1:A:4895:UNK:O    | 1:A:4898:UNK:CB  | 2.64                     | 0.46              |
| 1:B:90:VAL:HB     | 1:B:91:GLU:CD    | 2.41                     | 0.46              |
| 1:B:319:SER:HA    | 1:B:347:PHE:CE1  | 2.51                     | 0.46              |
| 1:B:474:ARG:O     | 1:B:478:PHE:HD1  | 1.97                     | 0.46              |
| 1:B:1000:ARG:C    | 1:B:1000:ARG:HD3 | 2.40                     | 0.46              |
| 1:B:1429:ASN:HB2  | 1:B:1547:LYS:CB  | 2.43                     | 0.46              |
| 1:C:426:ARG:HG2   | 1:C:502:HIS:HB2  | 1.97                     | 0.46              |
| 1:C:680:THR:HG21  | 1:C:785:ALA:HB2  | 1.96                     | 0.46              |
| 1:C:991:ASN:C     | 1:C:993:HIS:N    | 2.73                     | 0.46              |
| 1:C:1007:TYR:O    | 1:C:1008:SER:OG  | 2.30                     | 0.46              |
| 1:C:1109:LEU:HD13 | 1:C:1120:LEU:HB2 | 1.97                     | 0.46              |
| 1:C:2296:UNK:C    | 1:C:2352:UNK:CB  | 2.93                     | 0.46              |
| 1:D:139:GLU:CD    | 1:D:139:GLU:H    | 2.22                     | 0.46              |
| 1:D:206:CYS:HA    | 1:D:269:TRP:CE3  | 2.50                     | 0.46              |
| 1:D:457:GLU:C     | 1:D:460:GLN:HB2  | 2.41                     | 0.46              |
| 1:D:951:LYS:HG2   | 1:D:958:THR:O    | 2.16                     | 0.46              |
| 1:D:1007:TYR:CE1  | 1:D:1015:ALA:C   | 2.94                     | 0.46              |
| 1:D:1453:VAL:HA   | 1:D:1471:ALA:HB1 | 1.98                     | 0.46              |
| 1:A:90:VAL:HB     | 1:A:91:GLU:CD    | 2.41                     | 0.46              |
| 1:A:139:GLU:H     | 1:A:139:GLU:CD   | 2.22                     | 0.46              |
| 1:A:657:THR:CB    | 1:A:662:TRP:CZ2  | 2.91                     | 0.46              |
| 1:A:728:ARG:CD    | 1:A:1133:HIS:CD2 | 2.96                     | 0.46              |
| 1:A:855:PRO:HG3   | 1:A:994:ASN:CB   | 2.46                     | 0.46              |
| 1:A:887:ILE:HA    | 1:A:891:TRP:O    | 2.16                     | 0.46              |
| 1:A:1452:TRP:HZ2  | 1:A:1519:LEU:O   | 1.99                     | 0.46              |
| 1:A:1835:UNK:O    | 1:A:1838:UNK:N   | 2.49                     | 0.46              |
| 1:B:206:CYS:CB    | 1:B:271:GLY:C    | 2.89                     | 0.46              |
| 1:C:206:CYS:CB    | 1:C:271:GLY:C    | 2.89                     | 0.46              |
| 1:C:319:SER:HA    | 1:C:347:PHE:CE1  | 2.51                     | 0.46              |
| 1:C:728:ARG:CD    | 1:C:1133:HIS:CD2 | 2.96                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:753:PRO:CB    | 1:C:773:LEU:CD1   | 2.88                     | 0.46              |
| 1:C:1434:TYR:CD1  | 1:C:1570:LYS:HG3  | 2.48                     | 0.46              |
| 1:C:1441:ALA:HB1  | 1:C:1513:ASP:HA   | 1.97                     | 0.46              |
| 1:D:855:PRO:HG3   | 1:D:994:ASN:CB    | 2.46                     | 0.46              |
| 1:D:906:CYS:SG    | 1:D:907:LEU:N     | 2.89                     | 0.46              |
| 1:D:1434:TYR:HD1  | 1:D:1570:LYS:HB2  | 1.77                     | 0.46              |
| 1:D:1441:ALA:HB1  | 1:D:1513:ASP:HA   | 1.97                     | 0.46              |
| 1:D:1452:TRP:HB2  | 1:D:1548:LEU:HD22 | 1.98                     | 0.46              |
| 1:A:1002:ALA:N    | 1:A:1005:TRP:NE1  | 2.64                     | 0.46              |
| 1:B:1000:ARG:HD3  | 1:B:1016:ARG:HD2  | 1.98                     | 0.46              |
| 1:B:1007:TYR:CE1  | 1:B:1015:ALA:C    | 2.94                     | 0.46              |
| 1:B:5006:UNK:O    | 1:B:5009:UNK:N    | 2.49                     | 0.46              |
| 1:C:418:LEU:HA    | 1:C:421:PHE:CZ    | 2.50                     | 0.46              |
| 1:C:457:GLU:C     | 1:C:460:GLN:HB2   | 2.41                     | 0.46              |
| 1:C:948:ASP:CB    | 1:C:959:TYR:HE1   | 2.26                     | 0.46              |
| 1:D:2073:UNK:C    | 1:D:2094:UNK:CB   | 2.94                     | 0.46              |
| 1:D:3306:UNK:CB   | 1:D:3309:UNK:CB   | 2.94                     | 0.46              |
| 1:D:4905:UNK:N    | 1:D:4906:UNK:CA   | 2.78                     | 0.46              |
| 1:A:291:LEU:HD11  | 1:A:299:LEU:HD11  | 1.97                     | 0.46              |
| 1:A:728:ARG:NH1   | 1:A:1133:HIS:C    | 2.74                     | 0.46              |
| 1:A:991:ASN:C     | 1:A:993:HIS:N     | 2.73                     | 0.46              |
| 1:A:1001:VAL:CG1  | 1:A:1005:TRP:CE2  | 2.92                     | 0.46              |
| 1:A:3306:UNK:CB   | 1:A:3309:UNK:CB   | 2.94                     | 0.46              |
| 1:B:291:LEU:HD11  | 1:B:299:LEU:HD11  | 1.97                     | 0.46              |
| 1:B:457:GLU:C     | 1:B:460:GLN:HB2   | 2.41                     | 0.46              |
| 1:B:728:ARG:NH1   | 1:B:1133:HIS:C    | 2.74                     | 0.46              |
| 1:B:894:GLY:O     | 1:B:905:PRO:HA    | 2.16                     | 0.46              |
| 1:B:1452:TRP:HB2  | 1:B:1548:LEU:HD22 | 1.98                     | 0.46              |
| 1:C:75:VAL:C      | 1:C:79:GLN:NE2    | 2.73                     | 0.46              |
| 1:C:855:PRO:HG3   | 1:C:994:ASN:CB    | 2.46                     | 0.46              |
| 1:C:1002:ALA:N    | 1:C:1005:TRP:NE1  | 2.64                     | 0.46              |
| 1:C:1007:TYR:C    | 1:C:1008:SER:OG   | 2.56                     | 0.46              |
| 1:C:1016:ARG:HA   | 1:C:1017:ARG:NE   | 2.31                     | 0.46              |
| 1:C:1453:VAL:HA   | 1:C:1471:ALA:HB1  | 1.98                     | 0.46              |
| 1:C:2821:TRP:CD1  | 1:C:2939:ARG:HB3  | 2.51                     | 0.46              |
| 1:C:4855:UNK:O    | 1:C:4859:UNK:CA   | 2.62                     | 0.46              |
| 1:D:427:GLY:O     | 1:D:505:GLU:HG3   | 2.16                     | 0.46              |
| 1:D:887:ILE:HA    | 1:D:891:TRP:O     | 2.16                     | 0.46              |
| 1:D:991:ASN:O     | 1:D:994:ASN:N     | 2.49                     | 0.46              |
| 1:D:1437:VAL:HG23 | 1:D:1518:CYS:H    | 1.81                     | 0.46              |
| 1:A:426:ARG:HG2   | 1:A:502:HIS:HB2   | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1452:TRP:HB2  | 1:A:1548:LEU:HD22 | 1.98                     | 0.45              |
| 1:B:988:LEU:HD23  | 1:B:1039:LEU:HB2  | 1.97                     | 0.45              |
| 1:B:3306:UNK:HA   | 1:B:3309:UNK:CA   | 2.46                     | 0.45              |
| 1:B:4818:UNK:N    | 1:B:4821:UNK:CB   | 2.73                     | 0.45              |
| 1:C:424:LYS:NZ    | 1:C:506:TYR:CD1   | 2.83                     | 0.45              |
| 1:C:5006:UNK:O    | 1:C:5009:UNK:N    | 2.49                     | 0.45              |
| 1:D:74:SER:HB2    | 1:D:75:VAL:H      | 1.43                     | 0.45              |
| 1:D:90:VAL:HB     | 1:D:91:GLU:CD     | 2.41                     | 0.45              |
| 1:D:1000:ARG:HD3  | 1:D:1016:ARG:HD2  | 1.99                     | 0.45              |
| 1:D:4561:UNK:C    | 1:D:4565:UNK:CB   | 2.94                     | 0.45              |
| 1:D:4895:UNK:O    | 1:D:4898:UNK:CB   | 2.64                     | 0.45              |
| 1:A:77:ALA:C      | 1:A:80:GLU:HG2    | 2.41                     | 0.45              |
| 1:A:951:LYS:HG2   | 1:A:958:THR:O     | 2.16                     | 0.45              |
| 1:A:1016:ARG:HA   | 1:A:1017:ARG:NE   | 2.31                     | 0.45              |
| 1:A:1437:VAL:CB   | 1:A:1516:ILE:O    | 2.63                     | 0.45              |
| 1:A:1558:HIS:HD2  | 1:A:1559:GLN:H    | 1.60                     | 0.45              |
| 1:B:77:ALA:C      | 1:B:80:GLU:HG2    | 2.41                     | 0.45              |
| 1:B:1555:LEU:HB3  | 1:B:1556:PRO:CD   | 2.44                     | 0.45              |
| 1:B:3445:UNK:C    | 1:B:3447:UNK:H    | 2.30                     | 0.45              |
| 1:C:894:GLY:O     | 1:C:905:PRO:HA    | 2.17                     | 0.45              |
| 1:C:1429:ASN:CG   | 1:C:1546:THR:O    | 2.55                     | 0.45              |
| 1:C:1437:VAL:HG23 | 1:C:1518:CYS:H    | 1.81                     | 0.45              |
| 1:C:1452:TRP:HB2  | 1:C:1527:MET:HE1  | 1.98                     | 0.45              |
| 1:C:1452:TRP:HB2  | 1:C:1548:LEU:HD22 | 1.98                     | 0.45              |
| 1:C:2073:UNK:C    | 1:C:2094:UNK:CB   | 2.94                     | 0.45              |
| 1:D:77:ALA:C      | 1:D:80:GLU:HG2    | 2.41                     | 0.45              |
| 1:D:324:ASP:CB    | 1:D:325:THR:C     | 2.85                     | 0.45              |
| 1:D:988:LEU:HD23  | 1:D:1039:LEU:HB2  | 1.97                     | 0.45              |
| 1:D:1016:ARG:HA   | 1:D:1017:ARG:NE   | 2.31                     | 0.45              |
| 1:A:1000:ARG:HD3  | 1:A:1016:ARG:HD2  | 1.99                     | 0.45              |
| 1:A:3304:UNK:C    | 1:A:3306:UNK:N    | 2.77                     | 0.45              |
| 1:B:427:GLY:O     | 1:B:505:GLU:HG3   | 2.16                     | 0.45              |
| 1:B:1429:ASN:CB   | 1:B:1547:LYS:HB2  | 2.43                     | 0.45              |
| 1:C:3205:UNK:CA   | 1:C:3208:UNK:CB   | 2.84                     | 0.45              |
| 1:C:4561:UNK:C    | 1:C:4565:UNK:CB   | 2.94                     | 0.45              |
| 1:D:319:SER:HA    | 1:D:347:PHE:CE1   | 2.51                     | 0.45              |
| 1:D:426:ARG:CZ    | 1:D:796:ARG:NH2   | 2.71                     | 0.45              |
| 1:D:688:LEU:HA    | 1:D:776:LEU:O     | 2.15                     | 0.45              |
| 1:D:1001:VAL:HG13 | 1:D:1005:TRP:CE2  | 2.30                     | 0.45              |
| 1:D:1437:VAL:CG2  | 1:D:1518:CYS:CB   | 2.84                     | 0.45              |
| 1:A:469:ARG:HA    | 1:A:472:ARG:HH11  | 1.80                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1558:HIS:HD2  | 1:A:1559:GLN:HB2  | 1.81                     | 0.45              |
| 1:B:426:ARG:HG2   | 1:B:502:HIS:HB2   | 1.97                     | 0.45              |
| 1:B:1002:ALA:N    | 1:B:1005:TRP:NE1  | 2.64                     | 0.45              |
| 1:B:1016:ARG:HA   | 1:B:1017:ARG:NE   | 2.31                     | 0.45              |
| 1:B:4561:UNK:C    | 1:B:4565:UNK:CB   | 2.94                     | 0.45              |
| 1:B:4885:UNK:O    | 1:C:4585:UNK:O    | 2.14                     | 0.45              |
| 1:C:469:ARG:HA    | 1:C:472:ARG:HH11  | 1.79                     | 0.45              |
| 1:C:1429:ASN:HB2  | 1:C:1547:LYS:CD   | 2.45                     | 0.45              |
| 1:C:3445:UNK:C    | 1:C:3447:UNK:H    | 2.30                     | 0.45              |
| 1:C:4645:UNK:CA   | 1:C:4648:UNK:CB   | 2.86                     | 0.45              |
| 1:D:151:HIS:HB2   | 1:D:170:ILE:CG2   | 2.46                     | 0.45              |
| 1:D:206:CYS:CB    | 1:D:271:GLY:C     | 2.89                     | 0.45              |
| 1:D:1835:UNK:O    | 1:D:1838:UNK:N    | 2.49                     | 0.45              |
| 1:A:206:CYS:CB    | 1:A:271:GLY:C     | 2.89                     | 0.45              |
| 1:A:993:HIS:O     | 1:A:996:TRP:CD2   | 2.69                     | 0.45              |
| 1:A:5006:UNK:O    | 1:A:5009:UNK:N    | 2.49                     | 0.45              |
| 1:C:870:ILE:HD13  | 1:C:870:ILE:HA    | 1.78                     | 0.45              |
| 1:C:951:LYS:HG2   | 1:C:958:THR:O     | 2.16                     | 0.45              |
| 1:C:1000:ARG:HD3  | 1:C:1016:ARG:HD2  | 1.99                     | 0.45              |
| 1:C:1007:TYR:HE1  | 1:C:1015:ALA:CB   | 2.29                     | 0.45              |
| 1:C:1558:HIS:HD2  | 1:C:1559:GLN:HB2  | 1.81                     | 0.45              |
| 1:C:1835:UNK:O    | 1:C:1838:UNK:N    | 2.49                     | 0.45              |
| 1:D:469:ARG:HA    | 1:D:472:ARG:HH11  | 1.79                     | 0.45              |
| 1:D:728:ARG:CD    | 1:D:1133:HIS:CD2  | 2.96                     | 0.45              |
| 1:A:1001:VAL:HG13 | 1:A:1002:ALA:N    | 2.30                     | 0.45              |
| 1:A:3306:UNK:HA   | 1:A:3309:UNK:CA   | 2.46                     | 0.45              |
| 1:B:906:CYS:SG    | 1:B:907:LEU:N     | 2.89                     | 0.45              |
| 1:B:1429:ASN:HB2  | 1:B:1547:LYS:CD   | 2.45                     | 0.45              |
| 1:B:1453:VAL:HA   | 1:B:1471:ALA:HB1  | 1.98                     | 0.45              |
| 1:B:1462:MET:O    | 1:B:1555:LEU:HD22 | 2.17                     | 0.45              |
| 1:C:3268:UNK:N    | 1:C:3271:UNK:CB   | 2.67                     | 0.45              |
| 1:C:3306:UNK:CB   | 1:C:3309:UNK:CB   | 2.94                     | 0.45              |
| 1:D:1007:TYR:HE1  | 1:D:1015:ALA:C    | 2.25                     | 0.45              |
| 1:D:1109:LEU:HD13 | 1:D:1120:LEU:HB2  | 1.97                     | 0.45              |
| 1:D:2821:TRP:CD1  | 1:D:2939:ARG:HB3  | 2.51                     | 0.45              |
| 1:A:324:ASP:OD1   | 1:A:324:ASP:N     | 2.50                     | 0.45              |
| 1:A:458:GLU:N     | 1:A:460:GLN:HB2   | 2.32                     | 0.45              |
| 1:A:675:LEU:HD12  | 1:A:679:ALA:HB3   | 1.99                     | 0.45              |
| 1:A:4169:UNK:O    | 1:A:4172:UNK:CB   | 2.65                     | 0.45              |
| 1:A:4818:UNK:N    | 1:A:4821:UNK:CB   | 2.73                     | 0.45              |
| 1:B:1007:TYR:HE1  | 1:B:1015:ALA:CB   | 2.29                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:3317:UNK:CB  | 1:B:3323:UNK:CA   | 2.91                     | 0.45              |
| 1:C:90:VAL:HB    | 1:C:91:GLU:CD     | 2.41                     | 0.45              |
| 1:C:954:LYS:HZ2  | 1:C:955:LEU:HD11  | 1.81                     | 0.45              |
| 1:C:991:ASN:O    | 1:C:994:ASN:N     | 2.49                     | 0.45              |
| 1:D:745:SER:HB3  | 1:D:758:ARG:HB2   | 1.99                     | 0.45              |
| 1:D:5006:UNK:O   | 1:D:5009:UNK:N    | 2.49                     | 0.45              |
| 1:A:319:SER:HA   | 1:A:347:PHE:CE1   | 2.51                     | 0.45              |
| 1:A:1453:VAL:HA  | 1:A:1471:ALA:HB1  | 1.98                     | 0.45              |
| 1:B:332:GLU:OE1  | 1:B:332:GLU:CA    | 2.63                     | 0.45              |
| 1:B:951:LYS:HG2  | 1:B:958:THR:O     | 2.16                     | 0.45              |
| 1:B:1444:GLU:CB  | 1:B:1445:PRO:C    | 2.84                     | 0.45              |
| 1:B:1452:TRP:HZ2 | 1:B:1519:LEU:O    | 1.99                     | 0.45              |
| 1:B:1495:VAL:O   | 1:B:1495:VAL:HG12 | 2.16                     | 0.45              |
| 1:B:1558:HIS:HD2 | 1:B:1559:GLN:HB2  | 1.81                     | 0.45              |
| 1:C:353:SER:HB3  | 1:C:355:LEU:HG    | 1.99                     | 0.45              |
| 1:C:1007:TYR:HE1 | 1:C:1015:ALA:C    | 2.25                     | 0.45              |
| 1:C:4169:UNK:O   | 1:C:4172:UNK:CB   | 2.65                     | 0.45              |
| 1:D:675:LEU:HD12 | 1:D:679:ALA:HB3   | 1.99                     | 0.45              |
| 1:D:993:HIS:CE1  | 1:D:1020:ARG:CA   | 2.91                     | 0.45              |
| 1:D:1462:MET:O   | 1:D:1555:LEU:HD22 | 2.17                     | 0.45              |
| 1:D:1935:UNK:H   | 1:D:1938:UNK:CB   | 2.30                     | 0.45              |
| 1:A:745:SER:HB3  | 1:A:758:ARG:HB2   | 1.99                     | 0.45              |
| 1:A:1555:LEU:HB3 | 1:A:1556:PRO:CD   | 2.44                     | 0.45              |
| 1:A:3445:UNK:C   | 1:A:3447:UNK:H    | 2.30                     | 0.45              |
| 1:B:3306:UNK:CB  | 1:B:3309:UNK:CB   | 2.94                     | 0.45              |
| 1:B:4169:UNK:O   | 1:B:4172:UNK:CB   | 2.65                     | 0.45              |
| 1:C:906:CYS:SG   | 1:C:907:LEU:N     | 2.89                     | 0.45              |
| 1:D:1007:TYR:O   | 1:D:1008:SER:OG   | 2.30                     | 0.45              |
| 1:A:991:ASN:O    | 1:A:994:ASN:N     | 2.50                     | 0.45              |
| 1:A:2763:HIS:HE1 | 1:A:2790:MET:O    | 2.00                     | 0.45              |
| 1:B:350:HIS:HB2  | 1:B:378:LEU:CD2   | 2.47                     | 0.45              |
| 1:B:458:GLU:N    | 1:B:460:GLN:HB2   | 2.32                     | 0.45              |
| 1:B:1007:TYR:HE1 | 1:B:1015:ALA:C    | 2.25                     | 0.45              |
| 1:B:1452:TRP:HB2 | 1:B:1527:MET:HE1  | 1.98                     | 0.45              |
| 1:B:1835:UNK:O   | 1:B:1838:UNK:N    | 2.49                     | 0.45              |
| 1:B:3895:UNK:HA  | 1:B:3898:UNK:CB   | 2.47                     | 0.45              |
| 1:C:324:ASP:OD1  | 1:C:324:ASP:N     | 2.50                     | 0.45              |
| 1:C:675:LEU:HD12 | 1:C:679:ALA:HB3   | 1.99                     | 0.45              |
| 1:A:64:ILE:O     | 1:A:111:HIS:HE1   | 2.00                     | 0.44              |
| 1:B:768:PHE:HB2  | 1:B:771:PHE:CZ    | 2.53                     | 0.44              |
| 1:B:879:HIS:HE1  | 1:B:906:CYS:SG    | 2.39                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1437:VAL:HG23 | 1:B:1518:CYS:H    | 1.81                     | 0.44              |
| 1:C:1935:UNK:H    | 1:C:1938:UNK:CB   | 2.30                     | 0.44              |
| 1:D:64:ILE:O      | 1:D:111:HIS:HE1   | 2.00                     | 0.44              |
| 1:D:904:HIS:C     | 1:D:906:CYS:H     | 2.25                     | 0.44              |
| 1:D:3268:UNK:N    | 1:D:3271:UNK:CB   | 2.67                     | 0.44              |
| 1:A:246:TYR:CD1   | 1:A:375:LYS:HA    | 2.53                     | 0.44              |
| 1:A:353:SER:HB3   | 1:A:355:LEU:HG    | 1.98                     | 0.44              |
| 1:A:4585:UNK:O    | 1:D:4885:UNK:O    | 2.12                     | 0.44              |
| 1:B:528:SER:HA    | 1:B:531:ARG:HD3   | 1.99                     | 0.44              |
| 1:C:77:ALA:C      | 1:C:80:GLU:HG2    | 2.41                     | 0.44              |
| 1:C:768:PHE:HB2   | 1:C:771:PHE:CZ    | 2.53                     | 0.44              |
| 1:D:75:VAL:C      | 1:D:79:GLN:NE2    | 2.73                     | 0.44              |
| 1:D:458:GLU:N     | 1:D:460:GLN:HB2   | 2.32                     | 0.44              |
| 1:D:3205:UNK:HA   | 1:D:3208:UNK:N    | 2.32                     | 0.44              |
| 1:D:3445:UNK:C    | 1:D:3447:UNK:H    | 2.30                     | 0.44              |
| 1:A:332:GLU:OE1   | 1:A:332:GLU:CA    | 2.63                     | 0.44              |
| 1:A:1437:VAL:HG23 | 1:A:1518:CYS:H    | 1.81                     | 0.44              |
| 1:B:991:ASN:O     | 1:B:994:ASN:N     | 2.49                     | 0.44              |
| 1:C:265:LEU:HD12  | 1:C:265:LEU:HA    | 1.73                     | 0.44              |
| 1:C:427:GLY:O     | 1:C:505:GLU:HG3   | 2.16                     | 0.44              |
| 1:C:456:SER:OG    | 1:C:460:GLN:OE1   | 2.31                     | 0.44              |
| 1:D:353:SER:HB3   | 1:D:355:LEU:HG    | 1.98                     | 0.44              |
| 1:D:4169:UNK:O    | 1:D:4172:UNK:CB   | 2.65                     | 0.44              |
| 1:A:1007:TYR:O    | 1:A:1008:SER:OG   | 2.30                     | 0.44              |
| 1:A:1007:TYR:HE1  | 1:A:1015:ALA:C    | 2.25                     | 0.44              |
| 1:A:1495:VAL:O    | 1:A:1495:VAL:HG12 | 2.16                     | 0.44              |
| 1:A:4091:UNK:O    | 1:A:4094:UNK:N    | 2.51                     | 0.44              |
| 1:B:2763:HIS:HE1  | 1:B:2790:MET:O    | 2.00                     | 0.44              |
| 1:C:745:SER:HB3   | 1:C:758:ARG:HB2   | 1.99                     | 0.44              |
| 1:C:1462:MET:O    | 1:C:1555:LEU:HD22 | 2.17                     | 0.44              |
| 1:C:1476:MET:CE   | 1:C:1516:ILE:HD13 | 2.47                     | 0.44              |
| 1:D:894:GLY:O     | 1:D:905:PRO:HA    | 2.17                     | 0.44              |
| 1:D:1001:VAL:HG13 | 1:D:1002:ALA:N    | 2.30                     | 0.44              |
| 1:D:1004:GLY:CA   | 1:D:1015:ALA:CB   | 2.60                     | 0.44              |
| 1:D:2763:HIS:HE1  | 1:D:2790:MET:O    | 2.00                     | 0.44              |
| 1:D:3304:UNK:C    | 1:D:3306:UNK:N    | 2.77                     | 0.44              |
| 1:A:151:HIS:HB2   | 1:A:170:ILE:CG2   | 2.46                     | 0.44              |
| 1:A:350:HIS:HB2   | 1:A:378:LEU:CD2   | 2.48                     | 0.44              |
| 1:A:855:PRO:CG    | 1:A:994:ASN:O     | 2.58                     | 0.44              |
| 1:A:1020:ARG:HH12 | 1:A:1027:LEU:HG   | 1.15                     | 0.44              |
| 1:A:4898:UNK:CB   | 1:A:4899:UNK:C    | 2.96                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:26:ALA:HB2    | 1:B:182:LEU:HD21 | 1.99                     | 0.44              |
| 1:B:74:SER:HA     | 1:B:105:HIS:HA   | 2.00                     | 0.44              |
| 1:B:745:SER:HB3   | 1:B:758:ARG:HB2  | 1.99                     | 0.44              |
| 1:B:993:HIS:O     | 1:B:996:TRP:CD2  | 2.69                     | 0.44              |
| 1:C:458:GLU:N     | 1:C:460:GLN:HB2  | 2.32                     | 0.44              |
| 1:C:981:GLN:O     | 1:C:985:VAL:HG23 | 2.18                     | 0.44              |
| 1:D:324:ASP:OD1   | 1:D:324:ASP:N    | 2.50                     | 0.44              |
| 1:D:424:LYS:HZ3   | 1:D:505:GLU:HB2  | 1.79                     | 0.44              |
| 1:D:466:SER:O     | 1:D:469:ARG:HB2  | 2.17                     | 0.44              |
| 1:D:1002:ALA:N    | 1:D:1005:TRP:NE1 | 2.65                     | 0.44              |
| 1:D:1020:ARG:HH12 | 1:D:1027:LEU:HG  | 1.15                     | 0.44              |
| 1:A:768:PHE:HB2   | 1:A:771:PHE:CZ   | 2.53                     | 0.44              |
| 1:A:954:LYS:HZ2   | 1:A:955:LEU:HD11 | 1.82                     | 0.44              |
| 1:A:956:PRO:HD2   | 1:A:959:TYR:N    | 2.27                     | 0.44              |
| 1:A:1437:VAL:HB   | 1:A:1517:GLY:HA2 | 2.00                     | 0.44              |
| 1:A:1935:UNK:H    | 1:A:1938:UNK:CB  | 2.30                     | 0.44              |
| 1:A:3205:UNK:HA   | 1:A:3208:UNK:N   | 2.33                     | 0.44              |
| 1:B:324:ASP:OD1   | 1:B:324:ASP:N    | 2.50                     | 0.44              |
| 1:B:689:THR:HG22  | 1:B:778:PHE:HE2  | 1.83                     | 0.44              |
| 1:B:719:LEU:HD22  | 1:B:737:LEU:HD11 | 1.99                     | 0.44              |
| 1:B:1110:ARG:HG2  | 1:B:1112:ASP:H   | 1.83                     | 0.44              |
| 1:B:4898:UNK:CB   | 1:B:4899:UNK:C   | 2.96                     | 0.44              |
| 1:C:64:ILE:O      | 1:C:111:HIS:HE1  | 2.00                     | 0.44              |
| 1:C:157:ARG:NH2   | 1:C:164:ARG:HD2  | 2.33                     | 0.44              |
| 1:C:672:VAL:HG11  | 1:C:785:ALA:HB1  | 2.00                     | 0.44              |
| 1:C:904:HIS:C     | 1:C:906:CYS:H    | 2.25                     | 0.44              |
| 1:C:1495:VAL:HG12 | 1:C:1495:VAL:O   | 2.16                     | 0.44              |
| 1:D:90:VAL:HB     | 1:D:91:GLU:OE1   | 2.18                     | 0.44              |
| 1:D:689:THR:HG22  | 1:D:778:PHE:HE2  | 1.83                     | 0.44              |
| 1:D:719:LEU:HD22  | 1:D:737:LEU:HD11 | 1.99                     | 0.44              |
| 1:D:991:ASN:C     | 1:D:993:HIS:N    | 2.73                     | 0.44              |
| 1:A:370:GLY:O     | 1:A:371:VAL:HG23 | 2.18                     | 0.44              |
| 1:A:719:LEU:HD22  | 1:A:737:LEU:HD11 | 1.99                     | 0.44              |
| 1:A:758:ARG:HG2   | 1:A:763:PRO:HA   | 2.00                     | 0.44              |
| 1:B:64:ILE:O      | 1:B:111:HIS:HE1  | 2.00                     | 0.44              |
| 1:B:728:ARG:HH11  | 1:B:1134:LEU:HB2 | 1.83                     | 0.44              |
| 1:B:1813:UNK:O    | 1:B:1817:UNK:N   | 2.42                     | 0.44              |
| 1:B:4113:UNK:HA   | 1:B:4116:UNK:CA  | 2.48                     | 0.44              |
| 1:C:13:PHE:CE1    | 1:C:162:LYS:HB2  | 2.53                     | 0.44              |
| 1:C:689:THR:HG22  | 1:C:778:PHE:HE2  | 1.83                     | 0.44              |
| 1:C:3205:UNK:HA   | 1:C:3208:UNK:N   | 2.32                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:993:HIS:O    | 1:D:996:TRP:CD2   | 2.69                     | 0.44              |
| 1:A:70:GLU:CG    | 1:A:110:ARG:HB2   | 2.48                     | 0.44              |
| 1:A:265:LEU:HA   | 1:A:265:LEU:HD12  | 1.73                     | 0.44              |
| 1:A:689:THR:HG22 | 1:A:778:PHE:HE2   | 1.83                     | 0.44              |
| 1:A:904:HIS:C    | 1:A:906:CYS:H     | 2.25                     | 0.44              |
| 1:A:1004:GLY:N   | 1:A:1007:TYR:CE2  | 2.86                     | 0.44              |
| 1:A:1110:ARG:HG2 | 1:A:1112:ASP:H    | 1.83                     | 0.44              |
| 1:A:1471:ALA:C   | 1:A:1472:VAL:CG2  | 2.87                     | 0.44              |
| 1:A:3895:UNK:HA  | 1:A:3898:UNK:CB   | 2.47                     | 0.44              |
| 1:B:70:GLU:CG    | 1:B:110:ARG:HB2   | 2.47                     | 0.44              |
| 1:B:246:TYR:CD1  | 1:B:375:LYS:HA    | 2.53                     | 0.44              |
| 1:B:370:GLY:O    | 1:B:371:VAL:HG23  | 2.18                     | 0.44              |
| 1:B:675:LEU:HD12 | 1:B:679:ALA:HB3   | 1.99                     | 0.44              |
| 1:B:904:HIS:C    | 1:B:906:CYS:H     | 2.25                     | 0.44              |
| 1:C:466:SER:O    | 1:C:469:ARG:HB2   | 2.17                     | 0.44              |
| 1:C:993:HIS:O    | 1:C:996:TRP:CD2   | 2.69                     | 0.44              |
| 1:C:1110:ARG:HG2 | 1:C:1112:ASP:H    | 1.83                     | 0.44              |
| 1:C:1477:GLY:C   | 1:C:1509:ILE:HG22 | 2.39                     | 0.44              |
| 1:D:758:ARG:HG2  | 1:D:763:PRO:HA    | 2.00                     | 0.44              |
| 1:D:1110:ARG:HG2 | 1:D:1112:ASP:H    | 1.83                     | 0.44              |
| 1:D:3895:UNK:HA  | 1:D:3898:UNK:CB   | 2.47                     | 0.44              |
| 1:D:4898:UNK:CB  | 1:D:4899:UNK:C    | 2.96                     | 0.44              |
| 1:A:752:VAL:CB   | 1:A:753:PRO:C     | 2.85                     | 0.44              |
| 1:B:424:LYS:NZ   | 1:B:506:TYR:CD1   | 2.83                     | 0.44              |
| 1:B:753:PRO:CB   | 1:B:773:LEU:HD13  | 2.48                     | 0.44              |
| 1:B:3036:UNK:O   | 1:B:3039:UNK:N    | 2.51                     | 0.44              |
| 1:B:3304:UNK:C   | 1:B:3306:UNK:N    | 2.77                     | 0.44              |
| 1:C:90:VAL:HB    | 1:C:91:GLU:OE1    | 2.18                     | 0.44              |
| 1:C:350:HIS:HB2  | 1:C:378:LEU:CD2   | 2.47                     | 0.44              |
| 1:C:752:VAL:CB   | 1:C:753:PRO:C     | 2.85                     | 0.44              |
| 1:C:1007:TYR:CD2 | 1:C:1016:ARG:CZ   | 2.95                     | 0.44              |
| 1:D:672:VAL:HG11 | 1:D:785:ALA:HB1   | 2.00                     | 0.44              |
| 1:D:1471:ALA:C   | 1:D:1472:VAL:CG2  | 2.87                     | 0.44              |
| 1:A:466:SER:O    | 1:A:469:ARG:HB2   | 2.17                     | 0.43              |
| 1:B:752:VAL:CB   | 1:B:753:PRO:C     | 2.85                     | 0.43              |
| 1:C:719:LEU:HD22 | 1:C:737:LEU:HD11  | 1.99                     | 0.43              |
| 1:C:879:HIS:HE1  | 1:C:906:CYS:SG    | 2.39                     | 0.43              |
| 1:C:993:HIS:CE1  | 1:C:1020:ARG:CA   | 2.91                     | 0.43              |
| 1:C:3895:UNK:HA  | 1:C:3898:UNK:CB   | 2.47                     | 0.43              |
| 1:C:4898:UNK:CB  | 1:C:4899:UNK:C    | 2.96                     | 0.43              |
| 1:D:13:PHE:CE1   | 1:D:162:LYS:HB2   | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:350:HIS:HB2  | 1:D:378:LEU:CD2  | 2.47                     | 0.43              |
| 1:D:768:PHE:HB2  | 1:D:771:PHE:CZ   | 2.53                     | 0.43              |
| 1:A:74:SER:HA    | 1:A:105:HIS:HA   | 2.00                     | 0.43              |
| 1:A:323:LEU:CB   | 1:A:324:ASP:C    | 2.85                     | 0.43              |
| 1:A:445:LEU:HD23 | 1:A:521:LEU:CB   | 2.44                     | 0.43              |
| 1:A:728:ARG:HH11 | 1:A:1134:LEU:HB2 | 1.83                     | 0.43              |
| 1:A:753:PRO:CB   | 1:A:773:LEU:HD13 | 2.48                     | 0.43              |
| 1:A:953:THR:HG22 | 1:A:954:LYS:N    | 2.34                     | 0.43              |
| 1:A:981:GLN:O    | 1:A:985:VAL:HG23 | 2.18                     | 0.43              |
| 1:B:89:GLY:HA2   | 1:B:90:VAL:HG13  | 2.00                     | 0.43              |
| 1:B:466:SER:O    | 1:B:469:ARG:HB2  | 2.17                     | 0.43              |
| 1:B:1935:UNK:H   | 1:B:1938:UNK:CB  | 2.30                     | 0.43              |
| 1:B:4091:UNK:O   | 1:B:4094:UNK:N   | 2.51                     | 0.43              |
| 1:C:70:GLU:CG    | 1:C:110:ARG:HB2  | 2.48                     | 0.43              |
| 1:C:528:SER:HA   | 1:C:531:ARG:HD3  | 2.00                     | 0.43              |
| 1:C:3036:UNK:O   | 1:C:3039:UNK:N   | 2.51                     | 0.43              |
| 1:D:19:GLU:HG2   | 1:D:205:ILE:CG1  | 2.48                     | 0.43              |
| 1:D:26:ALA:HB2   | 1:D:182:LEU:HD21 | 2.00                     | 0.43              |
| 1:D:170:ILE:HD12 | 1:D:170:ILE:HA   | 1.93                     | 0.43              |
| 1:D:370:GLY:O    | 1:D:371:VAL:HG23 | 2.18                     | 0.43              |
| 1:D:756:SER:HB2  | 1:D:766:GLY:HA2  | 2.01                     | 0.43              |
| 1:D:4904:UNK:O   | 1:D:4905:UNK:C   | 2.66                     | 0.43              |
| 1:A:89:GLY:HA2   | 1:A:90:VAL:HG13  | 2.00                     | 0.43              |
| 1:A:157:ARG:NH2  | 1:A:164:ARG:HD2  | 2.32                     | 0.43              |
| 1:A:528:SER:HA   | 1:A:531:ARG:HD3  | 1.99                     | 0.43              |
| 1:A:894:GLY:O    | 1:A:905:PRO:HA   | 2.17                     | 0.43              |
| 1:A:1000:ARG:CD  | 1:A:1007:TYR:OH  | 2.66                     | 0.43              |
| 1:A:3036:UNK:O   | 1:A:3039:UNK:N   | 2.51                     | 0.43              |
| 1:A:4904:UNK:O   | 1:A:4905:UNK:C   | 2.66                     | 0.43              |
| 1:B:84:ASN:ND2   | 1:B:84:ASN:N     | 2.60                     | 0.43              |
| 1:B:157:ARG:NH2  | 1:B:164:ARG:HD2  | 2.33                     | 0.43              |
| 1:B:672:VAL:HG11 | 1:B:785:ALA:HB1  | 2.00                     | 0.43              |
| 1:B:981:GLN:O    | 1:B:985:VAL:HG23 | 2.18                     | 0.43              |
| 1:C:246:TYR:CD1  | 1:C:375:LYS:HA   | 2.53                     | 0.43              |
| 1:C:728:ARG:HD3  | 1:C:1133:HIS:CD2 | 2.54                     | 0.43              |
| 1:C:855:PRO:HA   | 1:C:994:ASN:CB   | 2.20                     | 0.43              |
| 1:C:1004:GLY:N   | 1:C:1007:TYR:CE2 | 2.86                     | 0.43              |
| 1:D:157:ARG:NH2  | 1:D:164:ARG:HD2  | 2.33                     | 0.43              |
| 1:D:246:TYR:CD1  | 1:D:375:LYS:HA   | 2.52                     | 0.43              |
| 1:D:275:ARG:HG3  | 1:D:278:GLN:HB2  | 2.00                     | 0.43              |
| 1:D:424:LYS:NZ   | 1:D:506:TYR:CD1  | 2.83                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:728:ARG:NH1  | 1:D:1119:GLU:HA   | 2.31                     | 0.43              |
| 1:D:753:PRO:CB   | 1:D:773:LEU:HD13  | 2.48                     | 0.43              |
| 1:D:953:THR:HG22 | 1:D:954:LYS:N     | 2.34                     | 0.43              |
| 1:D:981:GLN:O    | 1:D:985:VAL:HG23  | 2.18                     | 0.43              |
| 1:D:1004:GLY:N   | 1:D:1007:TYR:CE2  | 2.86                     | 0.43              |
| 1:A:13:PHE:CE1   | 1:A:162:LYS:HB2   | 2.53                     | 0.43              |
| 1:A:275:ARG:HG3  | 1:A:278:GLN:HB2   | 2.00                     | 0.43              |
| 1:A:317:ARG:HH12 | 1:A:322:LYS:CA    | 2.24                     | 0.43              |
| 1:A:988:LEU:CB   | 1:A:1039:LEU:HD22 | 2.47                     | 0.43              |
| 1:A:1007:TYR:CD2 | 1:A:1016:ARG:CZ   | 2.95                     | 0.43              |
| 1:B:20:VAL:HA    | 1:B:205:ILE:HG12  | 2.00                     | 0.43              |
| 1:B:3205:UNK:CA  | 1:B:3208:UNK:CB   | 2.84                     | 0.43              |
| 1:C:170:ILE:HD12 | 1:C:170:ILE:HA    | 1.93                     | 0.43              |
| 1:D:20:VAL:CA    | 1:D:205:ILE:HG12  | 2.49                     | 0.43              |
| 1:D:70:GLU:CG    | 1:D:110:ARG:HB2   | 2.48                     | 0.43              |
| 1:D:89:GLY:HA2   | 1:D:90:VAL:HG13   | 2.00                     | 0.43              |
| 1:A:75:VAL:C     | 1:A:79:GLN:NE2    | 2.73                     | 0.43              |
| 1:A:4103:UNK:C   | 1:A:4104:UNK:O    | 2.64                     | 0.43              |
| 1:B:20:VAL:CA    | 1:B:205:ILE:HG12  | 2.49                     | 0.43              |
| 1:B:46:LEU:HD23  | 1:B:46:LEU:HA     | 1.84                     | 0.43              |
| 1:B:50:GLU:HA    | 1:B:51:PRO:HD2    | 1.92                     | 0.43              |
| 1:B:353:SER:HB3  | 1:B:355:LEU:HG    | 1.98                     | 0.43              |
| 1:B:4904:UNK:O   | 1:B:4905:UNK:C    | 2.66                     | 0.43              |
| 1:C:2763:HIS:HE1 | 1:C:2790:MET:O    | 2.00                     | 0.43              |
| 1:C:4091:UNK:O   | 1:C:4094:UNK:N    | 2.51                     | 0.43              |
| 1:C:4904:UNK:O   | 1:C:4905:UNK:C    | 2.66                     | 0.43              |
| 1:D:728:ARG:HH11 | 1:D:1134:LEU:HB2  | 1.83                     | 0.43              |
| 1:D:752:VAL:HB   | 1:D:754:SER:CB    | 2.49                     | 0.43              |
| 1:D:1000:ARG:CD  | 1:D:1007:TYR:OH   | 2.67                     | 0.43              |
| 1:A:20:VAL:CA    | 1:A:205:ILE:HG12  | 2.49                     | 0.43              |
| 1:A:20:VAL:HA    | 1:A:205:ILE:HG12  | 2.00                     | 0.43              |
| 1:A:76:ARG:CA    | 1:A:79:GLN:CD     | 2.85                     | 0.43              |
| 1:A:672:VAL:HG11 | 1:A:785:ALA:HB1   | 2.00                     | 0.43              |
| 1:A:728:ARG:HD3  | 1:A:1133:HIS:CD2  | 2.53                     | 0.43              |
| 1:A:756:SER:HB2  | 1:A:766:GLY:HA2   | 2.01                     | 0.43              |
| 1:A:855:PRO:HA   | 1:A:994:ASN:CB    | 2.20                     | 0.43              |
| 1:A:1007:TYR:HE1 | 1:A:1015:ALA:CB   | 2.29                     | 0.43              |
| 1:B:323:LEU:CB   | 1:B:324:ASP:C     | 2.85                     | 0.43              |
| 1:B:728:ARG:HD3  | 1:B:1133:HIS:CD2  | 2.54                     | 0.43              |
| 1:B:756:SER:HB2  | 1:B:766:GLY:HA2   | 2.01                     | 0.43              |
| 1:B:1007:TYR:CD2 | 1:B:1016:ARG:CZ   | 2.95                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:20:VAL:CA     | 1:C:205:ILE:HG12  | 2.49                     | 0.43              |
| 1:C:329:ARG:NH1   | 1:C:329:ARG:CG    | 2.71                     | 0.43              |
| 1:D:576:UNK:CA    | 1:D:579:UNK:CB    | 2.92                     | 0.43              |
| 1:D:4091:UNK:O    | 1:D:4094:UNK:N    | 2.51                     | 0.43              |
| 1:A:221:ARG:NH2   | 1:A:259:LEU:HD11  | 2.34                     | 0.43              |
| 1:A:324:ASP:CB    | 1:A:325:THR:C     | 2.85                     | 0.43              |
| 1:A:426:ARG:CZ    | 1:A:796:ARG:NH2   | 2.71                     | 0.43              |
| 1:B:1000:ARG:CD   | 1:B:1007:TYR:OH   | 2.67                     | 0.43              |
| 1:B:1020:ARG:HH12 | 1:B:1027:LEU:HG   | 1.15                     | 0.43              |
| 1:B:1021:LEU:C    | 1:B:1022:VAL:CG1  | 2.84                     | 0.43              |
| 1:B:4232:UNK:H2   | 1:B:4235:UNK:CB   | 2.31                     | 0.43              |
| 1:C:73:LEU:HB2    | 1:C:78:LEU:HD22   | 1.60                     | 0.43              |
| 1:C:323:LEU:CB    | 1:C:324:ASP:C     | 2.85                     | 0.43              |
| 1:C:332:GLU:OE1   | 1:C:332:GLU:CA    | 2.63                     | 0.43              |
| 1:C:753:PRO:CB    | 1:C:773:LEU:HD13  | 2.48                     | 0.43              |
| 1:C:758:ARG:HG2   | 1:C:763:PRO:HA    | 2.00                     | 0.43              |
| 1:C:953:THR:HG22  | 1:C:954:LYS:N     | 2.34                     | 0.43              |
| 1:C:1076:ARG:HG2  | 1:C:1191:VAL:HG12 | 2.00                     | 0.43              |
| 1:D:528:SER:HA    | 1:D:531:ARG:HD3   | 1.99                     | 0.43              |
| 1:D:728:ARG:HD3   | 1:D:1133:HIS:CD2  | 2.54                     | 0.43              |
| 1:D:728:ARG:HA    | 1:D:729:PRO:HA    | 1.63                     | 0.43              |
| 1:D:1437:VAL:HB   | 1:D:1517:GLY:HA2  | 2.00                     | 0.43              |
| 1:D:3036:UNK:O    | 1:D:3039:UNK:N    | 2.51                     | 0.43              |
| 1:D:4232:UNK:H2   | 1:D:4235:UNK:CB   | 2.31                     | 0.43              |
| 1:A:728:ARG:NH1   | 1:A:1119:GLU:HA   | 2.31                     | 0.43              |
| 1:A:1476:MET:HE1  | 1:A:1516:ILE:HD13 | 1.93                     | 0.43              |
| 1:B:13:PHE:CE1    | 1:B:162:LYS:HB2   | 2.53                     | 0.43              |
| 1:B:1007:TYR:C    | 1:B:1008:SER:HG   | 2.26                     | 0.43              |
| 1:C:89:GLY:HA2    | 1:C:90:VAL:HG13   | 2.01                     | 0.43              |
| 1:C:445:LEU:HD23  | 1:C:521:LEU:CB    | 2.44                     | 0.43              |
| 1:C:956:PRO:CD    | 1:C:959:TYR:CD1   | 2.58                     | 0.43              |
| 1:C:3398:UNK:C    | 1:C:3401:UNK:N    | 2.82                     | 0.43              |
| 1:C:4103:UNK:C    | 1:C:4104:UNK:O    | 2.64                     | 0.43              |
| 1:D:368:ARG:HB3   | 1:D:369:LEU:HD22  | 2.01                     | 0.43              |
| 1:D:1022:VAL:HG22 | 1:D:1027:LEU:HD21 | 2.01                     | 0.43              |
| 1:A:424:LYS:HZ3   | 1:A:505:GLU:HB2   | 1.82                     | 0.43              |
| 1:A:870:ILE:HD13  | 1:A:870:ILE:HA    | 1.78                     | 0.43              |
| 1:B:76:ARG:CA     | 1:B:79:GLN:CD     | 2.85                     | 0.43              |
| 1:B:90:VAL:HB     | 1:B:91:GLU:OE1    | 2.18                     | 0.43              |
| 1:B:368:ARG:HB3   | 1:B:369:LEU:HD22  | 2.00                     | 0.43              |
| 1:B:1004:GLY:N    | 1:B:1007:TYR:CE2  | 2.86                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1076:ARG:HG2  | 1:B:1191:VAL:HG12 | 2.00                     | 0.43              |
| 1:C:370:GLY:O     | 1:C:371:VAL:HG23  | 2.18                     | 0.43              |
| 1:C:659:TYR:C     | 1:C:750:LEU:CD2   | 2.71                     | 0.43              |
| 1:C:756:SER:HB2   | 1:C:766:GLY:HA2   | 2.01                     | 0.43              |
| 1:C:4113:UNK:HA   | 1:C:4116:UNK:CA   | 2.48                     | 0.43              |
| 1:C:4232:UNK:H2   | 1:C:4235:UNK:CB   | 2.31                     | 0.43              |
| 1:C:4730:UNK:O    | 1:C:4731:UNK:C    | 2.66                     | 0.43              |
| 1:D:456:SER:OG    | 1:D:460:GLN:OE1   | 2.31                     | 0.43              |
| 1:D:1022:VAL:HG21 | 1:D:1027:LEU:HD23 | 2.01                     | 0.43              |
| 1:D:1076:ARG:HG2  | 1:D:1191:VAL:HG12 | 2.00                     | 0.43              |
| 1:A:26:ALA:HB2    | 1:A:182:LEU:HD21  | 2.00                     | 0.43              |
| 1:A:1462:MET:O    | 1:A:1555:LEU:HD22 | 2.17                     | 0.43              |
| 1:B:207:SER:OG    | 1:B:269:TRP:CE3   | 2.70                     | 0.43              |
| 1:B:758:ARG:HG2   | 1:B:763:PRO:HA    | 2.00                     | 0.43              |
| 1:B:773:LEU:HA    | 1:B:777:PHE:HZ    | 1.83                     | 0.43              |
| 1:B:1018:ASN:HA   | 1:B:1019:PRO:HD3  | 1.84                     | 0.43              |
| 1:C:1437:VAL:HB   | 1:C:1517:GLY:HA2  | 2.00                     | 0.43              |
| 1:D:369:LEU:HB3   | 1:D:370:GLY:HA2   | 2.01                     | 0.43              |
| 1:A:90:VAL:HB     | 1:A:91:GLU:OE1    | 2.18                     | 0.42              |
| 1:B:728:ARG:NH2   | 1:B:1119:GLU:C    | 2.77                     | 0.42              |
| 1:B:953:THR:HG22  | 1:B:954:LYS:N     | 2.34                     | 0.42              |
| 1:B:1521:ASP:C    | 1:B:1521:ASP:OD1  | 2.62                     | 0.42              |
| 1:C:151:HIS:HB2   | 1:C:170:ILE:CG2   | 2.46                     | 0.42              |
| 1:C:728:ARG:HA    | 1:C:729:PRO:HA    | 1.63                     | 0.42              |
| 1:C:1022:VAL:HG22 | 1:C:1027:LEU:HD21 | 2.01                     | 0.42              |
| 1:C:1437:VAL:CG2  | 1:C:1518:CYS:H    | 2.32                     | 0.42              |
| 1:D:332:GLU:OE1   | 1:D:332:GLU:CA    | 2.63                     | 0.42              |
| 1:D:1429:ASN:HB2  | 1:D:1547:LYS:CG   | 2.49                     | 0.42              |
| 1:D:2908:TYR:O    | 1:D:2916:LYS:HE2  | 2.19                     | 0.42              |
| 1:A:79:GLN:HE21   | 1:A:79:GLN:HB3    | 1.59                     | 0.42              |
| 1:A:728:ARG:NH2   | 1:A:1119:GLU:C    | 2.77                     | 0.42              |
| 1:A:1076:ARG:HG2  | 1:A:1191:VAL:HG12 | 2.00                     | 0.42              |
| 1:A:1492:CYS:SG   | 1:A:1539:PHE:HE1  | 2.39                     | 0.42              |
| 1:A:2908:TYR:O    | 1:A:2916:LYS:HE2  | 2.19                     | 0.42              |
| 1:B:728:ARG:NH1   | 1:B:1119:GLU:HA   | 2.31                     | 0.42              |
| 1:B:1429:ASN:O    | 1:B:1522:LEU:HD13 | 2.19                     | 0.42              |
| 1:B:1437:VAL:CG2  | 1:B:1518:CYS:H    | 2.32                     | 0.42              |
| 1:B:4797:UNK:O    | 1:B:4801:UNK:O    | 2.38                     | 0.42              |
| 1:C:26:ALA:HB2    | 1:C:182:LEU:HD21  | 2.00                     | 0.42              |
| 1:C:728:ARG:NH1   | 1:C:1119:GLU:HA   | 2.31                     | 0.42              |
| 1:D:77:ALA:CA     | 1:D:80:GLU:CG     | 2.90                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:81:MET:O      | 1:D:85:THR:HG23   | 2.19                     | 0.42              |
| 1:D:445:LEU:HD23  | 1:D:521:LEU:CB    | 2.44                     | 0.42              |
| 1:D:1437:VAL:CG2  | 1:D:1518:CYS:H    | 2.32                     | 0.42              |
| 1:A:12:GLN:NE2    | 1:A:164:ARG:HB3   | 2.34                     | 0.42              |
| 1:A:369:LEU:HB3   | 1:A:370:GLY:HA2   | 2.01                     | 0.42              |
| 1:A:681:HIS:CE1   | 1:A:719:LEU:HB2   | 2.55                     | 0.42              |
| 1:A:1022:VAL:HG21 | 1:A:1027:LEU:HD23 | 2.01                     | 0.42              |
| 1:A:4113:UNK:HA   | 1:A:4116:UNK:CA   | 2.48                     | 0.42              |
| 1:A:4232:UNK:H2   | 1:A:4235:UNK:CB   | 2.31                     | 0.42              |
| 1:B:110:ARG:HH21  | 1:B:115:ARG:HB3   | 1.84                     | 0.42              |
| 1:B:1437:VAL:HB   | 1:B:1517:GLY:HA2  | 2.00                     | 0.42              |
| 1:B:3205:UNK:HA   | 1:B:3208:UNK:N    | 2.33                     | 0.42              |
| 1:C:110:ARG:HH21  | 1:C:115:ARG:HB3   | 1.85                     | 0.42              |
| 1:C:275:ARG:HG3   | 1:C:278:GLN:HB2   | 2.00                     | 0.42              |
| 1:C:681:HIS:CE1   | 1:C:719:LEU:HB2   | 2.55                     | 0.42              |
| 1:C:728:ARG:HH11  | 1:C:1134:LEU:HB2  | 1.83                     | 0.42              |
| 1:C:1000:ARG:CD   | 1:C:1007:TYR:OH   | 2.66                     | 0.42              |
| 1:C:1022:VAL:HG21 | 1:C:1027:LEU:HD23 | 2.01                     | 0.42              |
| 1:B:12:GLN:NE2    | 1:B:164:ARG:HB3   | 2.34                     | 0.42              |
| 1:B:336:PRO:HA    | 1:B:337:PRO:HD2   | 1.93                     | 0.42              |
| 1:C:85:THR:O      | 1:C:89:GLY:N      | 2.51                     | 0.42              |
| 1:C:1018:ASN:HA   | 1:C:1019:PRO:HD3  | 1.84                     | 0.42              |
| 1:C:1477:GLY:C    | 1:C:1509:ILE:HG23 | 2.43                     | 0.42              |
| 1:C:4087:UNK:HA   | 1:C:4123:UNK:O    | 2.19                     | 0.42              |
| 1:D:728:ARG:NH2   | 1:D:1119:GLU:C    | 2.77                     | 0.42              |
| 1:D:752:VAL:CB    | 1:D:753:PRO:C     | 2.85                     | 0.42              |
| 1:D:3398:UNK:C    | 1:D:3401:UNK:N    | 2.82                     | 0.42              |
| 1:A:368:ARG:HB3   | 1:A:369:LEU:HD22  | 2.01                     | 0.42              |
| 1:A:752:VAL:HB    | 1:A:754:SER:CB    | 2.49                     | 0.42              |
| 1:A:773:LEU:O     | 1:A:775:GLY:N     | 2.53                     | 0.42              |
| 1:A:1020:ARG:NH2  | 1:A:1027:LEU:CD2  | 2.55                     | 0.42              |
| 1:A:4730:UNK:O    | 1:A:4731:UNK:C    | 2.66                     | 0.42              |
| 1:B:265:LEU:HD12  | 1:B:265:LEU:HA    | 1.73                     | 0.42              |
| 1:B:369:LEU:HB3   | 1:B:370:GLY:HA2   | 2.01                     | 0.42              |
| 1:C:20:VAL:HA     | 1:C:205:ILE:HG12  | 2.00                     | 0.42              |
| 1:D:20:VAL:HA     | 1:D:205:ILE:HG12  | 2.00                     | 0.42              |
| 1:D:81:MET:CE     | 1:D:85:THR:CG2    | 2.97                     | 0.42              |
| 1:D:998:ARG:NH2   | 1:D:1002:ALA:HB3  | 2.16                     | 0.42              |
| 1:D:1100:MET:SD   | 1:D:1194:LEU:HD13 | 2.60                     | 0.42              |
| 1:A:1100:MET:SD   | 1:A:1194:LEU:HD13 | 2.60                     | 0.42              |
| 1:A:1429:ASN:HB2  | 1:A:1547:LYS:CG   | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1465:ASP:CA   | 1:A:1553:PHE:CG   | 2.73                     | 0.42              |
| 1:A:3398:UNK:C    | 1:A:3401:UNK:N    | 2.82                     | 0.42              |
| 1:B:221:ARG:NH2   | 1:B:259:LEU:HD11  | 2.34                     | 0.42              |
| 1:B:752:VAL:HB    | 1:B:754:SER:CB    | 2.49                     | 0.42              |
| 1:B:1429:ASN:HB2  | 1:B:1547:LYS:CG   | 2.49                     | 0.42              |
| 1:B:1452:TRP:CZ2  | 1:B:1527:MET:HG2  | 2.54                     | 0.42              |
| 1:C:81:MET:CE     | 1:C:85:THR:CG2    | 2.97                     | 0.42              |
| 1:D:74:SER:HA     | 1:D:105:HIS:HA    | 2.00                     | 0.42              |
| 1:D:123:THR:HG23  | 1:D:134:ASP:OD2   | 2.20                     | 0.42              |
| 1:D:1444:GLU:N    | 1:D:1445:PRO:CA   | 2.82                     | 0.42              |
| 1:A:81:MET:CE     | 1:A:85:THR:CG2    | 2.97                     | 0.42              |
| 1:A:242:ARG:HB2   | 1:A:289:ARG:HH12  | 1.85                     | 0.42              |
| 1:A:727:ALA:CB    | 1:A:1119:GLU:CD   | 2.93                     | 0.42              |
| 1:A:1022:VAL:HG22 | 1:A:1027:LEU:HD21 | 2.01                     | 0.42              |
| 1:A:1437:VAL:CG2  | 1:A:1518:CYS:H    | 2.33                     | 0.42              |
| 1:B:75:VAL:C      | 1:B:79:GLN:NE2    | 2.73                     | 0.42              |
| 1:B:123:THR:HG23  | 1:B:134:ASP:OD2   | 2.20                     | 0.42              |
| 1:B:1100:MET:SD   | 1:B:1194:LEU:HD13 | 2.60                     | 0.42              |
| 1:C:19:GLU:HG2    | 1:C:205:ILE:CG1   | 2.48                     | 0.42              |
| 1:C:76:ARG:NH1    | 1:D:3930:UNK:O    | 2.44                     | 0.42              |
| 1:C:207:SER:OG    | 1:C:269:TRP:CE3   | 2.70                     | 0.42              |
| 1:C:1020:ARG:HH12 | 1:C:1027:LEU:HG   | 1.15                     | 0.42              |
| 1:C:1429:ASN:HB2  | 1:C:1547:LYS:CG   | 2.49                     | 0.42              |
| 1:C:1549:PHE:CG   | 1:C:1550:PRO:CD   | 3.03                     | 0.42              |
| 1:C:4797:UNK:O    | 1:C:4801:UNK:O    | 2.38                     | 0.42              |
| 1:D:681:HIS:CE1   | 1:D:719:LEU:HB2   | 2.55                     | 0.42              |
| 1:A:1429:ASN:O    | 1:A:1522:LEU:HD13 | 2.19                     | 0.42              |
| 1:A:1452:TRP:CZ2  | 1:A:1527:MET:HG2  | 2.55                     | 0.42              |
| 1:A:1549:PHE:CG   | 1:A:1550:PRO:CD   | 3.03                     | 0.42              |
| 1:A:4797:UNK:O    | 1:A:4801:UNK:O    | 2.38                     | 0.42              |
| 1:C:728:ARG:NH2   | 1:C:1119:GLU:C    | 2.77                     | 0.42              |
| 1:D:727:ALA:CB    | 1:D:1119:GLU:CD   | 2.93                     | 0.42              |
| 1:D:753:PRO:CG    | 1:D:773:LEU:HD12  | 2.07                     | 0.42              |
| 1:D:773:LEU:O     | 1:D:775:GLY:N     | 2.53                     | 0.42              |
| 1:D:1813:UNK:O    | 1:D:1817:UNK:N    | 2.42                     | 0.42              |
| 1:D:4665:UNK:O    | 1:D:4668:UNK:N    | 2.53                     | 0.42              |
| 1:A:81:MET:O      | 1:A:85:THR:HG23   | 2.19                     | 0.42              |
| 1:A:286:THR:HG21  | 1:A:481:GLU:OE2   | 2.20                     | 0.42              |
| 1:A:4087:UNK:HA   | 1:A:4123:UNK:O    | 2.19                     | 0.42              |
| 1:B:275:ARG:HG3   | 1:B:278:GLN:HB2   | 2.00                     | 0.42              |
| 1:B:681:HIS:CE1   | 1:B:719:LEU:HB2   | 2.55                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:1470:ARG:HG3  | 1:B:1497:GLY:HA2 | 2.02                     | 0.42              |
| 1:C:81:MET:O      | 1:C:85:THR:HG23  | 2.19                     | 0.42              |
| 1:C:369:LEU:HB3   | 1:C:370:GLY:HA2  | 2.01                     | 0.42              |
| 1:C:1521:ASP:C    | 1:C:1521:ASP:OD1 | 2.63                     | 0.42              |
| 1:C:2908:TYR:O    | 1:C:2916:LYS:HE2 | 2.19                     | 0.42              |
| 1:C:3894:UNK:O    | 1:C:3898:UNK:CA  | 2.68                     | 0.42              |
| 1:C:4898:UNK:CA   | 1:C:4899:UNK:C   | 2.98                     | 0.42              |
| 1:D:9:ASP:CG      | 1:D:11:VAL:H     | 2.28                     | 0.42              |
| 1:D:110:ARG:HH21  | 1:D:115:ARG:HB3  | 1.85                     | 0.42              |
| 1:D:4898:UNK:CA   | 1:D:4899:UNK:C   | 2.98                     | 0.42              |
| 1:A:379:HIS:CD2   | 1:A:381:GLU:H    | 2.38                     | 0.42              |
| 1:A:4665:UNK:O    | 1:A:4668:UNK:N   | 2.53                     | 0.42              |
| 1:B:379:HIS:CD2   | 1:B:381:GLU:H    | 2.38                     | 0.42              |
| 1:B:1429:ASN:CG   | 1:B:1546:THR:O   | 2.55                     | 0.42              |
| 1:B:1549:PHE:CD1  | 1:B:1550:PRO:O   | 2.73                     | 0.42              |
| 1:B:3305:UNK:O    | 1:B:3308:UNK:CB  | 2.68                     | 0.42              |
| 1:C:213:TYR:CD1   | 1:C:337:PRO:HB2  | 2.55                     | 0.42              |
| 1:C:1470:ARG:HG3  | 1:C:1497:GLY:HA2 | 2.02                     | 0.42              |
| 1:D:379:HIS:CD2   | 1:D:381:GLU:H    | 2.38                     | 0.42              |
| 1:D:1549:PHE:CD1  | 1:D:1550:PRO:O   | 2.73                     | 0.42              |
| 1:D:4807:UNK:O    | 1:D:4811:UNK:N   | 2.53                     | 0.42              |
| 1:A:213:TYR:CD1   | 1:A:337:PRO:HB2  | 2.55                     | 0.41              |
| 1:A:1444:GLU:CB   | 1:A:1445:PRO:C   | 2.84                     | 0.41              |
| 1:B:242:ARG:HB2   | 1:B:289:ARG:HH12 | 1.85                     | 0.41              |
| 1:B:3398:UNK:C    | 1:B:3401:UNK:N   | 2.82                     | 0.41              |
| 1:B:4898:UNK:CA   | 1:B:4899:UNK:C   | 2.98                     | 0.41              |
| 1:C:77:ALA:O      | 1:C:80:GLU:HG3   | 2.20                     | 0.41              |
| 1:C:221:ARG:NH2   | 1:C:259:LEU:HD11 | 2.34                     | 0.41              |
| 1:C:1083:VAL:HG13 | 1:C:1088:TRP:HB3 | 2.03                     | 0.41              |
| 1:C:1452:TRP:CZ2  | 1:C:1527:MET:HG2 | 2.55                     | 0.41              |
| 1:D:514:SER:O     | 1:D:518:ILE:HG13 | 2.20                     | 0.41              |
| 1:D:711:LEU:HD23  | 1:D:726:VAL:HG11 | 2.02                     | 0.41              |
| 1:D:1521:ASP:OD1  | 1:D:1521:ASP:C   | 2.62                     | 0.41              |
| 1:D:4797:UNK:O    | 1:D:4801:UNK:O   | 2.38                     | 0.41              |
| 1:A:1434:TYR:HD1  | 1:A:1570:LYS:HB2 | 1.77                     | 0.41              |
| 1:A:4232:UNK:O    | 1:A:4233:UNK:N   | 2.54                     | 0.41              |
| 1:B:727:ALA:CB    | 1:B:1119:GLU:CD  | 2.93                     | 0.41              |
| 1:B:993:HIS:CE1   | 1:B:1020:ARG:CA  | 2.91                     | 0.41              |
| 1:B:4797:UNK:C    | 1:B:4801:UNK:O   | 2.68                     | 0.41              |
| 1:C:50:GLU:HA     | 1:C:51:PRO:HD2   | 1.92                     | 0.41              |
| 1:C:467:LYS:HB3   | 1:C:467:LYS:HZ1  | 1.83                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:752:VAL:HB   | 1:C:754:SER:CB    | 2.49                     | 0.41              |
| 1:C:773:LEU:O    | 1:C:775:GLY:N     | 2.53                     | 0.41              |
| 1:C:1100:MET:SD  | 1:C:1194:LEU:HD13 | 2.60                     | 0.41              |
| 1:C:1429:ASN:O   | 1:C:1522:LEU:HD13 | 2.19                     | 0.41              |
| 1:D:1492:CYS:SG  | 1:D:1539:PHE:HE1  | 2.39                     | 0.41              |
| 1:D:1549:PHE:CG  | 1:D:1550:PRO:CD   | 3.03                     | 0.41              |
| 1:A:76:ARG:NH1   | 1:B:3930:UNK:O    | 2.43                     | 0.41              |
| 1:A:84:ASN:ND2   | 1:A:84:ASN:N      | 2.60                     | 0.41              |
| 1:A:206:CYS:HB3  | 1:A:271:GLY:HA3   | 2.02                     | 0.41              |
| 1:A:514:SER:O    | 1:A:518:ILE:HG13  | 2.20                     | 0.41              |
| 1:A:4797:UNK:C   | 1:A:4801:UNK:O    | 2.68                     | 0.41              |
| 1:B:19:GLU:HG2   | 1:B:205:ILE:CG1   | 2.48                     | 0.41              |
| 1:B:77:ALA:O     | 1:B:80:GLU:HG3    | 2.20                     | 0.41              |
| 1:B:213:TYR:CD1  | 1:B:337:PRO:HB2   | 2.55                     | 0.41              |
| 1:B:1441:ALA:CB  | 1:B:1513:ASP:HA   | 2.50                     | 0.41              |
| 1:B:1549:PHE:CG  | 1:B:1550:PRO:CD   | 3.03                     | 0.41              |
| 1:B:2908:TYR:O   | 1:B:2916:LYS:HE2  | 2.19                     | 0.41              |
| 1:B:4232:UNK:O   | 1:B:4233:UNK:N    | 2.54                     | 0.41              |
| 1:B:4665:UNK:O   | 1:B:4668:UNK:N    | 2.53                     | 0.41              |
| 1:B:4807:UNK:O   | 1:B:4811:UNK:N    | 2.53                     | 0.41              |
| 1:C:74:SER:HA    | 1:C:105:HIS:HA    | 2.00                     | 0.41              |
| 1:C:424:LYS:HZ1  | 1:C:505:GLU:CB    | 2.21                     | 0.41              |
| 1:C:3985:UNK:O   | 1:C:3988:UNK:CB   | 2.69                     | 0.41              |
| 1:D:221:ARG:NH2  | 1:D:259:LEU:HD11  | 2.34                     | 0.41              |
| 1:D:265:LEU:HD12 | 1:D:265:LEU:HA    | 1.73                     | 0.41              |
| 1:D:1429:ASN:HB2 | 1:D:1547:LYS:CD   | 2.45                     | 0.41              |
| 1:D:2285:UNK:C   | 1:D:2286:UNK:H2   | 2.29                     | 0.41              |
| 1:D:4087:UNK:HA  | 1:D:4123:UNK:O    | 2.19                     | 0.41              |
| 1:A:1441:ALA:CB  | 1:A:1513:ASP:HA   | 2.50                     | 0.41              |
| 1:A:1476:MET:CE  | 1:A:1516:ILE:HD13 | 2.47                     | 0.41              |
| 1:A:3305:UNK:O   | 1:A:3308:UNK:CB   | 2.68                     | 0.41              |
| 1:A:3930:UNK:O   | 1:D:76:ARG:NH1    | 2.42                     | 0.41              |
| 1:A:3984:UNK:C   | 1:A:3986:UNK:N    | 2.82                     | 0.41              |
| 1:A:4807:UNK:O   | 1:A:4811:UNK:N    | 2.53                     | 0.41              |
| 1:B:81:MET:O     | 1:B:85:THR:HG23   | 2.19                     | 0.41              |
| 1:B:81:MET:CE    | 1:B:85:THR:CG2    | 2.97                     | 0.41              |
| 1:B:514:SER:O    | 1:B:518:ILE:HG13  | 2.20                     | 0.41              |
| 1:B:998:ARG:NH2  | 1:B:1002:ALA:HB3  | 2.16                     | 0.41              |
| 1:B:3894:UNK:O   | 1:B:3898:UNK:CA   | 2.68                     | 0.41              |
| 1:B:4087:UNK:HA  | 1:B:4123:UNK:O    | 2.19                     | 0.41              |
| 1:B:4854:UNK:O   | 1:B:4857:UNK:N    | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:79:GLN:CG     | 1:C:80:GLU:N      | 2.75                     | 0.41              |
| 1:C:379:HIS:CD2   | 1:C:381:GLU:H     | 2.38                     | 0.41              |
| 1:C:1492:CYS:SG   | 1:C:1539:PHE:HE1  | 2.39                     | 0.41              |
| 1:C:1549:PHE:CD1  | 1:C:1550:PRO:O    | 2.73                     | 0.41              |
| 1:C:4665:UNK:O    | 1:C:4668:UNK:N    | 2.53                     | 0.41              |
| 1:C:4854:UNK:O    | 1:C:4857:UNK:N    | 2.54                     | 0.41              |
| 1:D:1429:ASN:O    | 1:D:1522:LEU:HD13 | 2.19                     | 0.41              |
| 1:D:1470:ARG:HG3  | 1:D:1497:GLY:HA2  | 2.02                     | 0.41              |
| 1:D:3984:UNK:C    | 1:D:3986:UNK:N    | 2.82                     | 0.41              |
| 1:A:166:GLY:O     | 1:B:384:MET:SD    | 2.79                     | 0.41              |
| 1:A:329:ARG:NH1   | 1:A:329:ARG:CG    | 2.71                     | 0.41              |
| 1:A:3985:UNK:O    | 1:A:3988:UNK:CB   | 2.69                     | 0.41              |
| 1:A:4730:UNK:C    | 1:A:4731:UNK:O    | 2.68                     | 0.41              |
| 1:B:299:LEU:HD13  | 1:B:378:LEU:HD11  | 2.03                     | 0.41              |
| 1:C:711:LEU:HD23  | 1:C:726:VAL:HG11  | 2.02                     | 0.41              |
| 1:C:767:VAL:HG12  | 1:C:768:PHE:CD2   | 2.56                     | 0.41              |
| 1:C:773:LEU:HA    | 1:C:777:PHE:HZ    | 1.83                     | 0.41              |
| 1:C:1444:GLU:CB   | 1:C:1445:PRO:C    | 2.84                     | 0.41              |
| 1:C:4797:UNK:C    | 1:C:4801:UNK:O    | 2.68                     | 0.41              |
| 1:D:79:GLN:HE21   | 1:D:79:GLN:HB3    | 1.59                     | 0.41              |
| 1:D:80:GLU:O      | 1:D:83:ALA:HB3    | 2.21                     | 0.41              |
| 1:D:84:ASN:ND2    | 1:D:84:ASN:N      | 2.60                     | 0.41              |
| 1:D:1452:TRP:CZ2  | 1:D:1527:MET:HG2  | 2.55                     | 0.41              |
| 1:A:80:GLU:O      | 1:A:83:ALA:HB3    | 2.21                     | 0.41              |
| 1:A:123:THR:HG23  | 1:A:134:ASP:OD2   | 2.20                     | 0.41              |
| 1:A:659:TYR:C     | 1:A:750:LEU:CD2   | 2.71                     | 0.41              |
| 1:A:1549:PHE:CD1  | 1:A:1550:PRO:O    | 2.73                     | 0.41              |
| 1:B:206:CYS:HB3   | 1:B:271:GLY:HA3   | 2.02                     | 0.41              |
| 1:B:458:GLU:HA    | 1:B:459:LEU:C     | 2.46                     | 0.41              |
| 1:B:988:LEU:CB    | 1:B:1039:LEU:HD22 | 2.47                     | 0.41              |
| 1:B:1083:VAL:HG13 | 1:B:1088:TRP:HB3  | 2.03                     | 0.41              |
| 1:C:165:VAL:HG21  | 1:C:204:PRO:HG3   | 2.03                     | 0.41              |
| 1:C:206:CYS:HB3   | 1:C:271:GLY:HA3   | 2.02                     | 0.41              |
| 1:C:1020:ARG:NH2  | 1:C:1027:LEU:CD2  | 2.55                     | 0.41              |
| 1:D:242:ARG:HB2   | 1:D:289:ARG:HH12  | 1.85                     | 0.41              |
| 1:D:767:VAL:HG12  | 1:D:768:PHE:CD2   | 2.56                     | 0.41              |
| 1:D:1477:GLY:C    | 1:D:1509:ILE:HG23 | 2.43                     | 0.41              |
| 1:A:1083:VAL:HG13 | 1:A:1088:TRP:HB3  | 2.03                     | 0.41              |
| 1:A:3900:UNK:O    | 1:A:3901:UNK:C    | 2.69                     | 0.41              |
| 1:A:4681:UNK:O    | 1:A:4685:UNK:N    | 2.54                     | 0.41              |
| 1:B:445:LEU:HD23  | 1:B:521:LEU:CB    | 2.44                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:767:VAL:HG12  | 1:B:768:PHE:CD2  | 2.56                     | 0.41              |
| 1:B:1020:ARG:O    | 1:B:1020:ARG:CD  | 2.67                     | 0.41              |
| 1:B:3985:UNK:O    | 1:B:3988:UNK:CB  | 2.69                     | 0.41              |
| 1:C:368:ARG:HB3   | 1:C:369:LEU:HD22 | 2.00                     | 0.41              |
| 1:C:727:ALA:CB    | 1:C:1119:GLU:CD  | 2.93                     | 0.41              |
| 1:C:3305:UNK:O    | 1:C:3308:UNK:CB  | 2.68                     | 0.41              |
| 1:D:286:THR:HG21  | 1:D:481:GLU:OE2  | 2.20                     | 0.41              |
| 1:D:1083:VAL:HG13 | 1:D:1088:TRP:HB3 | 2.02                     | 0.41              |
| 1:D:4232:UNK:O    | 1:D:4233:UNK:N   | 2.54                     | 0.41              |
| 1:D:4645:UNK:O    | 1:D:4648:UNK:N   | 2.54                     | 0.41              |
| 1:D:4681:UNK:O    | 1:D:4685:UNK:N   | 2.54                     | 0.41              |
| 1:A:458:GLU:HA    | 1:A:459:LEU:C    | 2.46                     | 0.41              |
| 1:A:671:VAL:HA    | 1:A:787:VAL:HG12 | 2.03                     | 0.41              |
| 1:A:767:VAL:HG12  | 1:A:768:PHE:CD2  | 2.56                     | 0.41              |
| 1:A:1521:ASP:C    | 1:A:1521:ASP:OD1 | 2.63                     | 0.41              |
| 1:A:4898:UNK:CA   | 1:A:4899:UNK:C   | 2.98                     | 0.41              |
| 1:B:286:THR:HG21  | 1:B:481:GLU:OE2  | 2.20                     | 0.41              |
| 1:B:575:UNK:O     | 1:B:579:UNK:CB   | 2.69                     | 0.41              |
| 1:B:864:PRO:HA    | 1:B:865:PRO:HD3  | 1.90                     | 0.41              |
| 1:B:954:LYS:HB2   | 1:B:971:ASP:HB2  | 2.03                     | 0.41              |
| 1:B:4681:UNK:O    | 1:B:4685:UNK:N   | 2.54                     | 0.41              |
| 1:C:123:THR:HG23  | 1:C:134:ASP:OD2  | 2.20                     | 0.41              |
| 1:C:4681:UNK:O    | 1:C:4685:UNK:N   | 2.54                     | 0.41              |
| 1:C:4807:UNK:O    | 1:C:4811:UNK:N   | 2.53                     | 0.41              |
| 1:D:77:ALA:O      | 1:D:80:GLU:HG3   | 2.20                     | 0.41              |
| 1:D:208:CYS:C     | 1:D:334:MET:HE2  | 2.46                     | 0.41              |
| 1:D:1465:ASP:CA   | 1:D:1553:PHE:CG  | 2.73                     | 0.41              |
| 1:A:46:LEU:HA     | 1:A:46:LEU:HD23  | 1.84                     | 0.41              |
| 1:A:77:ALA:O      | 1:A:80:GLU:HG3   | 2.20                     | 0.41              |
| 1:A:102:LEU:HB2   | 1:A:105:HIS:CD2  | 2.56                     | 0.41              |
| 1:A:110:ARG:HH21  | 1:A:115:ARG:HB3  | 1.85                     | 0.41              |
| 1:A:208:CYS:C     | 1:A:334:MET:HE2  | 2.46                     | 0.41              |
| 1:A:310:LYS:HD3   | 1:A:352:ALA:HB2  | 2.03                     | 0.41              |
| 1:A:321:GLU:N     | 1:A:321:GLU:CD   | 2.76                     | 0.41              |
| 1:A:322:LYS:HB2   | 1:A:322:LYS:HZ2  | 1.85                     | 0.41              |
| 1:A:411:TYR:OH    | 1:A:445:LEU:HD12 | 2.21                     | 0.41              |
| 1:A:544:UNK:O     | 1:A:547:UNK:CB   | 2.69                     | 0.41              |
| 1:A:954:LYS:HB2   | 1:A:971:ASP:HB2  | 2.03                     | 0.41              |
| 1:A:1017:ARG:C    | 1:A:1018:ASN:OD1 | 2.64                     | 0.41              |
| 1:A:1495:VAL:N    | 1:A:1540:PHE:CE1 | 2.89                     | 0.41              |
| 1:A:4854:UNK:O    | 1:A:4857:UNK:N   | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:5016:UNK:O    | 1:A:5017:UNK:C    | 2.69                     | 0.41              |
| 1:B:78:LEU:HG     | 1:B:78:LEU:H      | 1.67                     | 0.41              |
| 1:B:78:LEU:HD13   | 1:B:106:ALA:N     | 2.36                     | 0.41              |
| 1:B:85:THR:O      | 1:B:89:GLY:N      | 2.51                     | 0.41              |
| 1:B:102:LEU:HB2   | 1:B:105:HIS:CD2   | 2.56                     | 0.41              |
| 1:B:151:HIS:HB2   | 1:B:170:ILE:CG2   | 2.46                     | 0.41              |
| 1:B:341:TYR:HD1   | 1:B:390:LEU:O     | 2.04                     | 0.41              |
| 1:B:773:LEU:O     | 1:B:775:GLY:N     | 2.53                     | 0.41              |
| 1:B:1022:VAL:HG22 | 1:B:1027:LEU:HD21 | 2.01                     | 0.41              |
| 1:B:1476:MET:CE   | 1:B:1516:ILE:HD13 | 2.47                     | 0.41              |
| 1:B:3900:UNK:O    | 1:B:3901:UNK:C    | 2.69                     | 0.41              |
| 1:C:80:GLU:O      | 1:C:83:ALA:HB3    | 2.21                     | 0.41              |
| 1:C:102:LEU:HB2   | 1:C:105:HIS:CD2   | 2.56                     | 0.41              |
| 1:C:299:LEU:HD13  | 1:C:378:LEU:HD11  | 2.03                     | 0.41              |
| 1:C:310:LYS:HD3   | 1:C:352:ALA:HB2   | 2.03                     | 0.41              |
| 1:C:684:VAL:HG12  | 1:C:781:VAL:HG13  | 2.03                     | 0.41              |
| 1:C:954:LYS:HB2   | 1:C:971:ASP:HB2   | 2.03                     | 0.41              |
| 1:C:998:ARG:CD    | 1:C:999:ASP:CG    | 2.76                     | 0.41              |
| 1:C:3900:UNK:O    | 1:C:3901:UNK:C    | 2.69                     | 0.41              |
| 1:C:4645:UNK:O    | 1:C:4648:UNK:N    | 2.54                     | 0.41              |
| 1:C:4818:UNK:N    | 1:C:4821:UNK:CB   | 2.73                     | 0.41              |
| 1:C:5016:UNK:O    | 1:C:5017:UNK:C    | 2.69                     | 0.41              |
| 1:D:213:TYR:CD1   | 1:D:337:PRO:HB2   | 2.55                     | 0.41              |
| 1:D:424:LYS:NZ    | 1:D:506:TYR:CE1   | 2.89                     | 0.41              |
| 1:D:671:VAL:HA    | 1:D:787:VAL:HG12  | 2.03                     | 0.41              |
| 1:D:954:LYS:HB2   | 1:D:971:ASP:HB2   | 2.03                     | 0.41              |
| 1:D:994:ASN:CG    | 1:D:995:VAL:N     | 2.79                     | 0.41              |
| 1:D:1817:UNK:O    | 1:D:1818:UNK:CB   | 2.69                     | 0.41              |
| 1:D:3985:UNK:O    | 1:D:3988:UNK:CB   | 2.69                     | 0.41              |
| 1:D:4797:UNK:C    | 1:D:4801:UNK:O    | 2.68                     | 0.41              |
| 1:D:4818:UNK:N    | 1:D:4821:UNK:CB   | 2.73                     | 0.41              |
| 1:B:728:ARG:NH2   | 1:B:1119:GLU:HA   | 2.35                     | 0.41              |
| 1:B:3204:UNK:O    | 1:B:3207:UNK:CB   | 2.69                     | 0.41              |
| 1:C:242:ARG:HB2   | 1:C:289:ARG:HH12  | 1.85                     | 0.41              |
| 1:C:341:TYR:HD1   | 1:C:390:LEU:O     | 2.04                     | 0.41              |
| 1:C:514:SER:O     | 1:C:518:ILE:HG13  | 2.20                     | 0.41              |
| 1:C:567:UNK:O     | 1:C:568:UNK:C     | 2.69                     | 0.41              |
| 1:D:1495:VAL:N    | 1:D:1540:PHE:CE1  | 2.89                     | 0.41              |
| 1:A:575:UNK:O     | 1:A:579:UNK:CB    | 2.69                     | 0.40              |
| 1:A:728:ARG:NH2   | 1:A:1119:GLU:HA   | 2.35                     | 0.40              |
| 1:A:773:LEU:HA    | 1:A:777:PHE:HZ    | 1.83                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1817:UNK:O    | 1:A:1818:UNK:CB   | 2.69                     | 0.40              |
| 1:A:3802:UNK:O    | 1:A:3803:UNK:C    | 2.70                     | 0.40              |
| 1:B:411:TYR:OH    | 1:B:445:LEU:HD12  | 2.21                     | 0.40              |
| 1:B:544:UNK:O     | 1:B:547:UNK:CB    | 2.69                     | 0.40              |
| 1:B:1017:ARG:C    | 1:B:1018:ASN:OD1  | 2.64                     | 0.40              |
| 1:B:1495:VAL:N    | 1:B:1540:PHE:CE1  | 2.89                     | 0.40              |
| 1:C:76:ARG:CA     | 1:C:79:GLN:CD     | 2.85                     | 0.40              |
| 1:C:575:UNK:O     | 1:C:579:UNK:CB    | 2.69                     | 0.40              |
| 1:C:4232:UNK:O    | 1:C:4233:UNK:N    | 2.54                     | 0.40              |
| 1:C:4885:UNK:O    | 1:D:4585:UNK:O    | 2.14                     | 0.40              |
| 1:D:954:LYS:HZ2   | 1:D:955:LEU:HD11  | 1.86                     | 0.40              |
| 1:D:1131:ARG:HD3  | 1:D:1139:PHE:HB2  | 2.04                     | 0.40              |
| 1:D:4983:UNK:O    | 1:D:4984:UNK:C    | 2.69                     | 0.40              |
| 1:A:1444:GLU:N    | 1:A:1445:PRO:CA   | 2.82                     | 0.40              |
| 1:A:3204:UNK:O    | 1:A:3207:UNK:CB   | 2.69                     | 0.40              |
| 1:A:3982:UNK:O    | 1:A:3986:UNK:CB   | 2.70                     | 0.40              |
| 1:B:166:GLY:O     | 1:C:384:MET:SD    | 2.79                     | 0.40              |
| 1:B:424:LYS:NZ    | 1:B:506:TYR:CE1   | 2.90                     | 0.40              |
| 1:B:424:LYS:HZ3   | 1:B:505:GLU:HB2   | 1.81                     | 0.40              |
| 1:B:671:VAL:HA    | 1:B:787:VAL:HG12  | 2.03                     | 0.40              |
| 1:B:1022:VAL:HG21 | 1:B:1027:LEU:HD23 | 2.02                     | 0.40              |
| 1:B:3802:UNK:O    | 1:B:3803:UNK:C    | 2.70                     | 0.40              |
| 1:C:286:THR:HG21  | 1:C:481:GLU:OE2   | 2.20                     | 0.40              |
| 1:C:411:TYR:OH    | 1:C:445:LEU:HD12  | 2.21                     | 0.40              |
| 1:C:4983:UNK:O    | 1:C:4984:UNK:C    | 2.69                     | 0.40              |
| 1:D:76:ARG:CA     | 1:D:79:GLN:CD     | 2.85                     | 0.40              |
| 1:D:77:ALA:O      | 1:D:80:GLU:CG     | 2.70                     | 0.40              |
| 1:D:165:VAL:HG21  | 1:D:204:PRO:HG3   | 2.03                     | 0.40              |
| 1:D:411:TYR:OH    | 1:D:445:LEU:HD12  | 2.21                     | 0.40              |
| 1:D:3305:UNK:O    | 1:D:3308:UNK:CB   | 2.68                     | 0.40              |
| 1:A:75:VAL:CG1    | 1:A:76:ARG:N      | 2.73                     | 0.40              |
| 1:A:78:LEU:HD13   | 1:A:106:ALA:N     | 2.36                     | 0.40              |
| 1:A:299:LEU:HD13  | 1:A:378:LEU:HD11  | 2.03                     | 0.40              |
| 1:A:994:ASN:CG    | 1:A:995:VAL:N     | 2.79                     | 0.40              |
| 1:A:1001:VAL:CA   | 1:A:1005:TRP:CE2  | 3.01                     | 0.40              |
| 1:A:1470:ARG:HG3  | 1:A:1497:GLY:HA2  | 2.02                     | 0.40              |
| 1:B:208:CYS:C     | 1:B:334:MET:HE2   | 2.46                     | 0.40              |
| 1:B:310:LYS:HD3   | 1:B:352:ALA:HB2   | 2.03                     | 0.40              |
| 1:B:576:UNK:CA    | 1:B:579:UNK:CB    | 2.92                     | 0.40              |
| 1:B:3643:UNK:O    | 1:B:3644:UNK:C    | 2.70                     | 0.40              |
| 1:B:4120:UNK:O    | 1:B:4121:UNK:CB   | 2.70                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:4142:UNK:O   | 1:B:4145:UNK:CB  | 2.70                     | 0.40              |
| 1:C:77:ALA:O     | 1:C:80:GLU:CG    | 2.70                     | 0.40              |
| 1:C:166:GLY:O    | 1:D:384:MET:SD   | 2.79                     | 0.40              |
| 1:C:321:GLU:HG2  | 1:C:323:LEU:HD12 | 2.03                     | 0.40              |
| 1:C:458:GLU:HA   | 1:C:459:LEU:C    | 2.46                     | 0.40              |
| 1:C:855:PRO:HG3  | 1:C:994:ASN:CA   | 2.50                     | 0.40              |
| 1:C:1017:ARG:C   | 1:C:1018:ASN:OD1 | 2.64                     | 0.40              |
| 1:C:1131:ARG:HD3 | 1:C:1139:PHE:HB2 | 2.04                     | 0.40              |
| 1:C:4142:UNK:O   | 1:C:4145:UNK:CB  | 2.70                     | 0.40              |
| 1:C:4785:UNK:O   | 1:C:4788:UNK:N   | 2.54                     | 0.40              |
| 1:D:206:CYS:HB3  | 1:D:271:GLY:HA3  | 2.02                     | 0.40              |
| 1:D:323:LEU:CB   | 1:D:324:ASP:C    | 2.85                     | 0.40              |
| 1:D:661:LYS:C    | 1:D:662:TRP:CD1  | 3.00                     | 0.40              |
| 1:A:265:LEU:HD11 | 1:A:281:ARG:HH21 | 1.87                     | 0.40              |
| 1:A:773:LEU:HA   | 1:A:777:PHE:CE1  | 2.57                     | 0.40              |
| 1:A:1021:LEU:C   | 1:A:1022:VAL:CG1 | 2.84                     | 0.40              |
| 1:A:1141:ARG:HA  | 1:A:1142:PRO:HD3 | 1.89                     | 0.40              |
| 1:A:3397:UNK:O   | 1:A:3398:UNK:CB  | 2.70                     | 0.40              |
| 1:A:4120:UNK:O   | 1:A:4121:UNK:CB  | 2.70                     | 0.40              |
| 1:B:165:VAL:HG21 | 1:B:204:PRO:HG3  | 2.03                     | 0.40              |
| 1:B:317:ARG:HH12 | 1:B:322:LYS:CA   | 2.24                     | 0.40              |
| 1:B:870:ILE:HA   | 1:B:870:ILE:HD13 | 1.78                     | 0.40              |
| 1:B:4983:UNK:O   | 1:B:4984:UNK:C   | 2.69                     | 0.40              |
| 1:C:74:SER:HB2   | 1:C:75:VAL:H     | 1.43                     | 0.40              |
| 1:C:424:LYS:NZ   | 1:C:506:TYR:CE1  | 2.90                     | 0.40              |
| 1:C:1495:VAL:N   | 1:C:1540:PHE:CE1 | 2.89                     | 0.40              |
| 1:D:728:ARG:NH2  | 1:D:1119:GLU:HA  | 2.35                     | 0.40              |
| 1:D:1017:ARG:C   | 1:D:1018:ASN:OD1 | 2.64                     | 0.40              |
| 1:A:227:MET:HA   | 1:A:227:MET:HE2  | 2.03                     | 0.40              |
| 1:A:328:LYS:H    | 1:A:328:LYS:HG3  | 1.73                     | 0.40              |
| 1:A:1454:THR:CB  | 1:A:1455:PRO:CD  | 2.96                     | 0.40              |
| 1:A:3421:UNK:O   | 1:A:3422:UNK:CB  | 2.70                     | 0.40              |
| 1:A:4112:UNK:O   | 1:A:4115:UNK:CB  | 2.70                     | 0.40              |
| 1:A:4972:UNK:O   | 1:A:4975:UNK:CB  | 2.70                     | 0.40              |
| 1:B:265:LEU:HD11 | 1:B:281:ARG:HH21 | 1.87                     | 0.40              |
| 1:B:1437:VAL:N   | 1:B:1517:GLY:HA2 | 2.35                     | 0.40              |
| 1:B:1454:THR:CB  | 1:B:1455:PRO:CD  | 2.96                     | 0.40              |
| 1:B:2650:UNK:O   | 1:B:2651:UNK:CB  | 2.70                     | 0.40              |
| 1:B:4645:UNK:O   | 1:B:4648:UNK:N   | 2.54                     | 0.40              |
| 1:C:317:ARG:HH12 | 1:C:322:LYS:CA   | 2.24                     | 0.40              |
| 1:C:956:PRO:CD   | 1:C:956:PRO:O    | 2.70                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:988:LEU:O    | 1:C:988:LEU:HG  | 2.21                     | 0.40              |
| 1:C:3982:UNK:O   | 1:C:3986:UNK:CB | 2.70                     | 0.40              |
| 1:C:4120:UNK:O   | 1:C:4121:UNK:CB | 2.70                     | 0.40              |
| 1:C:4972:UNK:O   | 1:C:4975:UNK:CB | 2.70                     | 0.40              |
| 1:D:988:LEU:O    | 1:D:988:LEU:HG  | 2.21                     | 0.40              |
| 1:D:1000:ARG:NH2 | 1:D:1016:ARG:O  | 2.47                     | 0.40              |
| 1:D:2441:UNK:O   | 1:D:2442:UNK:CB | 2.70                     | 0.40              |
| 1:D:3888:UNK:O   | 1:D:3889:UNK:C  | 2.70                     | 0.40              |
| 1:D:4113:UNK:HA  | 1:D:4116:UNK:CA | 2.48                     | 0.40              |
| 1:D:4142:UNK:O   | 1:D:4145:UNK:CB | 2.70                     | 0.40              |
| 1:D:4859:UNK:O   | 1:D:4860:UNK:CB | 2.70                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|----------|-------------|----|
| 1   | A     | 1280/5037 (25%)  | 1177 (92%) | 70 (6%)  | 33 (3%)  | 4           | 25 |
| 1   | B     | 1280/5037 (25%)  | 1177 (92%) | 70 (6%)  | 33 (3%)  | 4           | 25 |
| 1   | C     | 1280/5037 (25%)  | 1177 (92%) | 70 (6%)  | 33 (3%)  | 4           | 25 |
| 1   | D     | 1280/5037 (25%)  | 1177 (92%) | 70 (6%)  | 33 (3%)  | 4           | 25 |
| All | All   | 5120/20148 (25%) | 4708 (92%) | 280 (6%) | 132 (3%) | 6           | 25 |

All (132) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 98  | HIS  |
| 1   | A     | 368 | ARG  |
| 1   | A     | 393 | CYS  |
| 1   | A     | 425 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 426  | ARG  |
| 1   | A     | 456  | SER  |
| 1   | A     | 507  | ALA  |
| 1   | A     | 774  | ASP  |
| 1   | A     | 957  | LYS  |
| 1   | A     | 1022 | VAL  |
| 1   | A     | 1023 | PRO  |
| 1   | A     | 1196 | PRO  |
| 1   | B     | 98   | HIS  |
| 1   | B     | 368  | ARG  |
| 1   | B     | 393  | CYS  |
| 1   | B     | 425  | PRO  |
| 1   | B     | 426  | ARG  |
| 1   | B     | 456  | SER  |
| 1   | B     | 507  | ALA  |
| 1   | B     | 774  | ASP  |
| 1   | B     | 957  | LYS  |
| 1   | B     | 1022 | VAL  |
| 1   | B     | 1023 | PRO  |
| 1   | B     | 1196 | PRO  |
| 1   | C     | 98   | HIS  |
| 1   | C     | 368  | ARG  |
| 1   | C     | 393  | CYS  |
| 1   | C     | 425  | PRO  |
| 1   | C     | 426  | ARG  |
| 1   | C     | 456  | SER  |
| 1   | C     | 507  | ALA  |
| 1   | C     | 774  | ASP  |
| 1   | C     | 957  | LYS  |
| 1   | C     | 1022 | VAL  |
| 1   | C     | 1023 | PRO  |
| 1   | C     | 1196 | PRO  |
| 1   | D     | 98   | HIS  |
| 1   | D     | 368  | ARG  |
| 1   | D     | 393  | CYS  |
| 1   | D     | 425  | PRO  |
| 1   | D     | 426  | ARG  |
| 1   | D     | 456  | SER  |
| 1   | D     | 507  | ALA  |
| 1   | D     | 774  | ASP  |
| 1   | D     | 957  | LYS  |
| 1   | D     | 1022 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 1023 | PRO  |
| 1   | D     | 1196 | PRO  |
| 1   | A     | 1137 | GLU  |
| 1   | B     | 1137 | GLU  |
| 1   | C     | 1137 | GLU  |
| 1   | D     | 1137 | GLU  |
| 1   | A     | 226  | HIS  |
| 1   | A     | 431  | PRO  |
| 1   | A     | 500  | ALA  |
| 1   | A     | 956  | PRO  |
| 1   | A     | 1537 | ASN  |
| 1   | B     | 226  | HIS  |
| 1   | B     | 431  | PRO  |
| 1   | B     | 500  | ALA  |
| 1   | B     | 956  | PRO  |
| 1   | B     | 1537 | ASN  |
| 1   | C     | 226  | HIS  |
| 1   | C     | 431  | PRO  |
| 1   | C     | 500  | ALA  |
| 1   | C     | 956  | PRO  |
| 1   | C     | 1537 | ASN  |
| 1   | D     | 226  | HIS  |
| 1   | D     | 431  | PRO  |
| 1   | D     | 500  | ALA  |
| 1   | D     | 956  | PRO  |
| 1   | D     | 1537 | ASN  |
| 1   | A     | 126  | SER  |
| 1   | A     | 674  | PHE  |
| 1   | A     | 726  | VAL  |
| 1   | A     | 728  | ARG  |
| 1   | A     | 905  | PRO  |
| 1   | A     | 1183 | GLU  |
| 1   | A     | 1555 | LEU  |
| 1   | B     | 126  | SER  |
| 1   | B     | 674  | PHE  |
| 1   | B     | 726  | VAL  |
| 1   | B     | 728  | ARG  |
| 1   | B     | 905  | PRO  |
| 1   | B     | 1183 | GLU  |
| 1   | B     | 1555 | LEU  |
| 1   | C     | 126  | SER  |
| 1   | C     | 674  | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 726  | VAL  |
| 1   | C     | 728  | ARG  |
| 1   | C     | 905  | PRO  |
| 1   | C     | 1183 | GLU  |
| 1   | C     | 1555 | LEU  |
| 1   | D     | 126  | SER  |
| 1   | D     | 674  | PHE  |
| 1   | D     | 726  | VAL  |
| 1   | D     | 728  | ARG  |
| 1   | D     | 905  | PRO  |
| 1   | D     | 1183 | GLU  |
| 1   | D     | 1555 | LEU  |
| 1   | A     | 30   | LYS  |
| 1   | A     | 367  | LEU  |
| 1   | A     | 461  | HIS  |
| 1   | B     | 30   | LYS  |
| 1   | B     | 367  | LEU  |
| 1   | B     | 461  | HIS  |
| 1   | C     | 30   | LYS  |
| 1   | C     | 367  | LEU  |
| 1   | C     | 461  | HIS  |
| 1   | D     | 30   | LYS  |
| 1   | D     | 367  | LEU  |
| 1   | D     | 461  | HIS  |
| 1   | A     | 373  | LYS  |
| 1   | A     | 437  | PRO  |
| 1   | B     | 373  | LYS  |
| 1   | B     | 437  | PRO  |
| 1   | C     | 373  | LYS  |
| 1   | C     | 437  | PRO  |
| 1   | D     | 373  | LYS  |
| 1   | D     | 437  | PRO  |
| 1   | A     | 430  | PRO  |
| 1   | B     | 430  | PRO  |
| 1   | C     | 430  | PRO  |
| 1   | D     | 225  | GLY  |
| 1   | D     | 430  | PRO  |
| 1   | A     | 225  | GLY  |
| 1   | B     | 225  | GLY  |
| 1   | C     | 225  | GLY  |
| 1   | A     | 89   | GLY  |
| 1   | B     | 89   | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 89  | GLY  |
| 1   | D     | 89  | GLY  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 1112/1410 (79%) | 1052 (95%) | 60 (5%)  | 20          | 41 |
| 1   | B     | 1112/1410 (79%) | 1052 (95%) | 60 (5%)  | 20          | 41 |
| 1   | C     | 1112/1410 (79%) | 1052 (95%) | 60 (5%)  | 20          | 41 |
| 1   | D     | 1112/1410 (79%) | 1052 (95%) | 60 (5%)  | 20          | 41 |
| All | All   | 4448/5640 (79%) | 4208 (95%) | 240 (5%) | 21          | 41 |

All (240) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | ASP  |
| 1   | A     | 10  | GLU  |
| 1   | A     | 11  | VAL  |
| 1   | A     | 12  | GLN  |
| 1   | A     | 74  | SER  |
| 1   | A     | 76  | ARG  |
| 1   | A     | 79  | GLN  |
| 1   | A     | 84  | ASN  |
| 1   | A     | 86  | VAL  |
| 1   | A     | 87  | GLU  |
| 1   | A     | 90  | VAL  |
| 1   | A     | 94  | GLN  |
| 1   | A     | 139 | GLU  |
| 1   | A     | 156 | GLN  |
| 1   | A     | 300 | VAL  |
| 1   | A     | 301 | VAL  |
| 1   | A     | 319 | SER  |
| 1   | A     | 321 | GLU  |
| 1   | A     | 322 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 323  | LEU  |
| 1   | A     | 324  | ASP  |
| 1   | A     | 328  | LYS  |
| 1   | A     | 329  | ARG  |
| 1   | A     | 330  | ASP  |
| 1   | A     | 332  | GLU  |
| 1   | A     | 338  | GLU  |
| 1   | A     | 365  | LYS  |
| 1   | A     | 367  | LEU  |
| 1   | A     | 368  | ARG  |
| 1   | A     | 369  | LEU  |
| 1   | A     | 372  | LEU  |
| 1   | A     | 373  | LYS  |
| 1   | A     | 422  | SER  |
| 1   | A     | 424  | LYS  |
| 1   | A     | 426  | ARG  |
| 1   | A     | 443  | LEU  |
| 1   | A     | 458  | GLU  |
| 1   | A     | 460  | GLN  |
| 1   | A     | 467  | LYS  |
| 1   | A     | 505  | GLU  |
| 1   | A     | 522  | LEU  |
| 1   | A     | 870  | ILE  |
| 1   | A     | 988  | LEU  |
| 1   | A     | 993  | HIS  |
| 1   | A     | 994  | ASN  |
| 1   | A     | 995  | VAL  |
| 1   | A     | 996  | TRP  |
| 1   | A     | 998  | ARG  |
| 1   | A     | 1000 | ARG  |
| 1   | A     | 1003 | GLN  |
| 1   | A     | 1006 | SER  |
| 1   | A     | 1008 | SER  |
| 1   | A     | 1016 | ARG  |
| 1   | A     | 1017 | ARG  |
| 1   | A     | 1018 | ASN  |
| 1   | A     | 1020 | ARG  |
| 1   | A     | 1021 | LEU  |
| 1   | A     | 1078 | GLU  |
| 1   | A     | 2738 | ARG  |
| 1   | A     | 2743 | LEU  |
| 1   | B     | 9    | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 10  | GLU  |
| 1   | B     | 11  | VAL  |
| 1   | B     | 12  | GLN  |
| 1   | B     | 74  | SER  |
| 1   | B     | 76  | ARG  |
| 1   | B     | 79  | GLN  |
| 1   | B     | 84  | ASN  |
| 1   | B     | 86  | VAL  |
| 1   | B     | 87  | GLU  |
| 1   | B     | 90  | VAL  |
| 1   | B     | 94  | GLN  |
| 1   | B     | 139 | GLU  |
| 1   | B     | 156 | GLN  |
| 1   | B     | 300 | VAL  |
| 1   | B     | 301 | VAL  |
| 1   | B     | 319 | SER  |
| 1   | B     | 321 | GLU  |
| 1   | B     | 322 | LYS  |
| 1   | B     | 323 | LEU  |
| 1   | B     | 324 | ASP  |
| 1   | B     | 328 | LYS  |
| 1   | B     | 329 | ARG  |
| 1   | B     | 330 | ASP  |
| 1   | B     | 332 | GLU  |
| 1   | B     | 338 | GLU  |
| 1   | B     | 365 | LYS  |
| 1   | B     | 367 | LEU  |
| 1   | B     | 368 | ARG  |
| 1   | B     | 369 | LEU  |
| 1   | B     | 372 | LEU  |
| 1   | B     | 373 | LYS  |
| 1   | B     | 422 | SER  |
| 1   | B     | 424 | LYS  |
| 1   | B     | 426 | ARG  |
| 1   | B     | 443 | LEU  |
| 1   | B     | 458 | GLU  |
| 1   | B     | 460 | GLN  |
| 1   | B     | 467 | LYS  |
| 1   | B     | 505 | GLU  |
| 1   | B     | 522 | LEU  |
| 1   | B     | 870 | ILE  |
| 1   | B     | 988 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 993  | HIS  |
| 1   | B     | 994  | ASN  |
| 1   | B     | 995  | VAL  |
| 1   | B     | 996  | TRP  |
| 1   | B     | 998  | ARG  |
| 1   | B     | 1000 | ARG  |
| 1   | B     | 1003 | GLN  |
| 1   | B     | 1006 | SER  |
| 1   | B     | 1008 | SER  |
| 1   | B     | 1016 | ARG  |
| 1   | B     | 1017 | ARG  |
| 1   | B     | 1018 | ASN  |
| 1   | B     | 1020 | ARG  |
| 1   | B     | 1021 | LEU  |
| 1   | B     | 1078 | GLU  |
| 1   | B     | 2738 | ARG  |
| 1   | B     | 2743 | LEU  |
| 1   | C     | 9    | ASP  |
| 1   | C     | 10   | GLU  |
| 1   | C     | 11   | VAL  |
| 1   | C     | 12   | GLN  |
| 1   | C     | 74   | SER  |
| 1   | C     | 76   | ARG  |
| 1   | C     | 79   | GLN  |
| 1   | C     | 84   | ASN  |
| 1   | C     | 86   | VAL  |
| 1   | C     | 87   | GLU  |
| 1   | C     | 90   | VAL  |
| 1   | C     | 94   | GLN  |
| 1   | C     | 139  | GLU  |
| 1   | C     | 156  | GLN  |
| 1   | C     | 300  | VAL  |
| 1   | C     | 301  | VAL  |
| 1   | C     | 319  | SER  |
| 1   | C     | 321  | GLU  |
| 1   | C     | 322  | LYS  |
| 1   | C     | 323  | LEU  |
| 1   | C     | 324  | ASP  |
| 1   | C     | 328  | LYS  |
| 1   | C     | 329  | ARG  |
| 1   | C     | 330  | ASP  |
| 1   | C     | 332  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 338  | GLU  |
| 1   | C     | 365  | LYS  |
| 1   | C     | 367  | LEU  |
| 1   | C     | 368  | ARG  |
| 1   | C     | 369  | LEU  |
| 1   | C     | 372  | LEU  |
| 1   | C     | 373  | LYS  |
| 1   | C     | 422  | SER  |
| 1   | C     | 424  | LYS  |
| 1   | C     | 426  | ARG  |
| 1   | C     | 443  | LEU  |
| 1   | C     | 458  | GLU  |
| 1   | C     | 460  | GLN  |
| 1   | C     | 467  | LYS  |
| 1   | C     | 505  | GLU  |
| 1   | C     | 522  | LEU  |
| 1   | C     | 870  | ILE  |
| 1   | C     | 988  | LEU  |
| 1   | C     | 993  | HIS  |
| 1   | C     | 994  | ASN  |
| 1   | C     | 995  | VAL  |
| 1   | C     | 996  | TRP  |
| 1   | C     | 998  | ARG  |
| 1   | C     | 1000 | ARG  |
| 1   | C     | 1003 | GLN  |
| 1   | C     | 1006 | SER  |
| 1   | C     | 1008 | SER  |
| 1   | C     | 1016 | ARG  |
| 1   | C     | 1017 | ARG  |
| 1   | C     | 1018 | ASN  |
| 1   | C     | 1020 | ARG  |
| 1   | C     | 1021 | LEU  |
| 1   | C     | 1078 | GLU  |
| 1   | C     | 2738 | ARG  |
| 1   | C     | 2743 | LEU  |
| 1   | D     | 9    | ASP  |
| 1   | D     | 10   | GLU  |
| 1   | D     | 11   | VAL  |
| 1   | D     | 12   | GLN  |
| 1   | D     | 74   | SER  |
| 1   | D     | 76   | ARG  |
| 1   | D     | 79   | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 84   | ASN  |
| 1   | D     | 86   | VAL  |
| 1   | D     | 87   | GLU  |
| 1   | D     | 90   | VAL  |
| 1   | D     | 94   | GLN  |
| 1   | D     | 139  | GLU  |
| 1   | D     | 156  | GLN  |
| 1   | D     | 300  | VAL  |
| 1   | D     | 301  | VAL  |
| 1   | D     | 319  | SER  |
| 1   | D     | 321  | GLU  |
| 1   | D     | 322  | LYS  |
| 1   | D     | 323  | LEU  |
| 1   | D     | 324  | ASP  |
| 1   | D     | 328  | LYS  |
| 1   | D     | 329  | ARG  |
| 1   | D     | 330  | ASP  |
| 1   | D     | 332  | GLU  |
| 1   | D     | 338  | GLU  |
| 1   | D     | 365  | LYS  |
| 1   | D     | 367  | LEU  |
| 1   | D     | 368  | ARG  |
| 1   | D     | 369  | LEU  |
| 1   | D     | 372  | LEU  |
| 1   | D     | 373  | LYS  |
| 1   | D     | 422  | SER  |
| 1   | D     | 424  | LYS  |
| 1   | D     | 426  | ARG  |
| 1   | D     | 443  | LEU  |
| 1   | D     | 458  | GLU  |
| 1   | D     | 460  | GLN  |
| 1   | D     | 467  | LYS  |
| 1   | D     | 505  | GLU  |
| 1   | D     | 522  | LEU  |
| 1   | D     | 870  | ILE  |
| 1   | D     | 988  | LEU  |
| 1   | D     | 993  | HIS  |
| 1   | D     | 994  | ASN  |
| 1   | D     | 995  | VAL  |
| 1   | D     | 996  | TRP  |
| 1   | D     | 998  | ARG  |
| 1   | D     | 1000 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 1003 | GLN  |
| 1   | D     | 1006 | SER  |
| 1   | D     | 1008 | SER  |
| 1   | D     | 1016 | ARG  |
| 1   | D     | 1017 | ARG  |
| 1   | D     | 1018 | ASN  |
| 1   | D     | 1020 | ARG  |
| 1   | D     | 1021 | LEU  |
| 1   | D     | 1078 | GLU  |
| 1   | D     | 2738 | ARG  |
| 1   | D     | 2743 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 79   | GLN  |
| 1   | A     | 84   | ASN  |
| 1   | A     | 94   | GLN  |
| 1   | A     | 111  | HIS  |
| 1   | A     | 151  | HIS  |
| 1   | A     | 197  | GLN  |
| 1   | A     | 273  | HIS  |
| 1   | A     | 284  | HIS  |
| 1   | A     | 350  | HIS  |
| 1   | A     | 380  | GLN  |
| 1   | A     | 383  | HIS  |
| 1   | A     | 395  | GLN  |
| 1   | A     | 412  | ASN  |
| 1   | A     | 413  | GLN  |
| 1   | A     | 475  | GLN  |
| 1   | A     | 479  | GLN  |
| 1   | A     | 489  | ASN  |
| 1   | A     | 720  | HIS  |
| 1   | A     | 797  | HIS  |
| 1   | A     | 879  | HIS  |
| 1   | A     | 911  | HIS  |
| 1   | A     | 1035 | ASN  |
| 1   | A     | 1201 | HIS  |
| 1   | A     | 1458 | HIS  |
| 1   | A     | 1558 | HIS  |
| 1   | A     | 1569 | GLN  |
| 1   | A     | 1571 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2780 | ASN  |
| 1   | A     | 2877 | GLN  |
| 1   | A     | 2931 | GLN  |
| 1   | B     | 79   | GLN  |
| 1   | B     | 84   | ASN  |
| 1   | B     | 94   | GLN  |
| 1   | B     | 111  | HIS  |
| 1   | B     | 151  | HIS  |
| 1   | B     | 197  | GLN  |
| 1   | B     | 226  | HIS  |
| 1   | B     | 273  | HIS  |
| 1   | B     | 284  | HIS  |
| 1   | B     | 350  | HIS  |
| 1   | B     | 380  | GLN  |
| 1   | B     | 395  | GLN  |
| 1   | B     | 412  | ASN  |
| 1   | B     | 413  | GLN  |
| 1   | B     | 475  | GLN  |
| 1   | B     | 479  | GLN  |
| 1   | B     | 489  | ASN  |
| 1   | B     | 720  | HIS  |
| 1   | B     | 797  | HIS  |
| 1   | B     | 879  | HIS  |
| 1   | B     | 911  | HIS  |
| 1   | B     | 1035 | ASN  |
| 1   | B     | 1158 | ASN  |
| 1   | B     | 1458 | HIS  |
| 1   | B     | 1558 | HIS  |
| 1   | B     | 2780 | ASN  |
| 1   | B     | 2877 | GLN  |
| 1   | B     | 2931 | GLN  |
| 1   | C     | 79   | GLN  |
| 1   | C     | 84   | ASN  |
| 1   | C     | 94   | GLN  |
| 1   | C     | 111  | HIS  |
| 1   | C     | 151  | HIS  |
| 1   | C     | 197  | GLN  |
| 1   | C     | 226  | HIS  |
| 1   | C     | 273  | HIS  |
| 1   | C     | 284  | HIS  |
| 1   | C     | 350  | HIS  |
| 1   | C     | 380  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 383  | HIS  |
| 1   | C     | 395  | GLN  |
| 1   | C     | 412  | ASN  |
| 1   | C     | 413  | GLN  |
| 1   | C     | 475  | GLN  |
| 1   | C     | 479  | GLN  |
| 1   | C     | 489  | ASN  |
| 1   | C     | 720  | HIS  |
| 1   | C     | 797  | HIS  |
| 1   | C     | 879  | HIS  |
| 1   | C     | 911  | HIS  |
| 1   | C     | 1035 | ASN  |
| 1   | C     | 1158 | ASN  |
| 1   | C     | 1458 | HIS  |
| 1   | C     | 1558 | HIS  |
| 1   | C     | 2773 | ASN  |
| 1   | C     | 2780 | ASN  |
| 1   | C     | 2877 | GLN  |
| 1   | C     | 2931 | GLN  |
| 1   | D     | 79   | GLN  |
| 1   | D     | 84   | ASN  |
| 1   | D     | 94   | GLN  |
| 1   | D     | 111  | HIS  |
| 1   | D     | 151  | HIS  |
| 1   | D     | 197  | GLN  |
| 1   | D     | 218  | HIS  |
| 1   | D     | 226  | HIS  |
| 1   | D     | 273  | HIS  |
| 1   | D     | 284  | HIS  |
| 1   | D     | 350  | HIS  |
| 1   | D     | 380  | GLN  |
| 1   | D     | 383  | HIS  |
| 1   | D     | 395  | GLN  |
| 1   | D     | 412  | ASN  |
| 1   | D     | 413  | GLN  |
| 1   | D     | 475  | GLN  |
| 1   | D     | 479  | GLN  |
| 1   | D     | 489  | ASN  |
| 1   | D     | 720  | HIS  |
| 1   | D     | 879  | HIS  |
| 1   | D     | 911  | HIS  |
| 1   | D     | 963  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 1035 | ASN  |
| 1   | D     | 1158 | ASN  |
| 1   | D     | 1201 | HIS  |
| 1   | D     | 1458 | HIS  |
| 1   | D     | 1558 | HIS  |
| 1   | D     | 2780 | ASN  |
| 1   | D     | 2877 | GLN  |
| 1   | D     | 2931 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | A     | 95               |
| 1   | B     | 95               |
| 1   | C     | 95               |
| 1   | D     | 95               |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 1863:UNK  | C      | 1935:UNK  | N      | 107.77       |
| 1     | B     | 1863:UNK  | C      | 1935:UNK  | N      | 107.77       |
| 1     | C     | 1863:UNK  | C      | 1935:UNK  | N      | 107.77       |
| 1     | D     | 1863:UNK  | C      | 1935:UNK  | N      | 107.77       |
| 1     | A     | 2939:ARG  | C      | 2953:UNK  | N      | 48.57        |
| 1     | B     | 2939:ARG  | C      | 2953:UNK  | N      | 48.57        |
| 1     | C     | 2939:ARG  | C      | 2953:UNK  | N      | 48.57        |
| 1     | D     | 2939:ARG  | C      | 2953:UNK  | N      | 48.57        |
| 1     | B     | 3872:UNK  | C      | 3874:UNK  | N      | 28.32        |
| 1     | D     | 3872:UNK  | C      | 3874:UNK  | N      | 28.32        |
| 1     | A     | 3872:UNK  | C      | 3874:UNK  | N      | 28.31        |
| 1     | C     | 3872:UNK  | C      | 3874:UNK  | N      | 28.31        |
| 1     | A     | 3444:UNK  | C      | 3445:UNK  | N      | 27.42        |
| 1     | B     | 3444:UNK  | C      | 3445:UNK  | N      | 27.42        |
| 1     | C     | 3444:UNK  | C      | 3445:UNK  | N      | 27.42        |
| 1     | D     | 3444:UNK  | C      | 3445:UNK  | N      | 27.42        |
| 1     | C     | 2715:UNK  | C      | 2734:ASN  | N      | 26.32        |
| 1     | A     | 2715:UNK  | C      | 2734:ASN  | N      | 26.31        |
| 1     | B     | 2715:UNK  | C      | 2734:ASN  | N      | 26.31        |
| 1     | D     | 2715:UNK  | C      | 2734:ASN  | N      | 26.31        |
| 1     | A     | 3217:UNK  | C      | 3220:UNK  | N      | 24.93        |
| 1     | C     | 3217:UNK  | C      | 3220:UNK  | N      | 24.93        |
| 1     | D     | 3217:UNK  | C      | 3220:UNK  | N      | 24.93        |
| 1     | B     | 3217:UNK  | C      | 3220:UNK  | N      | 24.92        |
| 1     | A     | 1948:UNK  | C      | 1953:UNK  | N      | 23.37        |
| 1     | B     | 1948:UNK  | C      | 1953:UNK  | N      | 23.37        |
| 1     | C     | 1948:UNK  | C      | 1953:UNK  | N      | 23.37        |
| 1     | D     | 1948:UNK  | C      | 1953:UNK  | N      | 23.37        |
| 1     | B     | 1676:UNK  | C      | 1705:UNK  | N      | 23.12        |
| 1     | A     | 1676:UNK  | C      | 1705:UNK  | N      | 23.11        |
| 1     | C     | 1676:UNK  | C      | 1705:UNK  | N      | 23.11        |
| 1     | D     | 1676:UNK  | C      | 1705:UNK  | N      | 23.11        |
| 1     | A     | 592:UNK   | C      | 649:PHE   | N      | 22.95        |
| 1     | B     | 592:UNK   | C      | 649:PHE   | N      | 22.95        |
| 1     | C     | 592:UNK   | C      | 649:PHE   | N      | 22.95        |
| 1     | D     | 592:UNK   | C      | 649:PHE   | N      | 22.95        |
| 1     | A     | 1977:UNK  | C      | 2003:UNK  | N      | 21.22        |
| 1     | B     | 1977:UNK  | C      | 2003:UNK  | N      | 21.22        |
| 1     | C     | 1977:UNK  | C      | 2003:UNK  | N      | 21.22        |
| 1     | D     | 1977:UNK  | C      | 2003:UNK  | N      | 21.22        |
| 1     | A     | 4272:UNK  | C      | 4545:UNK  | N      | 21.18        |
| 1     | B     | 4272:UNK  | C      | 4545:UNK  | N      | 21.18        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C     | 4272:UNK  | C      | 4545:UNK  | N      | 21.18        |
| 1     | D     | 4272:UNK  | C      | 4545:UNK  | N      | 21.18        |
| 1     | A     | 4741:UNK  | C      | 4770:UNK  | N      | 20.48        |
| 1     | B     | 4741:UNK  | C      | 4770:UNK  | N      | 20.48        |
| 1     | C     | 4741:UNK  | C      | 4770:UNK  | N      | 20.48        |
| 1     | D     | 4741:UNK  | C      | 4770:UNK  | N      | 20.48        |
| 1     | A     | 3653:UNK  | C      | 3656:UNK  | N      | 19.53        |
| 1     | B     | 3653:UNK  | C      | 3656:UNK  | N      | 19.53        |
| 1     | C     | 3653:UNK  | C      | 3656:UNK  | N      | 19.53        |
| 1     | D     | 3653:UNK  | C      | 3656:UNK  | N      | 19.53        |
| 1     | A     | 2442:UNK  | C      | 2450:UNK  | N      | 19.47        |
| 1     | B     | 2442:UNK  | C      | 2450:UNK  | N      | 19.47        |
| 1     | C     | 2442:UNK  | C      | 2450:UNK  | N      | 19.47        |
| 1     | D     | 2442:UNK  | C      | 2450:UNK  | N      | 19.47        |
| 1     | A     | 2569:UNK  | C      | 2571:UNK  | N      | 18.85        |
| 1     | B     | 2569:UNK  | C      | 2571:UNK  | N      | 18.85        |
| 1     | C     | 2569:UNK  | C      | 2571:UNK  | N      | 18.85        |
| 1     | D     | 2569:UNK  | C      | 2571:UNK  | N      | 18.85        |
| 1     | A     | 4585:UNK  | C      | 4644:UNK  | N      | 18.37        |
| 1     | B     | 4585:UNK  | C      | 4644:UNK  | N      | 18.37        |
| 1     | C     | 4585:UNK  | C      | 4644:UNK  | N      | 18.37        |
| 1     | D     | 4585:UNK  | C      | 4644:UNK  | N      | 18.37        |
| 1     | A     | 2397:UNK  | C      | 2420:UNK  | N      | 17.23        |
| 1     | B     | 2397:UNK  | C      | 2420:UNK  | N      | 17.23        |
| 1     | C     | 2397:UNK  | C      | 2420:UNK  | N      | 17.23        |
| 1     | D     | 2397:UNK  | C      | 2420:UNK  | N      | 17.23        |
| 1     | A     | 2474:UNK  | C      | 2498:UNK  | N      | 16.81        |
| 1     | B     | 2474:UNK  | C      | 2498:UNK  | N      | 16.81        |
| 1     | C     | 2474:UNK  | C      | 2498:UNK  | N      | 16.81        |
| 1     | D     | 2474:UNK  | C      | 2498:UNK  | N      | 16.81        |
| 1     | A     | 3589:UNK  | C      | 3592:UNK  | N      | 16.51        |
| 1     | B     | 3589:UNK  | C      | 3592:UNK  | N      | 16.51        |
| 1     | C     | 3589:UNK  | C      | 3592:UNK  | N      | 16.51        |
| 1     | D     | 3589:UNK  | C      | 3592:UNK  | N      | 16.51        |
| 1     | A     | 2109:UNK  | C      | 2114:UNK  | N      | 16.23        |
| 1     | B     | 2109:UNK  | C      | 2114:UNK  | N      | 16.23        |
| 1     | C     | 2109:UNK  | C      | 2114:UNK  | N      | 16.23        |
| 1     | D     | 2109:UNK  | C      | 2114:UNK  | N      | 16.23        |
| 1     | A     | 3734:UNK  | C      | 3766:UNK  | N      | 15.99        |
| 1     | B     | 3734:UNK  | C      | 3766:UNK  | N      | 15.99        |
| 1     | C     | 3734:UNK  | C      | 3766:UNK  | N      | 15.99        |
| 1     | D     | 3734:UNK  | C      | 3766:UNK  | N      | 15.99        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 3625:UNK  | C      | 3628:UNK  | N      | 15.59        |
| 1     | B     | 3625:UNK  | C      | 3628:UNK  | N      | 15.59        |
| 1     | C     | 3625:UNK  | C      | 3628:UNK  | N      | 15.59        |
| 1     | D     | 3625:UNK  | C      | 3628:UNK  | N      | 15.59        |
| 1     | A     | 2510:UNK  | C      | 2515:UNK  | N      | 15.37        |
| 1     | B     | 2510:UNK  | C      | 2515:UNK  | N      | 15.37        |
| 1     | C     | 2510:UNK  | C      | 2515:UNK  | N      | 15.37        |
| 1     | D     | 2510:UNK  | C      | 2515:UNK  | N      | 15.37        |
| 1     | A     | 3014:UNK  | C      | 3036:UNK  | N      | 15.36        |
| 1     | B     | 3014:UNK  | C      | 3036:UNK  | N      | 15.36        |
| 1     | C     | 3014:UNK  | C      | 3036:UNK  | N      | 15.36        |
| 1     | D     | 3014:UNK  | C      | 3036:UNK  | N      | 15.36        |
| 1     | A     | 4688:UNK  | C      | 4702:UNK  | N      | 15.17        |
| 1     | B     | 4688:UNK  | C      | 4702:UNK  | N      | 15.17        |
| 1     | C     | 4688:UNK  | C      | 4702:UNK  | N      | 15.17        |
| 1     | D     | 4688:UNK  | C      | 4702:UNK  | N      | 15.17        |
| 1     | A     | 2344:UNK  | C      | 2347:UNK  | N      | 15.07        |
| 1     | B     | 2344:UNK  | C      | 2347:UNK  | N      | 15.07        |
| 1     | C     | 2344:UNK  | C      | 2347:UNK  | N      | 15.07        |
| 1     | D     | 2344:UNK  | C      | 2347:UNK  | N      | 15.07        |
| 1     | D     | 4154:UNK  | C      | 4160:UNK  | N      | 14.95        |
| 1     | A     | 4154:UNK  | C      | 4160:UNK  | N      | 14.94        |
| 1     | B     | 4154:UNK  | C      | 4160:UNK  | N      | 14.94        |
| 1     | C     | 4154:UNK  | C      | 4160:UNK  | N      | 14.94        |
| 1     | A     | 3714:UNK  | C      | 3715:UNK  | N      | 14.51        |
| 1     | B     | 3714:UNK  | C      | 3715:UNK  | N      | 14.51        |
| 1     | C     | 3714:UNK  | C      | 3715:UNK  | N      | 14.51        |
| 1     | D     | 3714:UNK  | C      | 3715:UNK  | N      | 14.51        |
| 1     | A     | 2215:UNK  | C      | 2221:UNK  | N      | 14.24        |
| 1     | B     | 2215:UNK  | C      | 2221:UNK  | N      | 14.24        |
| 1     | C     | 2215:UNK  | C      | 2221:UNK  | N      | 14.24        |
| 1     | D     | 2215:UNK  | C      | 2221:UNK  | N      | 14.24        |
| 1     | A     | 2618:UNK  | C      | 2633:UNK  | N      | 13.98        |
| 1     | B     | 2618:UNK  | C      | 2633:UNK  | N      | 13.98        |
| 1     | D     | 2618:UNK  | C      | 2633:UNK  | N      | 13.98        |
| 1     | C     | 2618:UNK  | C      | 2633:UNK  | N      | 13.97        |
| 1     | A     | 3230:UNK  | C      | 3233:UNK  | N      | 13.83        |
| 1     | C     | 3230:UNK  | C      | 3233:UNK  | N      | 13.83        |
| 1     | D     | 3230:UNK  | C      | 3233:UNK  | N      | 13.83        |
| 1     | B     | 3230:UNK  | C      | 3233:UNK  | N      | 13.82        |
| 1     | A     | 2145:UNK  | C      | 2149:UNK  | N      | 13.72        |
| 1     | A     | 3854:UNK  | C      | 3857:UNK  | N      | 13.72        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 2145:UNK  | C      | 2149:UNK  | N      | 13.72        |
| 1     | B     | 3854:UNK  | C      | 3857:UNK  | N      | 13.72        |
| 1     | C     | 2145:UNK  | C      | 2149:UNK  | N      | 13.72        |
| 1     | C     | 3854:UNK  | C      | 3857:UNK  | N      | 13.72        |
| 1     | D     | 2145:UNK  | C      | 2149:UNK  | N      | 13.72        |
| 1     | D     | 3854:UNK  | C      | 3857:UNK  | N      | 13.72        |
| 1     | A     | 3283:UNK  | C      | 3288:UNK  | N      | 13.70        |
| 1     | B     | 3283:UNK  | C      | 3288:UNK  | N      | 13.70        |
| 1     | C     | 3283:UNK  | C      | 3288:UNK  | N      | 13.70        |
| 1     | D     | 3283:UNK  | C      | 3288:UNK  | N      | 13.70        |
| 1     | A     | 3102:UNK  | C      | 3133:UNK  | N      | 13.38        |
| 1     | B     | 3102:UNK  | C      | 3133:UNK  | N      | 13.38        |
| 1     | C     | 3102:UNK  | C      | 3133:UNK  | N      | 13.38        |
| 1     | D     | 3102:UNK  | C      | 3133:UNK  | N      | 13.38        |
| 1     | A     | 4993:UNK  | C      | 5006:UNK  | N      | 13.05        |
| 1     | B     | 4993:UNK  | C      | 5006:UNK  | N      | 13.05        |
| 1     | C     | 4993:UNK  | C      | 5006:UNK  | N      | 13.05        |
| 1     | D     | 4993:UNK  | C      | 5006:UNK  | N      | 13.05        |
| 1     | A     | 3935:UNK  | C      | 3941:UNK  | N      | 12.96        |
| 1     | B     | 3935:UNK  | C      | 3941:UNK  | N      | 12.96        |
| 1     | C     | 3935:UNK  | C      | 3941:UNK  | N      | 12.96        |
| 1     | D     | 3935:UNK  | C      | 3941:UNK  | N      | 12.96        |
| 1     | A     | 2173:UNK  | C      | 2195:UNK  | N      | 12.90        |
| 1     | B     | 2173:UNK  | C      | 2195:UNK  | N      | 12.90        |
| 1     | C     | 2173:UNK  | C      | 2195:UNK  | N      | 12.90        |
| 1     | D     | 2173:UNK  | C      | 2195:UNK  | N      | 12.90        |
| 1     | B     | 1827:UNK  | C      | 1835:UNK  | N      | 12.82        |
| 1     | A     | 1827:UNK  | C      | 1835:UNK  | N      | 12.81        |
| 1     | C     | 1827:UNK  | C      | 1835:UNK  | N      | 12.81        |
| 1     | D     | 1827:UNK  | C      | 1835:UNK  | N      | 12.81        |
| 1     | A     | 3151:UNK  | C      | 3154:UNK  | N      | 12.62        |
| 1     | A     | 3483:UNK  | C      | 3485:UNK  | N      | 12.62        |
| 1     | B     | 3151:UNK  | C      | 3154:UNK  | N      | 12.62        |
| 1     | B     | 3483:UNK  | C      | 3485:UNK  | N      | 12.62        |
| 1     | C     | 3151:UNK  | C      | 3154:UNK  | N      | 12.62        |
| 1     | C     | 3483:UNK  | C      | 3485:UNK  | N      | 12.62        |
| 1     | D     | 3151:UNK  | C      | 3154:UNK  | N      | 12.62        |
| 1     | D     | 3483:UNK  | C      | 3485:UNK  | N      | 12.62        |
| 1     | A     | 2046:UNK  | C      | 2061:UNK  | N      | 12.56        |
| 1     | A     | 3057:UNK  | C      | 3085:UNK  | N      | 12.56        |
| 1     | B     | 2046:UNK  | C      | 2061:UNK  | N      | 12.56        |
| 1     | B     | 3057:UNK  | C      | 3085:UNK  | N      | 12.56        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C     | 2046:UNK  | C      | 2061:UNK  | N      | 12.56        |
| 1     | C     | 3057:UNK  | C      | 3085:UNK  | N      | 12.56        |
| 1     | D     | 2046:UNK  | C      | 2061:UNK  | N      | 12.56        |
| 1     | D     | 3057:UNK  | C      | 3085:UNK  | N      | 12.56        |
| 1     | A     | 4031:UNK  | C      | 4040:UNK  | N      | 12.20        |
| 1     | B     | 4031:UNK  | C      | 4040:UNK  | N      | 12.20        |
| 1     | C     | 4031:UNK  | C      | 4040:UNK  | N      | 12.20        |
| 1     | D     | 4031:UNK  | C      | 4040:UNK  | N      | 12.20        |
| 1     | A     | 2971:UNK  | C      | 2995:UNK  | N      | 12.12        |
| 1     | B     | 2971:UNK  | C      | 2995:UNK  | N      | 12.12        |
| 1     | C     | 2971:UNK  | C      | 2995:UNK  | N      | 12.12        |
| 1     | D     | 2971:UNK  | C      | 2995:UNK  | N      | 12.12        |
| 1     | A     | 3463:UNK  | C      | 3465:UNK  | N      | 12.05        |
| 1     | B     | 3463:UNK  | C      | 3465:UNK  | N      | 12.05        |
| 1     | C     | 3463:UNK  | C      | 3465:UNK  | N      | 12.05        |
| 1     | D     | 3463:UNK  | C      | 3465:UNK  | N      | 12.05        |
| 1     | A     | 2651:UNK  | C      | 2669:UNK  | N      | 11.67        |
| 1     | B     | 2651:UNK  | C      | 2669:UNK  | N      | 11.67        |
| 1     | C     | 2651:UNK  | C      | 2669:UNK  | N      | 11.67        |
| 1     | D     | 2651:UNK  | C      | 2669:UNK  | N      | 11.67        |
| 1     | A     | 2245:UNK  | C      | 2285:UNK  | N      | 11.17        |
| 1     | B     | 2245:UNK  | C      | 2285:UNK  | N      | 11.17        |
| 1     | C     | 2245:UNK  | C      | 2285:UNK  | N      | 11.17        |
| 1     | D     | 2245:UNK  | C      | 2285:UNK  | N      | 11.17        |
| 1     | A     | 4246:UNK  | C      | 4252:UNK  | N      | 11.01        |
| 1     | B     | 4246:UNK  | C      | 4252:UNK  | N      | 11.01        |
| 1     | C     | 4246:UNK  | C      | 4252:UNK  | N      | 11.01        |
| 1     | D     | 4246:UNK  | C      | 4252:UNK  | N      | 11.01        |
| 1     | A     | 3610:UNK  | C      | 3612:UNK  | N      | 10.99        |
| 1     | B     | 3610:UNK  | C      | 3612:UNK  | N      | 10.99        |
| 1     | C     | 3610:UNK  | C      | 3612:UNK  | N      | 10.99        |
| 1     | D     | 3610:UNK  | C      | 3612:UNK  | N      | 10.99        |
| 1     | A     | 3370:UNK  | C      | 3376:UNK  | N      | 10.83        |
| 1     | B     | 3370:UNK  | C      | 3376:UNK  | N      | 10.83        |
| 1     | C     | 3370:UNK  | C      | 3376:UNK  | N      | 10.83        |
| 1     | D     | 3370:UNK  | C      | 3376:UNK  | N      | 10.83        |
| 1     | A     | 3559:UNK  | C      | 3561:UNK  | N      | 10.75        |
| 1     | B     | 3559:UNK  | C      | 3561:UNK  | N      | 10.75        |
| 1     | C     | 3559:UNK  | C      | 3561:UNK  | N      | 10.75        |
| 1     | D     | 3559:UNK  | C      | 3561:UNK  | N      | 10.75        |
| 1     | A     | 4860:UNK  | C      | 4884:UNK  | N      | 10.38        |
| 1     | B     | 4860:UNK  | C      | 4884:UNK  | N      | 10.38        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C     | 4860:UNK  | C      | 4884:UNK  | N      | 10.38        |
| 1     | D     | 4860:UNK  | C      | 4884:UNK  | N      | 10.38        |
| 1     | A     | 2364:UNK  | C      | 2376:UNK  | N      | 10.04        |
| 1     | B     | 2364:UNK  | C      | 2376:UNK  | N      | 10.04        |
| 1     | C     | 2364:UNK  | C      | 2376:UNK  | N      | 10.04        |
| 1     | D     | 2364:UNK  | C      | 2376:UNK  | N      | 10.04        |
| 1     | A     | 2594:UNK  | C      | 2597:UNK  | N      | 9.21         |
| 1     | B     | 2594:UNK  | C      | 2597:UNK  | N      | 9.21         |
| 1     | C     | 2594:UNK  | C      | 2597:UNK  | N      | 9.21         |
| 1     | D     | 2594:UNK  | C      | 2597:UNK  | N      | 9.21         |
| 1     | A     | 3803:UNK  | C      | 3804:UNK  | N      | 9.15         |
| 1     | B     | 3803:UNK  | C      | 3804:UNK  | N      | 9.15         |
| 1     | C     | 3803:UNK  | C      | 3804:UNK  | N      | 9.15         |
| 1     | D     | 3803:UNK  | C      | 3804:UNK  | N      | 9.15         |
| 1     | A     | 2534:UNK  | C      | 2546:UNK  | N      | 9.05         |
| 1     | B     | 2534:UNK  | C      | 2546:UNK  | N      | 9.05         |
| 1     | C     | 2534:UNK  | C      | 2546:UNK  | N      | 9.05         |
| 1     | D     | 2534:UNK  | C      | 2546:UNK  | N      | 9.05         |
| 1     | A     | 3180:UNK  | C      | 3182:UNK  | N      | 9.04         |
| 1     | B     | 3180:UNK  | C      | 3182:UNK  | N      | 9.04         |
| 1     | C     | 3180:UNK  | C      | 3182:UNK  | N      | 9.04         |
| 1     | D     | 3180:UNK  | C      | 3182:UNK  | N      | 9.04         |
| 1     | A     | 4957:UNK  | C      | 4972:UNK  | N      | 8.87         |
| 1     | B     | 4957:UNK  | C      | 4972:UNK  | N      | 8.87         |
| 1     | C     | 4957:UNK  | C      | 4972:UNK  | N      | 8.87         |
| 1     | D     | 4957:UNK  | C      | 4972:UNK  | N      | 8.87         |
| 1     | A     | 3840:UNK  | C      | 3842:UNK  | N      | 8.76         |
| 1     | B     | 3840:UNK  | C      | 3842:UNK  | N      | 8.76         |
| 1     | C     | 3840:UNK  | C      | 3842:UNK  | N      | 8.76         |
| 1     | D     | 3840:UNK  | C      | 3842:UNK  | N      | 8.76         |
| 1     | A     | 3245:UNK  | C      | 3247:UNK  | N      | 8.58         |
| 1     | B     | 3245:UNK  | C      | 3247:UNK  | N      | 8.58         |
| 1     | C     | 3245:UNK  | C      | 3247:UNK  | N      | 8.58         |
| 1     | D     | 3245:UNK  | C      | 3247:UNK  | N      | 8.58         |
| 1     | A     | 2308:UNK  | C      | 2327:UNK  | N      | 8.41         |
| 1     | B     | 2308:UNK  | C      | 2327:UNK  | N      | 8.41         |
| 1     | C     | 2308:UNK  | C      | 2327:UNK  | N      | 8.41         |
| 1     | D     | 2308:UNK  | C      | 2327:UNK  | N      | 8.41         |
| 1     | A     | 3422:UNK  | C      | 3425:UNK  | N      | 7.83         |
| 1     | B     | 3422:UNK  | C      | 3425:UNK  | N      | 7.83         |
| 1     | C     | 3422:UNK  | C      | 3425:UNK  | N      | 7.83         |
| 1     | D     | 3422:UNK  | C      | 3425:UNK  | N      | 7.83         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 2690:UNK  | C      | 2694:UNK  | N      | 7.71         |
| 1     | B     | 2690:UNK  | C      | 2694:UNK  | N      | 7.71         |
| 1     | C     | 2690:UNK  | C      | 2694:UNK  | N      | 7.71         |
| 1     | D     | 2690:UNK  | C      | 2694:UNK  | N      | 7.71         |
| 1     | A     | 4907:UNK  | C      | 4911:UNK  | N      | 7.54         |
| 1     | B     | 4907:UNK  | C      | 4911:UNK  | N      | 7.54         |
| 1     | C     | 4907:UNK  | C      | 4911:UNK  | N      | 7.54         |
| 1     | D     | 4907:UNK  | C      | 4911:UNK  | N      | 7.54         |
| 1     | A     | 3698:UNK  | C      | 3700:UNK  | N      | 7.48         |
| 1     | B     | 3698:UNK  | C      | 3700:UNK  | N      | 7.48         |
| 1     | C     | 3698:UNK  | C      | 3700:UNK  | N      | 7.48         |
| 1     | D     | 3698:UNK  | C      | 3700:UNK  | N      | 7.48         |
| 1     | A     | 4006:UNK  | C      | 4008:UNK  | N      | 7.43         |
| 1     | B     | 4006:UNK  | C      | 4008:UNK  | N      | 7.43         |
| 1     | C     | 4006:UNK  | C      | 4008:UNK  | N      | 7.43         |
| 1     | D     | 4006:UNK  | C      | 4008:UNK  | N      | 7.43         |
| 1     | A     | 552:UNK   | C      | 553:UNK   | N      | 7.41         |
| 1     | B     | 552:UNK   | C      | 553:UNK   | N      | 7.41         |
| 1     | C     | 552:UNK   | C      | 553:UNK   | N      | 7.41         |
| 1     | D     | 552:UNK   | C      | 553:UNK   | N      | 7.41         |
| 1     | A     | 3500:UNK  | C      | 3508:UNK  | N      | 7.40         |
| 1     | B     | 3500:UNK  | C      | 3508:UNK  | N      | 7.40         |
| 1     | C     | 3500:UNK  | C      | 3508:UNK  | N      | 7.40         |
| 1     | D     | 3500:UNK  | C      | 3508:UNK  | N      | 7.40         |
| 1     | A     | 2020:UNK  | C      | 2026:UNK  | N      | 7.30         |
| 1     | B     | 2020:UNK  | C      | 2026:UNK  | N      | 7.30         |
| 1     | C     | 2020:UNK  | C      | 2026:UNK  | N      | 7.30         |
| 1     | D     | 2020:UNK  | C      | 2026:UNK  | N      | 7.30         |
| 1     | A     | 3821:UNK  | C      | 3825:UNK  | N      | 6.85         |
| 1     | B     | 3821:UNK  | C      | 3825:UNK  | N      | 6.85         |
| 1     | C     | 3821:UNK  | C      | 3825:UNK  | N      | 6.85         |
| 1     | D     | 3821:UNK  | C      | 3825:UNK  | N      | 6.85         |
| 1     | A     | 3333:UNK  | C      | 3336:UNK  | N      | 6.72         |
| 1     | B     | 3333:UNK  | C      | 3336:UNK  | N      | 6.72         |
| 1     | C     | 3333:UNK  | C      | 3336:UNK  | N      | 6.72         |
| 1     | D     | 3333:UNK  | C      | 3336:UNK  | N      | 6.72         |
| 1     | A     | 4798:UNK  | C      | 4800:UNK  | N      | 6.71         |
| 1     | B     | 4798:UNK  | C      | 4800:UNK  | N      | 6.71         |
| 1     | C     | 4798:UNK  | C      | 4800:UNK  | N      | 6.71         |
| 1     | D     | 4798:UNK  | C      | 4800:UNK  | N      | 6.71         |
| 1     | B     | 3889:UNK  | C      | 3891:UNK  | N      | 6.66         |
| 1     | A     | 3889:UNK  | C      | 3891:UNK  | N      | 6.65         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C     | 3889:UNK  | C      | 3891:UNK  | N      | 6.65         |
| 1     | D     | 3889:UNK  | C      | 3891:UNK  | N      | 6.65         |
| 1     | A     | 3901:UNK  | C      | 3910:UNK  | N      | 6.54         |
| 1     | B     | 3901:UNK  | C      | 3910:UNK  | N      | 6.54         |
| 1     | C     | 3901:UNK  | C      | 3910:UNK  | N      | 6.54         |
| 1     | D     | 3901:UNK  | C      | 3910:UNK  | N      | 6.54         |
| 1     | A     | 2074:UNK  | C      | 2093:UNK  | N      | 6.50         |
| 1     | B     | 2074:UNK  | C      | 2093:UNK  | N      | 6.50         |
| 1     | C     | 2074:UNK  | C      | 2093:UNK  | N      | 6.50         |
| 1     | D     | 2074:UNK  | C      | 2093:UNK  | N      | 6.50         |
| 1     | A     | 3785:UNK  | C      | 3793:UNK  | N      | 6.41         |
| 1     | B     | 3785:UNK  | C      | 3793:UNK  | N      | 6.41         |
| 1     | C     | 3785:UNK  | C      | 3793:UNK  | N      | 6.41         |
| 1     | D     | 3785:UNK  | C      | 3793:UNK  | N      | 6.41         |
| 1     | A     | 3317:UNK  | C      | 3321:UNK  | N      | 5.85         |
| 1     | B     | 3317:UNK  | C      | 3321:UNK  | N      | 5.85         |
| 1     | C     | 3317:UNK  | C      | 3321:UNK  | N      | 5.85         |
| 1     | D     | 3317:UNK  | C      | 3321:UNK  | N      | 5.85         |
| 1     | A     | 1660:UNK  | C      | 1662:UNK  | N      | 5.79         |
| 1     | C     | 1660:UNK  | C      | 1662:UNK  | N      | 5.79         |
| 1     | D     | 1660:UNK  | C      | 1662:UNK  | N      | 5.79         |
| 1     | B     | 1660:UNK  | C      | 1662:UNK  | N      | 5.78         |
| 1     | A     | 4815:UNK  | C      | 4818:UNK  | N      | 5.71         |
| 1     | B     | 4815:UNK  | C      | 4818:UNK  | N      | 5.71         |
| 1     | C     | 4815:UNK  | C      | 4818:UNK  | N      | 5.71         |
| 1     | D     | 4815:UNK  | C      | 4818:UNK  | N      | 5.71         |
| 1     | A     | 4181:UNK  | C      | 4212:UNK  | N      | 5.70         |
| 1     | B     | 4181:UNK  | C      | 4212:UNK  | N      | 5.70         |
| 1     | C     | 4181:UNK  | C      | 4212:UNK  | N      | 5.70         |
| 1     | D     | 4181:UNK  | C      | 4212:UNK  | N      | 5.70         |
| 1     | A     | 4832:UNK  | C      | 4835:UNK  | N      | 5.56         |
| 1     | B     | 4832:UNK  | C      | 4835:UNK  | N      | 5.56         |
| 1     | C     | 4832:UNK  | C      | 4835:UNK  | N      | 5.56         |
| 1     | D     | 4832:UNK  | C      | 4835:UNK  | N      | 5.56         |
| 1     | A     | 3266:UNK  | C      | 3268:UNK  | N      | 5.23         |
| 1     | B     | 3266:UNK  | C      | 3268:UNK  | N      | 5.23         |
| 1     | C     | 3266:UNK  | C      | 3268:UNK  | N      | 5.23         |
| 1     | D     | 3266:UNK  | C      | 3268:UNK  | N      | 5.23         |
| 1     | A     | 1725:UNK  | C      | 1806:UNK  | N      | 5.21         |
| 1     | C     | 1725:UNK  | C      | 1806:UNK  | N      | 5.21         |
| 1     | D     | 1725:UNK  | C      | 1806:UNK  | N      | 5.21         |
| 1     | B     | 1725:UNK  | C      | 1806:UNK  | N      | 5.20         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 4224:UNK  | C      | 4232:UNK  | N      | 5.07         |
| 1     | B     | 4224:UNK  | C      | 4232:UNK  | N      | 5.07         |
| 1     | C     | 4224:UNK  | C      | 4232:UNK  | N      | 5.07         |
| 1     | D     | 4224:UNK  | C      | 4232:UNK  | N      | 5.07         |
| 1     | A     | 3350:UNK  | C      | 3352:UNK  | N      | 5.04         |
| 1     | B     | 3350:UNK  | C      | 3352:UNK  | N      | 5.04         |
| 1     | C     | 3350:UNK  | C      | 3352:UNK  | N      | 5.04         |
| 1     | D     | 3350:UNK  | C      | 3352:UNK  | N      | 5.04         |
| 1     | A     | 3967:UNK  | C      | 3975:UNK  | N      | 4.68         |
| 1     | B     | 3967:UNK  | C      | 3975:UNK  | N      | 4.68         |
| 1     | C     | 3967:UNK  | C      | 3975:UNK  | N      | 4.68         |
| 1     | D     | 3967:UNK  | C      | 3975:UNK  | N      | 4.68         |
| 1     | A     | 4051:UNK  | C      | 4055:UNK  | N      | 4.60         |
| 1     | B     | 4051:UNK  | C      | 4055:UNK  | N      | 4.60         |
| 1     | C     | 4051:UNK  | C      | 4055:UNK  | N      | 4.59         |
| 1     | D     | 4051:UNK  | C      | 4055:UNK  | N      | 4.59         |
| 1     | A     | 3570:UNK  | C      | 3574:UNK  | N      | 3.91         |
| 1     | B     | 3570:UNK  | C      | 3574:UNK  | N      | 3.91         |
| 1     | C     | 3570:UNK  | C      | 3574:UNK  | N      | 3.91         |
| 1     | D     | 3570:UNK  | C      | 3574:UNK  | N      | 3.91         |
| 1     | A     | 3398:UNK  | C      | 3400:UNK  | N      | 3.20         |
| 1     | B     | 3398:UNK  | C      | 3400:UNK  | N      | 3.20         |
| 1     | C     | 3398:UNK  | C      | 3400:UNK  | N      | 3.20         |
| 1     | D     | 3398:UNK  | C      | 3400:UNK  | N      | 3.20         |
| 1     | A     | 4232:UNK  | C      | 4233:UNK  | N      | 3.13         |
| 1     | B     | 4232:UNK  | C      | 4233:UNK  | N      | 3.13         |
| 1     | C     | 4232:UNK  | C      | 4233:UNK  | N      | 3.13         |
| 1     | D     | 4232:UNK  | C      | 4233:UNK  | N      | 3.13         |
| 1     | A     | 4712:UNK  | C      | 4718:UNK  | N      | 3.07         |
| 1     | B     | 4712:UNK  | C      | 4718:UNK  | N      | 3.07         |
| 1     | C     | 4712:UNK  | C      | 4718:UNK  | N      | 3.07         |
| 1     | D     | 4712:UNK  | C      | 4718:UNK  | N      | 3.07         |
| 1     | A     | 3445:UNK  | C      | 3447:UNK  | N      | 3.00         |
| 1     | B     | 3445:UNK  | C      | 3447:UNK  | N      | 3.00         |
| 1     | C     | 3445:UNK  | C      | 3447:UNK  | N      | 3.00         |
| 1     | D     | 3445:UNK  | C      | 3447:UNK  | N      | 3.00         |
| 1     | A     | 3673:UNK  | C      | 3680:UNK  | N      | 2.72         |
| 1     | B     | 3673:UNK  | C      | 3680:UNK  | N      | 2.72         |
| 1     | C     | 3673:UNK  | C      | 3680:UNK  | N      | 2.72         |
| 1     | D     | 3673:UNK  | C      | 3680:UNK  | N      | 2.72         |
| 1     | A     | 2285:UNK  | C      | 2286:UNK  | N      | 2.32         |
| 1     | B     | 2285:UNK  | C      | 2286:UNK  | N      | 2.32         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C     | 2285:UNK  | C      | 2286:UNK  | N      | 2.32         |
| 1     | D     | 2285:UNK  | C      | 2286:UNK  | N      | 2.32         |

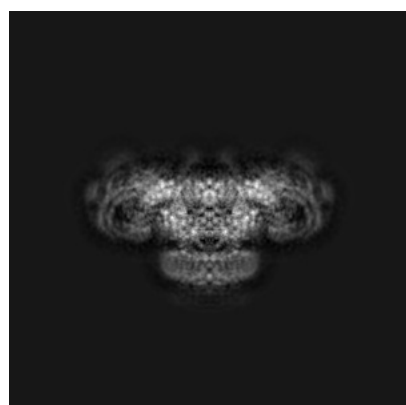
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2751. These allow visual inspection of the internal detail of the map and identification of artifacts.

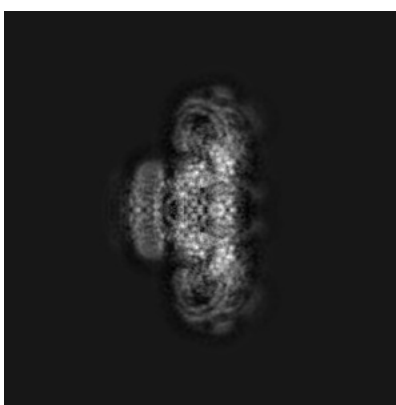
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

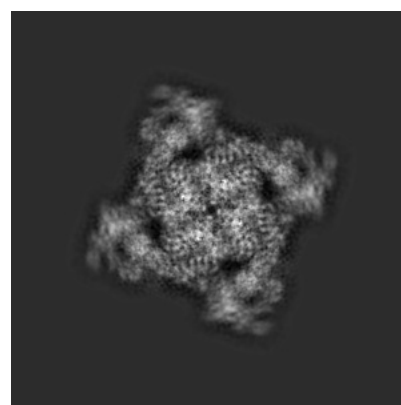
#### 6.1.1 Primary map



X



Y



Z

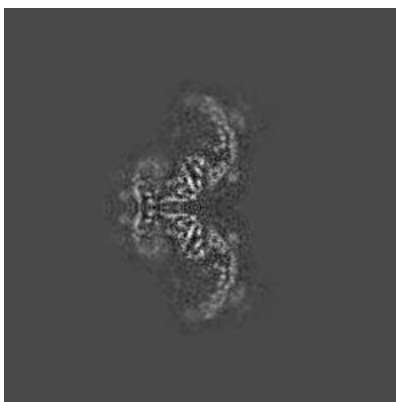
The images above show the map projected in three orthogonal directions.

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

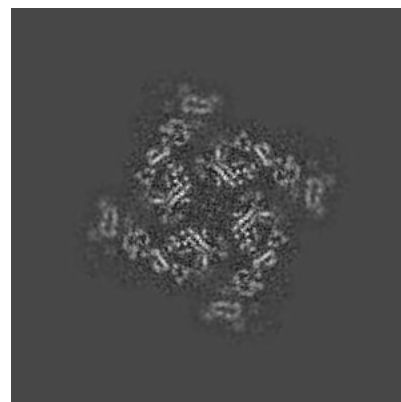
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

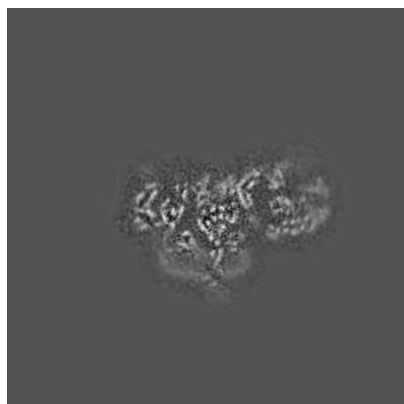


Z Index: 192

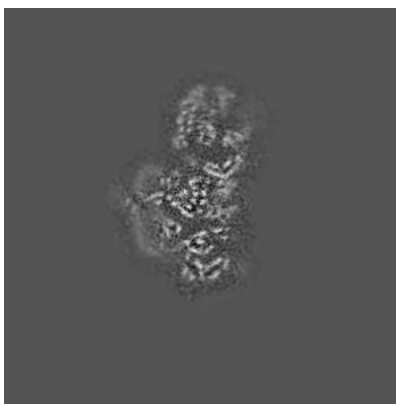
The images above show central slices of the map in three orthogonal directions.

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

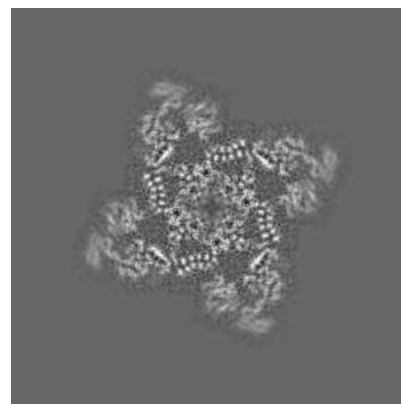
### 6.3.1 Primary map



X Index: 164



Y Index: 220

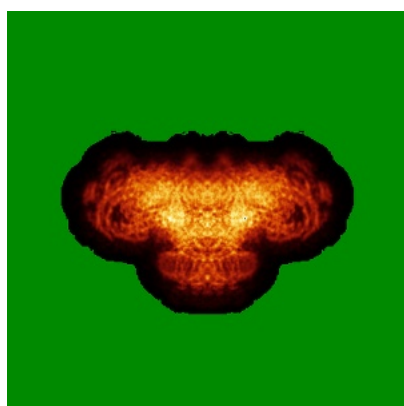


Z Index: 205

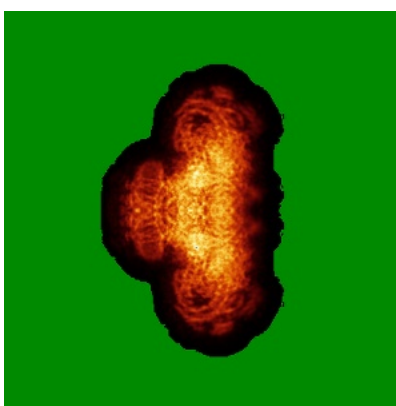
The images above show the largest variance slices of the map in three orthogonal directions.

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

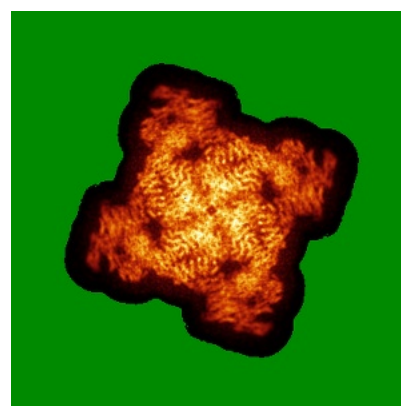
### 6.4.1 Primary map



X



Y

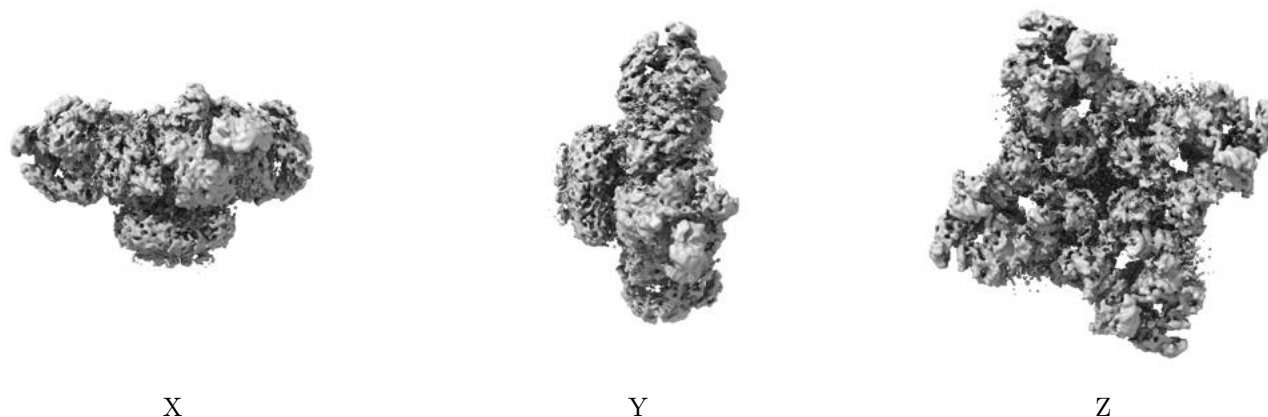


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.443. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

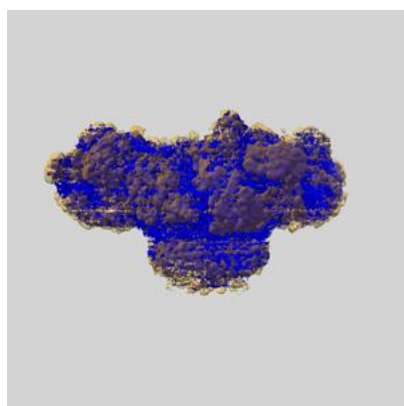
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

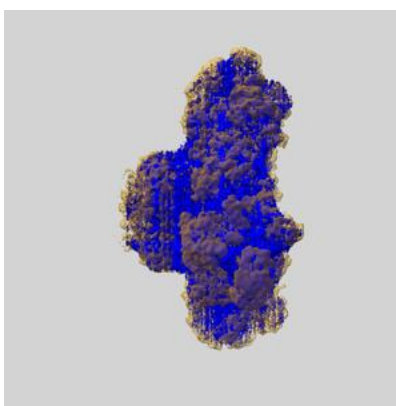
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

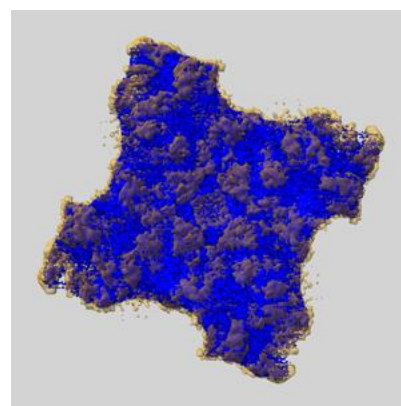
### 6.6.1 emd\_2751\_msk\_1.map [i](#)



X



Y

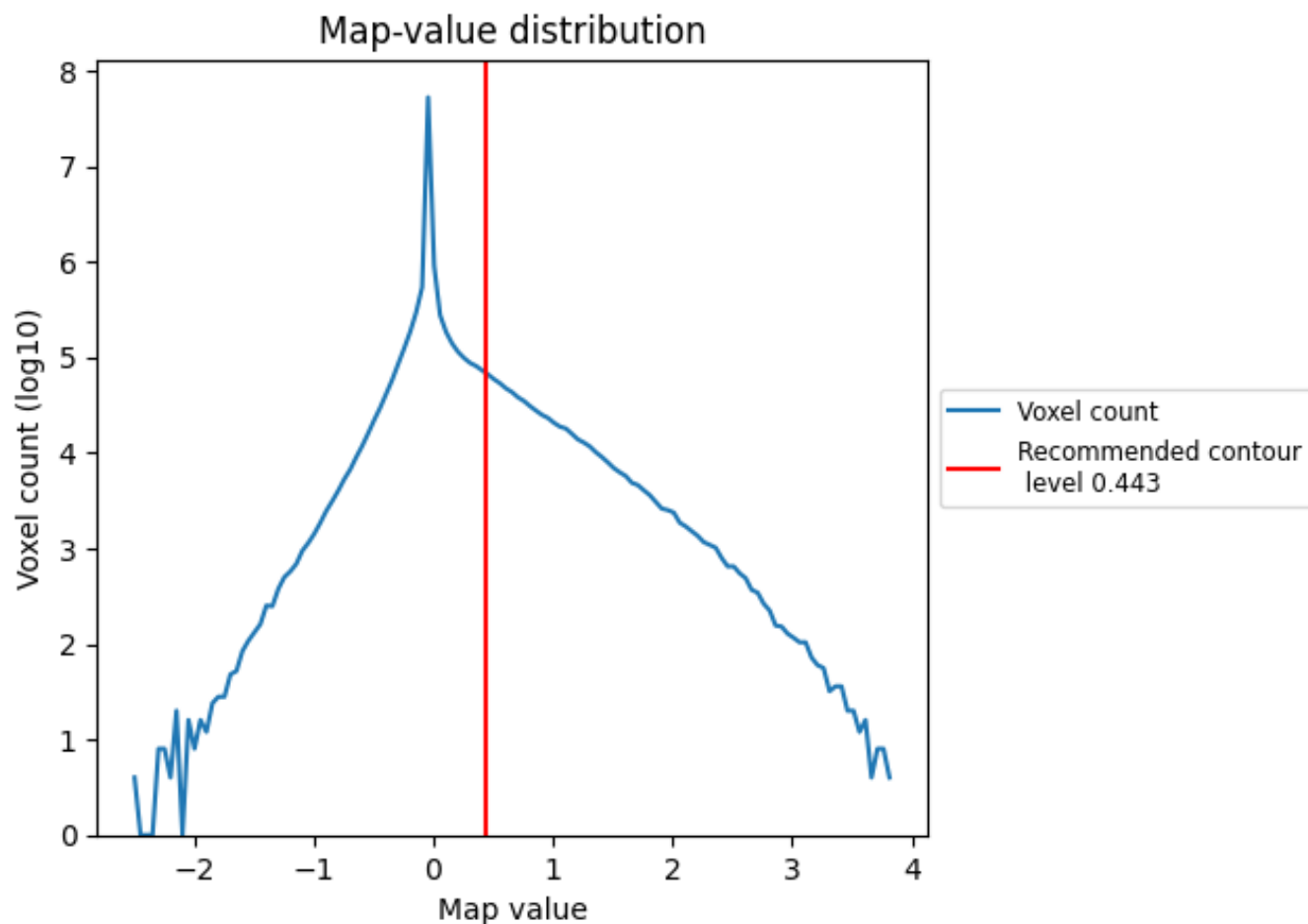


Z

## 7 Map analysis [i](#)

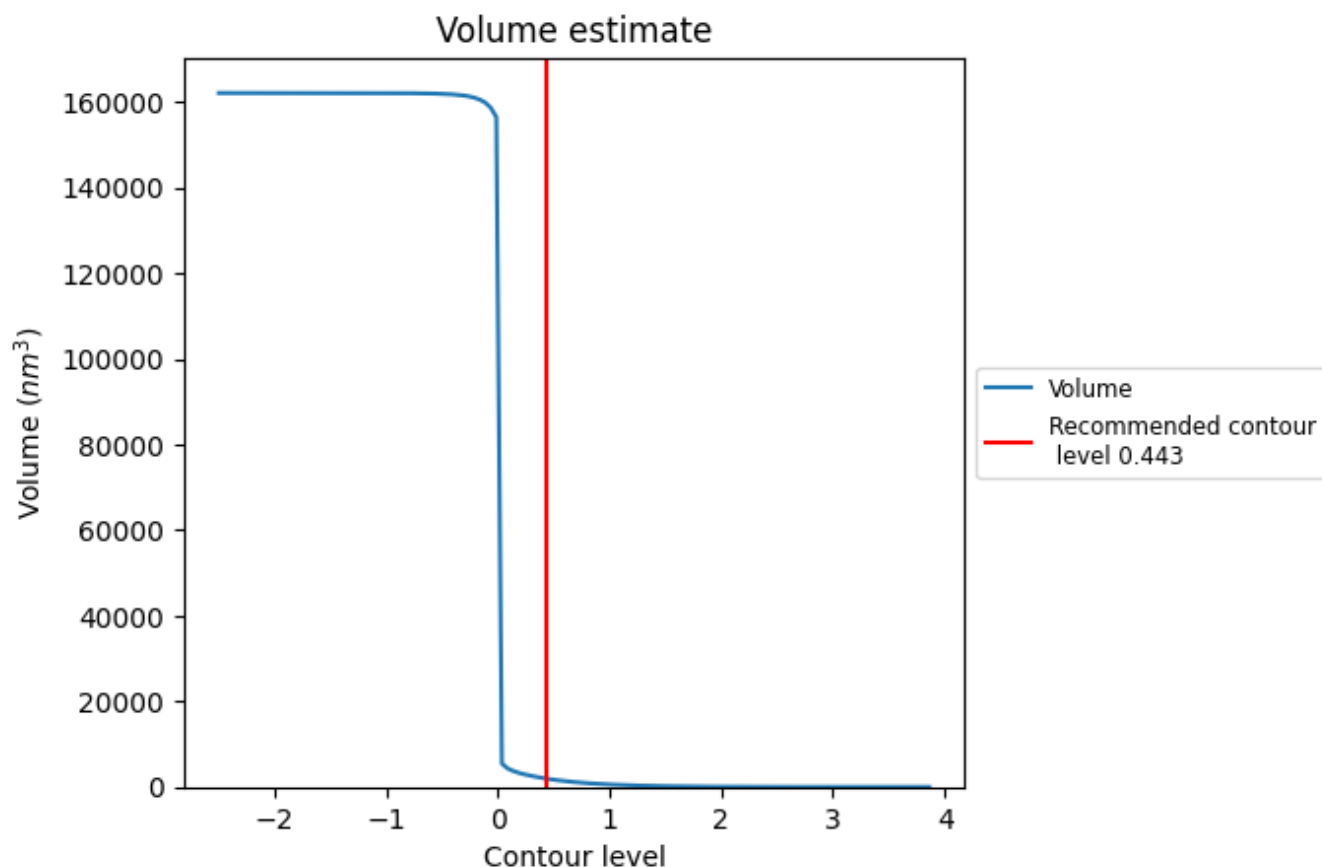
This section contains the results of statistical analysis of the map.

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



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

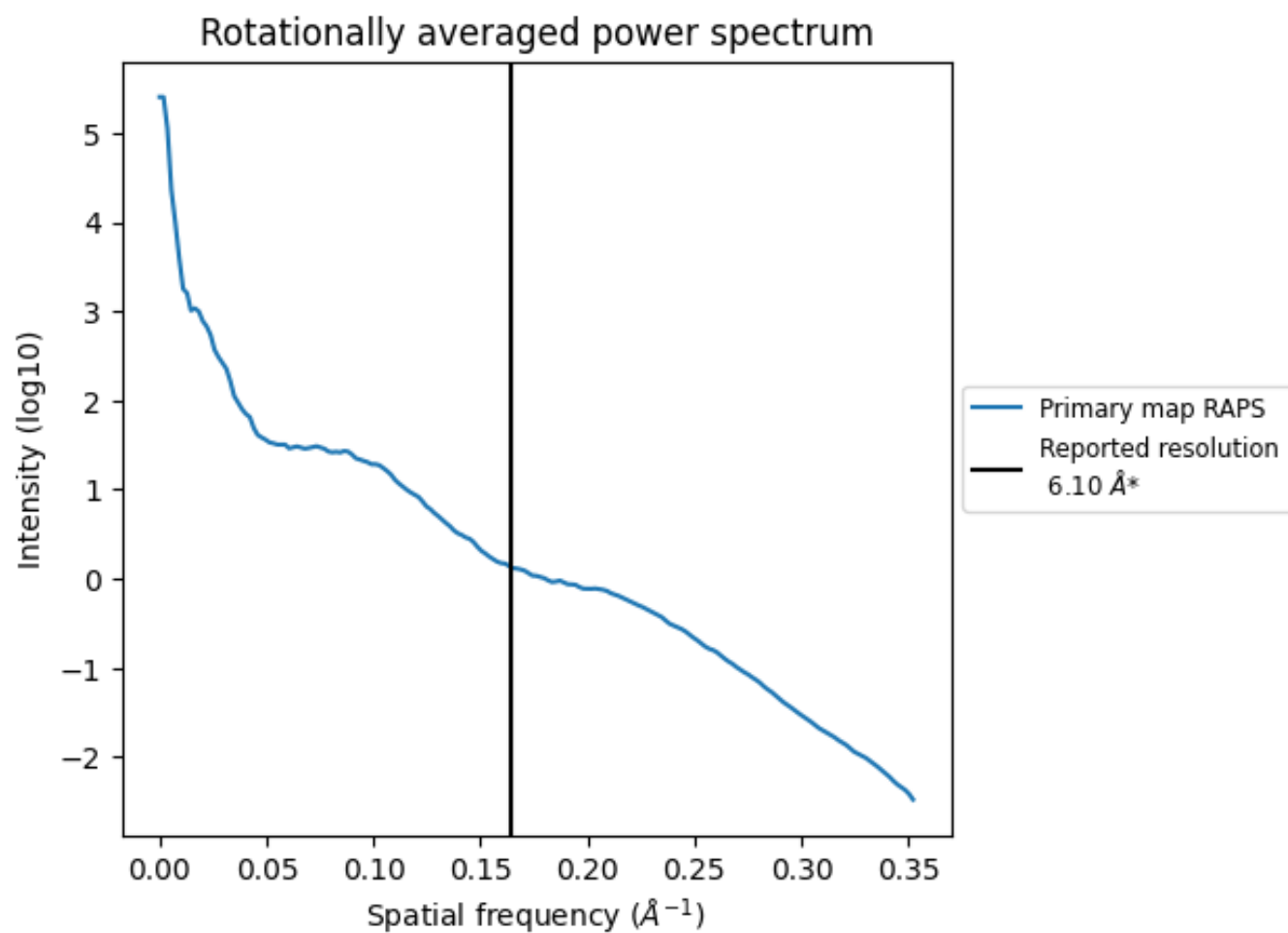
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1916 nm<sup>3</sup>; this corresponds to an approximate mass of 1731 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

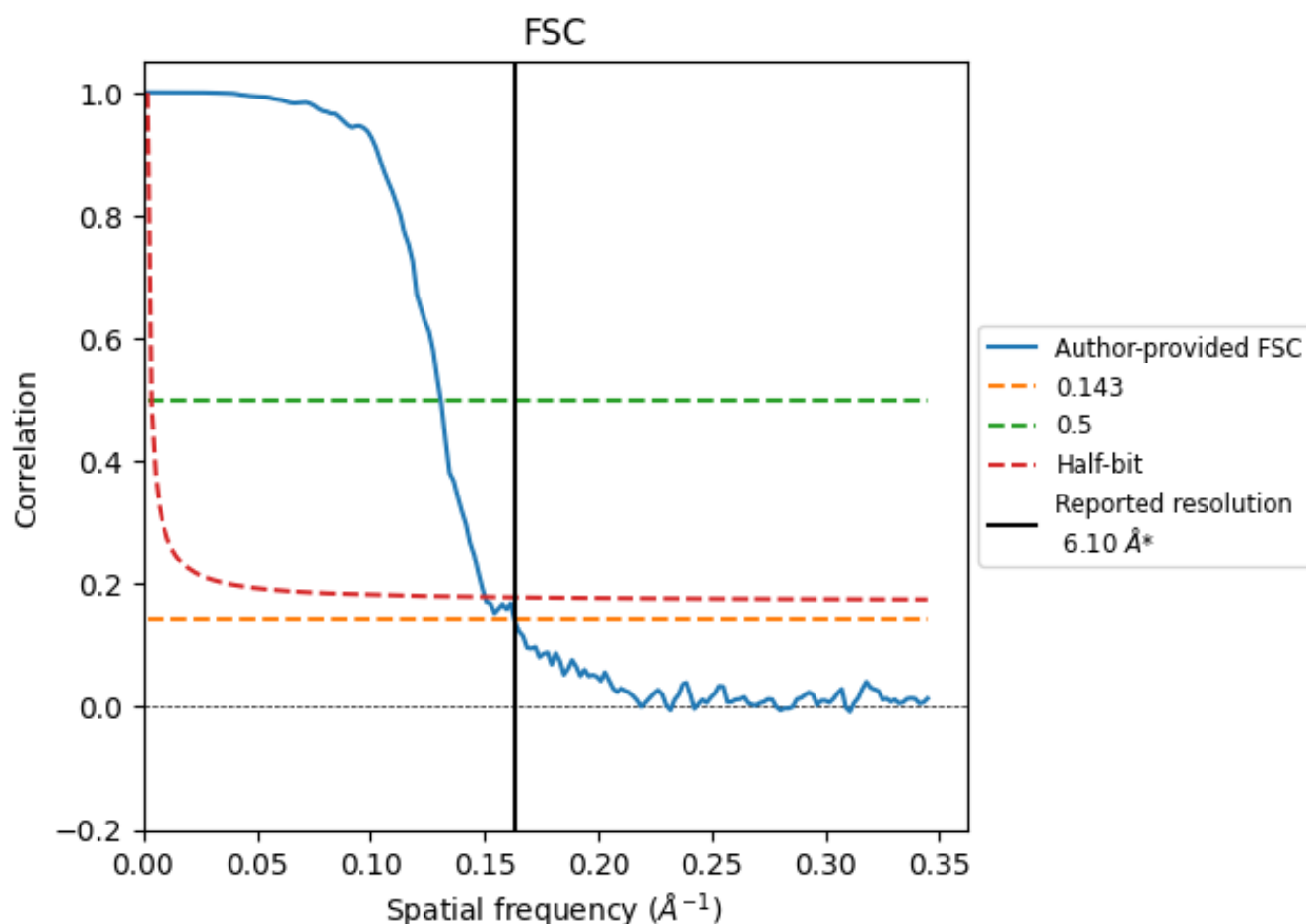


\*Reported resolution corresponds to spatial frequency of 0.164 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.164 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

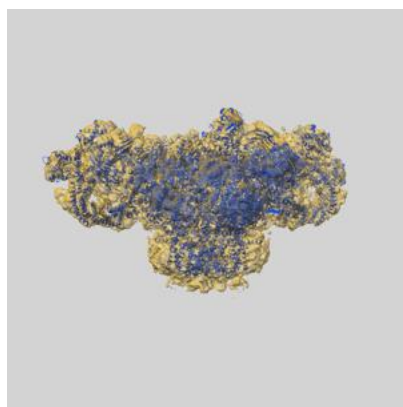
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | -                                  | -    | -        |
| Author-provided FSC curve | 6.12                               | 7.65 | 6.66     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

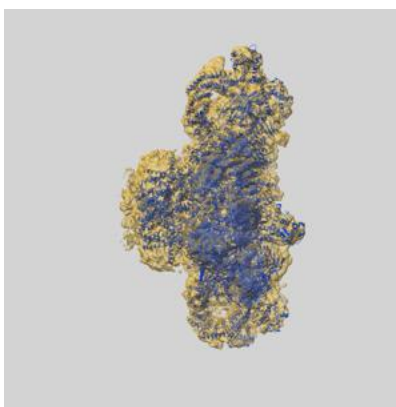
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2751 and PDB model 4UWA. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

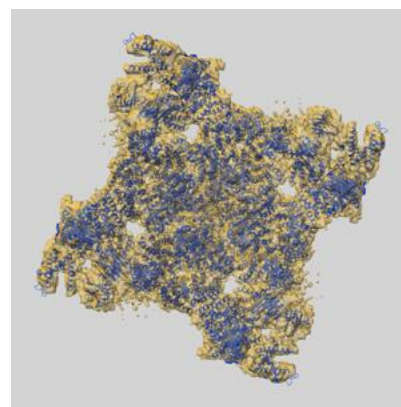
### 9.1 Map-model overlay [i](#)



X



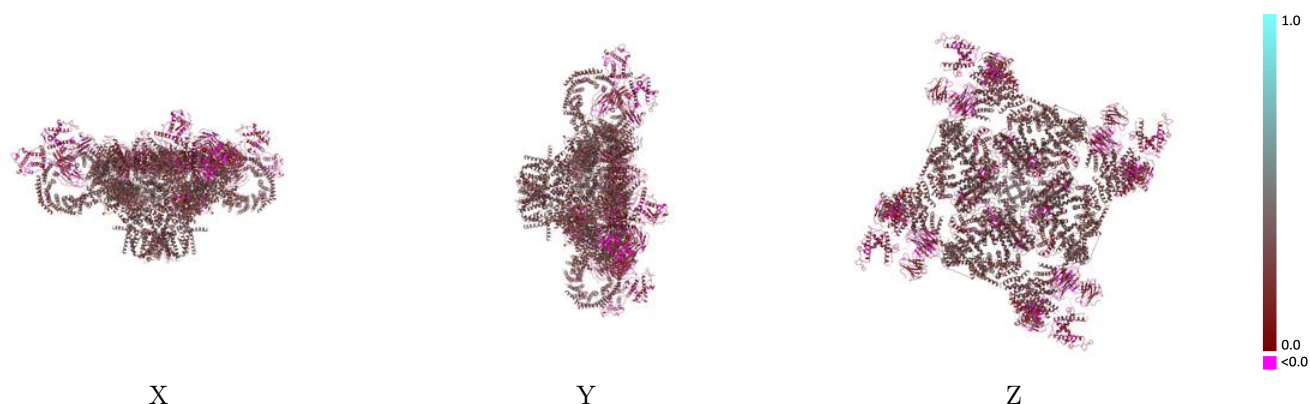
Y



Z

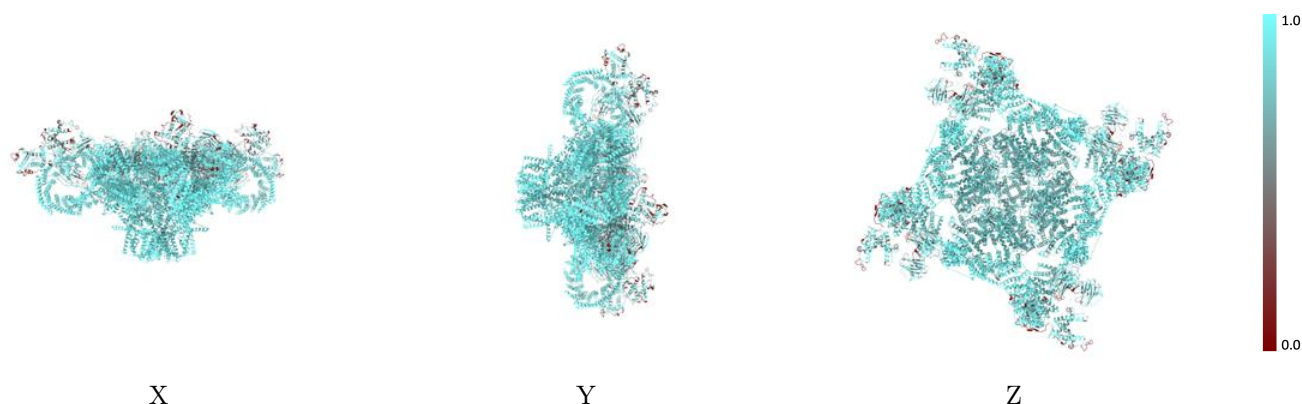
The images above show the 3D surface view of the map at the recommended contour level 0.443 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



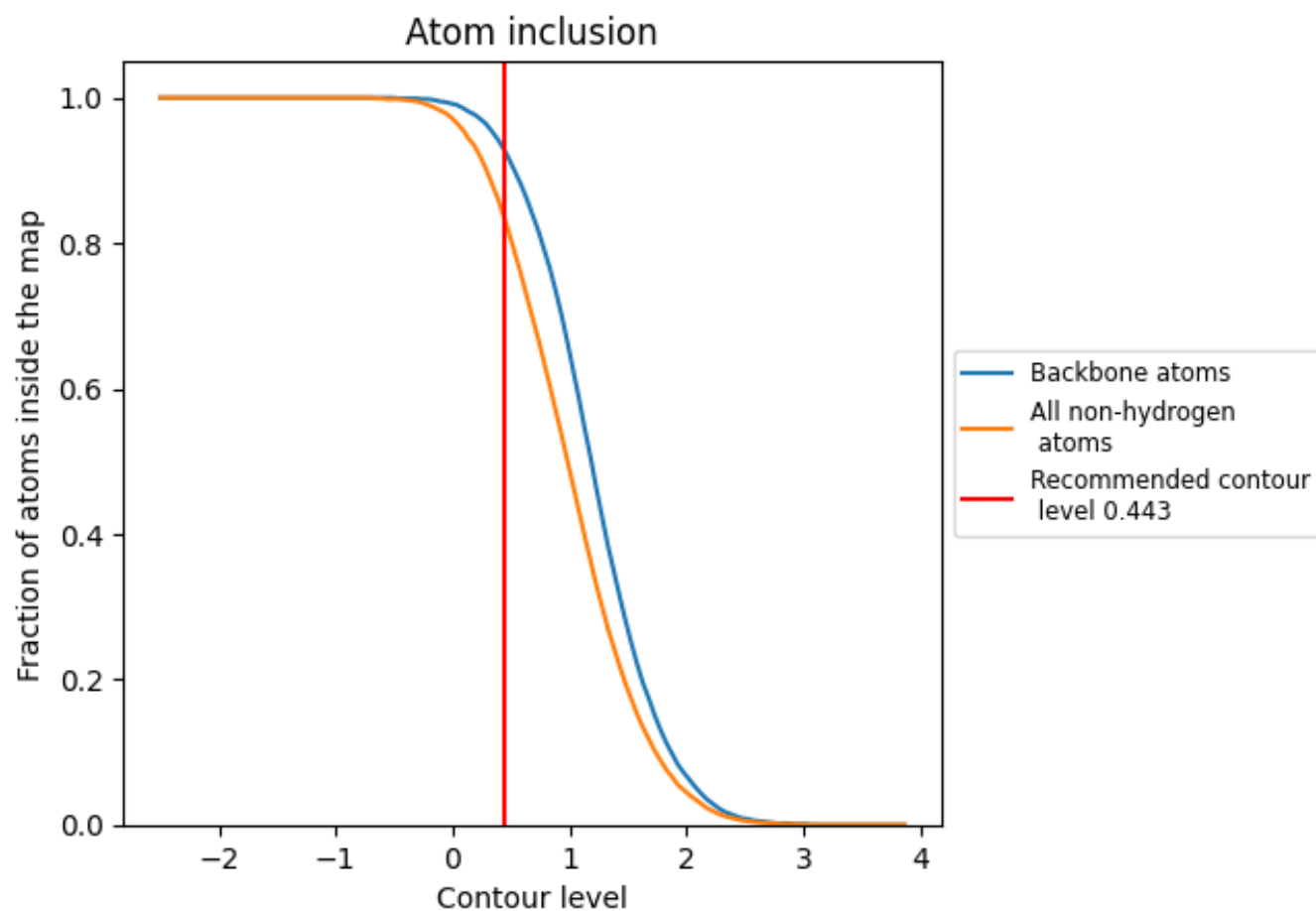
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.443).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.443) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.8340 | <div></div> 0.2080 |
| A     | <div></div> 0.8350 | <div></div> 0.2090 |
| B     | <div></div> 0.8340 | <div></div> 0.2080 |
| C     | <div></div> 0.8350 | <div></div> 0.2080 |
| D     | <div></div> 0.8340 | <div></div> 0.2080 |

