



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:28 AM UTC

PDB ID : 1BR1 / pdb\_00001br1  
Title : SMOOTH MUSCLE MYOSIN MOTOR DOMAIN-ESSENTIAL LIGHT CHAIN COMPLEX WITH MGADP.ALF4 BOUND AT THE ACTIVE SITE  
Authors : Dominguez, R.; Trybus, K.M.; Cohen, C.  
Deposited on : 1998-08-26  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

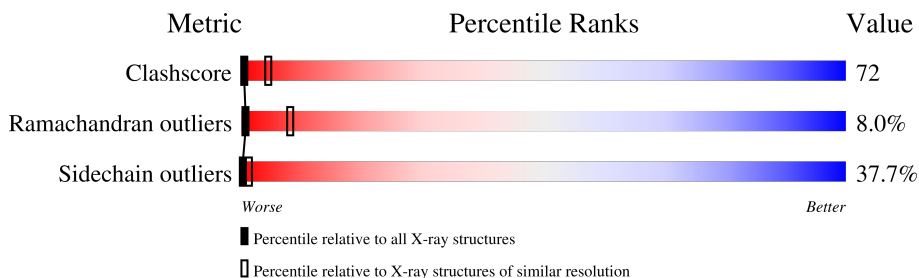
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1140 (3.54-3.46)                                      |
| Ramachandran outliers | 187476                      | 1113 (3.54-3.46)                                      |
| Sidechain outliers    | 187428                      | 1114 (3.54-3.46)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 820    |                  |
| 1   | C     | 820    |                  |
| 1   | E     | 820    |                  |
| 1   | G     | 820    |                  |
| 2   | B     | 150    |                  |
| 2   | D     | 150    |                  |
| 2   | F     | 150    |                  |
| 2   | H     | 150    |                  |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called MYOSIN.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 787      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6337  | 4036 | 1089 | 1183 | 29 |         |         |       |
| 1   | C     | 787      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6337  | 4036 | 1089 | 1183 | 29 |         |         |       |
| 1   | E     | 787      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6337  | 4036 | 1089 | 1183 | 29 |         |         |       |
| 1   | G     | 787      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6337  | 4036 | 1089 | 1183 | 29 |         |         |       |

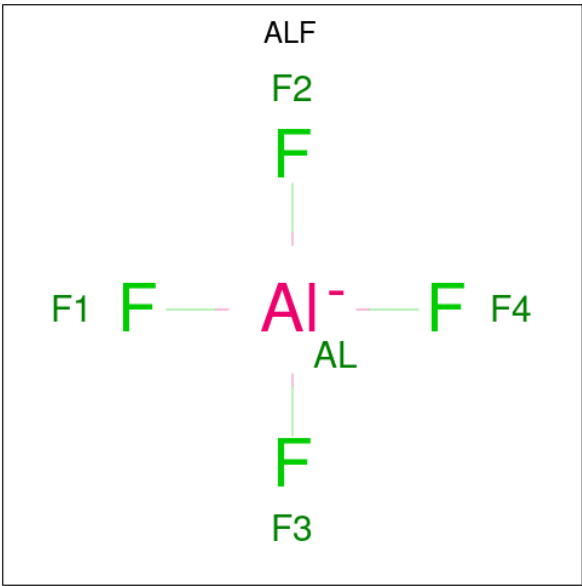
- Molecule 2 is a protein called MYOSIN.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2   | B     | 148      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1161  | 722 | 193 | 235 | 11 |         |         |       |
| 2   | D     | 148      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1161  | 722 | 193 | 235 | 11 |         |         |       |
| 2   | F     | 148      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1161  | 722 | 193 | 235 | 11 |         |         |       |
| 2   | H     | 148      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1161  | 722 | 193 | 235 | 11 |         |         |       |

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

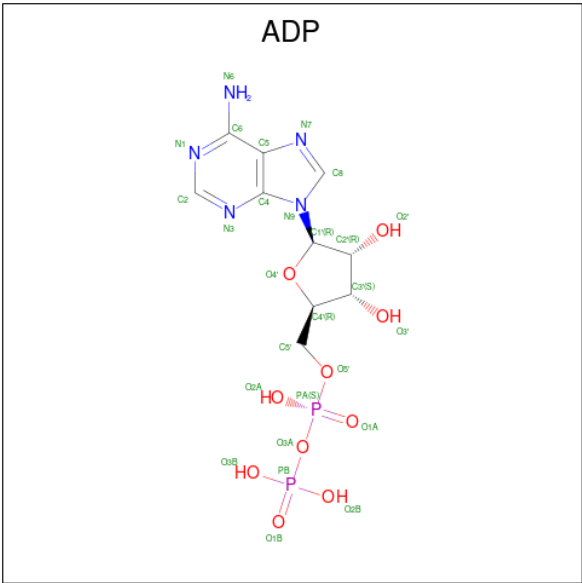
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | C     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | E     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | G     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula:  $\text{AlF}_4^-$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 4   | A     | 1        | Total | Al | F | 0       | 0       |
|     |       |          | 5     | 1  | 4 |         |         |
| 4   | C     | 1        | Total | Al | F | 0       | 0       |
|     |       |          | 5     | 1  | 4 |         |         |
| 4   | E     | 1        | Total | Al | F | 0       | 0       |
|     |       |          | 5     | 1  | 4 |         |         |
| 4   | G     | 1        | Total | Al | F | 0       | 0       |
|     |       |          | 5     | 1  | 4 |         |         |

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).

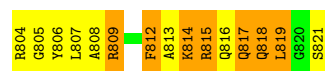
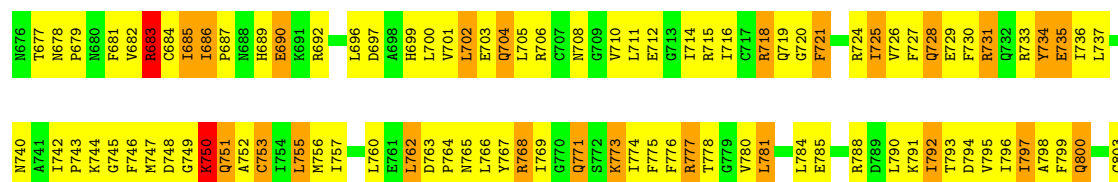


| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 5   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 5   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 5   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 5   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

- Molecule 6 is water.

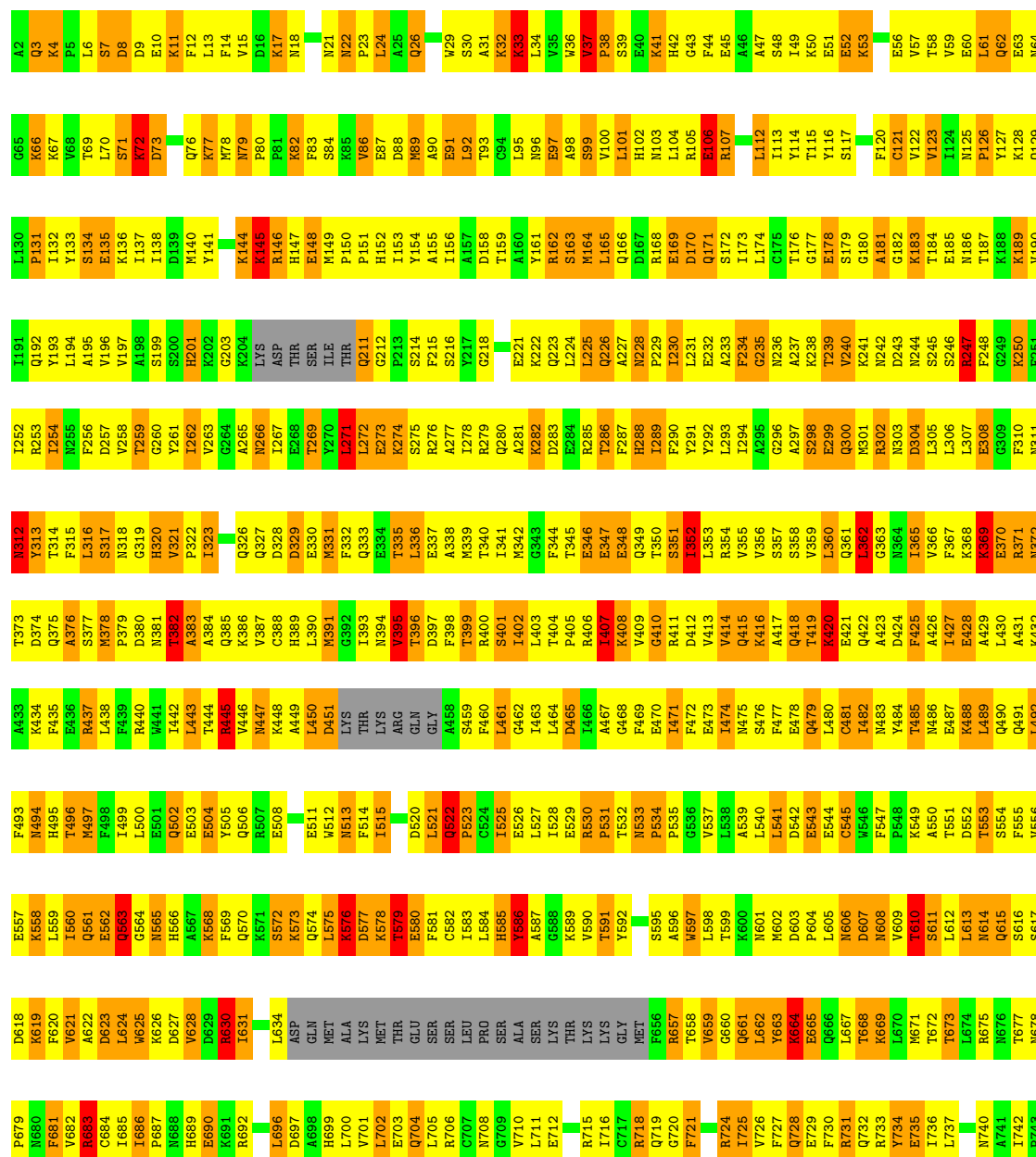
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 6   | A     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 6   | C     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 6   | E     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 6   | G     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |

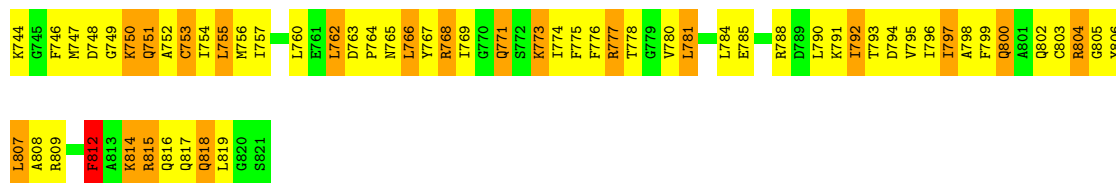




# Molecule 1: MYOSIN

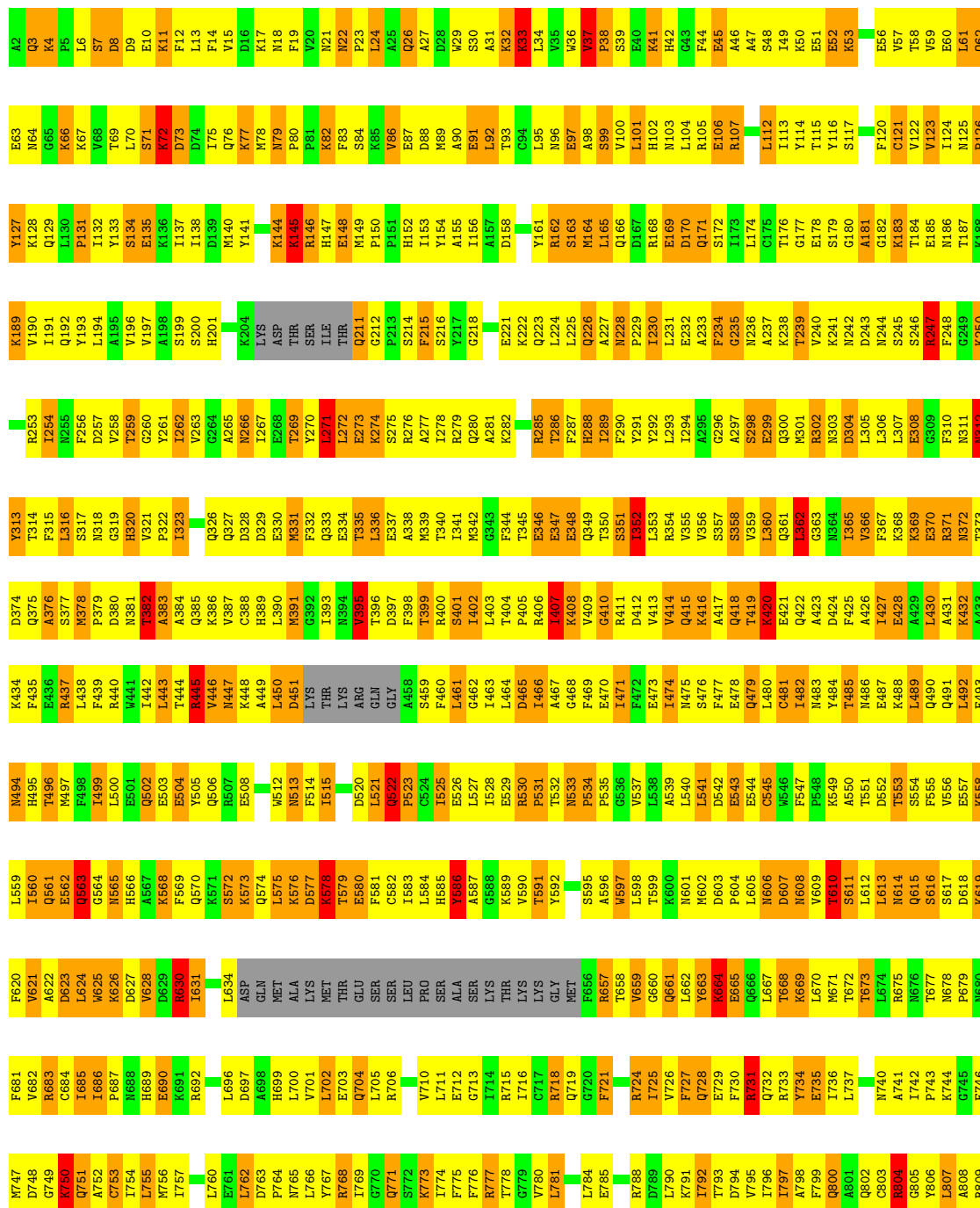
Chain C: 16% 50% 27%



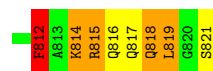


• Molecule 1: MYOSIN

Chain E: 16% 50% 27%

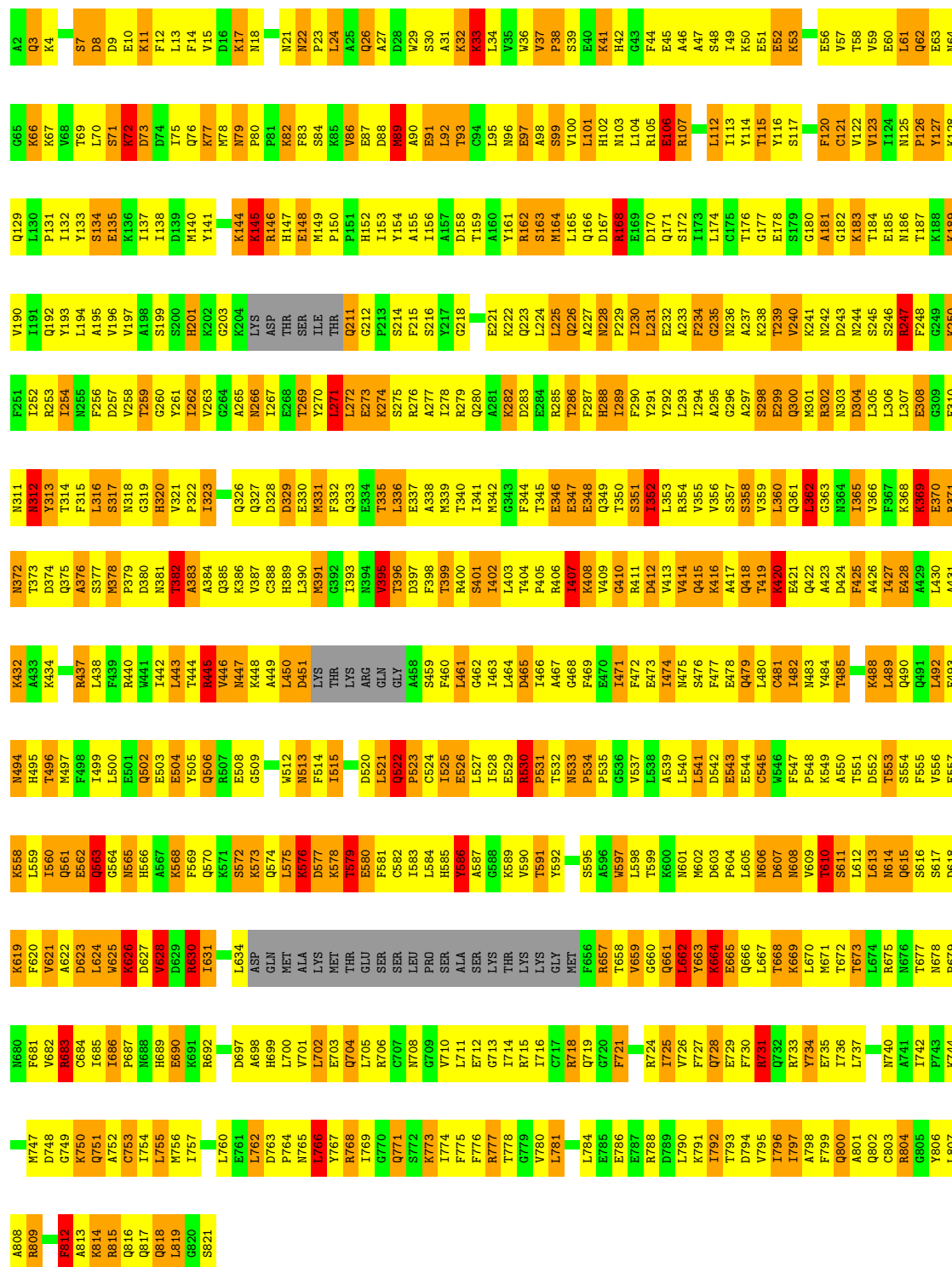




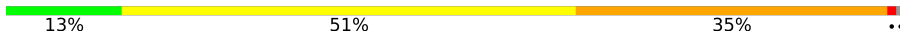


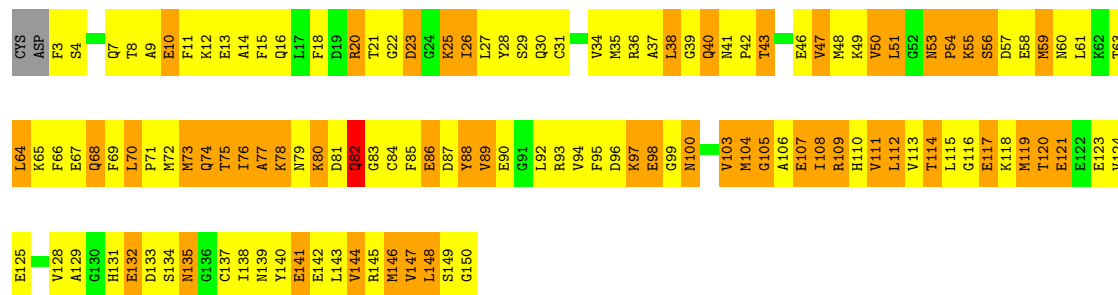
• Molecule 1: MYOSIN

Chain G: 16% 49% 26% . .

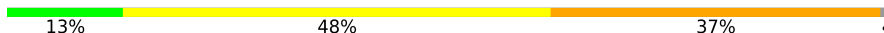


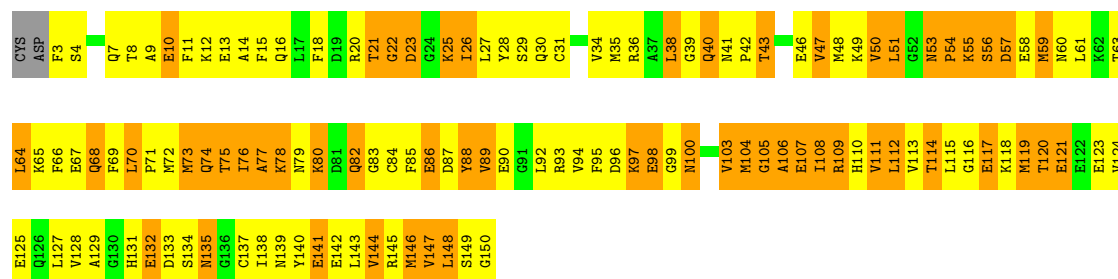
- Molecule 2: MYOSIN

Chain B: 

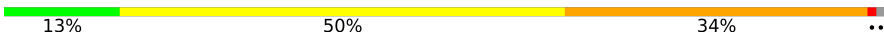


- Molecule 2: MYOSIN

Chain D: 



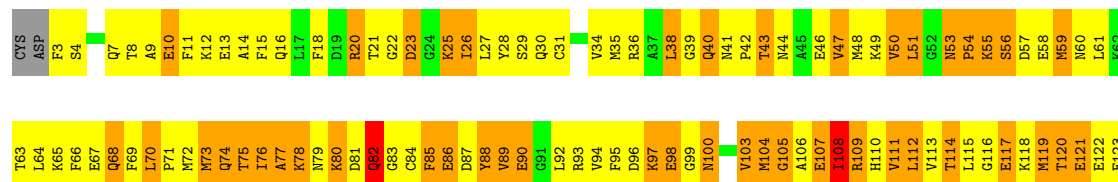
- Molecule 2: MYOSIN

Chain F: 



- Molecule 2: MYOSIN

Chain H: 



|      |      |  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|--|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| V124 | E125 |  | V128 | A129 | G130 | H131 | E132 | D133 | S134 | N135 | G136 | C137 | I138 | N139 | Y140 | E141 | E142 | L143 | V144 | R145 | M146 | V147 | L148 | S149 | G150 |
|------|------|--|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

## 4 Data and refinement statistics

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

| Property                                                 | Value                                            | Source    |
|----------------------------------------------------------|--------------------------------------------------|-----------|
| Space group                                              | P 1                                              | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 95.32Å 144.66Å 147.29Å<br>111.21° 106.10° 92.58° | Depositor |
| Resolution (Å)                                           | 10.00 – 3.50                                     | Depositor |
| % Data completeness<br>(in resolution range)             | 91.5 (10.00-3.50)                                | Depositor |
| $R_{merge}$                                              | (Not available)                                  | Depositor |
| $R_{sym}$                                                | 0.09                                             | Depositor |
| Refinement program                                       | X-PLOR 3.851                                     | Depositor |
| R, $R_{free}$                                            | 0.227 , 0.305                                    | Depositor |
| Estimated twinning fraction                              | No twinning to report.                           | Xtriage   |
| Total number of atoms                                    | 30132                                            | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 50.0                                             | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ALF, MG

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     | 0.64         | 3/6456 (0.0%)   | 1.02        | 27/8700 (0.3%)   |
| 1   | C     | 0.65         | 3/6456 (0.0%)   | 1.02        | 28/8700 (0.3%)   |
| 1   | E     | 0.64         | 3/6456 (0.0%)   | 1.01        | 27/8700 (0.3%)   |
| 1   | G     | 0.64         | 3/6456 (0.0%)   | 1.02        | 29/8700 (0.3%)   |
| 2   | B     | 0.46         | 0/1176          | 0.89        | 0/1575           |
| 2   | D     | 0.52         | 0/1176          | 0.89        | 1/1575 (0.1%)    |
| 2   | F     | 0.55         | 2/1176 (0.2%)   | 0.92        | 4/1575 (0.3%)    |
| 2   | H     | 0.61         | 0/1176          | 0.92        | 1/1575 (0.1%)    |
| All | All   | 0.63         | 14/30528 (0.0%) | 1.00        | 117/41100 (0.3%) |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | F     | 85  | PHE  | CA-C    | -5.71 | 1.45        | 1.52     |
| 2   | F     | 86  | GLU  | N-CA    | -5.52 | 1.39        | 1.46     |
| 1   | G     | 597 | TRP  | NE1-CE2 | -5.49 | 1.31        | 1.37     |
| 1   | E     | 597 | TRP  | NE1-CE2 | -5.45 | 1.31        | 1.37     |
| 1   | C     | 597 | TRP  | NE1-CE2 | -5.41 | 1.31        | 1.37     |
| 1   | A     | 597 | TRP  | NE1-CE2 | -5.38 | 1.31        | 1.37     |
| 1   | A     | 625 | TRP  | NE1-CE2 | -5.37 | 1.31        | 1.37     |
| 1   | E     | 625 | TRP  | NE1-CE2 | -5.37 | 1.31        | 1.37     |
| 1   | C     | 625 | TRP  | NE1-CE2 | -5.30 | 1.31        | 1.37     |
| 1   | G     | 625 | TRP  | NE1-CE2 | -5.25 | 1.31        | 1.37     |
| 1   | G     | 29  | TRP  | NE1-CE2 | -5.25 | 1.31        | 1.37     |
| 1   | E     | 29  | TRP  | NE1-CE2 | -5.24 | 1.31        | 1.37     |
| 1   | A     | 29  | TRP  | NE1-CE2 | -5.23 | 1.31        | 1.37     |
| 1   | C     | 29  | TRP  | NE1-CE2 | -5.22 | 1.31        | 1.37     |

All (117) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 817 | GLN  | OE1-CD-NE2 | -9.83 | 112.77      | 122.60   |
| 1   | A     | 669 | LYS  | N-CA-C     | -9.13 | 100.89      | 111.03   |
| 1   | C     | 669 | LYS  | N-CA-C     | -8.63 | 101.45      | 111.03   |
| 1   | E     | 669 | LYS  | N-CA-C     | -8.60 | 101.48      | 111.03   |
| 1   | G     | 669 | LYS  | N-CA-C     | -8.53 | 101.56      | 111.03   |
| 1   | C     | 97  | GLU  | N-CA-C     | -8.06 | 102.70      | 112.54   |
| 1   | C     | 312 | ASN  | N-CA-C     | -7.96 | 103.37      | 113.72   |
| 1   | G     | 668 | THR  | N-CA-C     | -7.89 | 103.87      | 113.97   |
| 1   | A     | 668 | THR  | N-CA-C     | -7.89 | 103.87      | 113.97   |
| 1   | E     | 312 | ASN  | N-CA-C     | -7.80 | 103.57      | 113.72   |
| 1   | G     | 312 | ASN  | N-CA-C     | -7.74 | 103.66      | 113.72   |
| 1   | C     | 668 | THR  | N-CA-C     | -7.73 | 104.00      | 113.50   |
| 1   | A     | 312 | ASN  | N-CA-C     | -7.46 | 104.03      | 113.72   |
| 1   | E     | 97  | GLU  | N-CA-C     | -7.41 | 103.50      | 112.54   |
| 1   | C     | 505 | TYR  | N-CA-C     | -7.36 | 103.33      | 111.36   |
| 1   | A     | 97  | GLU  | N-CA-C     | -7.36 | 103.56      | 112.54   |
| 1   | G     | 97  | GLU  | N-CA-C     | -7.33 | 103.59      | 112.54   |
| 1   | E     | 668 | THR  | N-CA-C     | -7.20 | 104.64      | 113.50   |
| 2   | F     | 22  | GLY  | N-CA-C     | 6.89  | 129.50      | 113.18   |
| 1   | A     | 817 | GLN  | CG-CD-NE2  | 6.71  | 126.46      | 116.40   |
| 1   | A     | 445 | ARG  | N-CA-C     | -6.67 | 103.18      | 112.45   |
| 1   | E     | 505 | TYR  | N-CA-C     | -6.45 | 104.25      | 111.28   |
| 1   | A     | 464 | LEU  | N-CA-C     | 6.44  | 119.02      | 108.52   |
| 1   | G     | 336 | LEU  | N-CA-C     | -6.38 | 104.25      | 111.07   |
| 1   | G     | 505 | TYR  | N-CA-C     | -6.37 | 104.42      | 111.36   |
| 1   | A     | 336 | LEU  | N-CA-C     | -6.37 | 104.26      | 111.07   |
| 1   | G     | 558 | LYS  | N-CA-C     | -6.33 | 104.38      | 111.28   |
| 1   | A     | 558 | LYS  | N-CA-C     | -6.29 | 104.42      | 111.28   |
| 1   | G     | 734 | TYR  | N-CA-C     | 6.27  | 119.65      | 112.57   |
| 1   | A     | 578 | LYS  | N-CA-C     | -6.25 | 105.48      | 113.23   |
| 1   | E     | 336 | LEU  | N-CA-C     | -6.19 | 104.45      | 111.07   |
| 1   | C     | 734 | TYR  | N-CA-C     | 6.19  | 119.56      | 112.57   |
| 1   | C     | 558 | LYS  | N-CA-C     | -6.18 | 104.54      | 111.28   |
| 1   | G     | 578 | LYS  | N-CA-C     | -6.18 | 105.56      | 113.23   |
| 1   | C     | 578 | LYS  | N-CA-C     | -6.17 | 105.58      | 113.23   |
| 1   | G     | 464 | LEU  | N-CA-C     | 6.14  | 118.54      | 108.52   |
| 1   | C     | 445 | ARG  | N-CA-C     | -6.11 | 103.96      | 112.45   |
| 1   | E     | 445 | ARG  | N-CA-C     | -6.08 | 104.00      | 112.45   |
| 1   | G     | 812 | PHE  | N-CA-C     | -6.06 | 103.32      | 112.04   |
| 1   | E     | 464 | LEU  | N-CA-C     | 6.03  | 118.34      | 108.52   |
| 1   | A     | 505 | TYR  | N-CA-C     | -6.02 | 104.72      | 111.28   |
| 1   | C     | 336 | LEU  | N-CA-C     | -5.99 | 104.66      | 111.07   |
| 1   | C     | 625 | TRP  | CB-CA-C    | -5.99 | 101.78      | 111.06   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | G     | 445 | ARG  | N-CA-C    | -5.97 | 104.15      | 112.45   |
| 1   | A     | 662 | LEU  | N-CA-C    | -5.96 | 104.71      | 111.14   |
| 1   | C     | 522 | GLN  | N-CA-C    | -5.90 | 105.98      | 113.77   |
| 1   | A     | 757 | ILE  | N-CA-C    | -5.87 | 104.07      | 112.35   |
| 1   | E     | 804 | ARG  | N-CA-C    | -5.87 | 104.96      | 111.71   |
| 1   | E     | 734 | TYR  | N-CA-C    | 5.84  | 119.17      | 112.57   |
| 1   | G     | 434 | LYS  | N-CA-C    | -5.82 | 105.07      | 111.82   |
| 1   | A     | 434 | LYS  | N-CA-C    | -5.81 | 105.08      | 111.82   |
| 1   | E     | 558 | LYS  | N-CA-C    | -5.80 | 104.95      | 111.28   |
| 1   | G     | 586 | TYR  | N-CA-C    | -5.78 | 105.33      | 112.90   |
| 1   | G     | 3   | GLN  | N-CA-C    | 5.73  | 118.58      | 109.81   |
| 1   | C     | 662 | LEU  | N-CA-C    | -5.72 | 104.95      | 111.07   |
| 1   | G     | 662 | LEU  | N-CA-C    | -5.71 | 104.96      | 111.07   |
| 1   | E     | 3   | GLN  | N-CA-C    | 5.70  | 118.53      | 109.81   |
| 1   | C     | 464 | LEU  | N-CA-C    | 5.63  | 117.69      | 108.52   |
| 1   | A     | 3   | GLN  | N-CA-C    | 5.61  | 118.39      | 109.81   |
| 1   | A     | 6   | LEU  | N-CA-C    | 5.58  | 118.06      | 109.07   |
| 1   | G     | 628 | VAL  | CB-CA-C   | -5.56 | 104.74      | 112.36   |
| 1   | E     | 434 | LYS  | N-CA-C    | -5.54 | 105.39      | 111.82   |
| 1   | E     | 430 | LEU  | N-CA-C    | -5.54 | 104.15      | 111.96   |
| 1   | C     | 3   | GLN  | N-CA-C    | 5.53  | 118.28      | 109.81   |
| 1   | C     | 812 | PHE  | N-CA-C    | -5.53 | 104.08      | 112.04   |
| 1   | E     | 191 | ILE  | N-CA-C    | -5.45 | 105.53      | 110.82   |
| 1   | C     | 630 | ARG  | NE-CZ-NH2 | 5.44  | 124.10      | 119.20   |
| 1   | E     | 124 | ILE  | N-CA-C    | 5.43  | 116.27      | 108.93   |
| 1   | G     | 630 | ARG  | NE-CZ-NH2 | 5.43  | 124.09      | 119.20   |
| 1   | A     | 285 | ARG  | NE-CZ-NH2 | 5.42  | 124.08      | 119.20   |
| 1   | E     | 578 | LYS  | N-CA-C    | -5.42 | 105.80      | 112.90   |
| 1   | C     | 804 | ARG  | N-CA-C    | -5.42 | 105.48      | 111.71   |
| 1   | A     | 247 | ARG  | NE-CZ-NH2 | 5.41  | 124.07      | 119.20   |
| 1   | E     | 285 | ARG  | NE-CZ-NH2 | 5.39  | 124.05      | 119.20   |
| 1   | A     | 630 | ARG  | NE-CZ-NH2 | 5.39  | 124.05      | 119.20   |
| 1   | C     | 247 | ARG  | NE-CZ-NH2 | 5.37  | 124.03      | 119.20   |
| 1   | E     | 630 | ARG  | NE-CZ-NH2 | 5.36  | 124.02      | 119.20   |
| 1   | C     | 586 | TYR  | N-CA-C    | -5.36 | 105.89      | 112.90   |
| 1   | E     | 586 | TYR  | N-CA-C    | -5.35 | 105.89      | 112.90   |
| 1   | E     | 812 | PHE  | N-CA-C    | -5.35 | 104.34      | 112.04   |
| 1   | G     | 285 | ARG  | NE-CZ-NH2 | 5.34  | 124.01      | 119.20   |
| 2   | F     | 108 | ILE  | N-CA-C    | -5.33 | 105.19      | 110.62   |
| 1   | E     | 522 | GLN  | N-CA-C    | -5.33 | 106.74      | 113.77   |
| 1   | A     | 279 | ARG  | NE-CZ-NH2 | 5.32  | 123.98      | 119.20   |
| 1   | C     | 285 | ARG  | NE-CZ-NH2 | 5.31  | 123.98      | 119.20   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | G     | 247 | ARG  | NE-CZ-NH2 | 5.31  | 123.98      | 119.20   |
| 1   | G     | 731 | ARG  | N-CA-C    | -5.30 | 106.88      | 113.19   |
| 1   | C     | 576 | LYS  | N-CA-C    | -5.30 | 106.89      | 113.19   |
| 1   | G     | 168 | ARG  | NE-CZ-NH2 | 5.30  | 123.97      | 119.20   |
| 1   | G     | 796 | ILE  | N-CA-C    | -5.29 | 105.34      | 110.42   |
| 2   | F     | 85  | PHE  | O-C-N     | 5.29  | 129.63      | 122.59   |
| 1   | A     | 522 | GLN  | N-CA-C    | -5.28 | 106.80      | 113.77   |
| 1   | A     | 734 | TYR  | N-CA-C    | 5.26  | 118.52      | 112.57   |
| 1   | E     | 247 | ARG  | NE-CZ-NH2 | 5.26  | 123.93      | 119.20   |
| 1   | E     | 731 | ARG  | N-CA-C    | -5.25 | 106.95      | 113.19   |
| 1   | A     | 576 | LYS  | N-CA-C    | -5.22 | 106.98      | 113.19   |
| 2   | D     | 106 | ALA  | N-CA-C    | -5.21 | 106.98      | 113.55   |
| 1   | G     | 522 | GLN  | N-CA-C    | -5.21 | 106.89      | 113.77   |
| 1   | G     | 766 | LEU  | N-CA-C    | -5.21 | 105.28      | 111.69   |
| 2   | F     | 106 | ALA  | N-CA-C    | -5.19 | 107.02      | 113.55   |
| 1   | E     | 37  | VAL  | CA-C-N    | 5.17  | 126.31      | 119.84   |
| 1   | E     | 37  | VAL  | C-N-CA    | 5.17  | 126.31      | 119.84   |
| 1   | C     | 6   | LEU  | N-CA-C    | 5.16  | 117.38      | 109.07   |
| 1   | G     | 576 | LYS  | N-CA-C    | -5.16 | 107.05      | 113.19   |
| 1   | C     | 766 | LEU  | N-CA-C    | -5.13 | 105.15      | 111.40   |
| 1   | C     | 434 | LYS  | N-CA-C    | -5.11 | 105.89      | 111.82   |
| 2   | H     | 108 | ILE  | N-CA-C    | -5.11 | 105.41      | 110.62   |
| 1   | A     | 586 | TYR  | N-CA-C    | -5.07 | 106.27      | 112.90   |
| 1   | A     | 547 | PHE  | CA-C-N    | 5.06  | 126.16      | 119.84   |
| 1   | A     | 547 | PHE  | C-N-CA    | 5.06  | 126.16      | 119.84   |
| 1   | G     | 698 | ALA  | N-CA-C    | 5.05  | 117.18      | 111.02   |
| 1   | C     | 681 | PHE  | N-CA-C    | 5.04  | 117.83      | 109.46   |
| 1   | G     | 530 | ARG  | CA-C-N    | 5.04  | 126.14      | 119.84   |
| 1   | G     | 530 | ARG  | C-N-CA    | 5.04  | 126.14      | 119.84   |
| 1   | E     | 6   | LEU  | N-CA-C    | 5.03  | 117.17      | 109.07   |
| 1   | C     | 37  | VAL  | CA-C-N    | 5.01  | 126.10      | 119.84   |
| 1   | C     | 37  | VAL  | C-N-CA    | 5.01  | 126.10      | 119.84   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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     | 6337  | 0        | 6346     | 929     | 5            |
| 1   | C     | 6337  | 0        | 6346     | 910     | 0            |
| 1   | E     | 6337  | 0        | 6346     | 913     | 4            |
| 1   | G     | 6337  | 0        | 6346     | 925     | 12           |
| 2   | B     | 1161  | 0        | 1126     | 172     | 0            |
| 2   | D     | 1161  | 0        | 1126     | 179     | 8            |
| 2   | F     | 1161  | 0        | 1126     | 180     | 5            |
| 2   | H     | 1161  | 0        | 1126     | 191     | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 5     | 0        | 0        | 1       | 0            |
| 4   | C     | 5     | 0        | 0        | 1       | 0            |
| 4   | E     | 5     | 0        | 0        | 1       | 0            |
| 4   | G     | 5     | 0        | 0        | 1       | 0            |
| 5   | A     | 27    | 0        | 12       | 1       | 0            |
| 5   | C     | 27    | 0        | 12       | 4       | 0            |
| 5   | E     | 27    | 0        | 12       | 4       | 0            |
| 5   | G     | 27    | 0        | 12       | 3       | 0            |
| 6   | A     | 2     | 0        | 0        | 0       | 0            |
| 6   | C     | 2     | 0        | 0        | 0       | 0            |
| 6   | E     | 2     | 0        | 0        | 0       | 0            |
| 6   | G     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 30132 | 0        | 29936    | 4315    | 17           |

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 72.

All (4315) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:89:VAL:HG12  | 2:F:144:VAL:HG21 | 1.29                     | 1.14              |
| 1:C:8:ASP:HA     | 1:C:11:LYS:HD2   | 1.31                     | 1.11              |
| 2:D:89:VAL:HG12  | 2:D:144:VAL:HG21 | 1.29                     | 1.10              |
| 1:A:8:ASP:HA     | 1:A:11:LYS:HD2   | 1.32                     | 1.09              |
| 1:G:8:ASP:HA     | 1:G:11:LYS:HD2   | 1.28                     | 1.08              |
| 1:C:628:VAL:HG13 | 1:C:631:ILE:HG13 | 1.33                     | 1.07              |
| 1:E:8:ASP:HA     | 1:E:11:LYS:HD2   | 1.31                     | 1.06              |
| 1:E:82:LYS:HG2   | 1:E:82:LYS:O     | 1.50                     | 1.06              |
| 1:C:628:VAL:HG13 | 1:C:631:ILE:CG1  | 1.85                     | 1.05              |
| 1:E:49:ILE:HA    | 1:E:59:VAL:HG22  | 1.36                     | 1.05              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:49:ILE:HA    | 1:A:59:VAL:HG22  | 1.40                     | 1.04              |
| 1:A:751:GLN:HG3  | 1:G:809:ARG:HB2  | 1.39                     | 1.03              |
| 1:G:82:LYS:O     | 1:G:82:LYS:HG2   | 1.58                     | 1.03              |
| 1:G:49:ILE:HA    | 1:G:59:VAL:HG22  | 1.41                     | 1.03              |
| 1:C:49:ILE:HA    | 1:C:59:VAL:HG22  | 1.37                     | 1.02              |
| 1:A:743:PRO:HG2  | 1:G:816:GLN:HB3  | 1.42                     | 1.01              |
| 1:C:610:THR:HG21 | 1:C:631:ILE:HG13 | 1.42                     | 1.01              |
| 1:E:79:ASN:HD22  | 1:E:80:PRO:HD2   | 1.21                     | 1.01              |
| 1:E:628:VAL:O    | 1:E:631:ILE:HG12 | 1.61                     | 1.01              |
| 2:B:89:VAL:HG12  | 2:B:144:VAL:HG21 | 1.43                     | 1.00              |
| 1:G:164:MET:HE1  | 1:G:256:PHE:HE2  | 1.25                     | 1.00              |
| 1:A:805:GLY:HA2  | 2:B:36:ARG:HG2   | 1.42                     | 1.00              |
| 1:A:541:LEU:HD23 | 1:A:601:ASN:HD22 | 1.25                     | 1.00              |
| 1:A:610:THR:HG21 | 1:A:631:ILE:HG13 | 1.42                     | 0.99              |
| 1:G:541:LEU:HD23 | 1:G:601:ASN:HD22 | 1.27                     | 0.99              |
| 1:G:419:THR:H    | 1:G:422:GLN:HE21 | 1.07                     | 0.99              |
| 1:C:805:GLY:HA2  | 2:D:36:ARG:HG2   | 1.42                     | 0.99              |
| 1:A:628:VAL:HG13 | 1:A:631:ILE:HG13 | 1.45                     | 0.99              |
| 1:E:541:LEU:HD23 | 1:E:601:ASN:HD22 | 1.23                     | 0.98              |
| 2:F:84:CYS:SG    | 2:F:86:GLU:HB2   | 2.04                     | 0.97              |
| 1:E:269:THR:HG21 | 1:E:443:LEU:HD13 | 1.44                     | 0.97              |
| 1:E:419:THR:H    | 1:E:422:GLN:HE21 | 1.04                     | 0.97              |
| 1:G:628:VAL:O    | 1:G:628:VAL:CG1  | 2.11                     | 0.97              |
| 1:C:269:THR:HG21 | 1:C:443:LEU:HD13 | 1.46                     | 0.97              |
| 1:C:541:LEU:HD23 | 1:C:601:ASN:HD22 | 1.28                     | 0.97              |
| 1:G:628:VAL:HG13 | 1:G:631:ILE:HG13 | 1.47                     | 0.97              |
| 1:G:164:MET:HE1  | 1:G:256:PHE:CE2  | 1.99                     | 0.97              |
| 1:G:269:THR:HG21 | 1:G:443:LEU:HD13 | 1.45                     | 0.97              |
| 1:G:678:ASN:HD22 | 1:G:679:PRO:HD2  | 1.26                     | 0.96              |
| 1:C:13:LEU:HD11  | 1:C:132:ILE:HB   | 1.44                     | 0.96              |
| 1:G:610:THR:HG21 | 1:G:631:ILE:HG13 | 1.48                     | 0.96              |
| 1:C:527:LEU:O    | 1:C:527:LEU:HD23 | 1.66                     | 0.96              |
| 1:C:678:ASN:HD22 | 1:C:679:PRO:HD2  | 1.28                     | 0.96              |
| 1:C:419:THR:H    | 1:C:422:GLN:HE21 | 1.09                     | 0.96              |
| 1:A:79:ASN:HD22  | 1:A:80:PRO:HD2   | 1.29                     | 0.95              |
| 1:C:628:VAL:CG1  | 1:C:628:VAL:O    | 2.14                     | 0.95              |
| 1:A:419:THR:H    | 1:A:422:GLN:HE21 | 1.06                     | 0.95              |
| 1:A:628:VAL:HG13 | 1:A:631:ILE:CG1  | 1.95                     | 0.95              |
| 1:C:82:LYS:HG2   | 1:C:82:LYS:O     | 1.64                     | 0.95              |
| 1:A:82:LYS:O     | 1:A:82:LYS:HG2   | 1.62                     | 0.95              |
| 2:F:84:CYS:O     | 2:F:87:ASP:N     | 1.99                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:610:THR:HG21 | 1:E:631:ILE:HG13 | 1.47                     | 0.94              |
| 1:A:13:LEU:HD11  | 1:A:132:ILE:HB   | 1.49                     | 0.94              |
| 1:C:36:TRP:NE1   | 1:C:78:MET:HG3   | 1.82                     | 0.94              |
| 1:A:678:ASN:HD22 | 1:A:679:PRO:HD2  | 1.32                     | 0.94              |
| 1:G:527:LEU:HD23 | 1:G:527:LEU:O    | 1.68                     | 0.94              |
| 1:G:36:TRP:NE1   | 1:G:78:MET:HG3   | 1.83                     | 0.93              |
| 1:A:269:THR:HG21 | 1:A:443:LEU:HD13 | 1.46                     | 0.93              |
| 1:E:678:ASN:HD22 | 1:E:679:PRO:HD2  | 1.30                     | 0.93              |
| 2:H:84:CYS:O     | 2:H:88:TYR:CD2   | 2.22                     | 0.93              |
| 1:G:628:VAL:HG13 | 1:G:631:ILE:CG1  | 1.99                     | 0.93              |
| 2:H:89:VAL:HG12  | 2:H:144:VAL:HG21 | 1.51                     | 0.93              |
| 1:A:527:LEU:O    | 1:A:527:LEU:HD23 | 1.68                     | 0.92              |
| 1:G:628:VAL:O    | 1:G:628:VAL:HG12 | 1.70                     | 0.92              |
| 1:E:471:ILE:O    | 1:E:471:ILE:HG12 | 1.70                     | 0.91              |
| 1:A:471:ILE:O    | 1:A:471:ILE:HG12 | 1.70                     | 0.91              |
| 1:A:628:VAL:O    | 1:A:631:ILE:HG12 | 1.71                     | 0.91              |
| 1:E:805:GLY:HA2  | 2:F:36:ARG:HG2   | 1.53                     | 0.90              |
| 1:G:471:ILE:O    | 1:G:471:ILE:HG12 | 1.67                     | 0.90              |
| 1:E:36:TRP:NE1   | 1:E:78:MET:HG3   | 1.86                     | 0.90              |
| 1:E:527:LEU:HD23 | 1:E:527:LEU:O    | 1.71                     | 0.90              |
| 1:C:345:THR:HB   | 1:C:348:GLU:HB2  | 1.54                     | 0.90              |
| 1:C:576:LYS:HA   | 1:C:579:THR:HA   | 1.53                     | 0.90              |
| 1:G:576:LYS:HA   | 1:G:579:THR:HA   | 1.53                     | 0.90              |
| 1:A:135:GLU:HB2  | 1:A:212:GLY:O    | 1.71                     | 0.90              |
| 1:C:79:ASN:HD22  | 1:C:80:PRO:HD2   | 1.37                     | 0.90              |
| 1:E:250:LYS:HE2  | 1:E:465:ASP:OD2  | 1.70                     | 0.90              |
| 1:A:345:THR:HB   | 1:A:348:GLU:HB2  | 1.53                     | 0.90              |
| 1:G:401:SER:HB3  | 1:G:608:ASN:HB3  | 1.54                     | 0.89              |
| 1:C:401:SER:HB3  | 1:C:608:ASN:HB3  | 1.54                     | 0.89              |
| 1:E:607:ASP:HA   | 1:E:610:THR:HB   | 1.54                     | 0.89              |
| 1:G:345:THR:HB   | 1:G:348:GLU:HB2  | 1.55                     | 0.89              |
| 1:A:36:TRP:NE1   | 1:A:78:MET:HG3   | 1.86                     | 0.89              |
| 1:E:401:SER:HB3  | 1:E:608:ASN:HB3  | 1.53                     | 0.89              |
| 1:A:576:LYS:HA   | 1:A:579:THR:HA   | 1.54                     | 0.89              |
| 1:G:377:SER:O    | 1:G:379:PRO:HD3  | 1.73                     | 0.89              |
| 1:E:419:THR:N    | 1:E:422:GLN:HE21 | 1.71                     | 0.88              |
| 1:G:79:ASN:HD22  | 1:G:80:PRO:HD2   | 1.37                     | 0.88              |
| 1:G:236:ASN:ND2  | 1:G:246:SER:HA   | 1.87                     | 0.88              |
| 2:H:26:ILE:HG23  | 2:H:30:GLN:HB2   | 1.54                     | 0.88              |
| 2:D:26:ILE:HG23  | 2:D:30:GLN:HB2   | 1.54                     | 0.88              |
| 1:A:401:SER:HB3  | 1:A:608:ASN:HB3  | 1.53                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:26:ILE:HG23  | 2:B:30:GLN:HB2   | 1.54                     | 0.88              |
| 1:C:13:LEU:CD1   | 1:C:132:ILE:HB   | 2.03                     | 0.88              |
| 1:E:135:GLU:HB2  | 1:E:212:GLY:O    | 1.72                     | 0.88              |
| 1:C:471:ILE:O    | 1:C:471:ILE:HG12 | 1.70                     | 0.88              |
| 1:G:230:ILE:HG22 | 1:G:231:LEU:HD23 | 1.56                     | 0.87              |
| 1:G:806:TYR:CD2  | 2:H:147:VAL:HA   | 2.10                     | 0.87              |
| 2:F:26:ILE:HG23  | 2:F:30:GLN:HB2   | 1.54                     | 0.87              |
| 1:C:250:LYS:HE2  | 1:C:465:ASP:OD2  | 1.74                     | 0.87              |
| 1:C:607:ASP:HA   | 1:C:610:THR:HB   | 1.56                     | 0.87              |
| 1:A:607:ASP:HA   | 1:A:610:THR:HB   | 1.55                     | 0.87              |
| 1:C:376:ALA:HB2  | 1:C:420:LYS:HB2  | 1.54                     | 0.87              |
| 1:E:659:VAL:HG12 | 1:E:660:GLY:N    | 1.90                     | 0.87              |
| 1:A:187:THR:HG23 | 1:A:463:ILE:HG21 | 1.56                     | 0.87              |
| 1:G:135:GLU:HB2  | 1:G:212:GLY:O    | 1.74                     | 0.87              |
| 1:E:236:ASN:ND2  | 1:E:246:SER:HA   | 1.91                     | 0.86              |
| 1:A:419:THR:N    | 1:A:422:GLN:HE21 | 1.73                     | 0.86              |
| 1:C:135:GLU:HB2  | 1:C:212:GLY:O    | 1.75                     | 0.85              |
| 1:C:377:SER:O    | 1:C:379:PRO:HD3  | 1.77                     | 0.85              |
| 1:C:331:MET:O    | 1:C:335:THR:HG23 | 1.76                     | 0.85              |
| 1:E:806:TYR:CD2  | 2:F:147:VAL:HA   | 2.12                     | 0.85              |
| 1:E:576:LYS:HA   | 1:E:579:THR:HA   | 1.56                     | 0.85              |
| 1:G:747:MET:HE3  | 1:G:752:ALA:HA   | 1.58                     | 0.85              |
| 1:A:625:TRP:O    | 1:A:627:ASP:N    | 2.10                     | 0.85              |
| 1:A:230:ILE:HG22 | 1:A:231:LEU:HD23 | 1.58                     | 0.84              |
| 1:G:187:THR:HG23 | 1:G:463:ILE:HG21 | 1.57                     | 0.84              |
| 1:E:814:LYS:HE3  | 1:E:818:GLN:HE22 | 1.42                     | 0.84              |
| 1:C:164:MET:HE1  | 1:C:256:PHE:HE2  | 1.43                     | 0.84              |
| 1:A:747:MET:HE3  | 1:A:752:ALA:HA   | 1.60                     | 0.84              |
| 1:C:747:MET:HE3  | 1:C:752:ALA:HA   | 1.59                     | 0.84              |
| 1:A:236:ASN:ND2  | 1:A:246:SER:HA   | 1.93                     | 0.84              |
| 1:E:79:ASN:HD22  | 1:E:80:PRO:CD    | 1.90                     | 0.84              |
| 1:E:345:THR:HB   | 1:E:348:GLU:HB2  | 1.57                     | 0.84              |
| 1:G:814:LYS:HE3  | 1:G:818:GLN:HE22 | 1.42                     | 0.84              |
| 1:G:250:LYS:HE2  | 1:G:465:ASP:OD2  | 1.77                     | 0.83              |
| 1:G:814:LYS:O    | 1:G:817:GLN:HG2  | 1.78                     | 0.83              |
| 1:E:331:MET:O    | 1:E:335:THR:HG23 | 1.78                     | 0.83              |
| 1:E:377:SER:O    | 1:E:379:PRO:HD3  | 1.77                     | 0.83              |
| 1:A:747:MET:HG3  | 1:G:812:PHE:CE2  | 2.13                     | 0.83              |
| 1:C:232:GLU:HA   | 1:C:236:ASN:OD1  | 1.78                     | 0.83              |
| 1:C:806:TYR:CD2  | 2:D:147:VAL:HA   | 2.13                     | 0.83              |
| 1:G:471:ILE:O    | 1:G:471:ILE:CG1  | 2.26                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:814:LYS:HE3  | 1:C:818:GLN:HE22 | 1.43                     | 0.83              |
| 1:E:582:CYS:SG   | 1:E:591:THR:HG23 | 2.18                     | 0.83              |
| 1:E:804:ARG:HG2  | 1:E:804:ARG:HH11 | 1.41                     | 0.83              |
| 1:A:232:GLU:HA   | 1:A:236:ASN:OD1  | 1.79                     | 0.83              |
| 1:E:576:LYS:O    | 1:E:579:THR:HG23 | 1.79                     | 0.83              |
| 1:A:471:ILE:O    | 1:A:471:ILE:CG1  | 2.26                     | 0.83              |
| 1:G:607:ASP:HA   | 1:G:610:THR:HB   | 1.57                     | 0.83              |
| 1:C:628:VAL:O    | 1:C:628:VAL:HG12 | 1.78                     | 0.83              |
| 1:E:62:GLN:HG3   | 1:E:62:GLN:O     | 1.78                     | 0.83              |
| 1:C:814:LYS:O    | 1:C:817:GLN:HG2  | 1.78                     | 0.82              |
| 1:A:576:LYS:O    | 1:A:579:THR:HG23 | 1.78                     | 0.82              |
| 1:C:419:THR:N    | 1:C:422:GLN:HE21 | 1.76                     | 0.82              |
| 1:A:377:SER:O    | 1:A:379:PRO:HD3  | 1.79                     | 0.82              |
| 1:A:37:VAL:HG12  | 1:A:38:PRO:HD2   | 1.61                     | 0.82              |
| 1:C:37:VAL:HG12  | 1:C:38:PRO:HD2   | 1.61                     | 0.82              |
| 1:C:62:GLN:O     | 1:C:62:GLN:HG3   | 1.79                     | 0.82              |
| 1:E:747:MET:HE3  | 1:E:752:ALA:HA   | 1.62                     | 0.82              |
| 1:E:232:GLU:HA   | 1:E:236:ASN:OD1  | 1.77                     | 0.82              |
| 1:E:493:PHE:O    | 1:E:497:MET:HB2  | 1.79                     | 0.82              |
| 1:G:419:THR:N    | 1:G:422:GLN:HE21 | 1.76                     | 0.82              |
| 2:H:83:GLY:HA3   | 2:H:88:TYR:OH    | 1.79                     | 0.82              |
| 1:C:471:ILE:O    | 1:C:471:ILE:CG1  | 2.28                     | 0.81              |
| 1:C:792:ILE:O    | 1:C:796:ILE:HG12 | 1.80                     | 0.81              |
| 1:E:424:ASP:HA   | 1:E:427:ILE:HG22 | 1.62                     | 0.81              |
| 1:A:751:GLN:OE1  | 1:G:813:ALA:CB   | 2.28                     | 0.81              |
| 1:C:236:ASN:ND2  | 1:C:246:SER:HA   | 1.95                     | 0.81              |
| 1:C:493:PHE:O    | 1:C:497:MET:HB2  | 1.80                     | 0.81              |
| 1:E:471:ILE:O    | 1:E:471:ILE:CG1  | 2.28                     | 0.81              |
| 1:C:230:ILE:HG22 | 1:C:231:LEU:HD23 | 1.63                     | 0.81              |
| 1:A:743:PRO:CG   | 1:G:816:GLN:HB3  | 2.09                     | 0.81              |
| 1:G:493:PHE:O    | 1:G:497:MET:HB2  | 1.80                     | 0.81              |
| 1:A:405:PRO:HB2  | 1:A:407:ILE:CG2  | 2.11                     | 0.81              |
| 1:E:418:GLN:HB3  | 1:E:422:GLN:HB2  | 1.63                     | 0.81              |
| 1:G:424:ASP:HA   | 1:G:427:ILE:HG22 | 1.61                     | 0.81              |
| 1:A:62:GLN:HG3   | 1:A:62:GLN:O     | 1.79                     | 0.81              |
| 2:D:58:GLU:HA    | 2:D:61:LEU:HD12  | 1.62                     | 0.81              |
| 2:B:58:GLU:HA    | 2:B:61:LEU:HD12  | 1.63                     | 0.81              |
| 2:F:58:GLU:HA    | 2:F:61:LEU:HD12  | 1.63                     | 0.81              |
| 1:G:232:GLU:HA   | 1:G:236:ASN:OD1  | 1.81                     | 0.81              |
| 2:H:58:GLU:HA    | 2:H:61:LEU:HD12  | 1.63                     | 0.80              |
| 1:A:540:LEU:HD12 | 1:A:559:LEU:HD12 | 1.63                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:352:ILE:HG21 | 1:E:442:ILE:HD11 | 1.63                     | 0.80              |
| 1:A:164:MET:HE1  | 1:A:256:PHE:HE2  | 1.43                     | 0.80              |
| 1:G:37:VAL:HG12  | 1:G:38:PRO:HD2   | 1.61                     | 0.80              |
| 1:G:418:GLN:HB3  | 1:G:422:GLN:HB2  | 1.62                     | 0.80              |
| 1:E:814:LYS:O    | 1:E:817:GLN:HG2  | 1.81                     | 0.80              |
| 1:A:437:ARG:HE   | 1:A:625:TRP:HA   | 1.47                     | 0.80              |
| 1:E:230:ILE:HG22 | 1:E:231:LEU:HD23 | 1.62                     | 0.80              |
| 1:G:161:TYR:O    | 1:G:165:LEU:HD12 | 1.81                     | 0.80              |
| 1:G:376:ALA:HB2  | 1:G:420:LYS:HB2  | 1.63                     | 0.80              |
| 1:A:628:VAL:O    | 1:A:628:VAL:CG1  | 2.30                     | 0.80              |
| 1:C:582:CYS:SG   | 1:C:591:THR:HG23 | 2.21                     | 0.80              |
| 1:G:62:GLN:HG3   | 1:G:62:GLN:O     | 1.80                     | 0.80              |
| 1:A:806:TYR:CD2  | 2:B:147:VAL:HA   | 2.16                     | 0.80              |
| 1:C:424:ASP:HA   | 1:C:427:ILE:HG22 | 1.64                     | 0.80              |
| 1:A:164:MET:HE1  | 1:A:256:PHE:CE2  | 2.17                     | 0.80              |
| 1:C:164:MET:HE1  | 1:C:256:PHE:CE2  | 2.17                     | 0.80              |
| 1:G:331:MET:O    | 1:G:335:THR:HG23 | 1.81                     | 0.80              |
| 2:H:85:PHE:CE1   | 2:H:145:ARG:HG2  | 2.15                     | 0.80              |
| 1:A:420:LYS:O    | 1:A:423:ALA:HB3  | 1.82                     | 0.80              |
| 2:D:114:THR:C    | 2:D:115:LEU:HD12 | 2.07                     | 0.80              |
| 1:E:792:ILE:O    | 1:E:796:ILE:HG12 | 1.82                     | 0.80              |
| 1:E:405:PRO:HB2  | 1:E:407:ILE:CG2  | 2.12                     | 0.79              |
| 2:H:114:THR:C    | 2:H:115:LEU:HD12 | 2.07                     | 0.79              |
| 1:A:424:ASP:HA   | 1:A:427:ILE:HG22 | 1.64                     | 0.79              |
| 1:E:164:MET:HE1  | 1:E:256:PHE:HE2  | 1.44                     | 0.79              |
| 1:A:259:THR:HB   | 1:A:261:TYR:CE1  | 2.18                     | 0.79              |
| 1:E:323:ILE:HG23 | 1:E:326:GLN:HB3  | 1.63                     | 0.79              |
| 1:A:331:MET:O    | 1:A:335:THR:HG23 | 1.82                     | 0.79              |
| 1:A:804:ARG:HH11 | 1:A:804:ARG:HG2  | 1.48                     | 0.79              |
| 1:C:272:LEU:C    | 1:C:272:LEU:HD12 | 2.08                     | 0.79              |
| 1:G:576:LYS:O    | 1:G:579:THR:HG23 | 1.82                     | 0.79              |
| 1:A:493:PHE:O    | 1:A:497:MET:HB2  | 1.82                     | 0.79              |
| 1:E:37:VAL:HG12  | 1:E:38:PRO:HD2   | 1.62                     | 0.79              |
| 1:G:420:LYS:O    | 1:G:423:ALA:HB3  | 1.83                     | 0.79              |
| 1:A:751:GLN:OE1  | 1:G:813:ALA:HB2  | 1.81                     | 0.79              |
| 1:C:187:THR:HG23 | 1:C:463:ILE:HG21 | 1.65                     | 0.79              |
| 1:G:502:GLN:HG2  | 1:G:512:TRP:HE1  | 1.47                     | 0.79              |
| 1:A:352:ILE:HG21 | 1:A:442:ILE:HD11 | 1.65                     | 0.79              |
| 1:A:558:LYS:O    | 1:A:561:GLN:HB3  | 1.82                     | 0.79              |
| 1:G:405:PRO:HB2  | 1:G:407:ILE:CG2  | 2.12                     | 0.79              |
| 1:G:437:ARG:HE   | 1:G:625:TRP:HA   | 1.47                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:148:GLU:O    | 1:A:149:MET:HG2  | 1.83                     | 0.78              |
| 1:A:582:CYS:SG   | 1:A:591:THR:HG23 | 2.23                     | 0.78              |
| 2:B:65:LYS:HD2   | 2:B:68:GLN:HE21  | 1.48                     | 0.78              |
| 1:C:558:LYS:O    | 1:C:561:GLN:HB3  | 1.83                     | 0.78              |
| 1:E:502:GLN:HG2  | 1:E:512:TRP:HE1  | 1.47                     | 0.78              |
| 1:E:690:GLU:HB3  | 1:E:692:ARG:HG3  | 1.65                     | 0.78              |
| 1:G:520:ASP:C    | 1:G:521:LEU:HD23 | 2.08                     | 0.78              |
| 1:E:407:ILE:HG13 | 1:E:414:VAL:O    | 1.84                     | 0.78              |
| 2:F:65:LYS:HD2   | 2:F:68:GLN:HE21  | 1.49                     | 0.78              |
| 1:A:244:ASN:ND2  | 1:A:244:ASN:O    | 2.17                     | 0.78              |
| 1:E:376:ALA:HB2  | 1:E:420:LYS:HB2  | 1.65                     | 0.78              |
| 1:A:376:ALA:HB2  | 1:A:420:LYS:HB2  | 1.65                     | 0.78              |
| 1:E:520:ASP:C    | 1:E:521:LEU:HD23 | 2.08                     | 0.78              |
| 1:G:558:LYS:O    | 1:G:561:GLN:HB3  | 1.82                     | 0.78              |
| 1:C:610:THR:CG2  | 1:C:628:VAL:HG11 | 2.14                     | 0.78              |
| 1:C:690:GLU:HB3  | 1:C:692:ARG:HG3  | 1.63                     | 0.78              |
| 2:F:84:CYS:SG    | 2:F:87:ASP:OD2   | 2.42                     | 0.78              |
| 1:A:323:ILE:HG23 | 1:A:326:GLN:HB3  | 1.65                     | 0.78              |
| 2:D:10:GLU:HA    | 2:D:13:GLU:HG3   | 1.66                     | 0.78              |
| 1:G:33:LYS:HB3   | 1:G:49:ILE:HB    | 1.64                     | 0.78              |
| 1:G:352:ILE:HG21 | 1:G:442:ILE:HD11 | 1.64                     | 0.78              |
| 1:E:272:LEU:C    | 1:E:272:LEU:HD12 | 2.08                     | 0.78              |
| 1:G:582:CYS:SG   | 1:G:591:THR:HG23 | 2.24                     | 0.78              |
| 1:G:272:LEU:C    | 1:G:272:LEU:HD12 | 2.09                     | 0.78              |
| 1:A:83:PHE:HB3   | 1:A:92:LEU:HD23  | 1.64                     | 0.77              |
| 1:C:418:GLN:HB3  | 1:C:422:GLN:HB2  | 1.65                     | 0.77              |
| 1:C:33:LYS:HB3   | 1:C:49:ILE:HB    | 1.66                     | 0.77              |
| 1:C:502:GLN:HG2  | 1:C:512:TRP:HE1  | 1.49                     | 0.77              |
| 1:G:148:GLU:O    | 1:G:149:MET:HG2  | 1.84                     | 0.77              |
| 1:A:418:GLN:HB3  | 1:A:422:GLN:HB2  | 1.65                     | 0.77              |
| 1:C:814:LYS:HG3  | 1:C:815:ARG:N    | 1.97                     | 0.77              |
| 1:A:610:THR:HG22 | 1:A:611:SER:N    | 2.00                     | 0.77              |
| 1:E:259:THR:HB   | 1:E:261:TYR:CE1  | 2.19                     | 0.77              |
| 1:G:659:VAL:HG12 | 1:G:660:GLY:N    | 1.98                     | 0.77              |
| 1:A:293:LEU:HD11 | 1:A:301:MET:HE1  | 1.67                     | 0.77              |
| 1:G:804:ARG:HG2  | 1:G:804:ARG:HH11 | 1.48                     | 0.77              |
| 1:C:437:ARG:HE   | 1:C:625:TRP:HA   | 1.49                     | 0.77              |
| 1:E:187:THR:HG23 | 1:E:463:ILE:HG21 | 1.64                     | 0.77              |
| 1:A:502:GLN:HG2  | 1:A:512:TRP:HE1  | 1.49                     | 0.77              |
| 1:C:405:PRO:HB2  | 1:C:407:ILE:CG2  | 2.14                     | 0.77              |
| 1:E:663:TYR:O    | 1:E:665:GLU:N    | 2.17                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:259:THR:HB   | 1:C:261:TYR:CE1  | 2.19                     | 0.77              |
| 2:D:65:LYS:HD2   | 2:D:68:GLN:HE21  | 1.48                     | 0.77              |
| 2:F:114:THR:C    | 2:F:115:LEU:HD12 | 2.10                     | 0.77              |
| 1:C:628:VAL:HG13 | 1:C:631:ILE:HG12 | 1.67                     | 0.77              |
| 1:E:164:MET:HE1  | 1:E:256:PHE:CE2  | 2.19                     | 0.77              |
| 2:H:65:LYS:HD2   | 2:H:68:GLN:HE21  | 1.48                     | 0.77              |
| 1:C:148:GLU:O    | 1:C:149:MET:HG2  | 1.85                     | 0.77              |
| 1:C:293:LEU:HD11 | 1:C:301:MET:HE1  | 1.66                     | 0.77              |
| 1:C:520:ASP:C    | 1:C:521:LEU:HD23 | 2.09                     | 0.77              |
| 1:E:558:LYS:O    | 1:E:561:GLN:HB3  | 1.84                     | 0.77              |
| 1:G:259:THR:HB   | 1:G:261:TYR:CE1  | 2.20                     | 0.77              |
| 1:A:690:GLU:HB3  | 1:A:692:ARG:HG3  | 1.65                     | 0.76              |
| 1:C:663:TYR:O    | 1:C:665:GLU:N    | 2.18                     | 0.76              |
| 1:C:659:VAL:HG12 | 1:C:660:GLY:N    | 1.98                     | 0.76              |
| 1:A:659:VAL:HG12 | 1:A:660:GLY:N    | 2.00                     | 0.76              |
| 1:C:79:ASN:OD1   | 1:C:92:LEU:HB3   | 1.84                     | 0.76              |
| 1:C:352:ILE:HG21 | 1:C:442:ILE:HD11 | 1.66                     | 0.76              |
| 1:C:540:LEU:HD12 | 1:C:559:LEU:HD12 | 1.67                     | 0.76              |
| 1:E:135:GLU:CD   | 1:E:215:PHE:HB2  | 2.11                     | 0.76              |
| 1:G:323:ILE:HG23 | 1:G:326:GLN:HB3  | 1.68                     | 0.76              |
| 1:A:814:LYS:HE3  | 1:A:818:GLN:HE22 | 1.47                     | 0.76              |
| 1:C:771:GLN:HE21 | 1:C:771:GLN:C    | 1.94                     | 0.76              |
| 1:C:804:ARG:HG2  | 1:C:804:ARG:HH11 | 1.50                     | 0.76              |
| 2:F:85:PHE:HA    | 2:F:89:VAL:HG13  | 1.65                     | 0.76              |
| 1:G:625:TRP:O    | 1:G:627:ASP:N    | 2.19                     | 0.76              |
| 1:A:135:GLU:CD   | 1:A:215:PHE:HB2  | 2.11                     | 0.76              |
| 2:B:114:THR:C    | 2:B:115:LEU:HD12 | 2.11                     | 0.76              |
| 2:D:141:GLU:O    | 2:D:145:ARG:HG3  | 1.85                     | 0.76              |
| 1:C:747:MET:HB3  | 1:C:752:ALA:HB2  | 1.67                     | 0.76              |
| 1:E:13:LEU:HD11  | 1:E:152:HIS:CD2  | 2.21                     | 0.76              |
| 1:E:293:LEU:HD11 | 1:E:301:MET:HE1  | 1.67                     | 0.76              |
| 1:C:576:LYS:O    | 1:C:579:THR:HG23 | 1.85                     | 0.76              |
| 1:G:690:GLU:HB3  | 1:G:692:ARG:HG3  | 1.65                     | 0.76              |
| 1:A:520:ASP:C    | 1:A:521:LEU:HD23 | 2.11                     | 0.76              |
| 2:H:10:GLU:HA    | 2:H:13:GLU:HG3   | 1.67                     | 0.76              |
| 2:B:10:GLU:HA    | 2:B:13:GLU:HG3   | 1.66                     | 0.75              |
| 1:E:80:PRO:HG2   | 1:E:83:PHE:CE2   | 2.20                     | 0.75              |
| 1:E:420:LYS:O    | 1:E:423:ALA:HB3  | 1.85                     | 0.75              |
| 1:E:44:PHE:CE2   | 1:E:702:LEU:HD21 | 2.21                     | 0.75              |
| 1:E:747:MET:HB3  | 1:E:752:ALA:HB2  | 1.65                     | 0.75              |
| 1:G:663:TYR:O    | 1:G:665:GLU:N    | 2.19                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:814:LYS:O    | 1:A:817:GLN:HG2  | 1.85                     | 0.75              |
| 1:E:30:SER:C     | 1:E:32:LYS:H     | 1.94                     | 0.75              |
| 1:C:610:THR:HG22 | 1:C:611:SER:N    | 2.01                     | 0.75              |
| 1:G:540:LEU:HD12 | 1:G:559:LEU:HD12 | 1.67                     | 0.75              |
| 1:C:114:TYR:CE2  | 1:C:153:ILE:HB   | 2.21                     | 0.75              |
| 1:C:420:LYS:O    | 1:C:423:ALA:HB3  | 1.87                     | 0.75              |
| 1:A:114:TYR:CE2  | 1:A:153:ILE:HB   | 2.21                     | 0.75              |
| 1:E:540:LEU:HD12 | 1:E:559:LEU:HD12 | 1.67                     | 0.75              |
| 2:D:112:LEU:HD13 | 2:D:119:MET:HE3  | 1.69                     | 0.75              |
| 1:G:747:MET:HB3  | 1:G:752:ALA:HB2  | 1.68                     | 0.75              |
| 2:F:10:GLU:HA    | 2:F:13:GLU:HG3   | 1.66                     | 0.75              |
| 1:G:114:TYR:CE2  | 1:G:153:ILE:HB   | 2.22                     | 0.75              |
| 1:G:135:GLU:CD   | 1:G:215:PHE:HB2  | 2.12                     | 0.75              |
| 1:E:552:ASP:O    | 1:E:556:VAL:HG23 | 1.87                     | 0.74              |
| 1:E:568:LYS:HD3  | 1:E:584:LEU:HB2  | 1.69                     | 0.74              |
| 1:G:79:ASN:HD22  | 1:G:80:PRO:CD    | 1.99                     | 0.74              |
| 1:G:293:LEU:HD11 | 1:G:301:MET:HE1  | 1.69                     | 0.74              |
| 1:E:148:GLU:O    | 1:E:149:MET:HG2  | 1.86                     | 0.74              |
| 2:F:85:PHE:O     | 2:F:86:GLU:C     | 2.28                     | 0.74              |
| 1:C:541:LEU:HD21 | 1:C:597:TRP:HB3  | 1.69                     | 0.74              |
| 1:E:134:SER:HB2  | 1:E:212:GLY:HA2  | 1.68                     | 0.74              |
| 1:E:244:ASN:O    | 1:E:244:ASN:ND2  | 2.20                     | 0.74              |
| 1:G:61:LEU:C     | 1:G:63:GLU:H     | 1.96                     | 0.74              |
| 1:G:244:ASN:O    | 1:G:244:ASN:ND2  | 2.20                     | 0.74              |
| 1:C:320:HIS:C    | 1:C:320:HIS:HD1  | 1.96                     | 0.74              |
| 1:E:619:LYS:O    | 1:E:622:ALA:HB3  | 1.87                     | 0.74              |
| 1:G:134:SER:HB2  | 1:G:212:GLY:HA2  | 1.69                     | 0.74              |
| 1:A:272:LEU:C    | 1:A:272:LEU:HD12 | 2.12                     | 0.74              |
| 1:A:771:GLN:HE21 | 1:A:771:GLN:C    | 1.95                     | 0.74              |
| 1:C:494:ASN:HD22 | 1:C:494:ASN:H    | 1.34                     | 0.74              |
| 1:G:30:SER:C     | 1:G:32:LYS:H     | 1.94                     | 0.74              |
| 1:A:30:SER:C     | 1:A:32:LYS:H     | 1.94                     | 0.74              |
| 1:A:79:ASN:HD22  | 1:A:80:PRO:CD    | 1.99                     | 0.74              |
| 1:C:135:GLU:CD   | 1:C:215:PHE:HB2  | 2.11                     | 0.74              |
| 1:C:628:VAL:HG22 | 1:C:631:ILE:HD11 | 1.70                     | 0.74              |
| 1:A:407:ILE:HG13 | 1:A:414:VAL:O    | 1.88                     | 0.73              |
| 1:E:320:HIS:HD1  | 1:E:320:HIS:C    | 1.96                     | 0.73              |
| 1:G:377:SER:C    | 1:G:379:PRO:HD3  | 2.13                     | 0.73              |
| 1:E:33:LYS:HB3   | 1:E:49:ILE:HB    | 1.67                     | 0.73              |
| 1:G:10:GLU:O     | 1:G:14:PHE:HB2   | 1.88                     | 0.73              |
| 1:G:610:THR:HG22 | 1:G:611:SER:N    | 2.01                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:678:ASN:ND2  | 1:G:679:PRO:HD2  | 2.03                     | 0.73              |
| 1:C:527:LEU:O    | 1:C:537:VAL:HG23 | 1.88                     | 0.73              |
| 1:C:715:ARG:O    | 1:C:719:GLN:HG2  | 1.86                     | 0.73              |
| 1:A:33:LYS:HB3   | 1:A:49:ILE:HB    | 1.70                     | 0.73              |
| 1:A:663:TYR:O    | 1:A:665:GLU:N    | 2.20                     | 0.73              |
| 1:C:323:ILE:HG23 | 1:C:326:GLN:HB3  | 1.69                     | 0.73              |
| 1:A:22:ASN:OD1   | 1:A:24:LEU:HB2   | 1.88                     | 0.73              |
| 2:B:141:GLU:O    | 2:B:145:ARG:HG3  | 1.88                     | 0.73              |
| 1:C:377:SER:C    | 1:C:379:PRO:HD3  | 2.14                     | 0.73              |
| 1:C:721:PHE:N    | 1:C:721:PHE:CD1  | 2.56                     | 0.73              |
| 1:C:234:PHE:HD1  | 1:C:289:ILE:HG21 | 1.51                     | 0.73              |
| 1:C:700:LEU:HD23 | 1:C:704:GLN:HE22 | 1.53                     | 0.73              |
| 1:G:407:ILE:HG13 | 1:G:414:VAL:O    | 1.87                     | 0.73              |
| 2:H:85:PHE:HB3   | 2:H:86:GLU:OE1   | 1.88                     | 0.73              |
| 1:A:792:ILE:O    | 1:A:796:ILE:HG12 | 1.89                     | 0.73              |
| 1:E:302:ARG:O    | 1:E:307:LEU:HD12 | 1.89                     | 0.73              |
| 1:E:114:TYR:CE2  | 1:E:153:ILE:HB   | 2.24                     | 0.73              |
| 1:E:715:ARG:O    | 1:E:719:GLN:HG2  | 1.89                     | 0.73              |
| 1:G:365:ILE:HD13 | 1:G:427:ILE:HD11 | 1.70                     | 0.73              |
| 1:A:715:ARG:O    | 1:A:719:GLN:HG2  | 1.89                     | 0.73              |
| 1:G:792:ILE:O    | 1:G:796:ILE:HG12 | 1.89                     | 0.73              |
| 1:G:814:LYS:HG3  | 1:G:815:ARG:N    | 2.04                     | 0.72              |
| 1:A:18:ASN:O     | 1:A:19:PHE:CD1   | 2.42                     | 0.72              |
| 1:C:30:SER:C     | 1:C:32:LYS:H     | 1.95                     | 0.72              |
| 1:C:313:TYR:HB2  | 1:C:316:LEU:CD1  | 2.20                     | 0.72              |
| 1:E:10:GLU:O     | 1:E:14:PHE:HB2   | 1.88                     | 0.72              |
| 1:C:628:VAL:O    | 1:C:631:ILE:HG12 | 1.89                     | 0.72              |
| 1:C:736:ILE:HG23 | 1:C:737:LEU:HD23 | 1.70                     | 0.72              |
| 1:A:302:ARG:O    | 1:A:307:LEU:HD12 | 1.89                     | 0.72              |
| 1:C:48:SER:C     | 1:C:59:VAL:HG13  | 2.15                     | 0.72              |
| 1:C:568:LYS:HD3  | 1:C:584:LEU:HB2  | 1.70                     | 0.72              |
| 1:E:243:ASP:HB3  | 1:E:323:ILE:HD11 | 1.71                     | 0.72              |
| 1:E:610:THR:HG22 | 1:E:611:SER:N    | 2.03                     | 0.72              |
| 2:D:65:LYS:O     | 2:D:68:GLN:HG3   | 1.90                     | 0.72              |
| 1:A:50:LYS:HE3   | 1:A:60:GLU:HB3   | 1.72                     | 0.72              |
| 1:A:568:LYS:HD3  | 1:A:584:LEU:HB2  | 1.72                     | 0.72              |
| 1:C:407:ILE:HD12 | 1:C:408:LYS:N    | 2.05                     | 0.72              |
| 1:A:10:GLU:O     | 1:A:14:PHE:HB2   | 1.90                     | 0.72              |
| 1:A:700:LEU:HD23 | 1:A:704:GLN:HE22 | 1.54                     | 0.72              |
| 1:A:13:LEU:CD1   | 1:A:132:ILE:HB   | 2.19                     | 0.72              |
| 1:C:79:ASN:HD22  | 1:C:80:PRO:CD    | 2.03                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:85:PHE:O     | 2:D:86:GLU:C     | 2.32                     | 0.72              |
| 1:E:161:TYR:O    | 1:E:165:LEU:HD12 | 1.89                     | 0.72              |
| 1:G:700:LEU:HD23 | 1:G:704:GLN:HE22 | 1.54                     | 0.72              |
| 1:A:407:ILE:HD12 | 1:A:408:LYS:N    | 2.04                     | 0.72              |
| 1:C:161:TYR:O    | 1:C:165:LEU:HD12 | 1.88                     | 0.72              |
| 2:F:112:LEU:HD13 | 2:F:119:MET:HE3  | 1.71                     | 0.72              |
| 2:H:141:GLU:O    | 2:H:145:ARG:HG3  | 1.88                     | 0.72              |
| 1:C:244:ASN:O    | 1:C:244:ASN:ND2  | 2.23                     | 0.71              |
| 2:F:65:LYS:O     | 2:F:68:GLN:HG3   | 1.89                     | 0.71              |
| 2:H:65:LYS:O     | 2:H:68:GLN:HG3   | 1.90                     | 0.71              |
| 2:H:112:LEU:HD13 | 2:H:119:MET:HE3  | 1.70                     | 0.71              |
| 2:B:65:LYS:O     | 2:B:68:GLN:HG3   | 1.90                     | 0.71              |
| 1:C:678:ASN:HD22 | 1:C:679:PRO:CD   | 2.02                     | 0.71              |
| 1:E:79:ASN:ND2   | 1:E:80:PRO:HD2   | 2.02                     | 0.71              |
| 1:E:399:THR:HG22 | 1:E:403:LEU:HD11 | 1.71                     | 0.71              |
| 1:G:320:HIS:HD1  | 1:G:320:HIS:C    | 1.97                     | 0.71              |
| 1:G:552:ASP:O    | 1:G:556:VAL:HG23 | 1.89                     | 0.71              |
| 1:E:541:LEU:HD23 | 1:E:601:ASN:ND2  | 2.03                     | 0.71              |
| 1:G:302:ARG:O    | 1:G:307:LEU:HD12 | 1.90                     | 0.71              |
| 2:B:4:SER:N      | 2:B:7:GLN:HE21   | 1.89                     | 0.71              |
| 1:C:10:GLU:O     | 1:C:14:PHE:HB2   | 1.89                     | 0.71              |
| 1:C:376:ALA:HB3  | 1:C:420:LYS:HA   | 1.72                     | 0.71              |
| 1:C:407:ILE:HD12 | 1:C:409:VAL:N    | 2.05                     | 0.71              |
| 1:C:796:ILE:HG22 | 1:C:800:GLN:OE1  | 1.90                     | 0.71              |
| 1:E:377:SER:C    | 1:E:379:PRO:HD3  | 2.14                     | 0.71              |
| 1:G:568:LYS:HD3  | 1:G:584:LEU:HB2  | 1.72                     | 0.71              |
| 2:B:86:GLU:H     | 2:B:86:GLU:CD    | 1.98                     | 0.71              |
| 1:A:48:SER:C     | 1:A:59:VAL:HG13  | 2.15                     | 0.71              |
| 1:A:61:LEU:C     | 1:A:63:GLU:H     | 1.96                     | 0.71              |
| 1:A:736:ILE:HG23 | 1:A:737:LEU:HD23 | 1.72                     | 0.71              |
| 1:C:134:SER:HB2  | 1:C:212:GLY:HA2  | 1.71                     | 0.71              |
| 1:C:302:ARG:O    | 1:C:307:LEU:HD12 | 1.89                     | 0.71              |
| 1:E:269:THR:CG2  | 1:E:443:LEU:HD13 | 2.19                     | 0.71              |
| 1:E:407:ILE:HD11 | 1:E:414:VAL:HB   | 1.73                     | 0.71              |
| 1:E:407:ILE:HD12 | 1:E:408:LYS:N    | 2.05                     | 0.71              |
| 1:A:399:THR:HG22 | 1:A:403:LEU:HD11 | 1.73                     | 0.71              |
| 1:C:535:PRO:HB2  | 1:C:540:LEU:HD21 | 1.73                     | 0.71              |
| 1:E:61:LEU:C     | 1:E:63:GLU:H     | 1.96                     | 0.71              |
| 1:E:409:VAL:HG22 | 1:E:634:LEU:HD12 | 1.73                     | 0.71              |
| 1:G:313:TYR:HB2  | 1:G:316:LEU:CD1  | 2.21                     | 0.71              |
| 1:G:715:ARG:O    | 1:G:719:GLN:HG2  | 1.91                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:377:SER:C    | 1:A:379:PRO:HD3  | 2.14                     | 0.71              |
| 1:C:50:LYS:HE3   | 1:C:60:GLU:HB3   | 1.73                     | 0.71              |
| 1:C:678:ASN:ND2  | 1:C:679:PRO:HD2  | 2.04                     | 0.71              |
| 1:E:50:LYS:HE3   | 1:E:60:GLU:HB3   | 1.72                     | 0.71              |
| 1:G:243:ASP:HB3  | 1:G:323:ILE:HD11 | 1.73                     | 0.71              |
| 1:C:306:LEU:HD12 | 1:C:390:LEU:HD21 | 1.72                     | 0.71              |
| 1:E:721:PHE:N    | 1:E:721:PHE:CD1  | 2.58                     | 0.71              |
| 1:G:234:PHE:HD1  | 1:G:289:ILE:HG21 | 1.55                     | 0.71              |
| 1:G:686:ILE:HD13 | 1:G:687:PRO:HD2  | 1.72                     | 0.71              |
| 1:G:771:GLN:HE21 | 1:G:771:GLN:C    | 1.99                     | 0.71              |
| 1:C:61:LEU:C     | 1:C:63:GLU:H     | 1.98                     | 0.71              |
| 1:C:365:ILE:HD13 | 1:C:427:ILE:HD11 | 1.73                     | 0.71              |
| 2:D:4:SER:N      | 2:D:7:GLN:HE21   | 1.89                     | 0.71              |
| 1:E:13:LEU:HD11  | 1:E:152:HIS:HD2  | 1.56                     | 0.71              |
| 1:E:481:CYS:O    | 1:E:484:TYR:HB3  | 1.91                     | 0.71              |
| 1:G:376:ALA:HB3  | 1:G:420:LYS:HA   | 1.71                     | 0.71              |
| 1:G:407:ILE:HD12 | 1:G:408:LYS:N    | 2.05                     | 0.71              |
| 1:G:721:PHE:CD1  | 1:G:721:PHE:N    | 2.58                     | 0.71              |
| 1:A:293:LEU:HD22 | 1:A:353:LEU:HD23 | 1.73                     | 0.70              |
| 1:A:619:LYS:O    | 1:A:622:ALA:HB3  | 1.91                     | 0.70              |
| 1:E:48:SER:C     | 1:E:59:VAL:HG13  | 2.16                     | 0.70              |
| 2:F:4:SER:N      | 2:F:7:GLN:HE21   | 1.88                     | 0.70              |
| 1:A:745:GLY:N    | 1:G:819:LEU:HD21 | 2.06                     | 0.70              |
| 1:G:8:ASP:CA     | 1:G:11:LYS:HD2   | 2.16                     | 0.70              |
| 1:G:50:LYS:HE3   | 1:G:60:GLU:HB3   | 1.71                     | 0.70              |
| 1:G:399:THR:HG22 | 1:G:403:LEU:HD11 | 1.73                     | 0.70              |
| 1:G:481:CYS:O    | 1:G:484:TYR:HB3  | 1.90                     | 0.70              |
| 1:E:199:SER:HB2  | 1:E:221:GLU:HG2  | 1.73                     | 0.70              |
| 1:E:242:ASN:OD1  | 1:E:244:ASN:N    | 2.23                     | 0.70              |
| 1:E:533:ASN:HB3  | 1:E:534:PRO:HD2  | 1.74                     | 0.70              |
| 1:E:627:ASP:O    | 1:E:627:ASP:OD1  | 2.08                     | 0.70              |
| 1:G:753:CYS:O    | 1:G:756:MET:HG3  | 1.91                     | 0.70              |
| 1:C:552:ASP:O    | 1:C:556:VAL:HG23 | 1.91                     | 0.70              |
| 1:E:313:TYR:HB2  | 1:E:316:LEU:CD1  | 2.21                     | 0.70              |
| 1:G:302:ARG:HH21 | 1:G:307:LEU:N    | 1.89                     | 0.70              |
| 1:A:721:PHE:N    | 1:A:721:PHE:CD1  | 2.57                     | 0.70              |
| 1:A:747:MET:HB3  | 1:A:752:ALA:HB2  | 1.73                     | 0.70              |
| 1:C:169:GLU:O    | 1:C:169:GLU:HG2  | 1.91                     | 0.70              |
| 1:C:689:HIS:CE1  | 1:C:700:LEU:HD11 | 2.27                     | 0.70              |
| 1:G:48:SER:C     | 1:G:59:VAL:HG13  | 2.16                     | 0.70              |
| 1:G:269:THR:CG2  | 1:G:443:LEU:HD13 | 2.22                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:306:LEU:HD12 | 1:A:390:LEU:HD21 | 1.74                     | 0.70              |
| 1:C:302:ARG:HH21 | 1:C:307:LEU:N    | 1.90                     | 0.70              |
| 1:E:302:ARG:HH21 | 1:E:307:LEU:N    | 1.88                     | 0.70              |
| 1:E:496:THR:HA   | 1:E:500:LEU:HD12 | 1.71                     | 0.70              |
| 1:A:320:HIS:C    | 1:A:320:HIS:HD1  | 1.99                     | 0.70              |
| 1:A:746:PHE:O    | 1:G:816:GLN:NE2  | 2.25                     | 0.70              |
| 1:G:199:SER:HB2  | 1:G:221:GLU:HG2  | 1.73                     | 0.70              |
| 2:B:83:GLY:HA3   | 2:B:88:TYR:CZ    | 2.27                     | 0.69              |
| 1:C:33:LYS:HD3   | 1:C:49:ILE:HD12  | 1.74                     | 0.69              |
| 1:C:271:LEU:HD21 | 1:C:663:TYR:CE1  | 2.26                     | 0.69              |
| 1:C:399:THR:HG22 | 1:C:403:LEU:HD11 | 1.73                     | 0.69              |
| 1:C:407:ILE:HD11 | 1:C:414:VAL:HB   | 1.74                     | 0.69              |
| 1:E:89:MET:C     | 1:E:91:GLU:H     | 1.98                     | 0.69              |
| 1:E:469:PHE:CE2  | 1:E:587:ALA:HB3  | 2.26                     | 0.69              |
| 2:F:141:GLU:O    | 2:F:145:ARG:HG3  | 1.91                     | 0.69              |
| 1:G:271:LEU:HD21 | 1:G:663:TYR:CE1  | 2.27                     | 0.69              |
| 2:H:4:SER:N      | 2:H:7:GLN:HE21   | 1.89                     | 0.69              |
| 1:A:269:THR:CG2  | 1:A:443:LEU:HD13 | 2.21                     | 0.69              |
| 1:A:365:ILE:HD13 | 1:A:427:ILE:HD11 | 1.72                     | 0.69              |
| 1:C:407:ILE:HG13 | 1:C:414:VAL:O    | 1.92                     | 0.69              |
| 1:C:494:ASN:HD22 | 1:C:494:ASN:N    | 1.90                     | 0.69              |
| 1:A:242:ASN:OD1  | 1:A:244:ASN:N    | 2.24                     | 0.69              |
| 1:A:814:LYS:HG3  | 1:A:815:ARG:N    | 2.06                     | 0.69              |
| 1:C:120:PHE:HD1  | 1:C:120:PHE:H    | 1.39                     | 0.69              |
| 1:C:199:SER:HB2  | 1:C:221:GLU:HG2  | 1.75                     | 0.69              |
| 1:C:243:ASP:HB3  | 1:C:323:ILE:HD11 | 1.74                     | 0.69              |
| 1:E:320:HIS:C    | 1:E:320:HIS:ND1  | 2.51                     | 0.69              |
| 1:E:771:GLN:HE21 | 1:E:771:GLN:C    | 2.00                     | 0.69              |
| 1:G:83:PHE:HB3   | 1:G:92:LEU:HD23  | 1.72                     | 0.69              |
| 1:A:552:ASP:O    | 1:A:556:VAL:HG23 | 1.92                     | 0.69              |
| 1:C:481:CYS:O    | 1:C:484:TYR:HB3  | 1.92                     | 0.69              |
| 2:D:4:SER:O      | 2:D:7:GLN:HG2    | 1.92                     | 0.69              |
| 1:E:182:GLY:HA2  | 5:E:998:ADP:PA   | 2.32                     | 0.69              |
| 1:E:814:LYS:HG3  | 1:E:815:ARG:N    | 2.07                     | 0.69              |
| 1:A:344:PHE:CE1  | 1:A:445:ARG:HB3  | 2.27                     | 0.69              |
| 1:A:494:ASN:H    | 1:A:494:ASN:HD22 | 1.39                     | 0.69              |
| 1:A:541:LEU:HD23 | 1:A:601:ASN:ND2  | 2.05                     | 0.69              |
| 1:C:407:ILE:CD1  | 1:C:409:VAL:HG23 | 2.22                     | 0.69              |
| 2:D:43:THR:O     | 2:D:47:VAL:HG23  | 1.93                     | 0.69              |
| 1:E:80:PRO:HD2   | 1:E:83:PHE:CD2   | 2.27                     | 0.69              |
| 1:E:250:LYS:CE   | 1:E:465:ASP:OD2  | 2.40                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:4:SER:O      | 2:F:7:GLN:HG2    | 1.92                     | 0.69              |
| 1:G:527:LEU:O    | 1:G:537:VAL:HG23 | 1.92                     | 0.69              |
| 1:A:678:ASN:HD22 | 1:A:679:PRO:CD   | 2.05                     | 0.69              |
| 1:C:407:ILE:HD13 | 1:C:409:VAL:HG23 | 1.74                     | 0.69              |
| 1:E:13:LEU:HD21  | 1:E:132:ILE:HD12 | 1.73                     | 0.69              |
| 1:G:44:PHE:CE2   | 1:G:702:LEU:HD21 | 2.28                     | 0.69              |
| 2:H:43:THR:O     | 2:H:47:VAL:HG23  | 1.93                     | 0.69              |
| 1:A:134:SER:HB2  | 1:A:212:GLY:HA2  | 1.74                     | 0.69              |
| 1:A:243:ASP:HB3  | 1:A:323:ILE:HD11 | 1.73                     | 0.69              |
| 1:A:628:VAL:HG13 | 1:A:631:ILE:HG12 | 1.74                     | 0.69              |
| 2:D:140:TYR:HD1  | 2:D:141:GLU:H    | 1.40                     | 0.69              |
| 1:E:419:THR:H    | 1:E:422:GLN:NE2  | 1.85                     | 0.69              |
| 1:A:361:GLN:C    | 1:A:363:GLY:H    | 1.99                     | 0.69              |
| 1:E:736:ILE:HG23 | 1:E:737:LEU:HD23 | 1.75                     | 0.69              |
| 2:F:25:LYS:HB3   | 2:F:63:THR:HB    | 1.74                     | 0.69              |
| 2:F:93:ARG:O     | 2:F:93:ARG:HG3   | 1.92                     | 0.69              |
| 1:G:812:PHE:C    | 1:G:814:LYS:H    | 1.99                     | 0.69              |
| 2:H:4:SER:O      | 2:H:7:GLN:HG2    | 1.92                     | 0.69              |
| 2:H:25:LYS:HB3   | 2:H:63:THR:HB    | 1.74                     | 0.69              |
| 1:A:161:TYR:O    | 1:A:165:LEU:HD12 | 1.93                     | 0.69              |
| 2:B:25:LYS:HB3   | 2:B:63:THR:HB    | 1.74                     | 0.69              |
| 2:B:36:ARG:HA    | 2:B:40:GLN:O     | 1.93                     | 0.69              |
| 1:C:320:HIS:C    | 1:C:320:HIS:ND1  | 2.50                     | 0.69              |
| 1:C:344:PHE:CE1  | 1:C:445:ARG:HB3  | 2.27                     | 0.69              |
| 1:C:700:LEU:CD2  | 1:C:704:GLN:HE22 | 2.06                     | 0.69              |
| 1:E:120:PHE:H    | 1:E:120:PHE:HD1  | 1.41                     | 0.69              |
| 1:E:700:LEU:HD23 | 1:E:704:GLN:HE22 | 1.57                     | 0.69              |
| 1:A:407:ILE:HD12 | 1:A:409:VAL:N    | 2.09                     | 0.69              |
| 1:E:97:GLU:OE2   | 1:E:702:LEU:HG   | 1.93                     | 0.69              |
| 1:E:313:TYR:HB2  | 1:E:316:LEU:HD11 | 1.75                     | 0.69              |
| 1:E:678:ASN:ND2  | 1:E:679:PRO:HD2  | 2.07                     | 0.69              |
| 1:G:320:HIS:C    | 1:G:320:HIS:ND1  | 2.51                     | 0.69              |
| 1:C:700:LEU:HD23 | 1:C:704:GLN:NE2  | 2.07                     | 0.68              |
| 2:F:43:THR:O     | 2:F:47:VAL:HG23  | 1.93                     | 0.68              |
| 1:G:678:ASN:HD22 | 1:G:679:PRO:CD   | 2.02                     | 0.68              |
| 1:A:199:SER:HB2  | 1:A:221:GLU:HG2  | 1.75                     | 0.68              |
| 1:A:301:MET:HA   | 1:A:304:ASP:HB2  | 1.75                     | 0.68              |
| 1:A:302:ARG:HH21 | 1:A:307:LEU:N    | 1.90                     | 0.68              |
| 1:A:450:LEU:N    | 1:A:450:LEU:HD23 | 2.09                     | 0.68              |
| 1:C:313:TYR:HB2  | 1:C:316:LEU:HD11 | 1.75                     | 0.68              |
| 1:C:527:LEU:HD12 | 1:C:566:HIS:CG   | 2.27                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:306:LEU:HD12 | 1:E:390:LEU:HD21 | 1.74                     | 0.68              |
| 1:A:33:LYS:HD3   | 1:A:49:ILE:HD12  | 1.75                     | 0.68              |
| 2:B:113:VAL:HG13 | 2:B:119:MET:O    | 1.93                     | 0.68              |
| 1:E:407:ILE:HD12 | 1:E:409:VAL:N    | 2.08                     | 0.68              |
| 1:E:535:PRO:HB2  | 1:E:540:LEU:HD21 | 1.75                     | 0.68              |
| 1:G:627:ASP:CG   | 1:G:627:ASP:O    | 2.37                     | 0.68              |
| 2:B:112:LEU:HD13 | 2:B:119:MET:HE3  | 1.74                     | 0.68              |
| 1:C:301:MET:HA   | 1:C:304:ASP:HB2  | 1.76                     | 0.68              |
| 2:D:25:LYS:HB3   | 2:D:63:THR:HB    | 1.74                     | 0.68              |
| 1:E:301:MET:HA   | 1:E:304:ASP:HB2  | 1.76                     | 0.68              |
| 1:E:437:ARG:HE   | 1:E:625:TRP:HA   | 1.57                     | 0.68              |
| 1:G:230:ILE:HG22 | 1:G:231:LEU:N    | 2.07                     | 0.68              |
| 1:A:313:TYR:HB2  | 1:A:316:LEU:CD1  | 2.23                     | 0.68              |
| 1:C:189:LYS:HD3  | 1:C:192:GLN:OE1  | 1.93                     | 0.68              |
| 1:C:293:LEU:HD22 | 1:C:353:LEU:HD23 | 1.75                     | 0.68              |
| 1:C:450:LEU:N    | 1:C:450:LEU:HD23 | 2.08                     | 0.68              |
| 1:C:628:VAL:HG13 | 1:C:628:VAL:O    | 1.94                     | 0.68              |
| 2:F:36:ARG:HA    | 2:F:40:GLN:O     | 1.93                     | 0.68              |
| 1:G:36:TRP:HE1   | 1:G:78:MET:HG3   | 1.58                     | 0.68              |
| 1:G:689:HIS:CE1  | 1:G:700:LEU:HD11 | 2.28                     | 0.68              |
| 1:G:736:ILE:HG23 | 1:G:737:LEU:HD23 | 1.73                     | 0.68              |
| 1:G:293:LEU:HD22 | 1:G:353:LEU:HD23 | 1.76                     | 0.68              |
| 1:G:490:GLN:O    | 1:G:494:ASN:ND2  | 2.26                     | 0.68              |
| 1:A:407:ILE:HD11 | 1:A:414:VAL:HB   | 1.75                     | 0.68              |
| 1:A:419:THR:H    | 1:A:422:GLN:NE2  | 1.87                     | 0.68              |
| 1:E:376:ALA:HB3  | 1:E:420:LYS:HA   | 1.75                     | 0.68              |
| 1:E:490:GLN:O    | 1:E:494:ASN:ND2  | 2.27                     | 0.68              |
| 1:G:306:LEU:HD12 | 1:G:390:LEU:HD21 | 1.74                     | 0.68              |
| 1:G:400:ARG:HG2  | 1:G:404:THR:OG1  | 1.93                     | 0.68              |
| 1:G:619:LYS:O    | 1:G:622:ALA:HB3  | 1.94                     | 0.68              |
| 2:H:85:PHE:CZ    | 2:H:145:ARG:HG2  | 2.28                     | 0.68              |
| 2:B:4:SER:O      | 2:B:7:GLN:HG2    | 1.92                     | 0.68              |
| 1:G:361:GLN:C    | 1:G:363:GLY:H    | 2.02                     | 0.68              |
| 1:A:13:LEU:HD21  | 1:A:132:ILE:CD1  | 2.24                     | 0.68              |
| 1:A:47:ALA:HA    | 1:A:62:GLN:H     | 1.59                     | 0.68              |
| 1:A:376:ALA:HB3  | 1:A:420:LYS:HA   | 1.75                     | 0.68              |
| 1:C:369:LYS:HZ2  | 1:C:420:LYS:HB3  | 1.57                     | 0.68              |
| 1:G:189:LYS:HD3  | 1:G:192:GLN:OE1  | 1.94                     | 0.68              |
| 1:G:313:TYR:HB2  | 1:G:316:LEU:HD11 | 1.76                     | 0.68              |
| 1:C:13:LEU:HD21  | 1:C:132:ILE:CD1  | 2.24                     | 0.68              |
| 1:C:469:PHE:CE2  | 1:C:587:ALA:HB3  | 2.29                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:555:PHE:CZ   | 1:C:559:LEU:HD13 | 2.28                     | 0.68              |
| 1:C:610:THR:HG23 | 1:C:628:VAL:HG21 | 1.76                     | 0.68              |
| 2:F:113:VAL:HG13 | 2:F:119:MET:O    | 1.94                     | 0.68              |
| 1:G:796:ILE:HG22 | 1:G:800:GLN:OE1  | 1.94                     | 0.68              |
| 1:A:57:VAL:O     | 1:A:69:THR:HG23  | 1.94                     | 0.67              |
| 1:A:145:LYS:HG3  | 1:A:146:ARG:HE   | 1.59                     | 0.67              |
| 2:B:43:THR:O     | 2:B:47:VAL:HG23  | 1.93                     | 0.67              |
| 1:C:13:LEU:HD21  | 1:C:132:ILE:HD12 | 1.75                     | 0.67              |
| 1:E:7:SER:HB3    | 1:E:10:GLU:OE1   | 1.95                     | 0.67              |
| 1:E:555:PHE:CZ   | 1:E:559:LEU:HD13 | 2.29                     | 0.67              |
| 1:G:407:ILE:HD11 | 1:G:414:VAL:HB   | 1.74                     | 0.67              |
| 1:C:361:GLN:C    | 1:C:363:GLY:H    | 2.02                     | 0.67              |
| 1:C:496:THR:HA   | 1:C:500:LEU:HD12 | 1.76                     | 0.67              |
| 1:C:533:ASN:HB3  | 1:C:534:PRO:HD2  | 1.75                     | 0.67              |
| 1:C:686:ILE:HD13 | 1:C:687:PRO:HD2  | 1.76                     | 0.67              |
| 1:E:242:ASN:OD1  | 1:E:242:ASN:C    | 2.37                     | 0.67              |
| 2:H:36:ARG:HA    | 2:H:40:GLN:O     | 1.93                     | 0.67              |
| 1:A:533:ASN:HB3  | 1:A:534:PRO:HD2  | 1.75                     | 0.67              |
| 1:C:490:GLN:O    | 1:C:494:ASN:ND2  | 2.27                     | 0.67              |
| 1:C:619:LYS:O    | 1:C:622:ALA:HB3  | 1.93                     | 0.67              |
| 2:D:93:ARG:HG3   | 2:D:93:ARG:O     | 1.94                     | 0.67              |
| 1:E:125:ASN:OD1  | 1:E:126:PRO:HD2  | 1.95                     | 0.67              |
| 1:E:527:LEU:HD12 | 1:E:566:HIS:CG   | 2.30                     | 0.67              |
| 2:F:43:THR:HG23  | 2:F:46:GLU:CD    | 2.20                     | 0.67              |
| 1:E:12:PHE:CD2   | 1:E:131:PRO:CD   | 2.78                     | 0.67              |
| 1:E:659:VAL:CG1  | 1:E:660:GLY:N    | 2.57                     | 0.67              |
| 1:G:344:PHE:CE1  | 1:G:445:ARG:HB3  | 2.30                     | 0.67              |
| 1:G:362:LEU:HD22 | 1:G:431:ALA:HB2  | 1.77                     | 0.67              |
| 1:A:689:HIS:CE1  | 1:A:700:LEU:HD11 | 2.29                     | 0.67              |
| 1:A:747:MET:SD   | 1:G:816:GLN:OE1  | 2.53                     | 0.67              |
| 1:G:33:LYS:HD3   | 1:G:49:ILE:HD12  | 1.75                     | 0.67              |
| 1:G:44:PHE:HE2   | 1:G:702:LEU:HD21 | 1.58                     | 0.67              |
| 1:G:409:VAL:HG22 | 1:G:634:LEU:HD12 | 1.76                     | 0.67              |
| 1:A:320:HIS:C    | 1:A:320:HIS:ND1  | 2.52                     | 0.67              |
| 1:C:362:LEU:HD23 | 1:C:427:ILE:HG13 | 1.76                     | 0.67              |
| 1:C:480:LEU:HD22 | 1:C:597:TRP:CH2  | 2.30                     | 0.67              |
| 1:C:552:ASP:O    | 1:C:555:PHE:HB3  | 1.94                     | 0.67              |
| 1:C:661:GLN:O    | 1:C:665:GLU:HB2  | 1.95                     | 0.67              |
| 1:E:169:GLU:O    | 1:E:169:GLU:HG2  | 1.94                     | 0.67              |
| 1:E:400:ARG:HG2  | 1:E:404:THR:OG1  | 1.94                     | 0.67              |
| 1:E:678:ASN:HD22 | 1:E:679:PRO:CD   | 2.05                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:301:MET:HA   | 1:G:304:ASP:HB2  | 1.77                     | 0.67              |
| 1:A:362:LEU:HD23 | 1:A:427:ILE:HG13 | 1.76                     | 0.67              |
| 1:A:407:ILE:HD13 | 1:A:409:VAL:HG23 | 1.76                     | 0.67              |
| 1:C:242:ASN:OD1  | 1:C:244:ASN:N    | 2.23                     | 0.67              |
| 2:D:43:THR:HG23  | 2:D:46:GLU:CD    | 2.20                     | 0.67              |
| 1:E:8:ASP:CA     | 1:E:11:LYS:HD2   | 2.19                     | 0.67              |
| 1:E:753:CYS:O    | 1:E:756:MET:HG3  | 1.95                     | 0.67              |
| 1:G:89:MET:C     | 1:G:91:GLU:H     | 2.02                     | 0.67              |
| 1:A:234:PHE:HD1  | 1:A:289:ILE:HG21 | 1.59                     | 0.67              |
| 1:A:556:VAL:HG12 | 1:A:560:ILE:HD11 | 1.77                     | 0.67              |
| 2:B:43:THR:HG23  | 2:B:46:GLU:CD    | 2.20                     | 0.67              |
| 1:C:812:PHE:C    | 1:C:814:LYS:H    | 2.03                     | 0.67              |
| 1:G:419:THR:H    | 1:G:422:GLN:NE2  | 1.89                     | 0.67              |
| 1:G:533:ASN:HB3  | 1:G:534:PRO:HD2  | 1.75                     | 0.67              |
| 1:G:628:VAL:HG13 | 1:G:631:ILE:HG12 | 1.76                     | 0.67              |
| 2:H:25:LYS:HA    | 2:H:64:LEU:O     | 1.95                     | 0.67              |
| 1:C:391:MET:HG2  | 1:C:613:LEU:CD2  | 2.25                     | 0.67              |
| 1:E:613:LEU:O    | 1:E:615:GLN:N    | 2.28                     | 0.67              |
| 2:F:128:VAL:HB   | 2:F:138:ILE:HD11 | 1.76                     | 0.67              |
| 1:G:555:PHE:CZ   | 1:G:559:LEU:HD13 | 2.29                     | 0.67              |
| 1:G:556:VAL:HG12 | 1:G:560:ILE:HD11 | 1.76                     | 0.67              |
| 2:B:31:CYS:O     | 2:B:35:MET:HG3   | 1.95                     | 0.66              |
| 1:C:89:MET:HE3   | 1:C:100:VAL:HG13 | 1.77                     | 0.66              |
| 1:E:796:ILE:HG22 | 1:E:800:GLN:OE1  | 1.95                     | 0.66              |
| 1:A:527:LEU:HD12 | 1:A:566:HIS:CG   | 2.30                     | 0.66              |
| 1:A:700:LEU:HD23 | 1:A:704:GLN:NE2  | 2.10                     | 0.66              |
| 2:D:36:ARG:HA    | 2:D:40:GLN:O     | 1.94                     | 0.66              |
| 1:A:169:GLU:O    | 1:A:169:GLU:HG2  | 1.93                     | 0.66              |
| 1:C:76:GLN:HB3   | 1:C:96:ASN:ND2   | 2.11                     | 0.66              |
| 1:C:391:MET:HE2  | 1:C:613:LEU:HD21 | 1.77                     | 0.66              |
| 2:D:31:CYS:O     | 2:D:35:MET:HG3   | 1.95                     | 0.66              |
| 1:E:47:ALA:HA    | 1:E:62:GLN:H     | 1.60                     | 0.66              |
| 1:E:271:LEU:HD21 | 1:E:663:TYR:CE1  | 2.31                     | 0.66              |
| 2:H:31:CYS:O     | 2:H:35:MET:HG3   | 1.94                     | 0.66              |
| 1:A:496:THR:HA   | 1:A:500:LEU:HD12 | 1.76                     | 0.66              |
| 2:B:25:LYS:HA    | 2:B:64:LEU:O     | 1.95                     | 0.66              |
| 1:E:230:ILE:HG22 | 1:E:231:LEU:N    | 2.11                     | 0.66              |
| 1:G:480:LEU:HD22 | 1:G:597:TRP:CH2  | 2.31                     | 0.66              |
| 1:G:700:LEU:HD23 | 1:G:704:GLN:NE2  | 2.09                     | 0.66              |
| 1:A:259:THR:HB   | 1:A:261:TYR:HE1  | 1.61                     | 0.66              |
| 1:C:97:GLU:OE2   | 1:C:702:LEU:HG   | 1.95                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:279:ARG:NH2  | 1:E:428:GLU:HG3  | 2.11                     | 0.66              |
| 1:E:362:LEU:HD22 | 1:E:431:ALA:HB2  | 1.77                     | 0.66              |
| 1:E:365:ILE:HD13 | 1:E:427:ILE:HD11 | 1.76                     | 0.66              |
| 1:G:7:SER:HB3    | 1:G:10:GLU:OE1   | 1.96                     | 0.66              |
| 1:C:556:VAL:HG12 | 1:C:560:ILE:HD11 | 1.76                     | 0.66              |
| 1:C:627:ASP:CG   | 1:C:627:ASP:O    | 2.37                     | 0.66              |
| 1:C:753:CYS:O    | 1:C:756:MET:HG3  | 1.95                     | 0.66              |
| 1:G:47:ALA:HA    | 1:G:62:GLN:H     | 1.60                     | 0.66              |
| 2:H:113:VAL:HG13 | 2:H:119:MET:O    | 1.95                     | 0.66              |
| 1:A:494:ASN:HD22 | 1:A:494:ASN:N    | 1.92                     | 0.66              |
| 1:C:362:LEU:HD22 | 1:C:431:ALA:HB2  | 1.78                     | 0.66              |
| 1:E:689:HIS:CE1  | 1:E:700:LEU:HD11 | 2.31                     | 0.66              |
| 1:G:527:LEU:HD12 | 1:G:566:HIS:CG   | 2.30                     | 0.66              |
| 2:H:43:THR:HG23  | 2:H:46:GLU:CD    | 2.20                     | 0.66              |
| 1:A:407:ILE:CD1  | 1:A:409:VAL:HG23 | 2.24                     | 0.66              |
| 1:A:747:MET:HB2  | 1:G:816:GLN:HE22 | 1.61                     | 0.66              |
| 1:C:57:VAL:C     | 1:C:69:THR:HG23  | 2.21                     | 0.66              |
| 1:C:269:THR:CG2  | 1:C:443:LEU:HD13 | 2.22                     | 0.66              |
| 1:C:728:GLN:CA   | 1:C:728:GLN:HE21 | 2.08                     | 0.66              |
| 1:G:57:VAL:C     | 1:G:69:THR:HG23  | 2.21                     | 0.66              |
| 1:G:57:VAL:O     | 1:G:69:THR:HG23  | 1.96                     | 0.66              |
| 1:G:227:ALA:C    | 1:G:229:PRO:HD2  | 2.20                     | 0.66              |
| 1:A:227:ALA:C    | 1:A:229:PRO:HD2  | 2.20                     | 0.66              |
| 1:A:527:LEU:O    | 1:A:537:VAL:HG23 | 1.95                     | 0.66              |
| 1:C:181:ALA:O    | 1:C:684:CYS:HB3  | 1.96                     | 0.66              |
| 1:E:607:ASP:CA   | 1:E:610:THR:HB   | 2.26                     | 0.66              |
| 2:F:31:CYS:O     | 2:F:35:MET:HG3   | 1.95                     | 0.66              |
| 2:F:44:ASN:HB2   | 2:F:117:GLU:CD   | 2.21                     | 0.66              |
| 1:G:407:ILE:HD13 | 1:G:409:VAL:HG23 | 1.78                     | 0.66              |
| 1:A:242:ASN:OD1  | 1:A:242:ASN:C    | 2.38                     | 0.66              |
| 1:E:302:ARG:NH2  | 1:E:303:ASN:HA   | 2.11                     | 0.66              |
| 1:E:586:TYR:HD1  | 1:E:586:TYR:H    | 1.44                     | 0.66              |
| 1:G:187:THR:HG23 | 1:G:463:ILE:CG2  | 2.26                     | 0.66              |
| 1:G:815:ARG:HA   | 1:G:818:GLN:CD   | 2.21                     | 0.66              |
| 2:B:93:ARG:HG3   | 2:B:93:ARG:O     | 1.94                     | 0.65              |
| 1:E:33:LYS:HD3   | 1:E:49:ILE:HD12  | 1.76                     | 0.65              |
| 1:E:293:LEU:HD22 | 1:E:353:LEU:HD23 | 1.77                     | 0.65              |
| 1:E:494:ASN:HD22 | 1:E:494:ASN:H    | 1.43                     | 0.65              |
| 2:F:25:LYS:HA    | 2:F:64:LEU:O     | 1.95                     | 0.65              |
| 1:G:407:ILE:CD1  | 1:G:409:VAL:HG23 | 2.26                     | 0.65              |
| 1:A:120:PHE:HD1  | 1:A:120:PHE:H    | 1.43                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:230:ILE:HG22 | 1:A:231:LEU:N    | 2.12                     | 0.65              |
| 1:A:678:ASN:ND2  | 1:A:679:PRO:HD2  | 2.10                     | 0.65              |
| 1:A:686:ILE:HD13 | 1:A:687:PRO:HD2  | 1.77                     | 0.65              |
| 1:C:613:LEU:O    | 1:C:615:GLN:N    | 2.28                     | 0.65              |
| 1:E:804:ARG:HG2  | 1:E:804:ARG:NH1  | 2.11                     | 0.65              |
| 1:G:407:ILE:HD12 | 1:G:409:VAL:N    | 2.10                     | 0.65              |
| 1:G:496:THR:HA   | 1:G:500:LEU:HD12 | 1.79                     | 0.65              |
| 1:G:586:TYR:H    | 1:G:586:TYR:HD1  | 1.44                     | 0.65              |
| 1:G:613:LEU:O    | 1:G:615:GLN:N    | 2.28                     | 0.65              |
| 1:A:522:GLN:N    | 1:A:523:PRO:HD2  | 2.11                     | 0.65              |
| 1:A:700:LEU:CD2  | 1:A:704:GLN:HE22 | 2.10                     | 0.65              |
| 1:G:247:ARG:HH11 | 1:G:247:ARG:HA   | 1.59                     | 0.65              |
| 2:H:93:ARG:HG3   | 2:H:93:ARG:O     | 1.97                     | 0.65              |
| 1:E:250:LYS:HG2  | 1:E:465:ASP:HB3  | 1.78                     | 0.65              |
| 1:E:344:PHE:CE1  | 1:E:445:ARG:HB3  | 2.30                     | 0.65              |
| 1:E:399:THR:HG22 | 1:E:403:LEU:CD1  | 2.26                     | 0.65              |
| 1:G:120:PHE:HD1  | 1:G:120:PHE:H    | 1.43                     | 0.65              |
| 1:A:189:LYS:HD3  | 1:A:192:GLN:OE1  | 1.95                     | 0.65              |
| 1:A:400:ARG:HG2  | 1:A:404:THR:OG1  | 1.97                     | 0.65              |
| 1:A:627:ASP:CG   | 1:A:627:ASP:O    | 2.38                     | 0.65              |
| 1:A:751:GLN:HG3  | 1:G:809:ARG:CB   | 2.22                     | 0.65              |
| 1:C:89:MET:C     | 1:C:91:GLU:H     | 2.05                     | 0.65              |
| 1:C:419:THR:H    | 1:C:422:GLN:NE2  | 1.90                     | 0.65              |
| 1:C:502:GLN:HG2  | 1:C:512:TRP:NE1  | 2.11                     | 0.65              |
| 1:E:247:ARG:HA   | 1:E:247:ARG:HH11 | 1.62                     | 0.65              |
| 1:E:628:VAL:HG13 | 1:E:631:ILE:HG13 | 1.78                     | 0.65              |
| 1:E:812:PHE:C    | 1:E:814:LYS:H    | 2.03                     | 0.65              |
| 2:H:85:PHE:HE1   | 2:H:145:ARG:HG2  | 1.61                     | 0.65              |
| 1:A:279:ARG:NH2  | 1:A:428:GLU:HG3  | 2.11                     | 0.65              |
| 1:A:728:GLN:CA   | 1:A:728:GLN:HE21 | 2.08                     | 0.65              |
| 2:D:25:LYS:HA    | 2:D:64:LEU:O     | 1.96                     | 0.65              |
| 1:E:323:ILE:CG2  | 1:E:326:GLN:HB3  | 2.27                     | 0.65              |
| 1:E:673:THR:O    | 1:E:677:THR:HG23 | 1.96                     | 0.65              |
| 2:F:84:CYS:O     | 2:F:85:PHE:C     | 2.40                     | 0.65              |
| 1:G:535:PRO:HB2  | 1:G:540:LEU:HD21 | 1.77                     | 0.65              |
| 2:H:55:LYS:HB2   | 2:H:58:GLU:OE2   | 1.96                     | 0.65              |
| 1:A:57:VAL:C     | 1:A:69:THR:HG23  | 2.21                     | 0.65              |
| 1:A:552:ASP:O    | 1:A:555:PHE:HB3  | 1.97                     | 0.65              |
| 2:B:38:LEU:HD12  | 2:B:73:MET:HE2   | 1.78                     | 0.65              |
| 1:C:400:ARG:HG2  | 1:C:404:THR:OG1  | 1.97                     | 0.65              |
| 1:C:527:LEU:HD23 | 1:C:537:VAL:HG23 | 1.79                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:480:LEU:HD22 | 1:E:597:TRP:CH2  | 2.32                     | 0.65              |
| 1:E:609:VAL:O    | 1:E:612:LEU:HB3  | 1.97                     | 0.65              |
| 1:E:700:LEU:HD23 | 1:E:704:GLN:NE2  | 2.12                     | 0.65              |
| 2:F:38:LEU:HD12  | 2:F:73:MET:HE2   | 1.78                     | 0.65              |
| 1:G:56:GLU:HG3   | 1:G:71:SER:HA    | 1.79                     | 0.65              |
| 1:G:313:TYR:HD2  | 1:G:360:LEU:HB3  | 1.61                     | 0.65              |
| 1:G:391:MET:HE2  | 1:G:613:LEU:HD21 | 1.77                     | 0.65              |
| 1:G:628:VAL:O    | 1:G:628:VAL:HG13 | 1.97                     | 0.65              |
| 1:A:313:TYR:HB2  | 1:A:316:LEU:HD11 | 1.78                     | 0.65              |
| 1:C:7:SER:HB3    | 1:C:10:GLU:OE1   | 1.96                     | 0.65              |
| 1:C:47:ALA:HA    | 1:C:62:GLN:H     | 1.61                     | 0.65              |
| 1:E:79:ASN:OD1   | 1:E:92:LEU:HB3   | 1.97                     | 0.65              |
| 1:E:407:ILE:CD1  | 1:E:409:VAL:HG23 | 2.26                     | 0.65              |
| 1:G:242:ASN:C    | 1:G:242:ASN:OD1  | 2.37                     | 0.65              |
| 1:G:552:ASP:O    | 1:G:555:PHE:HB3  | 1.97                     | 0.65              |
| 1:G:673:THR:O    | 1:G:677:THR:HG23 | 1.97                     | 0.65              |
| 1:A:370:GLU:O    | 1:A:374:ASP:N    | 2.29                     | 0.65              |
| 2:B:55:LYS:HB2   | 2:B:58:GLU:OE2   | 1.97                     | 0.65              |
| 1:C:405:PRO:HB2  | 1:C:407:ILE:HG23 | 1.79                     | 0.65              |
| 2:D:38:LEU:HD12  | 2:D:73:MET:HE2   | 1.78                     | 0.65              |
| 1:A:630:ARG:HH22 | 1:A:657:ARG:CB   | 2.10                     | 0.65              |
| 1:C:250:LYS:CE   | 1:C:465:ASP:OD2  | 2.44                     | 0.65              |
| 2:D:55:LYS:HB2   | 2:D:58:GLU:OE2   | 1.97                     | 0.65              |
| 2:D:113:VAL:HG13 | 2:D:119:MET:O    | 1.97                     | 0.65              |
| 1:E:671:MET:O    | 1:E:675:ARG:HD2  | 1.97                     | 0.65              |
| 1:G:469:PHE:CE2  | 1:G:587:ALA:HB3  | 2.32                     | 0.65              |
| 1:A:535:PRO:HB2  | 1:A:540:LEU:HD21 | 1.78                     | 0.64              |
| 1:C:60:GLU:HG3   | 1:C:66:LYS:O     | 1.97                     | 0.64              |
| 1:E:89:MET:HE1   | 1:E:104:LEU:HG   | 1.79                     | 0.64              |
| 1:E:407:ILE:HD13 | 1:E:409:VAL:HG23 | 1.79                     | 0.64              |
| 2:F:97:LYS:C     | 2:F:98:GLU:HG3   | 2.21                     | 0.64              |
| 1:G:158:ASP:HB2  | 1:G:193:TYR:OH   | 1.98                     | 0.64              |
| 1:G:502:GLN:HG2  | 1:G:512:TRP:NE1  | 2.12                     | 0.64              |
| 1:G:630:ARG:HH22 | 1:G:657:ARG:CB   | 2.10                     | 0.64              |
| 1:G:661:GLN:O    | 1:G:665:GLU:HB2  | 1.95                     | 0.64              |
| 1:A:181:ALA:O    | 1:A:684:CYS:HB3  | 1.98                     | 0.64              |
| 1:A:606:ASN:OD1  | 1:A:609:VAL:HG12 | 1.98                     | 0.64              |
| 1:C:586:TYR:HD1  | 1:C:586:TYR:H    | 1.44                     | 0.64              |
| 2:D:3:PHE:HA     | 2:D:7:GLN:HE21   | 1.63                     | 0.64              |
| 1:E:391:MET:HG2  | 1:E:613:LEU:CD2  | 2.27                     | 0.64              |
| 1:E:527:LEU:O    | 1:E:537:VAL:HG23 | 1.96                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:552:ASP:O    | 1:E:555:PHE:HB3  | 1.97                     | 0.64              |
| 2:F:3:PHE:HA     | 2:F:7:GLN:HE21   | 1.63                     | 0.64              |
| 1:G:33:LYS:HB3   | 1:G:49:ILE:CB    | 2.27                     | 0.64              |
| 1:A:79:ASN:ND2   | 1:A:80:PRO:HD2   | 2.09                     | 0.64              |
| 1:A:97:GLU:OE2   | 1:A:702:LEU:HG   | 1.96                     | 0.64              |
| 1:A:345:THR:HB   | 1:A:348:GLU:CB   | 2.27                     | 0.64              |
| 1:A:661:GLN:O    | 1:A:665:GLU:HB2  | 1.97                     | 0.64              |
| 1:C:419:THR:O    | 1:C:420:LYS:C    | 2.41                     | 0.64              |
| 1:E:502:GLN:HG2  | 1:E:512:TRP:NE1  | 2.11                     | 0.64              |
| 1:E:527:LEU:HG   | 1:E:563:GLN:HG3  | 1.79                     | 0.64              |
| 2:F:55:LYS:HB2   | 2:F:58:GLU:OE2   | 1.97                     | 0.64              |
| 1:A:419:THR:O    | 1:A:420:LYS:C    | 2.40                     | 0.64              |
| 1:A:530:ARG:HG2  | 1:A:534:PRO:O    | 1.98                     | 0.64              |
| 1:A:586:TYR:HD1  | 1:A:586:TYR:H    | 1.45                     | 0.64              |
| 2:D:83:GLY:HA3   | 2:D:88:TYR:CZ    | 2.33                     | 0.64              |
| 2:D:89:VAL:HG12  | 2:D:144:VAL:CG2  | 2.19                     | 0.64              |
| 2:F:89:VAL:HG12  | 2:F:144:VAL:CG2  | 2.19                     | 0.64              |
| 1:C:370:GLU:O    | 1:C:374:ASP:N    | 2.30                     | 0.64              |
| 1:A:342:MET:HE1  | 1:A:449:ALA:HB3  | 1.80                     | 0.64              |
| 1:A:613:LEU:O    | 1:A:615:GLN:N    | 2.31                     | 0.64              |
| 1:A:627:ASP:O    | 1:A:627:ASP:OD1  | 2.15                     | 0.64              |
| 1:G:803:CYS:CB   | 2:H:119:MET:HE1  | 2.28                     | 0.64              |
| 1:A:747:MET:HE1  | 1:A:755:LEU:HD22 | 1.78                     | 0.64              |
| 1:C:242:ASN:OD1  | 1:C:242:ASN:C    | 2.40                     | 0.64              |
| 1:C:606:ASN:OD1  | 1:C:609:VAL:HG12 | 1.98                     | 0.64              |
| 1:C:609:VAL:O    | 1:C:612:LEU:HB3  | 1.97                     | 0.64              |
| 1:E:405:PRO:HB2  | 1:E:407:ILE:HG23 | 1.78                     | 0.64              |
| 1:G:370:GLU:O    | 1:G:374:ASP:N    | 2.31                     | 0.64              |
| 1:G:667:LEU:HG   | 1:G:667:LEU:O    | 1.97                     | 0.64              |
| 1:A:187:THR:HG23 | 1:A:463:ILE:CG2  | 2.26                     | 0.64              |
| 1:C:409:VAL:HG22 | 1:C:634:LEU:HD12 | 1.79                     | 0.64              |
| 1:E:57:VAL:C     | 1:E:69:THR:HG23  | 2.22                     | 0.64              |
| 1:E:227:ALA:C    | 1:E:229:PRO:HD2  | 2.23                     | 0.64              |
| 1:G:97:GLU:OE2   | 1:G:702:LEU:HG   | 1.97                     | 0.64              |
| 1:G:391:MET:HG2  | 1:G:613:LEU:CD2  | 2.28                     | 0.64              |
| 1:A:405:PRO:HB2  | 1:A:407:ILE:HG23 | 1.79                     | 0.64              |
| 1:C:8:ASP:CA     | 1:C:11:LYS:HD2   | 2.17                     | 0.64              |
| 2:D:140:TYR:O    | 2:D:141:GLU:C    | 2.40                     | 0.64              |
| 2:D:140:TYR:CD1  | 2:D:141:GLU:HG2  | 2.32                     | 0.64              |
| 2:B:3:PHE:HA     | 2:B:7:GLN:HE21   | 1.63                     | 0.64              |
| 1:E:234:PHE:HD1  | 1:E:289:ILE:HG21 | 1.63                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:235:GLY:O    | 1:E:247:ARG:HB2  | 1.97                     | 0.64              |
| 1:G:181:ALA:O    | 1:G:684:CYS:HB3  | 1.97                     | 0.64              |
| 1:G:700:LEU:CD2  | 1:G:704:GLN:HE22 | 2.10                     | 0.64              |
| 1:A:502:GLN:HG2  | 1:A:512:TRP:NE1  | 2.12                     | 0.63              |
| 1:C:235:GLY:O    | 1:C:247:ARG:HB2  | 1.97                     | 0.63              |
| 1:E:181:ALA:O    | 1:E:684:CYS:HB3  | 1.98                     | 0.63              |
| 1:G:797:ILE:HG13 | 2:H:117:GLU:H    | 1.63                     | 0.63              |
| 1:A:391:MET:HE2  | 1:A:613:LEU:HD21 | 1.80                     | 0.63              |
| 1:A:481:CYS:O    | 1:A:484:TYR:HB3  | 1.97                     | 0.63              |
| 1:C:815:ARG:HA   | 1:C:818:GLN:CD   | 2.23                     | 0.63              |
| 1:G:399:THR:HG22 | 1:G:403:LEU:CD1  | 2.28                     | 0.63              |
| 1:A:362:LEU:HD22 | 1:A:431:ALA:HB2  | 1.79                     | 0.63              |
| 1:A:409:VAL:HG22 | 1:A:634:LEU:HD12 | 1.80                     | 0.63              |
| 1:A:671:MET:O    | 1:A:675:ARG:HD2  | 1.99                     | 0.63              |
| 1:C:247:ARG:HA   | 1:C:247:ARG:HH11 | 1.64                     | 0.63              |
| 1:C:663:TYR:OH   | 1:C:667:LEU:HD13 | 1.97                     | 0.63              |
| 1:E:494:ASN:HD22 | 1:E:494:ASN:N    | 1.96                     | 0.63              |
| 1:E:700:LEU:CD2  | 1:E:704:GLN:HE22 | 2.12                     | 0.63              |
| 2:H:55:LYS:O     | 2:H:58:GLU:HG2   | 1.98                     | 0.63              |
| 1:A:555:PHE:CZ   | 1:A:559:LEU:HD13 | 2.32                     | 0.63              |
| 1:A:673:THR:O    | 1:A:677:THR:HG23 | 1.98                     | 0.63              |
| 1:C:56:GLU:HG3   | 1:C:71:SER:HA    | 1.80                     | 0.63              |
| 2:D:35:MET:O     | 2:D:40:GLN:HB2   | 1.98                     | 0.63              |
| 1:E:328:ASP:HA   | 1:E:331:MET:HB2  | 1.78                     | 0.63              |
| 1:E:661:GLN:O    | 1:E:665:GLU:HB2  | 1.99                     | 0.63              |
| 1:G:235:GLY:O    | 1:G:247:ARG:HB2  | 1.97                     | 0.63              |
| 2:H:38:LEU:HD12  | 2:H:73:MET:HE2   | 1.78                     | 0.63              |
| 1:A:44:PHE:CE2   | 1:A:702:LEU:HD21 | 2.33                     | 0.63              |
| 1:A:158:ASP:HB2  | 1:A:193:TYR:OH   | 1.99                     | 0.63              |
| 1:A:399:THR:HG22 | 1:A:403:LEU:CD1  | 2.28                     | 0.63              |
| 1:A:743:PRO:CB   | 1:G:816:GLN:HB3  | 2.29                     | 0.63              |
| 1:E:60:GLU:HG3   | 1:E:66:LYS:O     | 1.99                     | 0.63              |
| 1:E:189:LYS:HD3  | 1:E:192:GLN:OE1  | 1.98                     | 0.63              |
| 1:E:193:TYR:CE1  | 1:E:197:VAL:HG21 | 2.33                     | 0.63              |
| 1:E:259:THR:HB   | 1:E:261:TYR:HE1  | 1.64                     | 0.63              |
| 1:G:541:LEU:HD23 | 1:G:601:ASN:ND2  | 2.07                     | 0.63              |
| 1:A:747:MET:HG3  | 1:G:812:PHE:HE2  | 1.62                     | 0.63              |
| 2:B:97:LYS:C     | 2:B:98:GLU:HG3   | 2.22                     | 0.63              |
| 1:C:437:ARG:HB3  | 1:C:624:LEU:HD23 | 1.81                     | 0.63              |
| 1:C:610:THR:CG2  | 1:C:628:VAL:CG1  | 2.77                     | 0.63              |
| 2:D:84:CYS:O     | 2:D:88:TYR:N     | 2.25                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:391:MET:HE2  | 1:E:613:LEU:HD21 | 1.80                     | 0.63              |
| 1:E:728:GLN:CA   | 1:E:728:GLN:HE21 | 2.10                     | 0.63              |
| 1:G:405:PRO:HB2  | 1:G:407:ILE:HG23 | 1.80                     | 0.63              |
| 1:A:628:VAL:O    | 1:A:628:VAL:HG12 | 1.99                     | 0.63              |
| 2:B:35:MET:O     | 2:B:40:GLN:HB2   | 1.98                     | 0.63              |
| 2:D:128:VAL:HB   | 2:D:138:ILE:HD11 | 1.79                     | 0.63              |
| 1:C:13:LEU:HG    | 1:C:132:ILE:HG21 | 1.81                     | 0.63              |
| 1:C:382:THR:O    | 1:C:385:GLN:HB3  | 1.99                     | 0.63              |
| 1:C:541:LEU:HD23 | 1:C:601:ASN:ND2  | 2.08                     | 0.63              |
| 1:G:345:THR:HB   | 1:G:348:GLU:CB   | 2.29                     | 0.63              |
| 1:G:362:LEU:HD23 | 1:G:427:ILE:HG13 | 1.80                     | 0.63              |
| 1:G:419:THR:O    | 1:G:420:LYS:C    | 2.41                     | 0.63              |
| 1:A:267:ILE:HD11 | 1:A:450:LEU:HD12 | 1.81                     | 0.63              |
| 1:A:753:CYS:O    | 1:A:756:MET:HG3  | 1.99                     | 0.63              |
| 1:A:788:ARG:HG2  | 1:A:788:ARG:HH11 | 1.64                     | 0.63              |
| 1:A:812:PHE:C    | 1:A:814:LYS:H    | 2.06                     | 0.63              |
| 1:C:57:VAL:O     | 1:C:69:THR:HG23  | 1.98                     | 0.63              |
| 1:C:279:ARG:NH2  | 1:C:428:GLU:HG3  | 2.13                     | 0.63              |
| 1:C:328:ASP:HA   | 1:C:331:MET:HB2  | 1.81                     | 0.63              |
| 1:E:419:THR:O    | 1:E:420:LYS:C    | 2.42                     | 0.63              |
| 2:F:70:LEU:N     | 2:F:71:PRO:HD2   | 2.14                     | 0.63              |
| 1:C:227:ALA:C    | 1:C:229:PRO:HD2  | 2.24                     | 0.62              |
| 1:C:345:THR:HB   | 1:C:348:GLU:CB   | 2.28                     | 0.62              |
| 1:E:667:LEU:HG   | 1:E:667:LEU:O    | 1.99                     | 0.62              |
| 2:F:72:MET:HA    | 2:F:75:THR:OG1   | 1.99                     | 0.62              |
| 1:G:747:MET:HE1  | 1:G:755:LEU:HD22 | 1.80                     | 0.62              |
| 1:A:305:LEU:HD22 | 1:A:354:ARG:HB3  | 1.81                     | 0.62              |
| 1:A:609:VAL:O    | 1:A:612:LEU:HB3  | 1.99                     | 0.62              |
| 1:A:686:ILE:HG22 | 1:A:700:LEU:HD21 | 1.80                     | 0.62              |
| 1:C:36:TRP:HE1   | 1:C:78:MET:HG3   | 1.59                     | 0.62              |
| 1:E:13:LEU:HD11  | 1:E:132:ILE:HB   | 1.81                     | 0.62              |
| 1:C:33:LYS:HB3   | 1:C:49:ILE:CB    | 2.29                     | 0.62              |
| 1:C:673:THR:O    | 1:C:677:THR:HG23 | 1.98                     | 0.62              |
| 2:F:84:CYS:O     | 2:F:88:TYR:N     | 2.32                     | 0.62              |
| 1:G:418:GLN:HB3  | 1:G:422:GLN:CB   | 2.28                     | 0.62              |
| 1:G:609:VAL:O    | 1:G:612:LEU:HB3  | 1.98                     | 0.62              |
| 1:C:313:TYR:HD2  | 1:C:360:LEU:HB3  | 1.63                     | 0.62              |
| 1:C:522:GLN:N    | 1:C:523:PRO:HD2  | 2.15                     | 0.62              |
| 1:C:527:LEU:HG   | 1:C:563:GLN:HG3  | 1.80                     | 0.62              |
| 1:C:607:ASP:CA   | 1:C:610:THR:HB   | 2.29                     | 0.62              |
| 1:E:313:TYR:HD2  | 1:E:360:LEU:HB3  | 1.65                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:370:GLU:O    | 1:E:374:ASP:N    | 2.32                     | 0.62              |
| 1:E:482:ILE:HG22 | 1:E:483:ASN:N    | 2.15                     | 0.62              |
| 1:G:278:ILE:HA   | 1:G:315:PHE:CD1  | 2.35                     | 0.62              |
| 1:G:450:LEU:N    | 1:G:450:LEU:HD23 | 2.13                     | 0.62              |
| 1:G:522:GLN:N    | 1:G:523:PRO:HD2  | 2.14                     | 0.62              |
| 1:G:606:ASN:OD1  | 1:G:609:VAL:HG12 | 2.00                     | 0.62              |
| 1:G:611:SER:O    | 1:G:615:GLN:NE2  | 2.32                     | 0.62              |
| 1:A:747:MET:HE1  | 1:A:755:LEU:CD2  | 2.29                     | 0.62              |
| 2:D:70:LEU:N     | 2:D:71:PRO:HD2   | 2.14                     | 0.62              |
| 1:E:57:VAL:O     | 1:E:69:THR:HG23  | 1.98                     | 0.62              |
| 1:G:60:GLU:HG3   | 1:G:66:LYS:O     | 1.99                     | 0.62              |
| 1:G:267:ILE:HD11 | 1:G:450:LEU:HD12 | 1.82                     | 0.62              |
| 1:A:266:ASN:HA   | 1:A:447:ASN:OD1  | 2.00                     | 0.62              |
| 1:A:302:ARG:NH2  | 1:A:303:ASN:HA   | 2.14                     | 0.62              |
| 1:A:418:GLN:HB3  | 1:A:422:GLN:CB   | 2.28                     | 0.62              |
| 1:C:250:LYS:HG2  | 1:C:465:ASP:HB3  | 1.80                     | 0.62              |
| 2:H:3:PHE:HA     | 2:H:7:GLN:HE21   | 1.63                     | 0.62              |
| 2:H:35:MET:O     | 2:H:40:GLN:HB2   | 1.98                     | 0.62              |
| 1:A:409:VAL:HB   | 1:A:414:VAL:HG21 | 1.82                     | 0.62              |
| 1:A:561:GLN:OE1  | 1:A:562:GLU:HG2  | 1.99                     | 0.62              |
| 1:C:302:ARG:NH2  | 1:C:303:ASN:HA   | 2.13                     | 0.62              |
| 1:E:382:THR:O    | 1:E:385:GLN:HB3  | 1.99                     | 0.62              |
| 2:F:84:CYS:C     | 2:F:86:GLU:N     | 2.51                     | 0.62              |
| 2:B:72:MET:HA    | 2:B:75:THR:OG1   | 2.00                     | 0.62              |
| 1:C:399:THR:HG22 | 1:C:403:LEU:CD1  | 2.29                     | 0.62              |
| 1:C:418:GLN:HB3  | 1:C:422:GLN:CB   | 2.30                     | 0.62              |
| 1:E:56:GLU:HG3   | 1:E:71:SER:HA    | 1.81                     | 0.62              |
| 1:E:278:ILE:HA   | 1:E:315:PHE:CD1  | 2.35                     | 0.62              |
| 1:E:527:LEU:HD11 | 1:E:569:PHE:HB2  | 1.81                     | 0.62              |
| 1:E:561:GLN:OE1  | 1:E:562:GLU:HG2  | 1.99                     | 0.62              |
| 1:E:815:ARG:HA   | 1:E:818:GLN:CD   | 2.24                     | 0.62              |
| 2:F:35:MET:O     | 2:F:40:GLN:HB2   | 1.98                     | 0.62              |
| 1:G:382:THR:O    | 1:G:385:GLN:HB3  | 2.00                     | 0.62              |
| 1:A:469:PHE:CE2  | 1:A:587:ALA:HB3  | 2.34                     | 0.62              |
| 1:A:803:CYS:CB   | 2:B:119:MET:HE1  | 2.29                     | 0.62              |
| 1:C:553:THR:O    | 1:C:557:GLU:HG2  | 2.00                     | 0.62              |
| 1:C:671:MET:O    | 1:C:675:ARG:HD2  | 1.99                     | 0.62              |
| 2:D:97:LYS:C     | 2:D:98:GLU:HG3   | 2.23                     | 0.62              |
| 1:E:469:PHE:CZ   | 1:E:587:ALA:HB3  | 2.35                     | 0.62              |
| 1:G:250:LYS:CE   | 1:G:465:ASP:OD2  | 2.47                     | 0.62              |
| 1:G:477:PHE:O    | 1:G:480:LEU:HB3  | 2.00                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:490:GLN:NE2  | 1:G:494:ASN:HD21 | 1.97                     | 0.62              |
| 2:H:84:CYS:C     | 2:H:88:TYR:CD2   | 2.77                     | 0.62              |
| 1:A:815:ARG:HA   | 1:A:818:GLN:CD   | 2.25                     | 0.62              |
| 1:C:158:ASP:HB2  | 1:C:193:TYR:OH   | 2.00                     | 0.62              |
| 2:D:4:SER:H      | 2:D:7:GLN:HE21   | 1.48                     | 0.62              |
| 1:A:323:ILE:CG2  | 1:A:326:GLN:HB3  | 2.29                     | 0.61              |
| 1:A:480:LEU:HD22 | 1:A:597:TRP:CH2  | 2.34                     | 0.61              |
| 2:B:70:LEU:N     | 2:B:71:PRO:HD2   | 2.14                     | 0.61              |
| 2:D:85:PHE:CD1   | 2:D:144:VAL:HG11 | 2.35                     | 0.61              |
| 1:E:158:ASP:HB2  | 1:E:193:TYR:OH   | 2.00                     | 0.61              |
| 1:A:60:GLU:HG3   | 1:A:66:LYS:O     | 2.00                     | 0.61              |
| 1:E:267:ILE:HD11 | 1:E:450:LEU:HD12 | 1.81                     | 0.61              |
| 1:E:310:PHE:CD2  | 1:E:320:HIS:HB2  | 2.35                     | 0.61              |
| 1:E:489:LEU:O    | 1:E:492:LEU:HB3  | 1.99                     | 0.61              |
| 1:E:568:LYS:CD   | 1:E:584:LEU:HB2  | 2.29                     | 0.61              |
| 1:G:305:LEU:HD22 | 1:G:354:ARG:HB3  | 1.81                     | 0.61              |
| 1:G:766:LEU:HB3  | 1:G:780:VAL:HG21 | 1.82                     | 0.61              |
| 1:A:747:MET:HG3  | 1:G:812:PHE:CZ   | 2.36                     | 0.61              |
| 2:D:125:GLU:O    | 2:D:129:ALA:HB2  | 2.00                     | 0.61              |
| 1:E:89:MET:HE3   | 1:E:100:VAL:HG13 | 1.81                     | 0.61              |
| 1:G:302:ARG:HH21 | 1:G:307:LEU:H    | 1.48                     | 0.61              |
| 1:G:302:ARG:NH2  | 1:G:303:ASN:HA   | 2.15                     | 0.61              |
| 2:H:70:LEU:N     | 2:H:71:PRO:HD2   | 2.15                     | 0.61              |
| 1:A:271:LEU:HD21 | 1:A:663:TYR:CE1  | 2.34                     | 0.61              |
| 1:C:362:LEU:HD21 | 1:C:430:LEU:HD23 | 1.81                     | 0.61              |
| 1:C:527:LEU:HD11 | 1:C:569:PHE:HB2  | 1.81                     | 0.61              |
| 1:C:705:LEU:HD22 | 1:C:710:VAL:HG21 | 1.82                     | 0.61              |
| 1:C:747:MET:HE1  | 1:C:755:LEU:HD22 | 1.81                     | 0.61              |
| 2:D:65:LYS:HD2   | 2:D:68:GLN:NE2   | 2.15                     | 0.61              |
| 1:E:52:GLU:HA    | 1:E:57:VAL:HG13  | 1.82                     | 0.61              |
| 1:E:686:ILE:HD13 | 1:E:687:PRO:HD2  | 1.82                     | 0.61              |
| 1:G:50:LYS:HE3   | 1:G:60:GLU:CB    | 2.30                     | 0.61              |
| 1:G:490:GLN:HE21 | 1:G:494:ASN:HD21 | 1.47                     | 0.61              |
| 1:G:541:LEU:HD21 | 1:G:597:TRP:HB3  | 1.82                     | 0.61              |
| 1:G:627:ASP:O    | 1:G:627:ASP:OD1  | 2.18                     | 0.61              |
| 1:G:686:ILE:HG22 | 1:G:700:LEU:HD21 | 1.80                     | 0.61              |
| 1:A:313:TYR:HD2  | 1:A:360:LEU:HB3  | 1.65                     | 0.61              |
| 1:C:561:GLN:OE1  | 1:C:562:GLU:HG2  | 2.00                     | 0.61              |
| 1:E:33:LYS:HB3   | 1:E:49:ILE:CB    | 2.31                     | 0.61              |
| 1:E:50:LYS:HE3   | 1:E:60:GLU:CB    | 2.30                     | 0.61              |
| 1:G:89:MET:HE1   | 1:G:104:LEU:HG   | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:242:ASN:OD1  | 1:G:244:ASN:N    | 2.29                     | 0.61              |
| 1:A:497:MET:HE3  | 1:A:497:MET:HA   | 1.81                     | 0.61              |
| 1:A:527:LEU:HD23 | 1:A:537:VAL:HG23 | 1.82                     | 0.61              |
| 2:B:55:LYS:O     | 2:B:58:GLU:HG2   | 2.01                     | 0.61              |
| 1:E:243:ASP:HB3  | 1:E:323:ILE:CD1  | 2.30                     | 0.61              |
| 1:E:305:LEU:HD22 | 1:E:354:ARG:HB3  | 1.83                     | 0.61              |
| 1:E:399:THR:O    | 1:E:403:LEU:HD12 | 2.00                     | 0.61              |
| 1:E:530:ARG:HG2  | 1:E:534:PRO:O    | 2.01                     | 0.61              |
| 1:E:747:MET:HE1  | 1:E:755:LEU:HD22 | 1.82                     | 0.61              |
| 1:A:243:ASP:HB3  | 1:A:323:ILE:CD1  | 2.31                     | 0.61              |
| 1:C:89:MET:HE2   | 1:C:104:LEU:HD21 | 1.81                     | 0.61              |
| 1:C:800:GLN:HA   | 2:D:119:MET:HE2  | 1.83                     | 0.61              |
| 2:D:84:CYS:SG    | 2:D:87:ASP:OD2   | 2.59                     | 0.61              |
| 1:E:23:PRO:HA    | 1:E:26:GLN:HB3   | 1.82                     | 0.61              |
| 1:E:362:LEU:HD23 | 1:E:427:ILE:HG13 | 1.82                     | 0.61              |
| 2:B:84:CYS:O     | 2:B:85:PHE:C     | 2.43                     | 0.61              |
| 1:C:89:MET:HE1   | 1:C:104:LEU:HG   | 1.82                     | 0.61              |
| 1:C:107:ARG:HH11 | 1:C:115:THR:HG23 | 1.66                     | 0.61              |
| 1:C:530:ARG:HG2  | 1:C:534:PRO:O    | 2.01                     | 0.61              |
| 1:C:803:CYS:CB   | 2:D:119:MET:HE1  | 2.30                     | 0.61              |
| 2:D:140:TYR:HD1  | 2:D:141:GLU:N    | 1.97                     | 0.61              |
| 2:D:140:TYR:CD1  | 2:D:141:GLU:N    | 2.68                     | 0.61              |
| 1:G:250:LYS:HG2  | 1:G:465:ASP:HB3  | 1.82                     | 0.61              |
| 2:H:72:MET:HA    | 2:H:75:THR:OG1   | 2.00                     | 0.61              |
| 1:A:541:LEU:HD21 | 1:A:597:TRP:HB3  | 1.83                     | 0.61              |
| 1:A:607:ASP:CA   | 1:A:610:THR:HB   | 2.28                     | 0.61              |
| 1:A:728:GLN:HE21 | 1:A:728:GLN:HA   | 1.66                     | 0.61              |
| 1:C:52:GLU:HA    | 1:C:57:VAL:HG13  | 1.81                     | 0.61              |
| 1:C:610:THR:HG22 | 1:C:628:VAL:HG11 | 1.82                     | 0.61              |
| 2:D:84:CYS:O     | 2:D:85:PHE:C     | 2.43                     | 0.61              |
| 1:E:556:VAL:HG12 | 1:E:560:ILE:HD11 | 1.82                     | 0.61              |
| 1:G:273:GLU:O    | 1:G:273:GLU:HG2  | 2.01                     | 0.61              |
| 1:G:328:ASP:HA   | 1:G:331:MET:HB2  | 1.81                     | 0.61              |
| 1:G:551:THR:N    | 1:G:554:SER:OG   | 2.32                     | 0.61              |
| 1:G:553:THR:O    | 1:G:557:GLU:HG2  | 2.01                     | 0.61              |
| 1:G:728:GLN:HE21 | 1:G:728:GLN:CA   | 2.12                     | 0.61              |
| 1:A:89:MET:C     | 1:A:91:GLU:H     | 2.09                     | 0.61              |
| 1:A:328:ASP:HA   | 1:A:331:MET:HB2  | 1.82                     | 0.61              |
| 1:A:551:THR:N    | 1:A:554:SER:OG   | 2.30                     | 0.61              |
| 2:B:4:SER:H      | 2:B:7:GLN:HE21   | 1.48                     | 0.61              |
| 1:E:450:LEU:HD23 | 1:E:450:LEU:N    | 2.15                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:553:THR:CG2  | 1:E:579:THR:HG21 | 2.31                     | 0.61              |
| 1:G:527:LEU:HD23 | 1:G:537:VAL:HG23 | 1.83                     | 0.61              |
| 1:A:405:PRO:HD2  | 1:A:417:ALA:HA   | 1.83                     | 0.60              |
| 1:C:747:MET:CG   | 1:C:751:GLN:HE22 | 2.14                     | 0.60              |
| 1:E:134:SER:CB   | 1:E:212:GLY:HA2  | 2.29                     | 0.60              |
| 2:F:4:SER:H      | 2:F:7:GLN:HE21   | 1.48                     | 0.60              |
| 1:G:279:ARG:NH2  | 1:G:428:GLU:HG3  | 2.16                     | 0.60              |
| 2:H:65:LYS:HD2   | 2:H:68:GLN:NE2   | 2.15                     | 0.60              |
| 1:A:145:LYS:CG   | 1:A:146:ARG:H    | 2.12                     | 0.60              |
| 1:A:362:LEU:HD21 | 1:A:430:LEU:HD23 | 1.83                     | 0.60              |
| 1:A:746:PHE:CE2  | 2:H:13:GLU:OE1   | 2.54                     | 0.60              |
| 1:C:125:ASN:OD1  | 1:C:126:PRO:HD2  | 2.02                     | 0.60              |
| 1:C:267:ILE:HD11 | 1:C:450:LEU:HD12 | 1.83                     | 0.60              |
| 2:D:55:LYS:O     | 2:D:58:GLU:HG2   | 2.00                     | 0.60              |
| 2:D:84:CYS:O     | 2:D:87:ASP:N     | 2.33                     | 0.60              |
| 1:E:418:GLN:HB3  | 1:E:422:GLN:CB   | 2.29                     | 0.60              |
| 1:E:478:GLU:OE1  | 1:E:478:GLU:N    | 2.21                     | 0.60              |
| 1:G:52:GLU:HA    | 1:G:57:VAL:HG13  | 1.84                     | 0.60              |
| 1:G:104:LEU:HD12 | 1:G:705:LEU:HD11 | 1.84                     | 0.60              |
| 1:G:323:ILE:CG2  | 1:G:326:GLN:HB3  | 2.31                     | 0.60              |
| 1:A:382:THR:O    | 1:A:385:GLN:HB3  | 2.01                     | 0.60              |
| 2:B:65:LYS:HD2   | 2:B:68:GLN:NE2   | 2.15                     | 0.60              |
| 1:C:230:ILE:HG22 | 1:C:231:LEU:N    | 2.15                     | 0.60              |
| 1:C:477:PHE:O    | 1:C:480:LEU:HB3  | 2.01                     | 0.60              |
| 2:D:72:MET:HA    | 2:D:75:THR:OG1   | 2.00                     | 0.60              |
| 1:E:145:LYS:HG3  | 1:E:146:ARG:HE   | 1.66                     | 0.60              |
| 1:G:342:MET:HE1  | 1:G:449:ALA:HB3  | 1.83                     | 0.60              |
| 1:G:712:GLU:H    | 1:G:712:GLU:CD   | 2.07                     | 0.60              |
| 1:G:807:LEU:O    | 1:G:807:LEU:HD23 | 2.01                     | 0.60              |
| 1:A:527:LEU:HD11 | 1:A:569:PHE:HB2  | 1.82                     | 0.60              |
| 1:A:721:PHE:N    | 1:A:721:PHE:HD1  | 1.99                     | 0.60              |
| 1:C:145:LYS:HG3  | 1:C:146:ARG:HE   | 1.66                     | 0.60              |
| 1:C:302:ARG:HH21 | 1:C:307:LEU:H    | 1.49                     | 0.60              |
| 1:C:568:LYS:CD   | 1:C:584:LEU:HB2  | 2.31                     | 0.60              |
| 1:E:302:ARG:HH21 | 1:E:307:LEU:H    | 1.47                     | 0.60              |
| 2:F:125:GLU:O    | 2:F:129:ALA:HB2  | 2.01                     | 0.60              |
| 1:G:480:LEU:HD11 | 1:G:528:ILE:HD12 | 1.83                     | 0.60              |
| 1:G:630:ARG:HH22 | 1:G:657:ARG:HB3  | 1.66                     | 0.60              |
| 2:B:140:TYR:CD1  | 2:B:141:GLU:HG2  | 2.37                     | 0.60              |
| 1:C:721:PHE:N    | 1:C:721:PHE:HD1  | 1.99                     | 0.60              |
| 1:E:533:ASN:CB   | 1:E:534:PRO:HD2  | 2.31                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:663:TYR:OH   | 1:E:667:LEU:HD13 | 2.01                     | 0.60              |
| 1:G:530:ARG:HG2  | 1:G:534:PRO:O    | 2.01                     | 0.60              |
| 1:A:533:ASN:O    | 1:A:534:PRO:C    | 2.45                     | 0.60              |
| 1:A:667:LEU:HG   | 1:A:667:LEU:O    | 2.01                     | 0.60              |
| 1:A:731:ARG:HG2  | 1:A:731:ARG:HH11 | 1.66                     | 0.60              |
| 1:C:50:LYS:HE3   | 1:C:60:GLU:CB    | 2.31                     | 0.60              |
| 1:C:259:THR:HB   | 1:C:261:TYR:HE1  | 1.63                     | 0.60              |
| 1:C:342:MET:HE1  | 1:C:449:ALA:HB3  | 1.83                     | 0.60              |
| 1:E:480:LEU:HD11 | 1:E:528:ILE:HD12 | 1.83                     | 0.60              |
| 1:G:145:LYS:HG3  | 1:G:146:ARG:HE   | 1.65                     | 0.60              |
| 1:A:36:TRP:HE1   | 1:A:78:MET:HG3   | 1.65                     | 0.60              |
| 1:A:391:MET:HG2  | 1:A:613:LEU:CD2  | 2.31                     | 0.60              |
| 1:E:361:GLN:C    | 1:E:363:GLY:H    | 2.07                     | 0.60              |
| 1:E:606:ASN:OD1  | 1:E:609:VAL:HG12 | 2.01                     | 0.60              |
| 1:E:711:LEU:HD22 | 1:E:711:LEU:N    | 2.17                     | 0.60              |
| 2:F:55:LYS:O     | 2:F:58:GLU:HG2   | 2.01                     | 0.60              |
| 1:G:23:PRO:HA    | 1:G:26:GLN:HB3   | 1.82                     | 0.60              |
| 1:G:482:ILE:HG22 | 1:G:483:ASN:N    | 2.15                     | 0.60              |
| 1:A:103:ASN:O    | 1:A:107:ARG:HG3  | 2.02                     | 0.60              |
| 1:A:568:LYS:CD   | 1:A:584:LEU:HB2  | 2.32                     | 0.60              |
| 1:A:804:ARG:HG2  | 1:A:804:ARG:NH1  | 2.15                     | 0.60              |
| 1:C:352:ILE:CG2  | 1:C:442:ILE:HD11 | 2.32                     | 0.60              |
| 1:C:469:PHE:CZ   | 1:C:587:ALA:HB3  | 2.37                     | 0.60              |
| 1:C:728:GLN:HE21 | 1:C:728:GLN:HA   | 1.67                     | 0.60              |
| 1:E:490:GLN:NE2  | 1:E:494:ASN:HD21 | 1.99                     | 0.60              |
| 1:E:663:TYR:C    | 1:E:665:GLU:H    | 2.10                     | 0.60              |
| 1:G:494:ASN:H    | 1:G:494:ASN:HD22 | 1.49                     | 0.60              |
| 1:G:561:GLN:OE1  | 1:G:562:GLU:HG2  | 2.01                     | 0.60              |
| 2:H:84:CYS:O     | 2:H:88:TYR:CG    | 2.54                     | 0.60              |
| 1:A:50:LYS:HE3   | 1:A:60:GLU:CB    | 2.32                     | 0.60              |
| 1:A:186:ASN:O    | 1:A:190:VAL:HG23 | 2.01                     | 0.60              |
| 1:C:568:LYS:HA   | 1:C:568:LYS:HE3  | 1.84                     | 0.60              |
| 1:G:382:THR:HA   | 1:G:385:GLN:OE1  | 2.01                     | 0.60              |
| 2:H:4:SER:H      | 2:H:7:GLN:HE21   | 1.49                     | 0.60              |
| 1:A:7:SER:HB3    | 1:A:10:GLU:OE1   | 2.00                     | 0.60              |
| 1:A:89:MET:HE1   | 1:A:104:LEU:HG   | 1.84                     | 0.60              |
| 2:B:140:TYR:CD1  | 2:B:141:GLU:N    | 2.70                     | 0.60              |
| 1:G:259:THR:HB   | 1:G:261:TYR:HE1  | 1.64                     | 0.60              |
| 1:G:416:LYS:HE2  | 1:G:417:ALA:H    | 1.66                     | 0.60              |
| 1:G:489:LEU:O    | 1:G:492:LEU:HB3  | 2.02                     | 0.60              |
| 1:A:527:LEU:HG   | 1:A:563:GLN:HG3  | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:663:TYR:OH   | 1:A:667:LEU:HD13 | 2.02                     | 0.59              |
| 1:A:745:GLY:CA   | 1:G:819:LEU:HD21 | 2.31                     | 0.59              |
| 1:G:186:ASN:O    | 1:G:190:VAL:HG23 | 2.02                     | 0.59              |
| 1:G:497:MET:HA   | 1:G:497:MET:HE3  | 1.82                     | 0.59              |
| 1:G:663:TYR:C    | 1:G:665:GLU:H    | 2.10                     | 0.59              |
| 1:C:405:PRO:HD2  | 1:C:417:ALA:HA   | 1.84                     | 0.59              |
| 1:C:703:GLU:O    | 1:C:706:ARG:HB2  | 2.02                     | 0.59              |
| 1:C:797:ILE:HG13 | 2:D:117:GLU:H    | 1.65                     | 0.59              |
| 1:E:12:PHE:CD2   | 1:E:131:PRO:HD2  | 2.37                     | 0.59              |
| 1:E:420:LYS:HD2  | 1:E:421:GLU:CD   | 2.27                     | 0.59              |
| 1:G:218:GLY:HA3  | 1:G:221:GLU:OE1  | 2.03                     | 0.59              |
| 2:B:85:PHE:CZ    | 2:B:145:ARG:CZ   | 2.85                     | 0.59              |
| 1:C:305:LEU:HD22 | 1:C:354:ARG:HB3  | 1.82                     | 0.59              |
| 1:E:176:THR:O    | 1:E:183:LYS:CD   | 2.50                     | 0.59              |
| 1:E:497:MET:HA   | 1:E:497:MET:HE3  | 1.84                     | 0.59              |
| 2:F:44:ASN:HD22  | 2:F:117:GLU:HB3  | 1.67                     | 0.59              |
| 1:G:13:LEU:HD11  | 1:G:132:ILE:HB   | 1.84                     | 0.59              |
| 1:G:254:ILE:O    | 1:G:460:PHE:HA   | 2.03                     | 0.59              |
| 1:G:527:LEU:HG   | 1:G:563:GLN:HG3  | 1.83                     | 0.59              |
| 1:A:347:GLU:C    | 1:A:349:GLN:H    | 2.11                     | 0.59              |
| 1:A:705:LEU:HD22 | 1:A:710:VAL:HG21 | 1.85                     | 0.59              |
| 1:C:145:LYS:CG   | 1:C:146:ARG:H    | 2.15                     | 0.59              |
| 1:C:271:LEU:HD21 | 1:C:663:TYR:CD1  | 2.36                     | 0.59              |
| 1:C:278:ILE:HA   | 1:C:315:PHE:CD1  | 2.37                     | 0.59              |
| 1:C:533:ASN:CB   | 1:C:534:PRO:HD2  | 2.32                     | 0.59              |
| 1:E:553:THR:HG23 | 1:E:579:THR:HG21 | 1.84                     | 0.59              |
| 1:E:686:ILE:HG22 | 1:E:700:LEU:HD21 | 1.84                     | 0.59              |
| 1:E:719:GLN:HA   | 1:E:719:GLN:NE2  | 2.17                     | 0.59              |
| 1:A:56:GLU:HG3   | 1:A:71:SER:HA    | 1.83                     | 0.59              |
| 1:A:399:THR:O    | 1:A:403:LEU:HD12 | 2.03                     | 0.59              |
| 1:C:36:TRP:CE2   | 1:C:78:MET:HG3   | 2.37                     | 0.59              |
| 1:C:489:LEU:O    | 1:C:492:LEU:HB3  | 2.03                     | 0.59              |
| 1:C:630:ARG:HH22 | 1:C:657:ARG:CB   | 2.15                     | 0.59              |
| 1:C:663:TYR:C    | 1:C:665:GLU:H    | 2.11                     | 0.59              |
| 1:G:13:LEU:HD11  | 1:G:152:HIS:HD2  | 1.68                     | 0.59              |
| 1:G:79:ASN:ND2   | 1:G:80:PRO:HD2   | 2.11                     | 0.59              |
| 1:G:568:LYS:HA   | 1:G:568:LYS:HE3  | 1.84                     | 0.59              |
| 1:G:671:MET:O    | 1:G:675:ARG:HD2  | 2.01                     | 0.59              |
| 1:G:703:GLU:O    | 1:G:706:ARG:HB2  | 2.03                     | 0.59              |
| 1:G:804:ARG:NH2  | 2:H:44:ASN:HD21  | 2.01                     | 0.59              |
| 2:B:131:HIS:CE1  | 2:B:146:MET:HE3  | 2.38                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:7:SER:O      | 1:C:11:LYS:HG3   | 2.03                     | 0.59              |
| 1:C:310:PHE:CD2  | 1:C:320:HIS:HB2  | 2.38                     | 0.59              |
| 2:D:85:PHE:O     | 2:D:87:ASP:N     | 2.36                     | 0.59              |
| 1:E:273:GLU:HG2  | 1:E:273:GLU:O    | 2.02                     | 0.59              |
| 1:E:533:ASN:O    | 1:E:534:PRO:C    | 2.44                     | 0.59              |
| 2:F:65:LYS:HD2   | 2:F:68:GLN:NE2   | 2.15                     | 0.59              |
| 1:G:731:ARG:HG2  | 1:G:731:ARG:HH11 | 1.68                     | 0.59              |
| 1:G:788:ARG:HG2  | 1:G:788:ARG:HH11 | 1.66                     | 0.59              |
| 1:A:100:VAL:O    | 1:A:104:LEU:HG   | 2.03                     | 0.59              |
| 1:C:13:LEU:HG    | 1:C:132:ILE:CG2  | 2.32                     | 0.59              |
| 1:E:527:LEU:HD23 | 1:E:537:VAL:HG23 | 1.83                     | 0.59              |
| 1:E:703:GLU:O    | 1:E:706:ARG:HB2  | 2.02                     | 0.59              |
| 1:E:788:ARG:HH11 | 1:E:788:ARG:HG2  | 1.68                     | 0.59              |
| 2:F:40:GLN:HB3   | 2:F:42:PRO:HD3   | 1.85                     | 0.59              |
| 2:F:80:LYS:H     | 2:F:80:LYS:HD2   | 1.67                     | 0.59              |
| 1:G:89:MET:HE3   | 1:G:100:VAL:HG13 | 1.84                     | 0.59              |
| 1:G:437:ARG:HB3  | 1:G:624:LEU:HD23 | 1.85                     | 0.59              |
| 1:A:104:LEU:HD12 | 1:A:705:LEU:HD11 | 1.85                     | 0.59              |
| 1:A:380:ASP:OD1  | 1:A:382:THR:HG23 | 2.02                     | 0.59              |
| 1:C:88:ASP:HB3   | 1:C:91:GLU:OE1   | 2.03                     | 0.59              |
| 1:C:581:PHE:HZ   | 1:C:597:TRP:CH2  | 2.21                     | 0.59              |
| 1:E:145:LYS:CG   | 1:E:146:ARG:H    | 2.15                     | 0.59              |
| 1:E:522:GLN:N    | 1:E:523:PRO:HD2  | 2.16                     | 0.59              |
| 1:G:420:LYS:HD2  | 1:G:421:GLU:CD   | 2.28                     | 0.59              |
| 1:G:469:PHE:CZ   | 1:G:587:ALA:HB3  | 2.38                     | 0.59              |
| 1:G:607:ASP:CA   | 1:G:610:THR:HB   | 2.31                     | 0.59              |
| 1:G:804:ARG:HG2  | 1:G:804:ARG:NH1  | 2.17                     | 0.59              |
| 2:H:97:LYS:C     | 2:H:98:GLU:HG3   | 2.28                     | 0.59              |
| 2:B:125:GLU:O    | 2:B:129:ALA:HB2  | 2.03                     | 0.59              |
| 1:C:659:VAL:CG1  | 1:C:660:GLY:N    | 2.65                     | 0.59              |
| 1:C:667:LEU:O    | 1:C:667:LEU:HG   | 2.02                     | 0.59              |
| 1:E:123:VAL:O    | 1:E:123:VAL:HG12 | 2.03                     | 0.59              |
| 1:E:437:ARG:HB3  | 1:E:624:LEU:HD23 | 1.85                     | 0.59              |
| 1:E:477:PHE:O    | 1:E:480:LEU:HB3  | 2.03                     | 0.59              |
| 1:A:23:PRO:HA    | 1:A:26:GLN:HB3   | 1.84                     | 0.59              |
| 1:A:702:LEU:O    | 1:A:706:ARG:HG3  | 2.02                     | 0.59              |
| 1:C:293:LEU:HD11 | 1:C:301:MET:CE   | 2.33                     | 0.59              |
| 1:C:482:ILE:HG22 | 1:C:483:ASN:N    | 2.18                     | 0.59              |
| 1:E:193:TYR:CZ   | 1:E:197:VAL:HG21 | 2.38                     | 0.59              |
| 1:E:568:LYS:CE   | 1:E:584:LEU:HB2  | 2.33                     | 0.59              |
| 1:E:803:CYS:CB   | 2:F:119:MET:HE1  | 2.33                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:89:MET:HE2   | 1:G:104:LEU:HD21 | 1.84                     | 0.59              |
| 2:H:131:HIS:CE1  | 2:H:146:MET:HE3  | 2.38                     | 0.59              |
| 1:A:52:GLU:HA    | 1:A:57:VAL:HG13  | 1.84                     | 0.58              |
| 1:A:490:GLN:O    | 1:A:494:ASN:ND2  | 2.36                     | 0.58              |
| 1:A:533:ASN:CB   | 1:A:534:PRO:HD2  | 2.33                     | 0.58              |
| 2:D:40:GLN:HB3   | 2:D:42:PRO:HD3   | 1.85                     | 0.58              |
| 1:G:242:ASN:ND2  | 1:G:245:SER:HA   | 2.18                     | 0.58              |
| 1:G:659:VAL:CG1  | 1:G:660:GLY:N    | 2.65                     | 0.58              |
| 2:H:86:GLU:OE1   | 2:H:86:GLU:N     | 2.34                     | 0.58              |
| 1:A:33:LYS:HB3   | 1:A:49:ILE:CB    | 2.32                     | 0.58              |
| 1:A:443:LEU:O    | 1:A:447:ASN:HB2  | 2.03                     | 0.58              |
| 1:A:607:ASP:HA   | 1:A:610:THR:CB   | 2.32                     | 0.58              |
| 1:A:630:ARG:HH22 | 1:A:657:ARG:HB3  | 1.67                     | 0.58              |
| 1:A:750:LYS:NZ   | 1:G:809:ARG:HH22 | 2.01                     | 0.58              |
| 1:A:763:ASP:HB3  | 1:A:766:LEU:HD11 | 1.85                     | 0.58              |
| 2:B:85:PHE:CE1   | 2:B:145:ARG:HG2  | 2.38                     | 0.58              |
| 1:E:22:ASN:OD1   | 1:E:24:LEU:HB2   | 2.01                     | 0.58              |
| 1:E:218:GLY:HA3  | 1:E:221:GLU:OE1  | 2.03                     | 0.58              |
| 1:E:382:THR:HA   | 1:E:385:GLN:OE1  | 2.02                     | 0.58              |
| 1:E:405:PRO:HD2  | 1:E:417:ALA:HA   | 1.85                     | 0.58              |
| 1:E:551:THR:N    | 1:E:554:SER:OG   | 2.33                     | 0.58              |
| 1:E:553:THR:O    | 1:E:557:GLU:HG2  | 2.02                     | 0.58              |
| 1:G:310:PHE:CD2  | 1:G:320:HIS:HB2  | 2.38                     | 0.58              |
| 1:G:361:GLN:C    | 1:G:363:GLY:N    | 2.59                     | 0.58              |
| 2:B:40:GLN:HB3   | 2:B:42:PRO:HD3   | 1.85                     | 0.58              |
| 1:E:138:ILE:HD13 | 1:E:154:TYR:CE2  | 2.38                     | 0.58              |
| 1:E:570:GLN:OE1  | 1:E:589:LYS:HE2  | 2.04                     | 0.58              |
| 1:G:721:PHE:CZ   | 1:G:768:ARG:HG2  | 2.37                     | 0.58              |
| 1:A:89:MET:HE2   | 1:A:104:LEU:HD21 | 1.86                     | 0.58              |
| 1:A:347:GLU:C    | 1:A:349:GLN:N    | 2.60                     | 0.58              |
| 2:B:104:MET:C    | 2:B:106:ALA:H    | 2.11                     | 0.58              |
| 1:C:243:ASP:HB3  | 1:C:323:ILE:CD1  | 2.32                     | 0.58              |
| 1:G:83:PHE:CE1   | 1:G:92:LEU:HA    | 2.38                     | 0.58              |
| 1:G:103:ASN:ND2  | 1:G:107:ARG:HD2  | 2.18                     | 0.58              |
| 1:G:123:VAL:O    | 1:G:123:VAL:HG12 | 2.03                     | 0.58              |
| 1:G:271:LEU:HD21 | 1:G:663:TYR:CD1  | 2.38                     | 0.58              |
| 1:G:362:LEU:HD21 | 1:G:430:LEU:HD23 | 1.84                     | 0.58              |
| 1:A:8:ASP:CA     | 1:A:11:LYS:HD2   | 2.20                     | 0.58              |
| 1:A:310:PHE:CD2  | 1:A:320:HIS:HB2  | 2.39                     | 0.58              |
| 1:A:437:ARG:HB3  | 1:A:624:LEU:HD23 | 1.85                     | 0.58              |
| 1:C:8:ASP:HA     | 1:C:11:LYS:CD    | 2.21                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:242:ASN:ND2  | 1:C:245:SER:HA   | 2.18                     | 0.58              |
| 1:E:731:ARG:HH11 | 1:E:731:ARG:HG2  | 1.67                     | 0.58              |
| 1:E:797:ILE:HG13 | 2:F:117:GLU:H    | 1.69                     | 0.58              |
| 1:G:22:ASN:OD1   | 1:G:24:LEU:HB2   | 2.04                     | 0.58              |
| 1:G:243:ASP:HB3  | 1:G:323:ILE:CD1  | 2.32                     | 0.58              |
| 1:G:533:ASN:CB   | 1:G:534:PRO:HD2  | 2.33                     | 0.58              |
| 1:G:712:GLU:OE1  | 1:G:712:GLU:N    | 2.35                     | 0.58              |
| 1:G:747:MET:HE1  | 1:G:755:LEU:CD2  | 2.33                     | 0.58              |
| 1:G:804:ARG:NH2  | 2:H:44:ASN:ND2   | 2.51                     | 0.58              |
| 1:A:89:MET:HE3   | 1:A:100:VAL:HG13 | 1.86                     | 0.58              |
| 2:B:140:TYR:O    | 2:B:141:GLU:C    | 2.45                     | 0.58              |
| 1:C:165:LEU:HD21 | 1:C:260:GLY:HA2  | 1.85                     | 0.58              |
| 1:C:788:ARG:HG2  | 1:C:788:ARG:HH11 | 1.67                     | 0.58              |
| 2:D:64:LEU:HD23  | 2:D:68:GLN:OE1   | 2.03                     | 0.58              |
| 1:E:712:GLU:H    | 1:E:712:GLU:CD   | 2.11                     | 0.58              |
| 1:G:369:LYS:HZ2  | 1:G:420:LYS:HB3  | 1.68                     | 0.58              |
| 1:G:416:LYS:HE2  | 1:G:417:ALA:N    | 2.18                     | 0.58              |
| 2:H:140:TYR:O    | 2:H:141:GLU:C    | 2.47                     | 0.58              |
| 1:A:361:GLN:O    | 1:A:363:GLY:N    | 2.36                     | 0.58              |
| 1:C:686:ILE:HG22 | 1:C:700:LEU:HD21 | 1.86                     | 0.58              |
| 1:C:747:MET:HE1  | 1:C:755:LEU:CD2  | 2.34                     | 0.58              |
| 1:E:711:LEU:H    | 1:E:711:LEU:CD2  | 2.17                     | 0.58              |
| 2:F:140:TYR:CD1  | 2:F:141:GLU:N    | 2.72                     | 0.58              |
| 1:G:568:LYS:CD   | 1:G:584:LEU:HB2  | 2.32                     | 0.58              |
| 2:H:125:GLU:O    | 2:H:129:ALA:HB2  | 2.03                     | 0.58              |
| 1:A:125:ASN:OD1  | 1:A:126:PRO:HD2  | 2.04                     | 0.58              |
| 1:A:302:ARG:HH21 | 1:A:307:LEU:H    | 1.49                     | 0.58              |
| 1:A:610:THR:HG23 | 1:A:628:VAL:CG2  | 2.33                     | 0.58              |
| 2:B:85:PHE:HE1   | 2:B:145:ARG:HG2  | 1.67                     | 0.58              |
| 1:E:165:LEU:HD21 | 1:E:260:GLY:HA2  | 1.85                     | 0.58              |
| 1:E:293:LEU:HA   | 1:E:332:PHE:CE1  | 2.39                     | 0.58              |
| 1:G:292:TYR:CE2  | 1:G:331:MET:HB3  | 2.39                     | 0.58              |
| 1:G:409:VAL:HB   | 1:G:414:VAL:HG21 | 1.85                     | 0.58              |
| 1:G:527:LEU:HD11 | 1:G:569:PHE:HB2  | 1.86                     | 0.58              |
| 2:H:40:GLN:HB3   | 2:H:42:PRO:HD3   | 1.85                     | 0.58              |
| 1:A:796:ILE:HG22 | 1:A:800:GLN:OE1  | 2.04                     | 0.58              |
| 1:C:265:ALA:HB3  | 1:C:450:LEU:HB3  | 1.86                     | 0.58              |
| 1:C:266:ASN:HA   | 1:C:447:ASN:OD1  | 2.04                     | 0.58              |
| 1:C:731:ARG:HG2  | 1:C:731:ARG:HH11 | 1.69                     | 0.58              |
| 1:E:254:ILE:O    | 1:E:460:PHE:HA   | 2.03                     | 0.58              |
| 1:E:362:LEU:HD21 | 1:E:430:LEU:HD23 | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:378:MET:HA   | 1:E:378:MET:HE3  | 1.86                     | 0.58              |
| 1:E:428:GLU:C    | 1:E:430:LEU:H    | 2.12                     | 0.58              |
| 1:E:611:SER:O    | 1:E:615:GLN:NE2  | 2.35                     | 0.58              |
| 2:F:131:HIS:CE1  | 2:F:146:MET:HE3  | 2.39                     | 0.58              |
| 1:G:37:VAL:CG1   | 1:G:38:PRO:HD2   | 2.34                     | 0.58              |
| 1:G:265:ALA:HB3  | 1:G:450:LEU:HB3  | 1.86                     | 0.58              |
| 2:H:64:LEU:HD23  | 2:H:68:GLN:OE1   | 2.04                     | 0.58              |
| 1:A:378:MET:HA   | 1:A:378:MET:HE3  | 1.85                     | 0.58              |
| 1:C:361:GLN:C    | 1:C:363:GLY:N    | 2.61                     | 0.58              |
| 2:D:80:LYS:H     | 2:D:80:LYS:HD2   | 1.68                     | 0.58              |
| 1:E:345:THR:HB   | 1:E:348:GLU:CB   | 2.29                     | 0.58              |
| 2:F:140:TYR:O    | 2:F:141:GLU:C    | 2.46                     | 0.58              |
| 1:G:705:LEU:HD22 | 1:G:710:VAL:HG21 | 1.84                     | 0.58              |
| 1:G:797:ILE:HG12 | 2:H:117:GLU:HG2  | 1.84                     | 0.58              |
| 2:H:14:ALA:CB    | 2:H:38:LEU:HD21  | 2.34                     | 0.58              |
| 1:A:293:LEU:HD11 | 1:A:301:MET:CE   | 2.34                     | 0.57              |
| 1:A:663:TYR:C    | 1:A:665:GLU:H    | 2.11                     | 0.57              |
| 1:A:703:GLU:O    | 1:A:706:ARG:HB2  | 2.02                     | 0.57              |
| 1:C:123:VAL:HG12 | 1:C:123:VAL:O    | 2.03                     | 0.57              |
| 1:C:273:GLU:HG2  | 1:C:273:GLU:O    | 2.03                     | 0.57              |
| 1:C:378:MET:HA   | 1:C:378:MET:HE3  | 1.85                     | 0.57              |
| 1:C:413:VAL:HG12 | 1:C:413:VAL:O    | 2.03                     | 0.57              |
| 1:E:265:ALA:HB3  | 1:E:450:LEU:HB3  | 1.86                     | 0.57              |
| 1:G:134:SER:CB   | 1:G:212:GLY:HA2  | 2.32                     | 0.57              |
| 2:B:140:TYR:HD1  | 2:B:141:GLU:N    | 2.02                     | 0.57              |
| 1:C:100:VAL:O    | 1:C:104:LEU:HG   | 2.03                     | 0.57              |
| 1:E:51:GLU:HG2   | 1:E:53:LYS:HE3   | 1.84                     | 0.57              |
| 1:G:50:LYS:HG3   | 1:G:67:LYS:HE3   | 1.86                     | 0.57              |
| 1:G:161:TYR:CZ   | 1:G:165:LEU:HD11 | 2.39                     | 0.57              |
| 1:G:266:ASN:HA   | 1:G:447:ASN:OD1  | 2.05                     | 0.57              |
| 1:G:380:ASP:OD1  | 1:G:382:THR:HG23 | 2.04                     | 0.57              |
| 1:A:13:LEU:HD21  | 1:A:132:ILE:HD13 | 1.86                     | 0.57              |
| 1:A:568:LYS:HA   | 1:A:568:LYS:HE3  | 1.85                     | 0.57              |
| 1:C:134:SER:CB   | 1:C:212:GLY:HA2  | 2.35                     | 0.57              |
| 1:C:187:THR:HG23 | 1:C:463:ILE:CG2  | 2.34                     | 0.57              |
| 1:C:267:ILE:HB   | 1:C:447:ASN:ND2  | 2.19                     | 0.57              |
| 1:C:323:ILE:CG2  | 1:C:326:GLN:HB3  | 2.33                     | 0.57              |
| 1:C:552:ASP:CG   | 1:C:596:ALA:H    | 2.12                     | 0.57              |
| 1:C:763:ASP:HB3  | 1:C:766:LEU:HD11 | 1.85                     | 0.57              |
| 1:C:803:CYS:O    | 1:C:807:LEU:HB2  | 2.05                     | 0.57              |
| 1:E:607:ASP:HA   | 1:E:610:THR:CB   | 2.31                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:807:LEU:HD23 | 1:E:807:LEU:O    | 2.04                     | 0.57              |
| 1:G:125:ASN:OD1  | 1:G:126:PRO:HD2  | 2.03                     | 0.57              |
| 1:G:769:ILE:HD13 | 1:G:774:ILE:HG12 | 1.85                     | 0.57              |
| 1:A:247:ARG:HH11 | 1:A:247:ARG:HA   | 1.68                     | 0.57              |
| 1:C:176:THR:O    | 1:C:183:LYS:CD   | 2.52                     | 0.57              |
| 1:E:89:MET:C     | 1:E:91:GLU:N     | 2.62                     | 0.57              |
| 1:E:369:LYS:NZ   | 1:E:420:LYS:HB3  | 2.19                     | 0.57              |
| 1:E:627:ASP:O    | 1:E:627:ASP:CG   | 2.48                     | 0.57              |
| 2:F:14:ALA:CB    | 2:F:38:LEU:HD21  | 2.35                     | 0.57              |
| 2:F:64:LEU:HD23  | 2:F:68:GLN:OE1   | 2.04                     | 0.57              |
| 1:G:405:PRO:HD2  | 1:G:417:ALA:HA   | 1.85                     | 0.57              |
| 1:G:413:VAL:O    | 1:G:413:VAL:HG12 | 2.04                     | 0.57              |
| 1:G:428:GLU:C    | 1:G:430:LEU:H    | 2.12                     | 0.57              |
| 1:G:721:PHE:N    | 1:G:721:PHE:HD1  | 2.01                     | 0.57              |
| 1:G:769:ILE:CD1  | 1:G:774:ILE:HG12 | 2.35                     | 0.57              |
| 1:A:13:LEU:HD21  | 1:A:132:ILE:HD12 | 1.86                     | 0.57              |
| 1:A:138:ILE:HD13 | 1:A:154:TYR:CE2  | 2.39                     | 0.57              |
| 1:A:477:PHE:O    | 1:A:480:LEU:HB3  | 2.04                     | 0.57              |
| 1:C:48:SER:O     | 1:C:59:VAL:HG13  | 2.04                     | 0.57              |
| 1:C:79:ASN:ND2   | 1:C:80:PRO:HD2   | 2.15                     | 0.57              |
| 1:C:797:ILE:HG22 | 1:C:798:ALA:N    | 2.19                     | 0.57              |
| 1:E:88:ASP:HB3   | 1:E:91:GLU:OE1   | 2.05                     | 0.57              |
| 1:E:298:SER:O    | 1:E:302:ARG:HB2  | 2.03                     | 0.57              |
| 1:G:32:LYS:C     | 1:G:34:LEU:H     | 2.12                     | 0.57              |
| 1:G:96:ASN:HB2   | 1:G:99:SER:OG    | 2.04                     | 0.57              |
| 1:G:165:LEU:HD21 | 1:G:260:GLY:HA2  | 1.87                     | 0.57              |
| 1:G:669:LYS:O    | 1:G:672:THR:HB   | 2.04                     | 0.57              |
| 1:G:814:LYS:HD2  | 1:G:818:GLN:OE1  | 2.04                     | 0.57              |
| 1:A:469:PHE:CZ   | 1:A:587:ALA:HB3  | 2.38                     | 0.57              |
| 1:A:711:LEU:CD2  | 1:A:711:LEU:H    | 2.18                     | 0.57              |
| 1:C:497:MET:HA   | 1:C:497:MET:HE3  | 1.86                     | 0.57              |
| 1:E:71:SER:C     | 1:E:73:ASP:H     | 2.12                     | 0.57              |
| 1:E:541:LEU:HD21 | 1:E:597:TRP:HB3  | 1.86                     | 0.57              |
| 1:E:581:PHE:HZ   | 1:E:597:TRP:CH2  | 2.23                     | 0.57              |
| 1:E:763:ASP:HB3  | 1:E:766:LEU:HD11 | 1.87                     | 0.57              |
| 1:G:275:SER:O    | 1:G:277:ALA:N    | 2.38                     | 0.57              |
| 1:G:352:ILE:CG2  | 1:G:442:ILE:HD11 | 2.34                     | 0.57              |
| 1:G:533:ASN:O    | 1:G:534:PRO:C    | 2.43                     | 0.57              |
| 1:A:88:ASP:HB3   | 1:A:91:GLU:OE1   | 2.03                     | 0.57              |
| 1:A:568:LYS:CE   | 1:A:584:LEU:HB2  | 2.35                     | 0.57              |
| 1:A:747:MET:CE   | 1:A:755:LEU:HD22 | 2.35                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:64:LEU:HD23  | 2:B:68:GLN:OE1   | 2.04                     | 0.57              |
| 1:C:382:THR:HA   | 1:C:385:GLN:OE1  | 2.05                     | 0.57              |
| 1:E:36:TRP:HE1   | 1:E:78:MET:HG3   | 1.65                     | 0.57              |
| 1:E:551:THR:H    | 1:E:554:SER:HG   | 1.52                     | 0.57              |
| 1:E:702:LEU:O    | 1:E:706:ARG:HG3  | 2.03                     | 0.57              |
| 1:G:33:LYS:CB    | 1:G:49:ILE:HB    | 2.34                     | 0.57              |
| 1:G:51:GLU:HG2   | 1:G:53:LYS:HE3   | 1.85                     | 0.57              |
| 1:G:79:ASN:OD1   | 1:G:92:LEU:HB3   | 2.04                     | 0.57              |
| 1:A:369:LYS:HZ2  | 1:A:420:LYS:HB3  | 1.69                     | 0.57              |
| 1:A:766:LEU:HB3  | 1:A:780:VAL:HG21 | 1.85                     | 0.57              |
| 1:C:64:ASN:C     | 1:C:66:LYS:H     | 2.13                     | 0.57              |
| 1:C:308:GLU:N    | 1:C:313:TYR:OH   | 2.38                     | 0.57              |
| 1:C:424:ASP:C    | 1:C:426:ALA:N    | 2.62                     | 0.57              |
| 1:C:804:ARG:HG2  | 1:C:804:ARG:NH1  | 2.18                     | 0.57              |
| 1:E:104:LEU:HD12 | 1:E:705:LEU:HD11 | 1.86                     | 0.57              |
| 1:G:182:GLY:HA2  | 5:G:998:ADP:PA   | 2.45                     | 0.57              |
| 1:G:259:THR:HB   | 1:G:261:TYR:CD1  | 2.40                     | 0.57              |
| 1:G:443:LEU:O    | 1:G:447:ASN:HB2  | 2.05                     | 0.57              |
| 2:H:110:HIS:O    | 2:H:113:VAL:N    | 2.26                     | 0.57              |
| 1:A:428:GLU:C    | 1:A:430:LEU:H    | 2.11                     | 0.57              |
| 1:A:611:SER:O    | 1:A:615:GLN:NE2  | 2.37                     | 0.57              |
| 1:C:293:LEU:HA   | 1:C:332:PHE:CE1  | 2.40                     | 0.57              |
| 1:C:527:LEU:HB2  | 1:C:566:HIS:NE2  | 2.20                     | 0.57              |
| 1:C:610:THR:HG23 | 1:C:628:VAL:CG2  | 2.34                     | 0.57              |
| 1:C:721:PHE:CZ   | 1:C:768:ARG:HG2  | 2.40                     | 0.57              |
| 1:E:271:LEU:HD21 | 1:E:663:TYR:CD1  | 2.39                     | 0.57              |
| 1:E:413:VAL:O    | 1:E:413:VAL:HG12 | 2.03                     | 0.57              |
| 1:G:702:LEU:O    | 1:G:706:ARG:HG3  | 2.05                     | 0.57              |
| 1:A:272:LEU:O    | 1:A:274:LYS:N    | 2.38                     | 0.57              |
| 1:A:570:GLN:OE1  | 1:A:589:LYS:HE2  | 2.04                     | 0.57              |
| 2:B:14:ALA:CB    | 2:B:38:LEU:HD21  | 2.35                     | 0.57              |
| 1:C:186:ASN:O    | 1:C:190:VAL:HG23 | 2.05                     | 0.57              |
| 1:E:44:PHE:HE2   | 1:E:702:LEU:HD21 | 1.70                     | 0.57              |
| 1:E:187:THR:HG23 | 1:E:463:ILE:CG2  | 2.32                     | 0.57              |
| 2:F:112:LEU:CD1  | 2:F:119:MET:HE3  | 2.35                     | 0.57              |
| 1:G:132:ILE:HD12 | 1:G:152:HIS:CD2  | 2.40                     | 0.57              |
| 1:G:145:LYS:CG   | 1:G:146:ARG:H    | 2.18                     | 0.57              |
| 2:H:40:GLN:C     | 2:H:42:PRO:HD3   | 2.30                     | 0.57              |
| 1:A:161:TYR:CZ   | 1:A:165:LEU:HD11 | 2.40                     | 0.56              |
| 1:A:273:GLU:O    | 1:A:273:GLU:HG2  | 2.05                     | 0.56              |
| 1:A:513:ASN:C    | 1:A:513:ASN:HD22 | 2.13                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:226:GLN:C    | 1:C:229:PRO:HD2  | 2.30                     | 0.56              |
| 1:C:347:GLU:C    | 1:C:349:GLN:N    | 2.62                     | 0.56              |
| 1:C:409:VAL:HB   | 1:C:414:VAL:HG21 | 1.87                     | 0.56              |
| 1:C:814:LYS:HD2  | 1:C:818:GLN:OE1  | 2.06                     | 0.56              |
| 1:G:312:ASN:HD22 | 1:G:312:ASN:N    | 2.03                     | 0.56              |
| 1:A:435:PHE:O    | 1:A:438:LEU:N    | 2.32                     | 0.56              |
| 1:A:553:THR:O    | 1:A:557:GLU:HG2  | 2.04                     | 0.56              |
| 1:A:750:LYS:HZ1  | 1:G:809:ARG:HH22 | 1.52                     | 0.56              |
| 1:A:797:ILE:HG22 | 1:A:798:ALA:N    | 2.19                     | 0.56              |
| 2:B:140:TYR:HD1  | 2:B:141:GLU:H    | 1.51                     | 0.56              |
| 1:C:32:LYS:C     | 1:C:34:LEU:H     | 2.13                     | 0.56              |
| 1:C:71:SER:C     | 1:C:73:ASP:H     | 2.13                     | 0.56              |
| 2:D:14:ALA:CB    | 2:D:38:LEU:HD21  | 2.35                     | 0.56              |
| 1:E:37:VAL:CG1   | 1:E:38:PRO:HD2   | 2.35                     | 0.56              |
| 1:E:424:ASP:C    | 1:E:426:ALA:N    | 2.63                     | 0.56              |
| 1:E:731:ARG:HG2  | 1:E:731:ARG:NH1  | 2.21                     | 0.56              |
| 1:E:747:MET:HE1  | 1:E:755:LEU:CD2  | 2.35                     | 0.56              |
| 1:G:542:ASP:O    | 1:G:545:CYS:HB3  | 2.05                     | 0.56              |
| 1:G:721:PHE:HB3  | 1:G:776:PHE:O    | 2.05                     | 0.56              |
| 1:G:728:GLN:HE21 | 1:G:728:GLN:HA   | 1.70                     | 0.56              |
| 1:A:226:GLN:C    | 1:A:229:PRO:HD2  | 2.30                     | 0.56              |
| 1:A:267:ILE:HB   | 1:A:447:ASN:ND2  | 2.20                     | 0.56              |
| 1:A:308:GLU:N    | 1:A:313:TYR:OH   | 2.38                     | 0.56              |
| 1:C:22:ASN:OD1   | 1:C:24:LEU:HB2   | 2.05                     | 0.56              |
| 1:C:265:ALA:N    | 1:C:450:LEU:O    | 2.39                     | 0.56              |
| 1:C:570:GLN:OE1  | 1:C:589:LYS:HE2  | 2.05                     | 0.56              |
| 1:C:807:LEU:O    | 1:C:807:LEU:HD23 | 2.06                     | 0.56              |
| 1:E:13:LEU:CD1   | 1:E:132:ILE:HB   | 2.35                     | 0.56              |
| 1:E:36:TRP:CE2   | 1:E:78:MET:HG3   | 2.40                     | 0.56              |
| 1:E:83:PHE:HB3   | 1:E:92:LEU:HD23  | 1.87                     | 0.56              |
| 1:E:541:LEU:CD2  | 1:E:601:ASN:HD22 | 2.09                     | 0.56              |
| 1:E:800:GLN:HA   | 2:F:119:MET:HE2  | 1.87                     | 0.56              |
| 1:G:36:TRP:CE2   | 1:G:78:MET:HG3   | 2.39                     | 0.56              |
| 1:G:66:LYS:HD3   | 1:G:67:LYS:H     | 1.70                     | 0.56              |
| 1:G:226:GLN:C    | 1:G:229:PRO:HD2  | 2.30                     | 0.56              |
| 1:G:278:ILE:HG13 | 1:G:279:ARG:N    | 2.20                     | 0.56              |
| 1:G:405:PRO:C    | 1:G:407:ILE:H    | 2.13                     | 0.56              |
| 1:G:568:LYS:CE   | 1:G:584:LEU:HB2  | 2.35                     | 0.56              |
| 1:G:812:PHE:C    | 1:G:814:LYS:N    | 2.62                     | 0.56              |
| 1:A:71:SER:C     | 1:A:73:ASP:H     | 2.13                     | 0.56              |
| 1:A:293:LEU:HA   | 1:A:332:PHE:CE1  | 2.40                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:788:ARG:HG2  | 1:A:788:ARG:NH1  | 2.20                     | 0.56              |
| 2:B:80:LYS:H     | 2:B:80:LYS:HD2   | 1.70                     | 0.56              |
| 1:E:107:ARG:HA   | 1:E:112:LEU:HD12 | 1.88                     | 0.56              |
| 1:E:527:LEU:HB2  | 1:E:566:HIS:NE2  | 2.21                     | 0.56              |
| 2:F:144:VAL:HG12 | 2:F:145:ARG:N    | 2.18                     | 0.56              |
| 1:G:42:HIS:C     | 1:G:44:PHE:H     | 2.14                     | 0.56              |
| 1:G:103:ASN:O    | 1:G:107:ARG:HG3  | 2.04                     | 0.56              |
| 1:G:308:GLU:N    | 1:G:313:TYR:OH   | 2.39                     | 0.56              |
| 1:A:420:LYS:HD2  | 1:A:421:GLU:CD   | 2.30                     | 0.56              |
| 1:A:478:GLU:OE1  | 1:A:478:GLU:N    | 2.24                     | 0.56              |
| 1:A:628:VAL:HG13 | 1:A:628:VAL:O    | 2.04                     | 0.56              |
| 1:C:42:HIS:C     | 1:C:44:PHE:H     | 2.14                     | 0.56              |
| 1:C:420:LYS:HD2  | 1:C:421:GLU:CD   | 2.31                     | 0.56              |
| 1:C:480:LEU:HD11 | 1:C:528:ILE:HD12 | 1.87                     | 0.56              |
| 1:C:551:THR:N    | 1:C:554:SER:OG   | 2.32                     | 0.56              |
| 1:C:712:GLU:CD   | 1:C:712:GLU:H    | 2.12                     | 0.56              |
| 1:E:409:VAL:HB   | 1:E:414:VAL:HG21 | 1.85                     | 0.56              |
| 1:G:228:ASN:N    | 1:G:229:PRO:HD2  | 2.21                     | 0.56              |
| 1:G:797:ILE:HG22 | 1:G:798:ALA:N    | 2.21                     | 0.56              |
| 2:H:95:PHE:O     | 2:H:103:VAL:HG13 | 2.06                     | 0.56              |
| 1:A:242:ASN:ND2  | 1:A:245:SER:HA   | 2.21                     | 0.56              |
| 1:A:278:ILE:HA   | 1:A:315:PHE:CD1  | 2.40                     | 0.56              |
| 1:C:259:THR:HB   | 1:C:261:TYR:CD1  | 2.41                     | 0.56              |
| 1:C:278:ILE:HG13 | 1:C:279:ARG:N    | 2.20                     | 0.56              |
| 1:C:409:VAL:HG13 | 1:C:634:LEU:CD1  | 2.35                     | 0.56              |
| 1:C:428:GLU:C    | 1:C:430:LEU:H    | 2.14                     | 0.56              |
| 2:D:55:LYS:HB2   | 2:D:58:GLU:CD    | 2.31                     | 0.56              |
| 1:E:30:SER:C     | 1:E:32:LYS:N     | 2.64                     | 0.56              |
| 1:E:186:ASN:O    | 1:E:190:VAL:HG23 | 2.05                     | 0.56              |
| 1:E:572:SER:CB   | 1:E:580:GLU:HG3  | 2.35                     | 0.56              |
| 1:E:669:LYS:O    | 1:E:672:THR:HB   | 2.05                     | 0.56              |
| 2:F:28:TYR:CD2   | 2:F:51:LEU:HD13  | 2.41                     | 0.56              |
| 2:F:40:GLN:C     | 2:F:42:PRO:HD3   | 2.31                     | 0.56              |
| 1:G:293:LEU:HA   | 1:G:332:PHE:CE1  | 2.40                     | 0.56              |
| 1:G:369:LYS:NZ   | 1:G:420:LYS:HB3  | 2.20                     | 0.56              |
| 1:G:543:GLU:C    | 1:G:545:CYS:H    | 2.14                     | 0.56              |
| 1:G:623:ASP:HA   | 1:G:626:LYS:HB3  | 1.87                     | 0.56              |
| 1:A:36:TRP:CE2   | 1:A:78:MET:HG3   | 2.40                     | 0.56              |
| 1:A:226:GLN:O    | 1:A:229:PRO:HG2  | 2.06                     | 0.56              |
| 1:A:800:GLN:HA   | 2:B:119:MET:HE2  | 1.86                     | 0.56              |
| 1:C:170:ASP:C    | 1:C:171:GLN:HG2  | 2.30                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:443:LEU:O    | 1:C:447:ASN:HB2  | 2.06                     | 0.56              |
| 1:C:490:GLN:NE2  | 1:C:494:ASN:HD21 | 2.03                     | 0.56              |
| 1:C:719:GLN:HA   | 1:C:719:GLN:NE2  | 2.21                     | 0.56              |
| 1:E:103:ASN:ND2  | 1:E:107:ARG:HD2  | 2.21                     | 0.56              |
| 1:E:145:LYS:HB3  | 1:E:148:GLU:HG3  | 1.88                     | 0.56              |
| 1:E:703:GLU:O    | 1:E:706:ARG:N    | 2.38                     | 0.56              |
| 1:E:742:ILE:HD11 | 1:E:756:MET:HG2  | 1.87                     | 0.56              |
| 1:G:525:ILE:O    | 1:G:529:GLU:N    | 2.38                     | 0.56              |
| 1:A:50:LYS:HG3   | 1:A:67:LYS:HE3   | 1.87                     | 0.56              |
| 1:A:480:LEU:HD11 | 1:A:528:ILE:HD12 | 1.86                     | 0.56              |
| 1:A:769:ILE:HD13 | 1:A:774:ILE:HG23 | 1.87                     | 0.56              |
| 2:B:85:PHE:HE1   | 2:B:145:ARG:CG   | 2.18                     | 0.56              |
| 1:C:164:MET:SD   | 1:C:256:PHE:CD2  | 2.99                     | 0.56              |
| 1:C:477:PHE:O    | 1:C:480:LEU:N    | 2.37                     | 0.56              |
| 2:D:131:HIS:CE1  | 2:D:146:MET:HE3  | 2.40                     | 0.56              |
| 1:E:308:GLU:N    | 1:E:313:TYR:OH   | 2.39                     | 0.56              |
| 1:E:405:PRO:C    | 1:E:407:ILE:H    | 2.14                     | 0.56              |
| 2:F:104:MET:C    | 2:F:106:ALA:H    | 2.13                     | 0.56              |
| 1:G:478:GLU:OE1  | 1:G:478:GLU:N    | 2.23                     | 0.56              |
| 1:A:369:LYS:NZ   | 1:A:420:LYS:HB3  | 2.20                     | 0.56              |
| 1:A:711:LEU:HD22 | 1:A:711:LEU:N    | 2.20                     | 0.56              |
| 1:A:742:ILE:HD11 | 1:A:756:MET:HG2  | 1.86                     | 0.56              |
| 1:C:145:LYS:HB3  | 1:C:148:GLU:HG3  | 1.88                     | 0.56              |
| 1:C:161:TYR:CZ   | 1:C:165:LEU:HD11 | 2.41                     | 0.56              |
| 1:C:305:LEU:HD12 | 1:C:307:LEU:HD11 | 1.87                     | 0.56              |
| 1:C:380:ASP:OD1  | 1:C:382:THR:HG23 | 2.06                     | 0.56              |
| 1:C:700:LEU:HD23 | 1:C:700:LEU:C    | 2.31                     | 0.56              |
| 2:D:35:MET:HE1   | 2:D:76:ILE:HG13  | 1.88                     | 0.56              |
| 2:D:40:GLN:C     | 2:D:42:PRO:HD3   | 2.31                     | 0.56              |
| 2:D:104:MET:C    | 2:D:106:ALA:H    | 2.14                     | 0.56              |
| 1:E:182:GLY:HA2  | 5:E:998:ADP:O1A  | 2.05                     | 0.56              |
| 1:E:490:GLN:HE21 | 1:E:494:ASN:HD21 | 1.51                     | 0.56              |
| 1:E:568:LYS:HA   | 1:E:568:LYS:HE3  | 1.87                     | 0.56              |
| 1:G:13:LEU:HD11  | 1:G:152:HIS:CD2  | 2.40                     | 0.56              |
| 1:G:107:ARG:HH11 | 1:G:115:THR:HG23 | 1.69                     | 0.56              |
| 1:G:145:LYS:HB3  | 1:G:148:GLU:HG3  | 1.87                     | 0.56              |
| 1:G:553:THR:CG2  | 1:G:579:THR:HG21 | 2.36                     | 0.56              |
| 1:G:747:MET:CG   | 1:G:751:GLN:HE22 | 2.18                     | 0.56              |
| 1:G:788:ARG:HG2  | 1:G:788:ARG:NH1  | 2.21                     | 0.56              |
| 2:H:28:TYR:CD2   | 2:H:51:LEU:HD13  | 2.41                     | 0.56              |
| 1:A:64:ASN:C     | 1:A:66:LYS:H     | 2.14                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:572:SER:HB3  | 1:A:580:GLU:O    | 2.06                     | 0.56              |
| 2:B:48:MET:HG3   | 2:B:53:ASN:HA    | 1.88                     | 0.56              |
| 2:B:55:LYS:HB2   | 2:B:58:GLU:CD    | 2.31                     | 0.56              |
| 1:E:80:PRO:HG2   | 1:E:83:PHE:HE2   | 1.68                     | 0.56              |
| 1:E:89:MET:HE2   | 1:E:104:LEU:HD21 | 1.88                     | 0.56              |
| 1:E:416:LYS:HE2  | 1:E:417:ALA:N    | 2.21                     | 0.56              |
| 1:G:71:SER:C     | 1:G:73:ASP:H     | 2.14                     | 0.56              |
| 1:G:145:LYS:HB3  | 1:G:148:GLU:CG   | 2.35                     | 0.56              |
| 1:G:164:MET:SD   | 1:G:256:PHE:CD2  | 2.99                     | 0.56              |
| 1:G:521:LEU:O    | 1:G:525:ILE:HG13 | 2.06                     | 0.56              |
| 1:G:763:ASP:HB3  | 1:G:766:LEU:HD11 | 1.88                     | 0.56              |
| 2:H:55:LYS:HB2   | 2:H:58:GLU:CD    | 2.31                     | 0.56              |
| 2:H:80:LYS:H     | 2:H:80:LYS:HD2   | 1.70                     | 0.56              |
| 1:A:44:PHE:HE2   | 1:A:702:LEU:HD21 | 1.69                     | 0.55              |
| 1:A:51:GLU:HG2   | 1:A:53:LYS:HE3   | 1.87                     | 0.55              |
| 1:A:275:SER:O    | 1:A:277:ALA:N    | 2.39                     | 0.55              |
| 1:A:382:THR:HA   | 1:A:385:GLN:OE1  | 2.06                     | 0.55              |
| 1:A:405:PRO:C    | 1:A:407:ILE:H    | 2.13                     | 0.55              |
| 1:A:807:LEU:O    | 1:A:807:LEU:HD23 | 2.07                     | 0.55              |
| 1:A:815:ARG:O    | 1:A:818:GLN:HG2  | 2.06                     | 0.55              |
| 1:C:298:SER:O    | 1:C:302:ARG:HB2  | 2.06                     | 0.55              |
| 1:C:525:ILE:O    | 1:C:529:GLU:N    | 2.38                     | 0.55              |
| 1:C:533:ASN:O    | 1:C:534:PRO:C    | 2.45                     | 0.55              |
| 1:C:771:GLN:HE21 | 1:C:771:GLN:CA   | 2.19                     | 0.55              |
| 1:C:815:ARG:NE   | 1:C:818:GLN:HE21 | 2.05                     | 0.55              |
| 1:E:361:GLN:C    | 1:E:363:GLY:N    | 2.64                     | 0.55              |
| 1:E:416:LYS:HE2  | 1:E:417:ALA:H    | 1.72                     | 0.55              |
| 1:E:721:PHE:HB3  | 1:E:776:PHE:O    | 2.06                     | 0.55              |
| 1:E:728:GLN:HE21 | 1:E:728:GLN:HA   | 1.69                     | 0.55              |
| 1:E:747:MET:CG   | 1:E:751:GLN:HE22 | 2.19                     | 0.55              |
| 2:F:48:MET:HG3   | 2:F:53:ASN:HA    | 1.88                     | 0.55              |
| 1:G:424:ASP:C    | 1:G:426:ALA:N    | 2.62                     | 0.55              |
| 1:G:803:CYS:O    | 1:G:807:LEU:HB2  | 2.06                     | 0.55              |
| 1:A:37:VAL:CG1   | 1:A:38:PRO:HD2   | 2.35                     | 0.55              |
| 1:A:361:GLN:C    | 1:A:363:GLY:N    | 2.58                     | 0.55              |
| 1:C:193:TYR:CE1  | 1:C:197:VAL:HG21 | 2.42                     | 0.55              |
| 1:E:164:MET:SD   | 1:E:256:PHE:CD2  | 3.00                     | 0.55              |
| 1:G:7:SER:O      | 1:G:11:LYS:HG3   | 2.06                     | 0.55              |
| 1:G:529:GLU:O    | 1:G:664:LYS:NZ   | 2.39                     | 0.55              |
| 1:A:48:SER:O     | 1:A:59:VAL:HG13  | 2.06                     | 0.55              |
| 1:C:23:PRO:HA    | 1:C:26:GLN:HB3   | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:33:LYS:CB    | 1:C:49:ILE:HB    | 2.36                     | 0.55              |
| 1:C:405:PRO:C    | 1:C:407:ILE:H    | 2.15                     | 0.55              |
| 1:C:553:THR:O    | 1:C:554:SER:C    | 2.48                     | 0.55              |
| 2:D:23:ASP:HB2   | 2:D:25:LYS:HD3   | 1.89                     | 0.55              |
| 1:E:256:PHE:CE1  | 1:E:262:ILE:HG13 | 2.42                     | 0.55              |
| 1:E:352:ILE:CG2  | 1:E:442:ILE:HD11 | 2.34                     | 0.55              |
| 1:G:88:ASP:HB3   | 1:G:91:GLU:OE1   | 2.05                     | 0.55              |
| 1:G:298:SER:O    | 1:G:302:ARG:HB2  | 2.06                     | 0.55              |
| 1:G:539:ALA:O    | 1:G:542:ASP:HB2  | 2.06                     | 0.55              |
| 1:G:658:THR:HG23 | 1:G:661:GLN:HB3  | 1.89                     | 0.55              |
| 2:H:140:TYR:CD1  | 2:H:141:GLU:HG2  | 2.41                     | 0.55              |
| 1:A:489:LEU:O    | 1:A:492:LEU:HB3  | 2.07                     | 0.55              |
| 1:A:731:ARG:HG2  | 1:A:731:ARG:NH1  | 2.21                     | 0.55              |
| 1:A:771:GLN:HE21 | 1:A:771:GLN:CA   | 2.17                     | 0.55              |
| 1:C:126:PRO:O    | 1:C:127:TYR:HB2  | 2.07                     | 0.55              |
| 1:C:153:ILE:HG23 | 1:C:154:TYR:N    | 2.21                     | 0.55              |
| 1:C:702:LEU:O    | 1:C:706:ARG:HG3  | 2.06                     | 0.55              |
| 2:D:28:TYR:CD2   | 2:D:51:LEU:HD13  | 2.41                     | 0.55              |
| 1:E:64:ASN:C     | 1:E:66:LYS:H     | 2.13                     | 0.55              |
| 1:E:312:ASN:N    | 1:E:312:ASN:HD22 | 2.04                     | 0.55              |
| 1:E:347:GLU:C    | 1:E:349:GLN:N    | 2.64                     | 0.55              |
| 1:E:788:ARG:HG2  | 1:E:788:ARG:NH1  | 2.22                     | 0.55              |
| 2:F:89:VAL:CG1   | 2:F:144:VAL:HG21 | 2.20                     | 0.55              |
| 1:G:140:MET:HE2  | 1:G:149:MET:HE1  | 1.87                     | 0.55              |
| 1:A:352:ILE:CG2  | 1:A:442:ILE:HD11 | 2.35                     | 0.55              |
| 1:A:541:LEU:CD2  | 1:A:601:ASN:HD22 | 2.11                     | 0.55              |
| 2:B:28:TYR:CD2   | 2:B:51:LEU:HD13  | 2.41                     | 0.55              |
| 1:C:239:THR:C    | 1:C:241:LYS:H    | 2.14                     | 0.55              |
| 1:C:669:LYS:O    | 1:C:672:THR:HB   | 2.06                     | 0.55              |
| 1:E:145:LYS:HB3  | 1:E:148:GLU:CG   | 2.36                     | 0.55              |
| 1:E:259:THR:HB   | 1:E:261:TYR:CD1  | 2.41                     | 0.55              |
| 1:E:293:LEU:HD11 | 1:E:301:MET:CE   | 2.36                     | 0.55              |
| 1:E:293:LEU:HD13 | 1:E:353:LEU:HD22 | 1.89                     | 0.55              |
| 1:E:418:GLN:CB   | 1:E:422:GLN:HB2  | 2.35                     | 0.55              |
| 1:E:443:LEU:O    | 1:E:447:ASN:HB2  | 2.06                     | 0.55              |
| 1:E:711:LEU:HD22 | 1:E:711:LEU:H    | 1.70                     | 0.55              |
| 1:G:152:HIS:CE1  | 1:G:154:TYR:CD2  | 2.95                     | 0.55              |
| 1:G:663:TYR:OH   | 1:G:667:LEU:HD13 | 2.06                     | 0.55              |
| 1:G:731:ARG:HG2  | 1:G:731:ARG:NH1  | 2.22                     | 0.55              |
| 1:G:802:GLN:HG3  | 2:H:88:TYR:OH    | 2.07                     | 0.55              |
| 2:H:35:MET:HE1   | 2:H:76:ILE:HG13  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:116:GLY:O    | 2:H:118:LYS:N    | 2.40                     | 0.55              |
| 2:H:140:TYR:CD1  | 2:H:141:GLU:N    | 2.73                     | 0.55              |
| 1:A:42:HIS:C     | 1:A:44:PHE:H     | 2.13                     | 0.55              |
| 1:A:170:ASP:C    | 1:A:171:GLN:HG2  | 2.31                     | 0.55              |
| 1:A:623:ASP:HA   | 1:A:626:LYS:HB3  | 1.88                     | 0.55              |
| 1:C:607:ASP:HA   | 1:C:610:THR:CB   | 2.34                     | 0.55              |
| 1:E:812:PHE:C    | 1:E:814:LYS:N    | 2.64                     | 0.55              |
| 2:F:55:LYS:HB2   | 2:F:58:GLU:CD    | 2.31                     | 0.55              |
| 1:G:30:SER:C     | 1:G:32:LYS:N     | 2.64                     | 0.55              |
| 1:G:293:LEU:HD13 | 1:G:353:LEU:HD22 | 1.88                     | 0.55              |
| 1:G:361:GLN:O    | 1:G:363:GLY:N    | 2.39                     | 0.55              |
| 1:G:409:VAL:HG13 | 1:G:634:LEU:CD1  | 2.37                     | 0.55              |
| 2:H:48:MET:HG3   | 2:H:53:ASN:HA    | 1.89                     | 0.55              |
| 2:H:76:ILE:O     | 2:H:79:ASN:ND2   | 2.40                     | 0.55              |
| 1:A:18:ASN:O     | 1:A:19:PHE:HD1   | 1.88                     | 0.55              |
| 1:A:107:ARG:CA   | 1:A:112:LEU:HD12 | 2.37                     | 0.55              |
| 1:A:418:GLN:CB   | 1:A:422:GLN:HB2  | 2.35                     | 0.55              |
| 1:A:553:THR:O    | 1:A:554:SER:C    | 2.49                     | 0.55              |
| 1:A:669:LYS:O    | 1:A:672:THR:HB   | 2.07                     | 0.55              |
| 1:A:743:PRO:HB3  | 1:G:816:GLN:O    | 2.07                     | 0.55              |
| 1:C:627:ASP:O    | 1:C:627:ASP:OD1  | 2.25                     | 0.55              |
| 1:E:32:LYS:C     | 1:E:34:LEU:H     | 2.15                     | 0.55              |
| 1:E:42:HIS:C     | 1:E:44:PHE:H     | 2.14                     | 0.55              |
| 1:E:380:ASP:OD1  | 1:E:382:THR:HG23 | 2.06                     | 0.55              |
| 1:E:721:PHE:N    | 1:E:721:PHE:HD1  | 2.02                     | 0.55              |
| 1:E:803:CYS:O    | 1:E:807:LEU:HB2  | 2.06                     | 0.55              |
| 1:E:814:LYS:HD2  | 1:E:818:GLN:OE1  | 2.07                     | 0.55              |
| 1:A:32:LYS:C     | 1:A:34:LEU:H     | 2.14                     | 0.55              |
| 1:A:123:VAL:O    | 1:A:123:VAL:HG12 | 2.04                     | 0.55              |
| 1:A:165:LEU:HD21 | 1:A:260:GLY:HA2  | 1.88                     | 0.55              |
| 1:A:312:ASN:HD22 | 1:A:312:ASN:N    | 2.05                     | 0.55              |
| 1:A:803:CYS:O    | 1:A:807:LEU:HB2  | 2.06                     | 0.55              |
| 2:B:40:GLN:C     | 2:B:42:PRO:HD3   | 2.31                     | 0.55              |
| 2:D:3:PHE:HA     | 2:D:7:GLN:NE2    | 2.22                     | 0.55              |
| 1:E:66:LYS:HD3   | 1:E:67:LYS:H     | 1.72                     | 0.55              |
| 1:E:409:VAL:HG13 | 1:E:634:LEU:CD1  | 2.36                     | 0.55              |
| 1:E:435:PHE:O    | 1:E:438:LEU:N    | 2.34                     | 0.55              |
| 1:E:529:GLU:O    | 1:E:664:LYS:NZ   | 2.40                     | 0.55              |
| 1:G:513:ASN:C    | 1:G:513:ASN:HD22 | 2.15                     | 0.55              |
| 1:A:250:LYS:HG2  | 1:A:465:ASP:OD2  | 2.07                     | 0.55              |
| 1:A:797:ILE:HG13 | 2:B:117:GLU:H    | 1.72                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:144:LYS:HG3  | 1:C:148:GLU:HB2  | 1.89                     | 0.55              |
| 1:C:407:ILE:HD12 | 1:C:409:VAL:H    | 1.72                     | 0.55              |
| 1:C:568:LYS:CE   | 1:C:584:LEU:HB2  | 2.36                     | 0.55              |
| 1:E:140:MET:HE2  | 1:E:149:MET:HE1  | 1.88                     | 0.55              |
| 1:E:226:GLN:O    | 1:E:229:PRO:HG2  | 2.07                     | 0.55              |
| 1:E:369:LYS:HZ2  | 1:E:420:LYS:HB3  | 1.72                     | 0.55              |
| 2:F:4:SER:H      | 2:F:7:GLN:NE2    | 2.04                     | 0.55              |
| 2:H:112:LEU:CD1  | 2:H:119:MET:HE3  | 2.37                     | 0.55              |
| 1:A:259:THR:HB   | 1:A:261:TYR:CD1  | 2.41                     | 0.55              |
| 1:A:265:ALA:HB3  | 1:A:450:LEU:HB3  | 1.88                     | 0.55              |
| 1:A:540:LEU:O    | 1:A:542:ASP:N    | 2.40                     | 0.55              |
| 1:C:815:ARG:O    | 1:C:818:GLN:HG2  | 2.07                     | 0.55              |
| 2:F:35:MET:HE1   | 2:F:76:ILE:HG13  | 1.89                     | 0.55              |
| 2:H:3:PHE:HA     | 2:H:7:GLN:NE2    | 2.22                     | 0.55              |
| 1:A:66:LYS:HD3   | 1:A:67:LYS:H     | 1.71                     | 0.54              |
| 1:A:347:GLU:O    | 1:A:349:GLN:N    | 2.40                     | 0.54              |
| 1:A:543:GLU:C    | 1:A:545:CYS:H    | 2.15                     | 0.54              |
| 2:B:3:PHE:HA     | 2:B:7:GLN:NE2    | 2.22                     | 0.54              |
| 1:C:61:LEU:HD12  | 1:C:64:ASN:HB3   | 1.89                     | 0.54              |
| 1:C:226:GLN:O    | 1:C:229:PRO:HG2  | 2.07                     | 0.54              |
| 1:C:347:GLU:C    | 1:C:349:GLN:H    | 2.15                     | 0.54              |
| 1:C:369:LYS:NZ   | 1:C:420:LYS:HB3  | 2.21                     | 0.54              |
| 1:E:61:LEU:HD12  | 1:E:64:ASN:HB3   | 1.88                     | 0.54              |
| 1:G:359:VAL:O    | 1:G:359:VAL:HG12 | 2.07                     | 0.54              |
| 1:G:378:MET:HA   | 1:G:378:MET:HE3  | 1.87                     | 0.54              |
| 1:G:494:ASN:HD22 | 1:G:494:ASN:N    | 2.04                     | 0.54              |
| 1:G:719:GLN:NE2  | 1:G:719:GLN:HA   | 2.22                     | 0.54              |
| 1:C:323:ILE:HG21 | 1:C:326:GLN:NE2  | 2.22                     | 0.54              |
| 1:C:376:ALA:CB   | 1:C:420:LYS:HB2  | 2.32                     | 0.54              |
| 1:C:405:PRO:HD2  | 1:C:416:LYS:O    | 2.06                     | 0.54              |
| 1:C:556:VAL:HG21 | 1:C:579:THR:HB   | 1.89                     | 0.54              |
| 1:E:13:LEU:HD21  | 1:E:132:ILE:CD1  | 2.37                     | 0.54              |
| 1:G:100:VAL:O    | 1:G:104:LEU:HG   | 2.08                     | 0.54              |
| 1:G:138:ILE:HD13 | 1:G:154:TYR:CE2  | 2.41                     | 0.54              |
| 1:G:347:GLU:C    | 1:G:349:GLN:N    | 2.64                     | 0.54              |
| 1:G:399:THR:O    | 1:G:403:LEU:HD12 | 2.06                     | 0.54              |
| 1:A:61:LEU:HD12  | 1:A:64:ASN:HB3   | 1.88                     | 0.54              |
| 1:A:103:ASN:ND2  | 1:A:107:ARG:HD2  | 2.22                     | 0.54              |
| 1:A:107:ARG:HA   | 1:A:112:LEU:HD12 | 1.89                     | 0.54              |
| 1:A:134:SER:CB   | 1:A:212:GLY:HA2  | 2.37                     | 0.54              |
| 1:A:218:GLY:HA3  | 1:A:221:GLU:OE1  | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:292:TYR:CE2  | 1:A:331:MET:HB3  | 2.42                     | 0.54              |
| 1:A:416:LYS:HE2  | 1:A:417:ALA:H    | 1.72                     | 0.54              |
| 1:A:527:LEU:HB2  | 1:A:566:HIS:NE2  | 2.23                     | 0.54              |
| 1:A:539:ALA:O    | 1:A:542:ASP:HB2  | 2.07                     | 0.54              |
| 1:C:529:GLU:O    | 1:C:664:LYS:NZ   | 2.40                     | 0.54              |
| 1:E:103:ASN:O    | 1:E:107:ARG:HG3  | 2.07                     | 0.54              |
| 1:E:290:PHE:CD1  | 1:E:360:LEU:HD11 | 2.43                     | 0.54              |
| 1:G:176:THR:O    | 1:G:183:LYS:CD   | 2.55                     | 0.54              |
| 1:C:107:ARG:CA   | 1:C:112:LEU:HD12 | 2.37                     | 0.54              |
| 1:C:312:ASN:HD22 | 1:C:312:ASN:N    | 2.05                     | 0.54              |
| 1:C:369:LYS:HG3  | 1:C:370:GLU:N    | 2.22                     | 0.54              |
| 1:C:478:GLU:HB2  | 1:C:479:GLN:OE1  | 2.07                     | 0.54              |
| 1:C:658:THR:HG23 | 1:C:661:GLN:HB3  | 1.89                     | 0.54              |
| 1:C:797:ILE:HG12 | 2:D:117:GLU:HG2  | 1.90                     | 0.54              |
| 1:E:100:VAL:O    | 1:E:104:LEU:HG   | 2.08                     | 0.54              |
| 1:E:199:SER:HB2  | 1:E:221:GLU:CG   | 2.37                     | 0.54              |
| 1:E:288:HIS:HB3  | 1:E:292:TYR:CE1  | 2.43                     | 0.54              |
| 1:E:630:ARG:HH22 | 1:E:657:ARG:HB3  | 1.73                     | 0.54              |
| 1:E:719:GLN:HA   | 1:E:719:GLN:HE21 | 1.72                     | 0.54              |
| 1:G:226:GLN:O    | 1:G:229:PRO:HG2  | 2.08                     | 0.54              |
| 2:H:83:GLY:HA3   | 2:H:88:TYR:CZ    | 2.42                     | 0.54              |
| 1:A:529:GLU:O    | 1:A:664:LYS:NZ   | 2.39                     | 0.54              |
| 1:A:766:LEU:O    | 1:A:777:ARG:HB2  | 2.08                     | 0.54              |
| 1:C:44:PHE:CE2   | 1:C:702:LEU:HD21 | 2.43                     | 0.54              |
| 1:C:267:ILE:HB   | 1:C:447:ASN:HD21 | 1.73                     | 0.54              |
| 1:C:269:THR:HG23 | 1:C:440:ARG:NH1  | 2.21                     | 0.54              |
| 1:C:278:ILE:O    | 1:C:279:ARG:HG3  | 2.07                     | 0.54              |
| 1:C:697:ASP:C    | 1:C:697:ASP:OD1  | 2.50                     | 0.54              |
| 1:E:495:HIS:ND1  | 1:E:499:ILE:HD12 | 2.23                     | 0.54              |
| 1:E:572:SER:HB3  | 1:E:580:GLU:O    | 2.08                     | 0.54              |
| 1:G:89:MET:C     | 1:G:91:GLU:N     | 2.63                     | 0.54              |
| 1:G:199:SER:HB2  | 1:G:221:GLU:CG   | 2.37                     | 0.54              |
| 1:G:267:ILE:H    | 1:G:447:ASN:HD21 | 1.55                     | 0.54              |
| 1:A:33:LYS:HB3   | 1:A:49:ILE:N     | 2.22                     | 0.54              |
| 1:C:50:LYS:HG3   | 1:C:67:LYS:HE3   | 1.89                     | 0.54              |
| 1:C:107:ARG:HA   | 1:C:112:LEU:HD12 | 1.88                     | 0.54              |
| 1:C:140:MET:HE2  | 1:C:149:MET:HE1  | 1.89                     | 0.54              |
| 1:C:269:THR:HG21 | 1:C:443:LEU:CD1  | 2.30                     | 0.54              |
| 1:E:269:THR:HG23 | 1:E:440:ARG:NH1  | 2.23                     | 0.54              |
| 1:E:342:MET:HE1  | 1:E:449:ALA:HB3  | 1.88                     | 0.54              |
| 1:E:766:LEU:O    | 1:E:777:ARG:HB2  | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:313:TYR:CD2  | 1:G:360:LEU:HB3  | 2.42                     | 0.54              |
| 1:G:370:GLU:O    | 1:G:374:ASP:HA   | 2.08                     | 0.54              |
| 1:G:514:PHE:CD1  | 1:G:515:ILE:N    | 2.76                     | 0.54              |
| 1:G:570:GLN:OE1  | 1:G:589:LYS:HE2  | 2.07                     | 0.54              |
| 2:H:4:SER:H      | 2:H:7:GLN:NE2    | 2.05                     | 0.54              |
| 2:H:104:MET:C    | 2:H:106:ALA:H    | 2.16                     | 0.54              |
| 1:A:482:ILE:HG22 | 1:A:483:ASN:N    | 2.20                     | 0.54              |
| 1:A:553:THR:CG2  | 1:A:579:THR:HG21 | 2.38                     | 0.54              |
| 1:C:103:ASN:ND2  | 1:C:107:ARG:HD2  | 2.23                     | 0.54              |
| 1:C:104:LEU:HD12 | 1:C:705:LEU:HD11 | 1.88                     | 0.54              |
| 1:C:145:LYS:HB3  | 1:C:148:GLU:CG   | 2.37                     | 0.54              |
| 1:C:290:PHE:CD1  | 1:C:360:LEU:HD11 | 2.42                     | 0.54              |
| 1:C:400:ARG:O    | 1:C:404:THR:N    | 2.40                     | 0.54              |
| 2:F:3:PHE:HA     | 2:F:7:GLN:NE2    | 2.22                     | 0.54              |
| 1:G:48:SER:O     | 1:G:59:VAL:HG13  | 2.08                     | 0.54              |
| 1:G:144:LYS:HG3  | 1:G:148:GLU:HB2  | 1.90                     | 0.54              |
| 1:A:126:PRO:O    | 1:A:127:TYR:HB2  | 2.07                     | 0.54              |
| 2:D:48:MET:HG3   | 2:D:53:ASN:HA    | 1.88                     | 0.54              |
| 2:D:89:VAL:CG1   | 2:D:144:VAL:HG21 | 2.20                     | 0.54              |
| 1:E:50:LYS:HG3   | 1:E:67:LYS:HE3   | 1.89                     | 0.54              |
| 1:E:797:ILE:HG22 | 1:E:798:ALA:N    | 2.21                     | 0.54              |
| 1:G:3:GLN:O      | 1:G:18:ASN:ND2   | 2.40                     | 0.54              |
| 1:G:298:SER:O    | 1:G:302:ARG:N    | 2.41                     | 0.54              |
| 1:G:527:LEU:HB2  | 1:G:566:HIS:NE2  | 2.21                     | 0.54              |
| 1:G:747:MET:CE   | 1:G:755:LEU:HD22 | 2.37                     | 0.54              |
| 1:G:762:LEU:HD13 | 1:G:766:LEU:CD1  | 2.38                     | 0.54              |
| 1:A:96:ASN:HB2   | 1:A:99:SER:OG    | 2.07                     | 0.54              |
| 1:A:239:THR:C    | 1:A:241:LYS:H    | 2.16                     | 0.54              |
| 1:A:490:GLN:NE2  | 1:A:494:ASN:HD21 | 2.06                     | 0.54              |
| 1:C:86:VAL:HG12  | 1:C:103:ASN:ND2  | 2.23                     | 0.54              |
| 1:C:257:ASP:C    | 1:C:257:ASP:OD1  | 2.50                     | 0.54              |
| 1:C:812:PHE:C    | 1:C:814:LYS:N    | 2.64                     | 0.54              |
| 2:D:55:LYS:O     | 2:D:56:SER:C     | 2.51                     | 0.54              |
| 2:D:144:VAL:HG12 | 2:D:145:ARG:N    | 2.23                     | 0.54              |
| 1:E:153:ILE:HG23 | 1:E:154:TYR:N    | 2.23                     | 0.54              |
| 1:E:370:GLU:O    | 1:E:374:ASP:HA   | 2.07                     | 0.54              |
| 1:E:721:PHE:CZ   | 1:E:768:ARG:HG2  | 2.42                     | 0.54              |
| 2:F:140:TYR:HD1  | 2:F:141:GLU:N    | 2.06                     | 0.54              |
| 1:G:815:ARG:O    | 1:G:818:GLN:HG2  | 2.08                     | 0.54              |
| 1:A:147:HIS:C    | 1:A:149:MET:H    | 2.15                     | 0.54              |
| 1:A:610:THR:HG23 | 1:A:628:VAL:HG21 | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:4:SER:H      | 2:B:7:GLN:NE2    | 2.05                     | 0.54              |
| 2:B:35:MET:HE1   | 2:B:76:ILE:HG13  | 1.89                     | 0.54              |
| 2:B:144:VAL:HG12 | 2:B:145:ARG:N    | 2.22                     | 0.54              |
| 1:C:802:GLN:NE2  | 2:D:88:TYR:OH    | 2.38                     | 0.54              |
| 2:D:4:SER:H      | 2:D:7:GLN:NE2    | 2.05                     | 0.54              |
| 1:E:266:ASN:HA   | 1:E:447:ASN:OD1  | 2.08                     | 0.54              |
| 1:E:275:SER:O    | 1:E:277:ALA:N    | 2.41                     | 0.54              |
| 1:E:586:TYR:CD1  | 1:E:587:ALA:N    | 2.76                     | 0.54              |
| 1:E:658:THR:HG23 | 1:E:661:GLN:HB3  | 1.90                     | 0.54              |
| 1:G:33:LYS:HB3   | 1:G:49:ILE:N     | 2.23                     | 0.54              |
| 1:A:278:ILE:HG13 | 1:A:279:ARG:N    | 2.21                     | 0.53              |
| 1:A:405:PRO:HD2  | 1:A:416:LYS:O    | 2.07                     | 0.53              |
| 1:A:745:GLY:H    | 1:G:819:LEU:HD21 | 1.73                     | 0.53              |
| 1:C:66:LYS:HD3   | 1:C:67:LYS:H     | 1.74                     | 0.53              |
| 1:C:382:THR:C    | 1:C:385:GLN:HB3  | 2.33                     | 0.53              |
| 1:C:747:MET:CE   | 1:C:755:LEU:HD22 | 2.39                     | 0.53              |
| 1:E:747:MET:CE   | 1:E:755:LEU:HD22 | 2.38                     | 0.53              |
| 1:G:145:LYS:CB   | 1:G:148:GLU:HG3  | 2.38                     | 0.53              |
| 1:G:359:VAL:O    | 1:G:359:VAL:CG1  | 2.56                     | 0.53              |
| 1:G:572:SER:HB3  | 1:G:580:GLU:O    | 2.08                     | 0.53              |
| 1:G:711:LEU:HD22 | 1:G:711:LEU:N    | 2.23                     | 0.53              |
| 2:H:98:GLU:O     | 2:H:100:ASN:N    | 2.41                     | 0.53              |
| 1:A:145:LYS:HB3  | 1:A:148:GLU:HG3  | 1.90                     | 0.53              |
| 1:A:228:ASN:N    | 1:A:229:PRO:HD2  | 2.23                     | 0.53              |
| 1:A:254:ILE:O    | 1:A:460:PHE:HA   | 2.08                     | 0.53              |
| 1:A:521:LEU:O    | 1:A:525:ILE:HG13 | 2.07                     | 0.53              |
| 1:C:271:LEU:HD21 | 1:C:663:TYR:CZ   | 2.44                     | 0.53              |
| 1:C:543:GLU:C    | 1:C:545:CYS:H    | 2.16                     | 0.53              |
| 2:D:112:LEU:CD1  | 2:D:119:MET:HE3  | 2.37                     | 0.53              |
| 1:E:80:PRO:HD2   | 1:E:83:PHE:HD2   | 1.71                     | 0.53              |
| 1:E:132:ILE:HD12 | 1:E:152:HIS:CD2  | 2.42                     | 0.53              |
| 1:E:226:GLN:C    | 1:E:229:PRO:HD2  | 2.32                     | 0.53              |
| 1:E:513:ASN:HD22 | 1:E:513:ASN:C    | 2.15                     | 0.53              |
| 1:G:61:LEU:HD12  | 1:G:64:ASN:HB3   | 1.90                     | 0.53              |
| 1:G:418:GLN:CB   | 1:G:422:GLN:HB2  | 2.35                     | 0.53              |
| 1:G:437:ARG:NH2  | 1:G:625:TRP:HE3  | 2.06                     | 0.53              |
| 2:H:92:LEU:HD13  | 2:H:108:ILE:HD11 | 1.90                     | 0.53              |
| 1:C:199:SER:HB2  | 1:C:221:GLU:CG   | 2.38                     | 0.53              |
| 1:C:514:PHE:CD1  | 1:C:515:ILE:N    | 2.76                     | 0.53              |
| 2:D:98:GLU:O     | 2:D:100:ASN:N    | 2.41                     | 0.53              |
| 1:E:292:TYR:CE2  | 1:E:331:MET:HB3  | 2.43                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:556:VAL:O    | 1:E:559:LEU:HB3  | 2.09                     | 0.53              |
| 2:F:23:ASP:HB2   | 2:F:25:LYS:HD3   | 1.90                     | 0.53              |
| 1:G:293:LEU:HD11 | 1:G:301:MET:CE   | 2.37                     | 0.53              |
| 1:A:267:ILE:HB   | 1:A:447:ASN:HD21 | 1.72                     | 0.53              |
| 1:A:305:LEU:HD12 | 1:A:307:LEU:HD11 | 1.90                     | 0.53              |
| 1:A:437:ARG:NH2  | 1:A:625:TRP:HE3  | 2.07                     | 0.53              |
| 1:A:610:THR:CG2  | 1:A:611:SER:N    | 2.70                     | 0.53              |
| 1:C:132:ILE:HD12 | 1:C:152:HIS:CD2  | 2.43                     | 0.53              |
| 1:C:292:TYR:CE2  | 1:C:331:MET:HB3  | 2.43                     | 0.53              |
| 1:C:361:GLN:O    | 1:C:363:GLY:N    | 2.41                     | 0.53              |
| 1:C:399:THR:O    | 1:C:403:LEU:HD12 | 2.08                     | 0.53              |
| 1:C:416:LYS:HE2  | 1:C:417:ALA:N    | 2.22                     | 0.53              |
| 1:C:556:VAL:O    | 1:C:559:LEU:HB3  | 2.09                     | 0.53              |
| 1:E:242:ASN:ND2  | 1:E:245:SER:HA   | 2.22                     | 0.53              |
| 1:E:797:ILE:HG12 | 2:F:117:GLU:HG2  | 1.89                     | 0.53              |
| 1:G:107:ARG:HA   | 1:G:112:LEU:HD12 | 1.90                     | 0.53              |
| 1:G:153:ILE:HG23 | 1:G:154:TYR:N    | 2.24                     | 0.53              |
| 1:G:628:VAL:O    | 1:G:631:ILE:HG12 | 2.09                     | 0.53              |
| 2:H:128:VAL:HB   | 2:H:138:ILE:HD11 | 1.89                     | 0.53              |
| 1:A:86:VAL:HG12  | 1:A:103:ASN:ND2  | 2.23                     | 0.53              |
| 1:A:344:PHE:HE1  | 1:A:445:ARG:HB3  | 1.72                     | 0.53              |
| 1:A:418:GLN:HA   | 1:A:422:GLN:NE2  | 2.23                     | 0.53              |
| 2:B:55:LYS:O     | 2:B:56:SER:C     | 2.51                     | 0.53              |
| 1:C:572:SER:HB3  | 1:C:580:GLU:O    | 2.09                     | 0.53              |
| 1:C:731:ARG:HG2  | 1:C:731:ARG:NH1  | 2.23                     | 0.53              |
| 1:C:766:LEU:O    | 1:C:777:ARG:HB2  | 2.08                     | 0.53              |
| 1:E:13:LEU:CD1   | 1:E:152:HIS:CD2  | 2.90                     | 0.53              |
| 1:E:553:THR:O    | 1:E:554:SER:C    | 2.49                     | 0.53              |
| 1:G:581:PHE:HZ   | 1:G:597:TRP:CH2  | 2.25                     | 0.53              |
| 1:A:107:ARG:HB3  | 1:A:112:LEU:HD12 | 1.89                     | 0.53              |
| 1:A:298:SER:O    | 1:A:302:ARG:N    | 2.40                     | 0.53              |
| 1:A:370:GLU:O    | 1:A:374:ASP:HA   | 2.07                     | 0.53              |
| 1:C:51:GLU:HG2   | 1:C:53:LYS:HE3   | 1.89                     | 0.53              |
| 1:C:89:MET:C     | 1:C:91:GLU:N     | 2.66                     | 0.53              |
| 1:C:407:ILE:CD1  | 1:C:409:VAL:H    | 2.22                     | 0.53              |
| 1:E:382:THR:C    | 1:E:385:GLN:HB3  | 2.33                     | 0.53              |
| 1:E:733:ARG:HG2  | 1:E:734:TYR:CE1  | 2.44                     | 0.53              |
| 1:G:342:MET:HE3  | 1:G:342:MET:O    | 2.08                     | 0.53              |
| 1:G:630:ARG:HH12 | 1:G:657:ARG:HB3  | 1.73                     | 0.53              |
| 1:A:36:TRP:HB2   | 1:A:76:GLN:HB2   | 1.91                     | 0.53              |
| 1:A:369:LYS:HG3  | 1:A:370:GLU:N    | 2.24                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:416:LYS:HE2  | 1:A:417:ALA:N    | 2.23                     | 0.53              |
| 1:A:712:GLU:OE1  | 1:A:712:GLU:N    | 2.35                     | 0.53              |
| 1:C:138:ILE:HD13 | 1:C:154:TYR:CE2  | 2.43                     | 0.53              |
| 1:C:275:SER:O    | 1:C:277:ALA:N    | 2.41                     | 0.53              |
| 1:C:293:LEU:HD13 | 1:C:353:LEU:HD22 | 1.90                     | 0.53              |
| 1:E:33:LYS:CB    | 1:E:49:ILE:HB    | 2.38                     | 0.53              |
| 1:G:553:THR:HG23 | 1:G:579:THR:HG21 | 1.90                     | 0.53              |
| 1:A:271:LEU:HD21 | 1:A:663:TYR:CD1  | 2.44                     | 0.53              |
| 1:A:298:SER:O    | 1:A:302:ARG:HB2  | 2.08                     | 0.53              |
| 1:A:388:CYS:SG   | 1:A:393:ILE:HD11 | 2.49                     | 0.53              |
| 1:A:424:ASP:C    | 1:A:426:ALA:N    | 2.63                     | 0.53              |
| 1:A:721:PHE:CZ   | 1:A:768:ARG:HG2  | 2.44                     | 0.53              |
| 1:A:743:PRO:HB3  | 1:G:816:GLN:C    | 2.33                     | 0.53              |
| 2:B:30:GLN:O     | 2:B:31:CYS:C     | 2.52                     | 0.53              |
| 2:B:116:GLY:O    | 2:B:118:LYS:N    | 2.41                     | 0.53              |
| 1:C:36:TRP:HE1   | 1:C:78:MET:HA    | 1.74                     | 0.53              |
| 1:C:193:TYR:CZ   | 1:C:197:VAL:HG21 | 2.43                     | 0.53              |
| 1:C:254:ILE:O    | 1:C:460:PHE:HA   | 2.09                     | 0.53              |
| 1:E:525:ILE:O    | 1:E:529:GLU:N    | 2.39                     | 0.53              |
| 2:F:30:GLN:O     | 2:F:31:CYS:C     | 2.52                     | 0.53              |
| 2:F:55:LYS:O     | 2:F:56:SER:C     | 2.51                     | 0.53              |
| 1:G:437:ARG:NH2  | 1:G:625:TRP:CE3  | 2.77                     | 0.53              |
| 2:H:94:VAL:HG12  | 2:H:94:VAL:O     | 2.07                     | 0.53              |
| 2:B:76:ILE:O     | 2:B:79:ASN:ND2   | 2.42                     | 0.53              |
| 1:C:490:GLN:HE21 | 1:C:494:ASN:HD21 | 1.55                     | 0.53              |
| 1:C:788:ARG:HG2  | 1:C:788:ARG:NH1  | 2.24                     | 0.53              |
| 1:E:96:ASN:HB2   | 1:E:99:SER:OG    | 2.09                     | 0.53              |
| 1:E:305:LEU:HD12 | 1:E:307:LEU:HD11 | 1.91                     | 0.53              |
| 1:E:618:ASP:CG   | 1:E:621:VAL:HG23 | 2.34                     | 0.53              |
| 1:G:87:GLU:OE1   | 1:G:107:ARG:NH2  | 2.42                     | 0.53              |
| 1:G:107:ARG:CA   | 1:G:112:LEU:HD12 | 2.39                     | 0.53              |
| 1:G:267:ILE:N    | 1:G:447:ASN:HD21 | 2.07                     | 0.53              |
| 1:G:351:SER:O    | 1:G:354:ARG:HG2  | 2.09                     | 0.53              |
| 1:G:572:SER:CB   | 1:G:580:GLU:HG3  | 2.39                     | 0.53              |
| 1:G:697:ASP:C    | 1:G:697:ASP:OD1  | 2.52                     | 0.53              |
| 1:G:766:LEU:O    | 1:G:777:ARG:HB2  | 2.09                     | 0.53              |
| 2:H:23:ASP:HB2   | 2:H:25:LYS:HD3   | 1.91                     | 0.53              |
| 2:H:55:LYS:O     | 2:H:56:SER:C     | 2.51                     | 0.53              |
| 1:C:33:LYS:HB3   | 1:C:49:ILE:N     | 2.24                     | 0.53              |
| 1:C:88:ASP:O     | 1:C:91:GLU:N     | 2.42                     | 0.53              |
| 1:C:313:TYR:HB2  | 1:C:316:LEU:HD12 | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:347:GLU:O    | 1:C:349:GLN:N    | 2.42                     | 0.53              |
| 1:C:742:ILE:HD11 | 1:C:756:MET:HG2  | 1.91                     | 0.53              |
| 1:E:199:SER:HB2  | 1:E:221:GLU:CD   | 2.34                     | 0.53              |
| 1:E:480:LEU:HD11 | 1:E:528:ILE:CD1  | 2.38                     | 0.53              |
| 1:E:700:LEU:HD23 | 1:E:700:LEU:C    | 2.34                     | 0.53              |
| 2:F:76:ILE:O     | 2:F:79:ASN:ND2   | 2.42                     | 0.53              |
| 2:F:92:LEU:HD13  | 2:F:108:ILE:HD11 | 1.91                     | 0.53              |
| 2:F:140:TYR:CD1  | 2:F:141:GLU:HG2  | 2.44                     | 0.53              |
| 1:G:64:ASN:C     | 1:G:66:LYS:H     | 2.15                     | 0.53              |
| 1:G:313:TYR:HB2  | 1:G:316:LEU:HD12 | 1.91                     | 0.53              |
| 1:A:33:LYS:CB    | 1:A:49:ILE:HB    | 2.37                     | 0.52              |
| 1:A:267:ILE:N    | 1:A:447:ASN:HD21 | 2.07                     | 0.52              |
| 1:A:542:ASP:O    | 1:A:545:CYS:HB3  | 2.09                     | 0.52              |
| 1:A:711:LEU:H    | 1:A:711:LEU:HD22 | 1.73                     | 0.52              |
| 1:C:551:THR:O    | 1:C:552:ASP:C    | 2.52                     | 0.52              |
| 1:C:630:ARG:HH22 | 1:C:657:ARG:HB3  | 1.73                     | 0.52              |
| 1:G:36:TRP:HE1   | 1:G:78:MET:HA    | 1.75                     | 0.52              |
| 1:G:199:SER:HB2  | 1:G:221:GLU:CD   | 2.34                     | 0.52              |
| 1:G:290:PHE:CD1  | 1:G:360:LEU:HD11 | 2.45                     | 0.52              |
| 1:G:361:GLN:HB3  | 1:G:387:VAL:HG22 | 1.90                     | 0.52              |
| 1:A:176:THR:O    | 1:A:183:LYS:CD   | 2.58                     | 0.52              |
| 1:A:290:PHE:CD1  | 1:A:360:LEU:HD11 | 2.44                     | 0.52              |
| 1:A:400:ARG:O    | 1:A:404:THR:N    | 2.40                     | 0.52              |
| 1:A:622:ALA:O    | 1:A:626:LYS:N    | 2.40                     | 0.52              |
| 1:A:658:THR:HG23 | 1:A:661:GLN:HB3  | 1.91                     | 0.52              |
| 1:C:228:ASN:N    | 1:C:229:PRO:HD2  | 2.25                     | 0.52              |
| 1:C:286:THR:HB   | 1:C:290:PHE:HD2  | 1.75                     | 0.52              |
| 1:C:351:SER:C    | 1:C:353:LEU:H    | 2.18                     | 0.52              |
| 1:C:437:ARG:NH2  | 1:C:625:TRP:HE3  | 2.07                     | 0.52              |
| 2:D:30:GLN:O     | 2:D:31:CYS:C     | 2.52                     | 0.52              |
| 1:E:347:GLU:C    | 1:E:349:GLN:H    | 2.15                     | 0.52              |
| 1:E:574:GLN:C    | 1:E:576:LYS:HE3  | 2.33                     | 0.52              |
| 1:G:286:THR:HB   | 1:G:290:PHE:HD2  | 1.74                     | 0.52              |
| 1:G:551:THR:O    | 1:G:552:ASP:C    | 2.53                     | 0.52              |
| 1:A:351:SER:O    | 1:A:354:ARG:HG2  | 2.09                     | 0.52              |
| 1:A:449:ALA:C    | 1:A:451:ASP:H    | 2.17                     | 0.52              |
| 1:A:553:THR:HG23 | 1:A:579:THR:HG21 | 1.91                     | 0.52              |
| 1:A:712:GLU:CD   | 1:A:712:GLU:H    | 2.10                     | 0.52              |
| 1:A:812:PHE:C    | 1:A:814:LYS:N    | 2.68                     | 0.52              |
| 2:B:23:ASP:HB2   | 2:B:25:LYS:HD3   | 1.90                     | 0.52              |
| 1:C:199:SER:HB2  | 1:C:221:GLU:CD   | 2.33                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:218:GLY:HA3  | 1:C:221:GLU:OE1  | 2.09                     | 0.52              |
| 1:C:572:SER:CB   | 1:C:580:GLU:HG3  | 2.39                     | 0.52              |
| 1:E:161:TYR:CZ   | 1:E:165:LEU:HD11 | 2.45                     | 0.52              |
| 1:E:521:LEU:O    | 1:E:525:ILE:HG13 | 2.09                     | 0.52              |
| 1:E:705:LEU:HD22 | 1:E:710:VAL:HG21 | 1.90                     | 0.52              |
| 2:F:95:PHE:O     | 2:F:103:VAL:HG13 | 2.10                     | 0.52              |
| 1:G:351:SER:C    | 1:G:353:LEU:H    | 2.18                     | 0.52              |
| 1:G:540:LEU:O    | 1:G:542:ASP:N    | 2.43                     | 0.52              |
| 2:H:105:GLY:O    | 2:H:109:ARG:NH1  | 2.42                     | 0.52              |
| 1:A:164:MET:SD   | 1:A:256:PHE:CD2  | 3.03                     | 0.52              |
| 1:A:525:ILE:O    | 1:A:529:GLU:N    | 2.40                     | 0.52              |
| 1:A:604:PRO:O    | 1:A:605:LEU:HB2  | 2.09                     | 0.52              |
| 1:A:610:THR:CG2  | 1:A:628:VAL:HG11 | 2.39                     | 0.52              |
| 1:C:33:LYS:HB2   | 1:C:48:SER:OG    | 2.08                     | 0.52              |
| 1:C:419:THR:O    | 1:C:421:GLU:N    | 2.42                     | 0.52              |
| 1:C:803:CYS:HB2  | 2:D:119:MET:HE1  | 1.91                     | 0.52              |
| 2:D:108:ILE:HG22 | 2:D:109:ARG:N    | 2.23                     | 0.52              |
| 1:E:145:LYS:CB   | 1:E:148:GLU:HG3  | 2.40                     | 0.52              |
| 1:E:170:ASP:C    | 1:E:171:GLN:HG2  | 2.34                     | 0.52              |
| 1:E:349:GLN:O    | 1:E:350:THR:C    | 2.53                     | 0.52              |
| 1:E:351:SER:C    | 1:E:353:LEU:N    | 2.67                     | 0.52              |
| 1:E:543:GLU:C    | 1:E:545:CYS:H    | 2.16                     | 0.52              |
| 1:G:199:SER:CB   | 1:G:221:GLU:HG2  | 2.39                     | 0.52              |
| 1:G:288:HIS:HB3  | 1:G:292:TYR:CE1  | 2.44                     | 0.52              |
| 1:G:563:GLN:O    | 1:G:565:ASN:N    | 2.42                     | 0.52              |
| 2:H:144:VAL:HG12 | 2:H:145:ARG:N    | 2.24                     | 0.52              |
| 1:A:7:SER:O      | 1:A:11:LYS:HG3   | 2.09                     | 0.52              |
| 1:A:132:ILE:HD12 | 1:A:152:HIS:CD2  | 2.43                     | 0.52              |
| 1:A:278:ILE:O    | 1:A:279:ARG:HG3  | 2.09                     | 0.52              |
| 1:A:551:THR:H    | 1:A:554:SER:HG   | 1.55                     | 0.52              |
| 1:C:61:LEU:C     | 1:C:63:GLU:N     | 2.66                     | 0.52              |
| 1:C:405:PRO:HG2  | 1:C:416:LYS:HG3  | 1.92                     | 0.52              |
| 1:C:521:LEU:O    | 1:C:525:ILE:HG13 | 2.09                     | 0.52              |
| 1:C:575:LEU:C    | 1:C:577:ASP:H    | 2.18                     | 0.52              |
| 1:E:298:SER:O    | 1:E:302:ARG:N    | 2.41                     | 0.52              |
| 1:E:400:ARG:O    | 1:E:404:THR:N    | 2.38                     | 0.52              |
| 1:E:542:ASP:O    | 1:E:545:CYS:HB3  | 2.10                     | 0.52              |
| 1:G:267:ILE:HB   | 1:G:447:ASN:ND2  | 2.24                     | 0.52              |
| 1:G:269:THR:HG23 | 1:G:440:ARG:NH1  | 2.24                     | 0.52              |
| 1:G:382:THR:C    | 1:G:385:GLN:HB3  | 2.34                     | 0.52              |
| 1:G:449:ALA:C    | 1:G:451:ASP:H    | 2.16                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:30:GLN:O     | 2:H:31:CYS:C     | 2.53                     | 0.52              |
| 1:A:144:LYS:HG3  | 1:A:148:GLU:HB2  | 1.90                     | 0.52              |
| 1:A:413:VAL:O    | 1:A:413:VAL:HG12 | 2.08                     | 0.52              |
| 1:A:437:ARG:NH2  | 1:A:625:TRP:CE3  | 2.78                     | 0.52              |
| 1:A:495:HIS:ND1  | 1:A:499:ILE:HD12 | 2.25                     | 0.52              |
| 1:C:267:ILE:N    | 1:C:447:ASN:HD21 | 2.08                     | 0.52              |
| 1:C:449:ALA:C    | 1:C:451:ASP:H    | 2.18                     | 0.52              |
| 2:D:120:THR:HG23 | 2:D:123:GLU:CD   | 2.34                     | 0.52              |
| 1:E:269:THR:CG2  | 1:E:443:LEU:CD1  | 2.87                     | 0.52              |
| 1:E:313:TYR:CD2  | 1:E:360:LEU:HB3  | 2.44                     | 0.52              |
| 1:E:337:GLU:O    | 1:E:340:THR:OG1  | 2.27                     | 0.52              |
| 2:F:44:ASN:HB2   | 2:F:117:GLU:OE2  | 2.10                     | 0.52              |
| 1:G:305:LEU:HD12 | 1:G:307:LEU:HD11 | 1.92                     | 0.52              |
| 1:G:369:LYS:HG3  | 1:G:370:GLU:N    | 2.25                     | 0.52              |
| 1:G:574:GLN:C    | 1:G:576:LYS:HE3  | 2.35                     | 0.52              |
| 2:H:120:THR:HG23 | 2:H:123:GLU:CD   | 2.34                     | 0.52              |
| 1:A:114:TYR:HE2  | 1:A:153:ILE:HB   | 1.70                     | 0.52              |
| 1:A:349:GLN:O    | 1:A:350:THR:C    | 2.53                     | 0.52              |
| 1:A:551:THR:H    | 1:A:554:SER:CB   | 2.23                     | 0.52              |
| 1:A:586:TYR:CD1  | 1:A:587:ALA:N    | 2.78                     | 0.52              |
| 1:C:521:LEU:HD23 | 1:C:521:LEU:N    | 2.24                     | 0.52              |
| 1:C:574:GLN:C    | 1:C:576:LYS:HE3  | 2.35                     | 0.52              |
| 1:C:721:PHE:CE2  | 1:C:768:ARG:HG2  | 2.45                     | 0.52              |
| 1:E:815:ARG:O    | 1:E:818:GLN:HG2  | 2.10                     | 0.52              |
| 1:A:140:MET:HE2  | 1:A:149:MET:HE1  | 1.91                     | 0.52              |
| 1:A:235:GLY:O    | 1:A:247:ARG:HB2  | 2.10                     | 0.52              |
| 1:A:803:CYS:HB2  | 2:B:119:MET:HE1  | 1.92                     | 0.52              |
| 1:A:814:LYS:HD2  | 1:A:818:GLN:OE1  | 2.09                     | 0.52              |
| 1:C:152:HIS:CE1  | 1:C:154:TYR:CD2  | 2.98                     | 0.52              |
| 1:E:521:LEU:HD23 | 1:E:521:LEU:N    | 2.25                     | 0.52              |
| 1:E:539:ALA:O    | 1:E:542:ASP:HB2  | 2.10                     | 0.52              |
| 1:G:307:LEU:HA   | 1:G:313:TYR:OH   | 2.10                     | 0.52              |
| 1:A:269:THR:HG23 | 1:A:440:ARG:NH1  | 2.24                     | 0.52              |
| 1:C:607:ASP:OD1  | 1:C:607:ASP:N    | 2.31                     | 0.52              |
| 1:C:815:ARG:NE   | 1:C:818:GLN:NE2  | 2.58                     | 0.52              |
| 2:D:66:PHE:CE1   | 2:D:70:LEU:HB2   | 2.45                     | 0.52              |
| 1:E:405:PRO:HD2  | 1:E:416:LYS:O    | 2.10                     | 0.52              |
| 1:E:805:GLY:CA   | 2:F:36:ARG:HG2   | 2.32                     | 0.52              |
| 2:F:15:PHE:O     | 2:F:18:PHE:HB2   | 2.10                     | 0.52              |
| 1:G:271:LEU:HD21 | 1:G:663:TYR:CZ   | 2.45                     | 0.52              |
| 1:G:604:PRO:O    | 1:G:605:LEU:HB2  | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:815:ARG:NE   | 1:G:818:GLN:HE21 | 2.08                     | 0.52              |
| 2:H:85:PHE:HD1   | 2:H:148:LEU:CD2  | 2.23                     | 0.52              |
| 1:A:248:PHE:CD1  | 1:A:248:PHE:O    | 2.62                     | 0.52              |
| 1:A:572:SER:CB   | 1:A:580:GLU:HG3  | 2.40                     | 0.52              |
| 1:C:562:GLU:OE1  | 1:C:562:GLU:HA   | 2.10                     | 0.52              |
| 1:E:89:MET:O     | 1:E:91:GLU:N     | 2.43                     | 0.52              |
| 1:E:287:PHE:O    | 1:E:288:HIS:C    | 2.52                     | 0.52              |
| 1:G:480:LEU:HD11 | 1:G:528:ILE:CD1  | 2.40                     | 0.52              |
| 1:G:657:ARG:HB2  | 1:G:657:ARG:HH11 | 1.75                     | 0.52              |
| 2:H:110:HIS:O    | 2:H:111:VAL:C    | 2.53                     | 0.52              |
| 1:A:193:TYR:CE1  | 1:A:197:VAL:HG21 | 2.44                     | 0.51              |
| 1:A:351:SER:C    | 1:A:353:LEU:N    | 2.68                     | 0.51              |
| 1:A:700:LEU:HD23 | 1:A:700:LEU:C    | 2.35                     | 0.51              |
| 2:B:112:LEU:CD1  | 2:B:119:MET:HE3  | 2.39                     | 0.51              |
| 1:C:37:VAL:CG1   | 1:C:38:PRO:HD2   | 2.34                     | 0.51              |
| 1:C:267:ILE:H    | 1:C:447:ASN:HD21 | 1.58                     | 0.51              |
| 1:C:610:THR:CG2  | 1:C:631:ILE:HG13 | 2.29                     | 0.51              |
| 1:C:703:GLU:O    | 1:C:706:ARG:N    | 2.39                     | 0.51              |
| 2:D:15:PHE:O     | 2:D:18:PHE:HB2   | 2.10                     | 0.51              |
| 2:D:64:LEU:HD21  | 2:D:72:MET:HE1   | 1.91                     | 0.51              |
| 1:E:33:LYS:HB2   | 1:E:48:SER:OG    | 2.10                     | 0.51              |
| 1:E:224:LEU:HD12 | 1:E:224:LEU:O    | 2.09                     | 0.51              |
| 1:E:228:ASN:N    | 1:E:229:PRO:HD2  | 2.24                     | 0.51              |
| 1:E:369:LYS:HG3  | 1:E:370:GLU:N    | 2.25                     | 0.51              |
| 1:E:418:GLN:HA   | 1:E:422:GLN:NE2  | 2.24                     | 0.51              |
| 1:E:630:ARG:HH22 | 1:E:657:ARG:CB   | 2.24                     | 0.51              |
| 2:F:116:GLY:O    | 2:F:118:LYS:N    | 2.44                     | 0.51              |
| 1:G:521:LEU:HD23 | 1:G:521:LEU:N    | 2.25                     | 0.51              |
| 2:H:15:PHE:O     | 2:H:18:PHE:HB2   | 2.10                     | 0.51              |
| 1:A:33:LYS:HB2   | 1:A:48:SER:OG    | 2.10                     | 0.51              |
| 1:A:184:THR:O    | 1:A:185:GLU:C    | 2.53                     | 0.51              |
| 1:A:293:LEU:HD13 | 1:A:353:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:514:PHE:CD1  | 1:A:515:ILE:N    | 2.78                     | 0.51              |
| 1:A:721:PHE:HB3  | 1:A:776:PHE:O    | 2.10                     | 0.51              |
| 2:B:94:VAL:O     | 2:B:94:VAL:HG12  | 2.10                     | 0.51              |
| 1:C:114:TYR:HE2  | 1:C:153:ILE:HB   | 1.74                     | 0.51              |
| 1:C:352:ILE:HG21 | 1:C:442:ILE:CD1  | 2.39                     | 0.51              |
| 1:C:513:ASN:HD22 | 1:C:513:ASN:C    | 2.18                     | 0.51              |
| 1:E:278:ILE:HG13 | 1:E:279:ARG:N    | 2.26                     | 0.51              |
| 1:E:351:SER:O    | 1:E:353:LEU:N    | 2.43                     | 0.51              |
| 1:E:430:LEU:HB2  | 1:E:605:LEU:HD11 | 1.91                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:514:PHE:CD1  | 1:E:515:ILE:N    | 2.79                     | 0.51              |
| 1:E:545:CYS:O    | 1:E:602:MET:HE1  | 2.10                     | 0.51              |
| 1:E:628:VAL:O    | 1:E:628:VAL:CG1  | 2.56                     | 0.51              |
| 1:E:712:GLU:OE1  | 1:E:712:GLU:N    | 2.38                     | 0.51              |
| 2:F:64:LEU:HD21  | 2:F:72:MET:HE1   | 1.92                     | 0.51              |
| 1:G:269:THR:CG2  | 1:G:443:LEU:CD1  | 2.88                     | 0.51              |
| 1:G:541:LEU:CD2  | 1:G:601:ASN:HD22 | 2.12                     | 0.51              |
| 1:A:100:VAL:HG21 | 1:A:711:LEU:CD1  | 2.40                     | 0.51              |
| 1:A:361:GLN:HB3  | 1:A:387:VAL:HG22 | 1.92                     | 0.51              |
| 1:A:382:THR:C    | 1:A:385:GLN:HB3  | 2.35                     | 0.51              |
| 1:A:562:GLU:OE1  | 1:A:562:GLU:HA   | 2.09                     | 0.51              |
| 1:A:625:TRP:C    | 1:A:627:ASP:H    | 2.19                     | 0.51              |
| 1:A:815:ARG:NE   | 1:A:818:GLN:NE2  | 2.58                     | 0.51              |
| 2:B:66:PHE:CE1   | 2:B:70:LEU:HB2   | 2.45                     | 0.51              |
| 2:B:74:GLN:O     | 2:B:75:THR:C     | 2.53                     | 0.51              |
| 1:C:145:LYS:CB   | 1:C:148:GLU:HG3  | 2.40                     | 0.51              |
| 1:C:756:MET:O    | 1:C:760:LEU:HG   | 2.10                     | 0.51              |
| 1:E:36:TRP:HE1   | 1:E:78:MET:HA    | 1.76                     | 0.51              |
| 1:E:61:LEU:C     | 1:E:63:GLU:N     | 2.65                     | 0.51              |
| 1:E:232:GLU:O    | 1:E:236:ASN:HB2  | 2.10                     | 0.51              |
| 1:E:361:GLN:HB3  | 1:E:387:VAL:HG22 | 1.93                     | 0.51              |
| 1:E:663:TYR:C    | 1:E:665:GLU:N    | 2.66                     | 0.51              |
| 1:G:495:HIS:ND1  | 1:G:499:ILE:HD12 | 2.24                     | 0.51              |
| 1:G:495:HIS:CD2  | 1:G:500:LEU:HG   | 2.45                     | 0.51              |
| 1:G:556:VAL:HG21 | 1:G:579:THR:HB   | 1.93                     | 0.51              |
| 1:G:700:LEU:HD23 | 1:G:700:LEU:C    | 2.34                     | 0.51              |
| 1:A:152:HIS:CE1  | 1:A:154:TYR:CD2  | 2.99                     | 0.51              |
| 1:A:327:GLN:HG2  | 1:A:330:GLU:HG2  | 1.93                     | 0.51              |
| 1:A:359:VAL:O    | 1:A:359:VAL:HG12 | 2.10                     | 0.51              |
| 1:C:256:PHE:CE1  | 1:C:262:ILE:HG13 | 2.46                     | 0.51              |
| 1:C:416:LYS:HE2  | 1:C:417:ALA:H    | 1.74                     | 0.51              |
| 2:D:8:THR:O      | 2:D:12:LYS:HG3   | 2.10                     | 0.51              |
| 1:E:107:ARG:CA   | 1:E:112:LEU:HD12 | 2.41                     | 0.51              |
| 1:E:272:LEU:O    | 1:E:274:LYS:N    | 2.42                     | 0.51              |
| 1:E:628:VAL:HG13 | 1:E:631:ILE:CG1  | 2.40                     | 0.51              |
| 2:F:94:VAL:O     | 2:F:94:VAL:HG12  | 2.10                     | 0.51              |
| 2:F:98:GLU:O     | 2:F:100:ASN:N    | 2.44                     | 0.51              |
| 2:H:64:LEU:HD21  | 2:H:72:MET:HE1   | 1.92                     | 0.51              |
| 2:H:85:PHE:HD1   | 2:H:148:LEU:HD23 | 1.75                     | 0.51              |
| 2:H:87:ASP:O     | 2:H:90:GLU:HB3   | 2.11                     | 0.51              |
| 1:A:145:LYS:HB3  | 1:A:148:GLU:CG   | 2.39                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:193:TYR:CZ   | 1:A:197:VAL:HG21 | 2.46                     | 0.51              |
| 1:A:307:LEU:HA   | 1:A:313:TYR:OH   | 2.10                     | 0.51              |
| 1:A:495:HIS:CD2  | 1:A:500:LEU:HG   | 2.46                     | 0.51              |
| 1:A:556:VAL:O    | 1:A:559:LEU:HB3  | 2.11                     | 0.51              |
| 1:C:80:PRO:HD2   | 1:C:83:PHE:CD2   | 2.45                     | 0.51              |
| 1:C:177:GLY:O    | 1:C:183:LYS:NZ   | 2.44                     | 0.51              |
| 1:C:370:GLU:O    | 1:C:374:ASP:HA   | 2.11                     | 0.51              |
| 1:C:586:TYR:CD1  | 1:C:587:ALA:N    | 2.79                     | 0.51              |
| 1:C:618:ASP:CG   | 1:C:621:VAL:HG23 | 2.35                     | 0.51              |
| 1:C:628:VAL:CG1  | 1:C:631:ILE:HG13 | 2.23                     | 0.51              |
| 1:C:762:LEU:HD13 | 1:C:766:LEU:CD1  | 2.41                     | 0.51              |
| 1:E:508:GLU:HG3  | 1:E:775:PHE:HE1  | 1.76                     | 0.51              |
| 1:E:766:LEU:HB3  | 1:E:780:VAL:HG21 | 1.93                     | 0.51              |
| 1:E:815:ARG:NE   | 1:E:818:GLN:HE21 | 2.09                     | 0.51              |
| 2:F:3:PHE:CA     | 2:F:7:GLN:HE21   | 2.23                     | 0.51              |
| 2:F:120:THR:HG23 | 2:F:123:GLU:CD   | 2.36                     | 0.51              |
| 1:G:77:LYS:H     | 1:G:77:LYS:HD2   | 1.75                     | 0.51              |
| 1:G:107:ARG:HB3  | 1:G:112:LEU:HD12 | 1.92                     | 0.51              |
| 1:G:347:GLU:C    | 1:G:349:GLN:H    | 2.16                     | 0.51              |
| 1:A:199:SER:HB2  | 1:A:221:GLU:CG   | 2.40                     | 0.51              |
| 1:A:657:ARG:HB2  | 1:A:657:ARG:HH11 | 1.76                     | 0.51              |
| 1:A:751:GLN:CD   | 1:G:813:ALA:HB2  | 2.36                     | 0.51              |
| 1:C:120:PHE:CD1  | 1:C:120:PHE:N    | 2.74                     | 0.51              |
| 1:C:184:THR:O    | 1:C:185:GLU:C    | 2.54                     | 0.51              |
| 1:C:351:SER:C    | 1:C:353:LEU:N    | 2.67                     | 0.51              |
| 1:E:36:TRP:HB2   | 1:E:76:GLN:HB2   | 1.92                     | 0.51              |
| 1:E:477:PHE:O    | 1:E:480:LEU:N    | 2.41                     | 0.51              |
| 2:F:108:ILE:HG22 | 2:F:109:ARG:N    | 2.26                     | 0.51              |
| 1:G:610:THR:HG23 | 1:G:628:VAL:HG21 | 1.93                     | 0.51              |
| 1:G:711:LEU:H    | 1:G:711:LEU:CD2  | 2.24                     | 0.51              |
| 1:A:584:LEU:N    | 1:A:584:LEU:HD23 | 2.25                     | 0.51              |
| 1:C:176:THR:O    | 1:C:183:LYS:HD2  | 2.10                     | 0.51              |
| 1:E:166:GLN:HE22 | 2:F:107:GLU:HG2  | 1.75                     | 0.51              |
| 1:E:313:TYR:HB2  | 1:E:316:LEU:HD12 | 1.92                     | 0.51              |
| 1:E:351:SER:C    | 1:E:353:LEU:H    | 2.17                     | 0.51              |
| 1:E:562:GLU:OE1  | 1:E:562:GLU:HA   | 2.10                     | 0.51              |
| 1:E:771:GLN:HE21 | 1:E:771:GLN:CA   | 2.24                     | 0.51              |
| 1:G:88:ASP:O     | 1:G:91:GLU:N     | 2.44                     | 0.51              |
| 1:G:232:GLU:O    | 1:G:236:ASN:HB2  | 2.11                     | 0.51              |
| 1:G:400:ARG:O    | 1:G:404:THR:N    | 2.38                     | 0.51              |
| 1:G:401:SER:O    | 1:G:606:ASN:ND2  | 2.43                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:442:ILE:O    | 1:G:445:ARG:N    | 2.38                     | 0.51              |
| 1:G:553:THR:O    | 1:G:554:SER:C    | 2.54                     | 0.51              |
| 1:G:800:GLN:HA   | 2:H:119:MET:HE2  | 1.93                     | 0.51              |
| 1:G:802:GLN:NE2  | 2:H:88:TYR:OH    | 2.40                     | 0.51              |
| 1:G:806:TYR:CB   | 2:H:147:VAL:HG12 | 2.41                     | 0.51              |
| 1:A:153:ILE:HG23 | 1:A:154:TYR:N    | 2.25                     | 0.51              |
| 1:A:359:VAL:O    | 1:A:359:VAL:CG1  | 2.59                     | 0.51              |
| 1:A:521:LEU:HD23 | 1:A:521:LEU:N    | 2.26                     | 0.51              |
| 1:A:747:MET:CG   | 1:A:751:GLN:HE22 | 2.22                     | 0.51              |
| 1:C:107:ARG:HB3  | 1:C:112:LEU:HD12 | 1.92                     | 0.51              |
| 1:C:298:SER:O    | 1:C:302:ARG:N    | 2.42                     | 0.51              |
| 1:C:542:ASP:O    | 1:C:545:CYS:HB3  | 2.11                     | 0.51              |
| 1:E:22:ASN:O     | 1:E:22:ASN:ND2   | 2.44                     | 0.51              |
| 1:E:121:CYS:SG   | 1:E:156:ILE:HD11 | 2.50                     | 0.51              |
| 1:G:239:THR:C    | 1:G:241:LYS:H    | 2.18                     | 0.51              |
| 1:G:797:ILE:CG1  | 2:H:117:GLU:HG2  | 2.41                     | 0.51              |
| 2:H:35:MET:HE3   | 2:H:73:MET:HA    | 1.93                     | 0.51              |
| 2:H:74:GLN:O     | 2:H:75:THR:C     | 2.53                     | 0.51              |
| 1:A:409:VAL:HG13 | 1:A:634:LEU:CD1  | 2.40                     | 0.51              |
| 1:C:103:ASN:O    | 1:C:107:ARG:HG3  | 2.11                     | 0.51              |
| 1:C:313:TYR:CD2  | 1:C:360:LEU:HB3  | 2.44                     | 0.51              |
| 1:C:407:ILE:CD1  | 1:C:409:VAL:N    | 2.72                     | 0.51              |
| 1:E:31:ALA:O     | 1:E:33:LYS:N     | 2.44                     | 0.51              |
| 1:E:76:GLN:HB3   | 1:E:96:ASN:ND2   | 2.26                     | 0.51              |
| 1:E:152:HIS:CE1  | 1:E:153:ILE:HG22 | 2.46                     | 0.51              |
| 1:E:540:LEU:O    | 1:E:542:ASP:N    | 2.44                     | 0.51              |
| 1:E:697:ASP:C    | 1:E:697:ASP:OD1  | 2.51                     | 0.51              |
| 1:G:147:HIS:C    | 1:G:149:MET:H    | 2.19                     | 0.51              |
| 1:G:282:LYS:O    | 1:G:283:ASP:HB2  | 2.10                     | 0.51              |
| 1:G:349:GLN:O    | 1:G:350:THR:C    | 2.54                     | 0.51              |
| 1:G:405:PRO:HD2  | 1:G:416:LYS:O    | 2.11                     | 0.51              |
| 1:G:721:PHE:CE2  | 1:G:768:ARG:HG2  | 2.45                     | 0.51              |
| 2:H:3:PHE:CA     | 2:H:7:GLN:HE21   | 2.24                     | 0.51              |
| 1:A:743:PRO:HB2  | 1:G:816:GLN:HG2  | 1.93                     | 0.51              |
| 1:C:306:LEU:HD22 | 1:C:386:LYS:HD3  | 1.93                     | 0.51              |
| 1:C:381:ASN:O    | 1:C:382:THR:C    | 2.54                     | 0.51              |
| 2:D:74:GLN:O     | 2:D:75:THR:C     | 2.53                     | 0.51              |
| 1:E:296:GLY:HA3  | 1:E:332:PHE:CG   | 2.46                     | 0.51              |
| 2:F:66:PHE:CE1   | 2:F:70:LEU:HB2   | 2.46                     | 0.51              |
| 1:G:256:PHE:CE1  | 1:G:262:ILE:HG13 | 2.46                     | 0.51              |
| 1:G:545:CYS:O    | 1:G:602:MET:HE1  | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:725:ILE:HD13 | 1:G:730:PHE:HB2  | 1.93                     | 0.51              |
| 1:A:166:GLN:HE22 | 2:B:107:GLU:HG2  | 1.76                     | 0.50              |
| 1:A:250:LYS:HG2  | 1:A:465:ASP:HB3  | 1.93                     | 0.50              |
| 1:A:574:GLN:C    | 1:A:576:LYS:HE3  | 2.37                     | 0.50              |
| 1:A:581:PHE:HZ   | 1:A:597:TRP:CH2  | 2.30                     | 0.50              |
| 1:A:610:THR:CG2  | 1:A:631:ILE:HG13 | 2.28                     | 0.50              |
| 1:A:815:ARG:NE   | 1:A:818:GLN:HE21 | 2.09                     | 0.50              |
| 2:B:120:THR:HG23 | 2:B:123:GLU:CD   | 2.35                     | 0.50              |
| 1:C:288:HIS:HB3  | 1:C:292:TYR:CE1  | 2.46                     | 0.50              |
| 1:C:437:ARG:NH2  | 1:C:628:VAL:HG23 | 2.26                     | 0.50              |
| 1:C:663:TYR:C    | 1:C:665:GLU:N    | 2.66                     | 0.50              |
| 1:E:286:THR:HB   | 1:E:290:PHE:HD2  | 1.76                     | 0.50              |
| 1:E:657:ARG:HH11 | 1:E:657:ARG:HB2  | 1.75                     | 0.50              |
| 2:F:8:THR:O      | 2:F:12:LYS:HG3   | 2.10                     | 0.50              |
| 1:G:381:ASN:O    | 1:G:382:THR:C    | 2.54                     | 0.50              |
| 1:G:405:PRO:O    | 1:G:407:ILE:HG23 | 2.11                     | 0.50              |
| 1:A:337:GLU:O    | 1:A:340:THR:OG1  | 2.28                     | 0.50              |
| 1:A:480:LEU:HD11 | 1:A:528:ILE:CD1  | 2.40                     | 0.50              |
| 1:A:663:TYR:C    | 1:A:665:GLU:N    | 2.69                     | 0.50              |
| 1:A:697:ASP:C    | 1:A:697:ASP:OD1  | 2.55                     | 0.50              |
| 1:A:733:ARG:HG2  | 1:A:734:TYR:CE1  | 2.47                     | 0.50              |
| 2:B:128:VAL:HB   | 2:B:138:ILE:HD11 | 1.92                     | 0.50              |
| 1:C:539:ALA:O    | 1:C:542:ASP:HB2  | 2.11                     | 0.50              |
| 2:D:95:PHE:O     | 2:D:103:VAL:HG13 | 2.10                     | 0.50              |
| 1:E:100:VAL:HG21 | 1:E:711:LEU:CD1  | 2.41                     | 0.50              |
| 1:E:144:LYS:HG3  | 1:E:148:GLU:HB2  | 1.92                     | 0.50              |
| 1:G:265:ALA:N    | 1:G:450:LEU:O    | 2.45                     | 0.50              |
| 1:G:771:GLN:HE21 | 1:G:771:GLN:CA   | 2.20                     | 0.50              |
| 2:H:8:THR:O      | 2:H:12:LYS:HG3   | 2.10                     | 0.50              |
| 2:H:105:GLY:O    | 2:H:109:ARG:HB2  | 2.10                     | 0.50              |
| 2:H:139:ASN:HD21 | 2:H:141:GLU:HG3  | 1.76                     | 0.50              |
| 1:A:449:ALA:C    | 1:A:451:ASP:N    | 2.69                     | 0.50              |
| 2:B:15:PHE:O     | 2:B:18:PHE:HB2   | 2.10                     | 0.50              |
| 1:C:31:ALA:O     | 1:C:33:LYS:N     | 2.44                     | 0.50              |
| 1:C:311:ASN:HD22 | 1:C:311:ASN:N    | 2.10                     | 0.50              |
| 1:C:404:THR:OG1  | 1:C:404:THR:O    | 2.28                     | 0.50              |
| 1:C:657:ARG:HH11 | 1:C:657:ARG:HB2  | 1.75                     | 0.50              |
| 1:C:766:LEU:HB3  | 1:C:780:VAL:HG21 | 1.94                     | 0.50              |
| 2:D:3:PHE:CA     | 2:D:7:GLN:HE21   | 2.24                     | 0.50              |
| 2:D:35:MET:HE3   | 2:D:73:MET:HA    | 1.92                     | 0.50              |
| 1:E:126:PRO:O    | 1:E:127:TYR:HB2  | 2.09                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:161:TYR:O    | 1:E:161:TYR:CG   | 2.64                     | 0.50              |
| 1:E:267:ILE:HB   | 1:E:447:ASN:ND2  | 2.26                     | 0.50              |
| 1:E:442:ILE:O    | 1:E:445:ARG:N    | 2.39                     | 0.50              |
| 2:F:74:GLN:O     | 2:F:75:THR:C     | 2.53                     | 0.50              |
| 1:G:430:LEU:HB2  | 1:G:605:LEU:HD11 | 1.92                     | 0.50              |
| 1:G:630:ARG:HH22 | 1:G:657:ARG:HB2  | 1.76                     | 0.50              |
| 2:H:66:PHE:CE1   | 2:H:70:LEU:HB2   | 2.45                     | 0.50              |
| 1:A:61:LEU:C     | 1:A:63:GLU:N     | 2.64                     | 0.50              |
| 1:A:287:PHE:O    | 1:A:288:HIS:C    | 2.54                     | 0.50              |
| 1:A:381:ASN:O    | 1:A:382:THR:C    | 2.55                     | 0.50              |
| 1:A:659:VAL:CG1  | 1:A:660:GLY:N    | 2.67                     | 0.50              |
| 1:A:719:GLN:NE2  | 1:A:719:GLN:HA   | 2.26                     | 0.50              |
| 1:A:763:ASP:HB3  | 1:A:766:LEU:CD1  | 2.42                     | 0.50              |
| 2:B:3:PHE:CA     | 2:B:7:GLN:HE21   | 2.23                     | 0.50              |
| 1:C:83:PHE:HB3   | 1:C:92:LEU:HD23  | 1.94                     | 0.50              |
| 1:C:269:THR:CG2  | 1:C:443:LEU:CD1  | 2.88                     | 0.50              |
| 1:C:540:LEU:O    | 1:C:542:ASP:N    | 2.45                     | 0.50              |
| 2:D:35:MET:SD    | 2:D:76:ILE:HD12  | 2.51                     | 0.50              |
| 2:D:48:MET:HE1   | 2:D:59:MET:HE1   | 1.94                     | 0.50              |
| 2:D:55:LYS:H     | 2:D:58:GLU:CG    | 2.25                     | 0.50              |
| 1:E:14:PHE:HE2   | 1:E:140:MET:HE1  | 1.77                     | 0.50              |
| 1:E:401:SER:O    | 1:E:606:ASN:ND2  | 2.45                     | 0.50              |
| 1:E:563:GLN:O    | 1:E:565:ASN:N    | 2.44                     | 0.50              |
| 2:F:48:MET:HE1   | 2:F:59:MET:HE1   | 1.94                     | 0.50              |
| 1:A:269:THR:CG2  | 1:A:443:LEU:CD1  | 2.88                     | 0.50              |
| 2:B:48:MET:HE1   | 2:B:59:MET:HE1   | 1.94                     | 0.50              |
| 1:C:351:SER:O    | 1:C:354:ARG:HG2  | 2.11                     | 0.50              |
| 1:C:409:VAL:HG13 | 1:C:634:LEU:HD11 | 1.94                     | 0.50              |
| 2:D:139:ASN:HD21 | 2:D:141:GLU:HG3  | 1.77                     | 0.50              |
| 1:G:31:ALA:O     | 1:G:33:LYS:N     | 2.45                     | 0.50              |
| 1:G:36:TRP:HB2   | 1:G:76:GLN:HB2   | 1.92                     | 0.50              |
| 1:G:236:ASN:ND2  | 1:G:246:SER:CA   | 2.70                     | 0.50              |
| 1:G:269:THR:HG21 | 1:G:443:LEU:CD1  | 2.30                     | 0.50              |
| 2:H:35:MET:SD    | 2:H:76:ILE:HD12  | 2.51                     | 0.50              |
| 1:A:134:SER:O    | 1:A:135:GLU:C    | 2.55                     | 0.50              |
| 1:A:478:GLU:HB2  | 1:A:479:GLN:OE1  | 2.12                     | 0.50              |
| 2:B:135:ASN:HB2  | 2:B:137:CYS:SG   | 2.52                     | 0.50              |
| 1:C:102:HIS:O    | 1:C:105:ARG:N    | 2.45                     | 0.50              |
| 1:E:58:THR:HA    | 1:E:69:THR:OG1   | 2.12                     | 0.50              |
| 1:E:267:ILE:HB   | 1:E:447:ASN:HD21 | 1.77                     | 0.50              |
| 2:F:35:MET:SD    | 2:F:76:ILE:HD12  | 2.51                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:533:ASN:O    | 1:G:535:PRO:N    | 2.45                     | 0.50              |
| 1:A:145:LYS:HG3  | 1:A:146:ARG:NE   | 2.26                     | 0.50              |
| 1:A:253:ARG:O    | 1:A:265:ALA:HA   | 2.11                     | 0.50              |
| 1:A:313:TYR:CD2  | 1:A:360:LEU:HB3  | 2.45                     | 0.50              |
| 1:A:326:GLN:HG3  | 1:A:331:MET:HE3  | 1.93                     | 0.50              |
| 1:A:544:GLU:OE1  | 1:A:550:ALA:HB1  | 2.11                     | 0.50              |
| 2:B:68:GLN:O     | 2:B:71:PRO:HG2   | 2.12                     | 0.50              |
| 1:C:199:SER:CB   | 1:C:221:GLU:HG2  | 2.40                     | 0.50              |
| 1:C:735:GLU:HA   | 1:C:756:MET:HE1  | 1.94                     | 0.50              |
| 1:C:767:TYR:CD1  | 1:C:767:TYR:C    | 2.90                     | 0.50              |
| 2:D:36:ARG:O     | 2:D:39:GLY:N     | 2.44                     | 0.50              |
| 2:D:76:ILE:O     | 2:D:79:ASN:ND2   | 2.44                     | 0.50              |
| 1:E:7:SER:O      | 1:E:11:LYS:HG3   | 2.11                     | 0.50              |
| 1:E:33:LYS:HB3   | 1:E:49:ILE:N     | 2.27                     | 0.50              |
| 1:E:184:THR:O    | 1:E:185:GLU:C    | 2.55                     | 0.50              |
| 1:E:265:ALA:N    | 1:E:450:LEU:O    | 2.44                     | 0.50              |
| 1:E:351:SER:O    | 1:E:354:ARG:HG2  | 2.12                     | 0.50              |
| 1:G:622:ALA:O    | 1:G:626:LYS:N    | 2.44                     | 0.50              |
| 1:A:145:LYS:CB   | 1:A:148:GLU:HG3  | 2.41                     | 0.50              |
| 1:A:293:LEU:O    | 1:A:297:ALA:HB2  | 2.12                     | 0.50              |
| 1:A:533:ASN:O    | 1:A:535:PRO:N    | 2.45                     | 0.50              |
| 2:B:35:MET:SD    | 2:B:76:ILE:HD12  | 2.51                     | 0.50              |
| 1:C:152:HIS:CE1  | 1:C:153:ILE:HG22 | 2.46                     | 0.50              |
| 1:C:232:GLU:O    | 1:C:236:ASN:HB2  | 2.11                     | 0.50              |
| 1:C:442:ILE:O    | 1:C:445:ARG:N    | 2.38                     | 0.50              |
| 1:C:569:PHE:CD2  | 1:C:570:GLN:N    | 2.80                     | 0.50              |
| 1:E:44:PHE:HD2   | 1:E:101:LEU:HD23 | 1.77                     | 0.50              |
| 1:E:107:ARG:HH11 | 1:E:115:THR:HG23 | 1.77                     | 0.50              |
| 1:E:551:THR:O    | 1:E:552:ASP:C    | 2.55                     | 0.50              |
| 1:E:728:GLN:O    | 1:E:728:GLN:NE2  | 2.44                     | 0.50              |
| 1:G:278:ILE:O    | 1:G:279:ARG:HG3  | 2.11                     | 0.50              |
| 1:G:351:SER:O    | 1:G:353:LEU:N    | 2.45                     | 0.50              |
| 1:G:586:TYR:CD1  | 1:G:587:ALA:N    | 2.79                     | 0.50              |
| 1:G:703:GLU:O    | 1:G:706:ARG:N    | 2.39                     | 0.50              |
| 1:G:733:ARG:HG2  | 1:G:734:TYR:CE1  | 2.46                     | 0.50              |
| 1:G:806:TYR:HB3  | 2:H:147:VAL:HG12 | 1.93                     | 0.50              |
| 1:G:815:ARG:NE   | 1:G:818:GLN:NE2  | 2.60                     | 0.50              |
| 2:H:48:MET:HE1   | 2:H:59:MET:HE1   | 1.94                     | 0.50              |
| 1:A:174:LEU:HD12 | 1:A:681:PHE:CE1  | 2.47                     | 0.50              |
| 1:A:267:ILE:H    | 1:A:447:ASN:HD21 | 1.60                     | 0.50              |
| 1:A:313:TYR:HB2  | 1:A:316:LEU:HD12 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:630:ARG:HH22 | 1:A:657:ARG:HB2  | 1.76                     | 0.50              |
| 2:B:64:LEU:HD21  | 2:B:72:MET:HE1   | 1.92                     | 0.50              |
| 1:C:13:LEU:HD11  | 1:C:152:HIS:HD2  | 1.77                     | 0.50              |
| 1:C:96:ASN:HB2   | 1:C:99:SER:OG    | 2.12                     | 0.50              |
| 1:C:166:GLN:HE22 | 2:D:107:GLU:HG2  | 1.77                     | 0.50              |
| 1:C:437:ARG:NH2  | 1:C:625:TRP:CE3  | 2.80                     | 0.50              |
| 1:C:553:THR:CG2  | 1:C:579:THR:HG21 | 2.41                     | 0.50              |
| 1:E:145:LYS:HG3  | 1:E:146:ARG:H    | 1.76                     | 0.50              |
| 1:E:359:VAL:O    | 1:E:359:VAL:HG12 | 2.11                     | 0.50              |
| 1:E:407:ILE:HD12 | 1:E:409:VAL:H    | 1.76                     | 0.50              |
| 1:E:742:ILE:CD1  | 1:E:756:MET:HE3  | 2.41                     | 0.50              |
| 1:G:575:LEU:C    | 1:G:577:ASP:H    | 2.19                     | 0.50              |
| 1:G:584:LEU:N    | 1:G:584:LEU:HD23 | 2.26                     | 0.50              |
| 2:H:96:ASP:O     | 2:H:98:GLU:N     | 2.45                     | 0.50              |
| 1:A:405:PRO:O    | 1:A:407:ILE:HG23 | 2.12                     | 0.49              |
| 1:A:504:GLU:OE2  | 1:A:508:GLU:HG2  | 2.12                     | 0.49              |
| 2:B:35:MET:HE3   | 2:B:73:MET:HA    | 1.93                     | 0.49              |
| 2:B:36:ARG:O     | 2:B:39:GLY:N     | 2.44                     | 0.49              |
| 1:C:147:HIS:C    | 1:C:149:MET:H    | 2.20                     | 0.49              |
| 1:C:495:HIS:CD2  | 1:C:500:LEU:HG   | 2.46                     | 0.49              |
| 1:C:814:LYS:O    | 1:C:818:GLN:OE1  | 2.30                     | 0.49              |
| 2:D:68:GLN:O     | 2:D:71:PRO:HG2   | 2.12                     | 0.49              |
| 1:E:333:GLN:O    | 1:E:337:GLU:HG3  | 2.12                     | 0.49              |
| 1:E:522:GLN:OE1  | 1:E:525:ILE:HD12 | 2.12                     | 0.49              |
| 1:E:533:ASN:O    | 1:E:535:PRO:N    | 2.45                     | 0.49              |
| 1:G:164:MET:HE3  | 1:G:461:LEU:HD12 | 1.94                     | 0.49              |
| 1:G:446:VAL:HG12 | 1:G:447:ASN:N    | 2.26                     | 0.49              |
| 1:A:224:LEU:HD12 | 1:A:224:LEU:O    | 2.12                     | 0.49              |
| 1:A:320:HIS:ND1  | 1:A:320:HIS:O    | 2.39                     | 0.49              |
| 1:A:351:SER:C    | 1:A:353:LEU:H    | 2.19                     | 0.49              |
| 1:A:419:THR:O    | 1:A:421:GLU:N    | 2.44                     | 0.49              |
| 2:B:64:LEU:HD21  | 2:B:72:MET:CE    | 2.42                     | 0.49              |
| 1:C:141:TYR:CE1  | 1:C:149:MET:HB3  | 2.47                     | 0.49              |
| 1:C:326:GLN:HG3  | 1:C:331:MET:HE3  | 1.92                     | 0.49              |
| 1:C:544:GLU:OE1  | 1:C:550:ALA:HB1  | 2.12                     | 0.49              |
| 1:C:719:GLN:HA   | 1:C:719:GLN:HE21 | 1.75                     | 0.49              |
| 2:D:64:LEU:HD21  | 2:D:72:MET:CE    | 2.42                     | 0.49              |
| 2:F:76:ILE:O     | 2:F:78:LYS:N     | 2.46                     | 0.49              |
| 2:F:97:LYS:HG2   | 2:F:98:GLU:HG3   | 1.94                     | 0.49              |
| 1:G:76:GLN:OE1   | 1:G:98:ALA:HB2   | 2.11                     | 0.49              |
| 1:G:83:PHE:HE2   | 1:G:93:THR:HG1   | 1.57                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:166:GLN:HE22 | 2:H:107:GLU:HG2  | 1.76                     | 0.49              |
| 1:G:299:GLU:O    | 1:G:302:ARG:CB   | 2.60                     | 0.49              |
| 1:G:543:GLU:C    | 1:G:545:CYS:N    | 2.69                     | 0.49              |
| 1:G:607:ASP:OD1  | 1:G:607:ASP:N    | 2.31                     | 0.49              |
| 2:H:68:GLN:O     | 2:H:71:PRO:HG2   | 2.12                     | 0.49              |
| 1:A:351:SER:O    | 1:A:353:LEU:N    | 2.46                     | 0.49              |
| 2:B:8:THR:O      | 2:B:12:LYS:HG3   | 2.10                     | 0.49              |
| 2:B:85:PHE:O     | 2:B:86:GLU:C     | 2.54                     | 0.49              |
| 1:C:224:LEU:HD12 | 1:C:224:LEU:O    | 2.12                     | 0.49              |
| 1:C:344:PHE:HE1  | 1:C:445:ARG:HB3  | 1.72                     | 0.49              |
| 1:G:58:THR:HA    | 1:G:69:THR:OG1   | 2.12                     | 0.49              |
| 1:G:424:ASP:O    | 1:G:426:ALA:N    | 2.46                     | 0.49              |
| 1:A:199:SER:HB2  | 1:A:221:GLU:CD   | 2.37                     | 0.49              |
| 1:A:232:GLU:O    | 1:A:236:ASN:HB2  | 2.12                     | 0.49              |
| 1:C:293:LEU:O    | 1:C:297:ALA:HB2  | 2.12                     | 0.49              |
| 1:C:418:GLN:HA   | 1:C:422:GLN:NE2  | 2.26                     | 0.49              |
| 1:C:721:PHE:HB3  | 1:C:776:PHE:O    | 2.11                     | 0.49              |
| 2:D:94:VAL:O     | 2:D:94:VAL:HG12  | 2.12                     | 0.49              |
| 1:E:176:THR:O    | 1:E:183:LYS:HD2  | 2.13                     | 0.49              |
| 1:E:199:SER:CB   | 1:E:221:GLU:HG2  | 2.39                     | 0.49              |
| 1:E:239:THR:C    | 1:E:241:LYS:H    | 2.19                     | 0.49              |
| 1:G:128:LYS:HG2  | 1:G:129:GLN:N    | 2.27                     | 0.49              |
| 1:G:145:LYS:HG3  | 1:G:146:ARG:H    | 1.77                     | 0.49              |
| 1:G:407:ILE:CG1  | 1:G:414:VAL:O    | 2.60                     | 0.49              |
| 1:G:449:ALA:C    | 1:G:451:ASP:N    | 2.68                     | 0.49              |
| 1:G:477:PHE:O    | 1:G:480:LEU:N    | 2.43                     | 0.49              |
| 1:G:610:THR:HG23 | 1:G:628:VAL:CG2  | 2.42                     | 0.49              |
| 2:H:36:ARG:O     | 2:H:39:GLY:N     | 2.44                     | 0.49              |
| 2:H:64:LEU:HD21  | 2:H:72:MET:CE    | 2.42                     | 0.49              |
| 1:A:551:THR:O    | 1:A:552:ASP:C    | 2.55                     | 0.49              |
| 1:A:610:THR:CG2  | 1:A:628:VAL:CG1  | 2.90                     | 0.49              |
| 1:C:747:MET:CG   | 1:C:751:GLN:NE2  | 2.75                     | 0.49              |
| 1:C:747:MET:HG2  | 1:C:751:GLN:NE2  | 2.27                     | 0.49              |
| 2:D:92:LEU:HD13  | 2:D:108:ILE:HD11 | 1.93                     | 0.49              |
| 1:E:327:GLN:HG2  | 1:E:330:GLU:HG2  | 1.94                     | 0.49              |
| 1:E:359:VAL:O    | 1:E:359:VAL:CG1  | 2.59                     | 0.49              |
| 1:E:381:ASN:O    | 1:E:382:THR:C    | 2.55                     | 0.49              |
| 1:E:478:GLU:HB2  | 1:E:479:GLN:OE1  | 2.12                     | 0.49              |
| 2:F:35:MET:HE3   | 2:F:73:MET:HA    | 1.93                     | 0.49              |
| 1:G:310:PHE:O    | 1:G:311:ASN:HB2  | 2.13                     | 0.49              |
| 1:G:551:THR:H    | 1:G:554:SER:CB   | 2.25                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:80:PRO:HD2   | 1:A:83:PHE:CD2   | 2.48                     | 0.49              |
| 1:A:313:TYR:N    | 1:A:313:TYR:CD1  | 2.81                     | 0.49              |
| 2:B:104:MET:O    | 2:B:106:ALA:N    | 2.46                     | 0.49              |
| 1:C:261:TYR:CD1  | 1:C:261:TYR:N    | 2.80                     | 0.49              |
| 1:C:307:LEU:HA   | 1:C:313:TYR:OH   | 2.11                     | 0.49              |
| 1:C:418:GLN:CB   | 1:C:422:GLN:HB2  | 2.36                     | 0.49              |
| 1:E:449:ALA:C    | 1:E:451:ASP:H    | 2.18                     | 0.49              |
| 1:E:495:HIS:CD2  | 1:E:500:LEU:HG   | 2.47                     | 0.49              |
| 1:E:572:SER:HB2  | 1:E:580:GLU:HG3  | 1.94                     | 0.49              |
| 2:F:92:LEU:C     | 2:F:94:VAL:H     | 2.20                     | 0.49              |
| 1:G:100:VAL:HG21 | 1:G:711:LEU:CD1  | 2.42                     | 0.49              |
| 1:G:237:ALA:HA   | 1:G:288:HIS:CD2  | 2.48                     | 0.49              |
| 1:G:556:VAL:O    | 1:G:559:LEU:HB3  | 2.12                     | 0.49              |
| 1:G:742:ILE:HD11 | 1:G:756:MET:HG2  | 1.94                     | 0.49              |
| 2:H:131:HIS:NE2  | 2:H:146:MET:HE3  | 2.28                     | 0.49              |
| 1:A:250:LYS:HE2  | 1:A:465:ASP:OD2  | 2.11                     | 0.49              |
| 1:A:430:LEU:HB2  | 1:A:605:LEU:HD11 | 1.95                     | 0.49              |
| 1:A:545:CYS:HA   | 1:A:598:LEU:HD22 | 1.94                     | 0.49              |
| 1:A:563:GLN:O    | 1:A:565:ASN:N    | 2.46                     | 0.49              |
| 1:A:767:TYR:O    | 1:A:768:ARG:HD3  | 2.12                     | 0.49              |
| 2:B:143:LEU:O    | 2:B:147:VAL:HG22 | 2.13                     | 0.49              |
| 1:C:351:SER:O    | 1:C:353:LEU:N    | 2.45                     | 0.49              |
| 1:C:435:PHE:O    | 1:C:438:LEU:N    | 2.37                     | 0.49              |
| 1:C:575:LEU:C    | 1:C:577:ASP:N    | 2.70                     | 0.49              |
| 1:C:630:ARG:HH22 | 1:C:657:ARG:HB2  | 1.78                     | 0.49              |
| 1:E:556:VAL:HG21 | 1:E:579:THR:HB   | 1.93                     | 0.49              |
| 1:G:103:ASN:HD21 | 1:G:107:ARG:HD2  | 1.77                     | 0.49              |
| 1:G:280:GLN:N    | 1:G:280:GLN:NE2  | 2.61                     | 0.49              |
| 1:G:329:ASP:OD1  | 1:G:329:ASP:N    | 2.42                     | 0.49              |
| 1:G:351:SER:C    | 1:G:353:LEU:N    | 2.66                     | 0.49              |
| 1:G:354:ARG:HG3  | 1:G:355:VAL:N    | 2.28                     | 0.49              |
| 1:G:418:GLN:HA   | 1:G:422:GLN:NE2  | 2.27                     | 0.49              |
| 2:H:55:LYS:H     | 2:H:58:GLU:CG    | 2.26                     | 0.49              |
| 2:H:85:PHE:O     | 2:H:88:TYR:HB2   | 2.13                     | 0.49              |
| 1:A:128:LYS:HG2  | 1:A:129:GLN:N    | 2.27                     | 0.49              |
| 1:A:575:LEU:C    | 1:A:577:ASP:N    | 2.71                     | 0.49              |
| 1:C:13:LEU:HD11  | 1:C:152:HIS:CD2  | 2.48                     | 0.49              |
| 1:C:313:TYR:N    | 1:C:313:TYR:CD1  | 2.81                     | 0.49              |
| 1:C:401:SER:O    | 1:C:606:ASN:ND2  | 2.45                     | 0.49              |
| 1:C:543:GLU:C    | 1:C:545:CYS:N    | 2.70                     | 0.49              |
| 1:C:563:GLN:O    | 1:C:565:ASN:N    | 2.46                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:54:PRO:HB2   | 2:D:59:MET:HG2   | 1.95                     | 0.49              |
| 1:E:88:ASP:O     | 1:E:91:GLU:N     | 2.45                     | 0.49              |
| 1:E:174:LEU:HD12 | 1:E:681:PHE:CE1  | 2.48                     | 0.49              |
| 1:E:347:GLU:O    | 1:E:349:GLN:N    | 2.44                     | 0.49              |
| 1:E:405:PRO:HG2  | 1:E:416:LYS:HG3  | 1.95                     | 0.49              |
| 1:E:489:LEU:C    | 1:E:489:LEU:HD12 | 2.38                     | 0.49              |
| 1:E:551:THR:H    | 1:E:554:SER:CB   | 2.26                     | 0.49              |
| 2:F:68:GLN:O     | 2:F:71:PRO:HG2   | 2.12                     | 0.49              |
| 1:G:311:ASN:HD22 | 1:G:311:ASN:N    | 2.11                     | 0.49              |
| 1:G:618:ASP:CG   | 1:G:621:VAL:HG23 | 2.38                     | 0.49              |
| 2:H:54:PRO:HB2   | 2:H:59:MET:HG2   | 1.95                     | 0.49              |
| 1:A:401:SER:O    | 1:A:606:ASN:ND2  | 2.46                     | 0.49              |
| 1:A:703:GLU:O    | 1:A:706:ARG:N    | 2.38                     | 0.49              |
| 2:B:83:GLY:HA3   | 2:B:88:TYR:CE2   | 2.47                     | 0.49              |
| 1:C:36:TRP:NE1   | 1:C:78:MET:HA    | 2.27                     | 0.49              |
| 1:C:361:GLN:HB3  | 1:C:387:VAL:HG22 | 1.94                     | 0.49              |
| 1:C:725:ILE:HD13 | 1:C:730:PHE:HB2  | 1.95                     | 0.49              |
| 1:E:345:THR:HG22 | 1:E:346:GLU:HG2  | 1.94                     | 0.49              |
| 1:G:184:THR:O    | 1:G:185:GLU:C    | 2.55                     | 0.49              |
| 1:G:520:ASP:OD1  | 1:G:523:PRO:HD2  | 2.12                     | 0.49              |
| 2:H:135:ASN:HB2  | 2:H:137:CYS:SG   | 2.52                     | 0.49              |
| 1:A:553:THR:HG22 | 1:A:557:GLU:OE2  | 2.13                     | 0.49              |
| 1:A:556:VAL:O    | 1:A:560:ILE:HG12 | 2.13                     | 0.49              |
| 2:B:95:PHE:O     | 2:B:103:VAL:HG13 | 2.13                     | 0.49              |
| 2:B:124:VAL:O    | 2:B:128:VAL:HG22 | 2.13                     | 0.49              |
| 1:C:299:GLU:O    | 1:C:302:ARG:CB   | 2.61                     | 0.49              |
| 2:D:76:ILE:O     | 2:D:78:LYS:N     | 2.45                     | 0.49              |
| 2:D:105:GLY:O    | 2:D:109:ARG:NH1  | 2.46                     | 0.49              |
| 1:E:48:SER:O     | 1:E:59:VAL:HG13  | 2.12                     | 0.49              |
| 1:E:618:ASP:HB3  | 1:E:621:VAL:HG23 | 1.95                     | 0.49              |
| 2:F:139:ASN:HD21 | 2:F:141:GLU:HG3  | 1.77                     | 0.49              |
| 1:G:424:ASP:C    | 1:G:426:ALA:H    | 2.20                     | 0.49              |
| 1:G:425:PHE:O    | 1:G:425:PHE:CD1  | 2.66                     | 0.49              |
| 1:G:475:ASN:HB2  | 1:G:592:TYR:HA   | 1.95                     | 0.49              |
| 1:G:478:GLU:HB2  | 1:G:479:GLN:OE1  | 2.12                     | 0.49              |
| 1:G:562:GLU:HA   | 1:G:562:GLU:OE1  | 2.12                     | 0.49              |
| 1:A:345:THR:HG22 | 1:A:346:GLU:HG2  | 1.94                     | 0.48              |
| 1:A:511:GLU:HG3  | 2:H:85:PHE:CD2   | 2.48                     | 0.48              |
| 1:A:575:LEU:C    | 1:A:577:ASP:H    | 2.19                     | 0.48              |
| 1:A:623:ASP:OD1  | 1:A:623:ASP:N    | 2.45                     | 0.48              |
| 2:B:105:GLY:O    | 2:B:109:ARG:HB2  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:36:TRP:HB2   | 1:C:76:GLN:HB2   | 1.94                     | 0.48              |
| 1:C:199:SER:HB2  | 1:C:221:GLU:OE2  | 2.13                     | 0.48              |
| 1:C:430:LEU:HB2  | 1:C:605:LEU:HD11 | 1.95                     | 0.48              |
| 1:C:613:LEU:C    | 1:C:615:GLN:N    | 2.71                     | 0.48              |
| 1:E:145:LYS:HB2  | 1:E:145:LYS:HE3  | 1.58                     | 0.48              |
| 1:E:147:HIS:C    | 1:E:149:MET:H    | 2.18                     | 0.48              |
| 1:E:237:ALA:HA   | 1:E:288:HIS:CD2  | 2.47                     | 0.48              |
| 1:E:256:PHE:HE1  | 1:E:262:ILE:HG13 | 1.78                     | 0.48              |
| 1:E:261:TYR:CD1  | 1:E:261:TYR:N    | 2.79                     | 0.48              |
| 1:E:397:ASP:O    | 1:E:398:PHE:C    | 2.56                     | 0.48              |
| 1:G:120:PHE:CD1  | 1:G:120:PHE:N    | 2.75                     | 0.48              |
| 1:G:337:GLU:O    | 1:G:340:THR:OG1  | 2.28                     | 0.48              |
| 1:G:504:GLU:OE2  | 1:G:508:GLU:HG2  | 2.12                     | 0.48              |
| 2:H:41:ASN:N     | 2:H:42:PRO:HD3   | 2.28                     | 0.48              |
| 1:A:145:LYS:HG3  | 1:A:146:ARG:H    | 1.76                     | 0.48              |
| 1:A:152:HIS:CE1  | 1:A:154:TYR:CG   | 3.02                     | 0.48              |
| 1:A:247:ARG:HH22 | 1:A:470:GLU:CD   | 2.22                     | 0.48              |
| 1:A:286:THR:HB   | 1:A:290:PHE:HD2  | 1.77                     | 0.48              |
| 2:B:76:ILE:O     | 2:B:78:LYS:N     | 2.46                     | 0.48              |
| 1:E:419:THR:O    | 1:E:421:GLU:N    | 2.46                     | 0.48              |
| 1:E:543:GLU:C    | 1:E:545:CYS:N    | 2.71                     | 0.48              |
| 1:E:659:VAL:HG12 | 1:E:660:GLY:H    | 1.71                     | 0.48              |
| 1:G:171:GLN:HA   | 1:G:678:ASN:H    | 1.78                     | 0.48              |
| 1:G:211:GLN:HG3  | 1:G:214:SER:HB2  | 1.95                     | 0.48              |
| 1:G:551:THR:H    | 1:G:554:SER:HG   | 1.56                     | 0.48              |
| 1:G:682:VAL:O    | 1:G:682:VAL:HG12 | 2.11                     | 0.48              |
| 1:G:814:LYS:O    | 1:G:818:GLN:OE1  | 2.31                     | 0.48              |
| 2:H:124:VAL:O    | 2:H:128:VAL:HG22 | 2.13                     | 0.48              |
| 1:A:36:TRP:HE1   | 1:A:78:MET:HA    | 1.77                     | 0.48              |
| 1:A:288:HIS:HB3  | 1:A:292:TYR:CE1  | 2.48                     | 0.48              |
| 1:A:296:GLY:HA3  | 1:A:332:PHE:CG   | 2.48                     | 0.48              |
| 1:A:520:ASP:OD1  | 1:A:523:PRO:HD2  | 2.14                     | 0.48              |
| 1:A:742:ILE:CD1  | 1:A:756:MET:HE3  | 2.44                     | 0.48              |
| 2:B:98:GLU:O     | 2:B:100:ASN:N    | 2.45                     | 0.48              |
| 2:B:108:ILE:HG22 | 2:B:109:ARG:N    | 2.27                     | 0.48              |
| 1:C:138:ILE:HG21 | 1:C:196:VAL:HG11 | 1.95                     | 0.48              |
| 1:C:237:ALA:HA   | 1:C:288:HIS:CD2  | 2.49                     | 0.48              |
| 1:C:280:GLN:NE2  | 1:C:315:PHE:O    | 2.45                     | 0.48              |
| 1:C:437:ARG:NE   | 1:C:625:TRP:HA   | 2.24                     | 0.48              |
| 1:C:527:LEU:HD12 | 1:C:566:HIS:CD2  | 2.48                     | 0.48              |
| 1:C:533:ASN:O    | 1:C:535:PRO:N    | 2.46                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:584:LEU:N    | 1:C:584:LEU:HD23 | 2.27                     | 0.48              |
| 2:D:97:LYS:HG2   | 2:D:98:GLU:HG3   | 1.95                     | 0.48              |
| 1:E:307:LEU:HA   | 1:E:313:TYR:OH   | 2.13                     | 0.48              |
| 1:E:320:HIS:ND1  | 1:E:320:HIS:O    | 2.40                     | 0.48              |
| 1:E:361:GLN:O    | 1:E:363:GLY:N    | 2.46                     | 0.48              |
| 1:E:756:MET:O    | 1:E:760:LEU:HG   | 2.14                     | 0.48              |
| 1:E:806:TYR:CG   | 2:F:147:VAL:HG12 | 2.47                     | 0.48              |
| 1:G:89:MET:O     | 1:G:91:GLU:N     | 2.47                     | 0.48              |
| 1:G:327:GLN:HG2  | 1:G:330:GLU:HG2  | 1.95                     | 0.48              |
| 1:A:31:ALA:O     | 1:A:33:LYS:N     | 2.46                     | 0.48              |
| 1:A:39:SER:C     | 1:A:41:LYS:H     | 2.22                     | 0.48              |
| 1:A:490:GLN:HE21 | 1:A:494:ASN:HD21 | 1.59                     | 0.48              |
| 1:C:58:THR:HA    | 1:C:69:THR:OG1   | 2.13                     | 0.48              |
| 1:C:64:ASN:C     | 1:C:66:LYS:N     | 2.71                     | 0.48              |
| 2:D:41:ASN:N     | 2:D:42:PRO:HD3   | 2.28                     | 0.48              |
| 1:E:311:ASN:N    | 1:E:311:ASN:HD22 | 2.11                     | 0.48              |
| 1:E:352:ILE:HG21 | 1:E:442:ILE:CD1  | 2.41                     | 0.48              |
| 1:E:356:VAL:O    | 1:E:360:LEU:HD12 | 2.13                     | 0.48              |
| 1:E:389:HIS:HD1  | 1:E:389:HIS:C    | 2.21                     | 0.48              |
| 1:E:578:LYS:C    | 1:E:579:THR:OG1  | 2.56                     | 0.48              |
| 1:E:742:ILE:HD13 | 1:E:756:MET:HE3  | 1.95                     | 0.48              |
| 1:E:803:CYS:HB2  | 2:F:119:MET:HE1  | 1.94                     | 0.48              |
| 1:G:607:ASP:HA   | 1:G:610:THR:CB   | 2.35                     | 0.48              |
| 1:G:756:MET:O    | 1:G:760:LEU:HG   | 2.14                     | 0.48              |
| 1:G:803:CYS:HB2  | 2:H:119:MET:HE1  | 1.94                     | 0.48              |
| 1:A:299:GLU:O    | 1:A:302:ARG:CB   | 2.60                     | 0.48              |
| 1:A:382:THR:OG1  | 1:A:383:ALA:N    | 2.46                     | 0.48              |
| 1:A:405:PRO:HG2  | 1:A:416:LYS:HG3  | 1.95                     | 0.48              |
| 1:A:556:VAL:HG21 | 1:A:579:THR:HB   | 1.95                     | 0.48              |
| 1:A:746:PHE:CD2  | 2:H:13:GLU:OE1   | 2.67                     | 0.48              |
| 1:A:797:ILE:HG12 | 2:B:117:GLU:HG2  | 1.94                     | 0.48              |
| 1:C:33:LYS:O     | 1:C:48:SER:HA    | 2.12                     | 0.48              |
| 1:C:362:LEU:HD12 | 1:C:387:VAL:HG13 | 1.96                     | 0.48              |
| 1:C:424:ASP:C    | 1:C:426:ALA:H    | 2.21                     | 0.48              |
| 1:C:491:GLN:OE1  | 1:C:521:LEU:HG   | 2.14                     | 0.48              |
| 1:C:553:THR:HG23 | 1:C:579:THR:HG21 | 1.94                     | 0.48              |
| 2:D:10:GLU:HA    | 2:D:13:GLU:CG    | 2.42                     | 0.48              |
| 1:E:257:ASP:C    | 1:E:257:ASP:OD1  | 2.54                     | 0.48              |
| 1:E:278:ILE:O    | 1:E:279:ARG:HG3  | 2.13                     | 0.48              |
| 1:E:313:TYR:N    | 1:E:313:TYR:CD1  | 2.81                     | 0.48              |
| 1:E:349:GLN:HA   | 1:E:352:ILE:HG13 | 1.94                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:575:LEU:HA   | 1:E:577:ASP:OD2  | 2.13                     | 0.48              |
| 1:E:719:GLN:HE21 | 1:E:719:GLN:CA   | 2.26                     | 0.48              |
| 2:F:76:ILE:O     | 2:F:77:ALA:C     | 2.57                     | 0.48              |
| 1:G:114:TYR:HE2  | 1:G:153:ILE:HB   | 1.74                     | 0.48              |
| 1:G:167:ASP:O    | 1:G:168:ARG:C    | 2.56                     | 0.48              |
| 1:G:565:ASN:CG   | 1:G:565:ASN:O    | 2.56                     | 0.48              |
| 1:G:776:PHE:CD2  | 1:G:781:LEU:HD22 | 2.48                     | 0.48              |
| 1:A:30:SER:C     | 1:A:32:LYS:N     | 2.64                     | 0.48              |
| 1:A:58:THR:HA    | 1:A:69:THR:OG1   | 2.13                     | 0.48              |
| 1:A:199:SER:CB   | 1:A:221:GLU:HG2  | 2.42                     | 0.48              |
| 1:A:370:GLU:O    | 1:A:374:ASP:CA   | 2.61                     | 0.48              |
| 1:A:625:TRP:C    | 1:A:627:ASP:N    | 2.68                     | 0.48              |
| 1:C:145:LYS:HG3  | 1:C:146:ARG:H    | 1.76                     | 0.48              |
| 1:C:333:GLN:O    | 1:C:337:GLU:HG3  | 2.13                     | 0.48              |
| 2:D:76:ILE:O     | 2:D:77:ALA:C     | 2.56                     | 0.48              |
| 2:D:92:LEU:C     | 2:D:94:VAL:H     | 2.22                     | 0.48              |
| 1:E:7:SER:N      | 1:E:10:GLU:OE1   | 2.43                     | 0.48              |
| 1:E:86:VAL:HG12  | 1:E:103:ASN:ND2  | 2.28                     | 0.48              |
| 1:E:102:HIS:O    | 1:E:105:ARG:N    | 2.47                     | 0.48              |
| 1:E:199:SER:HB2  | 1:E:221:GLU:OE2  | 2.13                     | 0.48              |
| 1:E:299:GLU:O    | 1:E:302:ARG:CB   | 2.61                     | 0.48              |
| 1:E:584:LEU:HD23 | 1:E:584:LEU:N    | 2.29                     | 0.48              |
| 1:E:607:ASP:O    | 1:E:610:THR:HB   | 2.13                     | 0.48              |
| 1:G:389:HIS:HD1  | 1:G:389:HIS:C    | 2.21                     | 0.48              |
| 1:G:613:LEU:C    | 1:G:615:GLN:N    | 2.72                     | 0.48              |
| 1:G:623:ASP:OD1  | 1:G:623:ASP:N    | 2.46                     | 0.48              |
| 1:G:719:GLN:HA   | 1:G:719:GLN:HE21 | 1.78                     | 0.48              |
| 2:H:128:VAL:HG23 | 2:H:129:ALA:N    | 2.28                     | 0.48              |
| 1:A:161:TYR:O    | 1:A:161:TYR:CG   | 2.67                     | 0.48              |
| 1:A:618:ASP:CG   | 1:A:621:VAL:HG23 | 2.38                     | 0.48              |
| 1:A:621:VAL:HG12 | 1:A:625:TRP:CD1  | 2.49                     | 0.48              |
| 1:C:128:LYS:HG2  | 1:C:129:GLN:N    | 2.28                     | 0.48              |
| 1:C:272:LEU:O    | 1:C:274:LYS:N    | 2.45                     | 0.48              |
| 1:C:395:VAL:O    | 1:C:396:THR:C    | 2.56                     | 0.48              |
| 1:C:630:ARG:HH12 | 1:C:657:ARG:HB3  | 1.78                     | 0.48              |
| 1:C:663:TYR:CZ   | 1:C:667:LEU:HD13 | 2.48                     | 0.48              |
| 1:C:711:LEU:N    | 1:C:711:LEU:HD22 | 2.28                     | 0.48              |
| 1:C:763:ASP:HB3  | 1:C:766:LEU:CD1  | 2.44                     | 0.48              |
| 1:E:36:TRP:NE1   | 1:E:78:MET:HA    | 2.29                     | 0.48              |
| 1:G:182:GLY:HA2  | 5:G:998:ADP:O1A  | 2.13                     | 0.48              |
| 1:G:344:PHE:HE1  | 1:G:445:ARG:HB3  | 1.77                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:428:GLU:C    | 1:G:430:LEU:N    | 2.72                     | 0.48              |
| 1:G:544:GLU:OE1  | 1:G:550:ALA:HB1  | 2.14                     | 0.48              |
| 1:G:566:HIS:CE1  | 1:G:568:LYS:HB2  | 2.48                     | 0.48              |
| 1:A:280:GLN:NE2  | 1:A:315:PHE:O    | 2.43                     | 0.48              |
| 1:A:479:GLN:OE1  | 1:A:479:GLN:N    | 2.47                     | 0.48              |
| 2:B:41:ASN:N     | 2:B:42:PRO:HD3   | 2.28                     | 0.48              |
| 1:C:495:HIS:ND1  | 1:C:499:ILE:HD12 | 2.28                     | 0.48              |
| 1:C:520:ASP:OD1  | 1:C:523:PRO:HD2  | 2.14                     | 0.48              |
| 1:E:13:LEU:CD1   | 1:E:152:HIS:HD2  | 2.23                     | 0.48              |
| 1:E:180:GLY:O    | 1:E:182:GLY:N    | 2.47                     | 0.48              |
| 1:E:407:ILE:CD1  | 1:E:409:VAL:H    | 2.27                     | 0.48              |
| 1:E:735:GLU:HA   | 1:E:756:MET:HE1  | 1.96                     | 0.48              |
| 1:G:141:TYR:CE1  | 1:G:149:MET:HB3  | 2.49                     | 0.48              |
| 1:G:610:THR:CG2  | 1:G:628:VAL:HG11 | 2.44                     | 0.48              |
| 1:A:321:VAL:HG13 | 1:A:322:PRO:HD2  | 1.96                     | 0.48              |
| 1:A:362:LEU:CD2  | 1:A:427:ILE:HG13 | 2.43                     | 0.48              |
| 1:A:494:ASN:N    | 1:A:494:ASN:ND2  | 2.61                     | 0.48              |
| 1:A:545:CYS:O    | 1:A:602:MET:HE1  | 2.13                     | 0.48              |
| 1:A:725:ILE:HD13 | 1:A:730:PHE:HB2  | 1.94                     | 0.48              |
| 2:B:55:LYS:H     | 2:B:58:GLU:CG    | 2.26                     | 0.48              |
| 1:C:551:THR:H    | 1:C:554:SER:CB   | 2.26                     | 0.48              |
| 1:C:610:THR:HG21 | 1:C:628:VAL:CG1  | 2.43                     | 0.48              |
| 1:C:806:TYR:CB   | 2:D:147:VAL:HG12 | 2.44                     | 0.48              |
| 1:E:77:LYS:H     | 1:E:77:LYS:HD2   | 1.79                     | 0.48              |
| 1:E:88:ASP:O     | 1:E:91:GLU:HB2   | 2.14                     | 0.48              |
| 1:E:293:LEU:O    | 1:E:297:ALA:HB2  | 2.13                     | 0.48              |
| 1:E:432:LYS:HE2  | 1:E:432:LYS:HB2  | 1.74                     | 0.48              |
| 1:E:762:LEU:HD13 | 1:E:766:LEU:CD1  | 2.43                     | 0.48              |
| 1:G:89:MET:HA    | 1:G:92:LEU:HD12  | 1.94                     | 0.48              |
| 1:G:152:HIS:CE1  | 1:G:154:TYR:CG   | 3.02                     | 0.48              |
| 1:G:223:GLN:C    | 1:G:225:LEU:N    | 2.71                     | 0.48              |
| 1:C:133:TYR:HB3  | 1:C:154:TYR:OH   | 2.14                     | 0.48              |
| 1:C:391:MET:HB3  | 1:C:393:ILE:HG12 | 1.95                     | 0.48              |
| 1:C:797:ILE:CG1  | 2:D:117:GLU:HG2  | 2.44                     | 0.48              |
| 1:E:64:ASN:C     | 1:E:66:LYS:N     | 2.71                     | 0.48              |
| 1:E:211:GLN:HG3  | 1:E:214:SER:HB2  | 1.95                     | 0.48              |
| 1:E:565:ASN:O    | 1:E:565:ASN:CG   | 2.56                     | 0.48              |
| 1:E:721:PHE:CE2  | 1:E:768:ARG:HG2  | 2.49                     | 0.48              |
| 2:F:64:LEU:HD21  | 2:F:72:MET:CE    | 2.42                     | 0.48              |
| 2:F:69:PHE:CZ    | 2:F:73:MET:HG2   | 2.49                     | 0.48              |
| 1:G:36:TRP:NE1   | 1:G:78:MET:HA    | 2.29                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:318:ASN:O    | 1:G:319:GLY:C    | 2.57                     | 0.48              |
| 1:G:333:GLN:O    | 1:G:337:GLU:HG3  | 2.14                     | 0.48              |
| 1:G:347:GLU:O    | 1:G:349:GLN:N    | 2.47                     | 0.48              |
| 2:H:140:TYR:HD1  | 2:H:141:GLU:N    | 2.11                     | 0.48              |
| 1:A:89:MET:C     | 1:A:91:GLU:N     | 2.70                     | 0.47              |
| 1:A:107:ARG:HH11 | 1:A:115:THR:HG23 | 1.79                     | 0.47              |
| 1:A:389:HIS:C    | 1:A:389:HIS:HD1  | 2.22                     | 0.47              |
| 1:A:428:GLU:C    | 1:A:430:LEU:N    | 2.72                     | 0.47              |
| 1:A:630:ARG:HH12 | 1:A:657:ARG:HB3  | 1.77                     | 0.47              |
| 2:B:54:PRO:HB2   | 2:B:59:MET:HG2   | 1.95                     | 0.47              |
| 2:B:69:PHE:CZ    | 2:B:73:MET:HG2   | 2.49                     | 0.47              |
| 1:C:321:VAL:HG13 | 1:C:322:PRO:HD2  | 1.96                     | 0.47              |
| 1:C:513:ASN:O    | 1:C:515:ILE:HD12 | 2.14                     | 0.47              |
| 1:E:149:MET:HB3  | 1:E:150:PRO:HD2  | 1.96                     | 0.47              |
| 1:E:189:LYS:O    | 1:E:192:GLN:HB3  | 2.14                     | 0.47              |
| 1:G:126:PRO:O    | 1:G:127:TYR:HB2  | 2.13                     | 0.47              |
| 1:G:134:SER:O    | 1:G:135:GLU:C    | 2.56                     | 0.47              |
| 1:G:767:TYR:O    | 1:G:768:ARG:HD3  | 2.14                     | 0.47              |
| 1:A:89:MET:HA    | 1:A:92:LEU:HD12  | 1.96                     | 0.47              |
| 1:C:389:HIS:C    | 1:C:389:HIS:HD1  | 2.21                     | 0.47              |
| 1:C:551:THR:O    | 1:C:554:SER:N    | 2.47                     | 0.47              |
| 1:C:618:ASP:HB3  | 1:C:621:VAL:HG23 | 1.96                     | 0.47              |
| 1:C:742:ILE:CD1  | 1:C:756:MET:HE3  | 2.44                     | 0.47              |
| 1:E:39:SER:C     | 1:E:41:LYS:H     | 2.22                     | 0.47              |
| 1:E:402:ILE:HG22 | 1:E:403:LEU:HG   | 1.96                     | 0.47              |
| 1:E:508:GLU:HG3  | 1:E:775:PHE:CE1  | 2.49                     | 0.47              |
| 1:E:776:PHE:CD2  | 1:E:781:LEU:HD22 | 2.50                     | 0.47              |
| 2:F:41:ASN:N     | 2:F:42:PRO:HD3   | 2.28                     | 0.47              |
| 1:G:60:GLU:OE1   | 1:G:67:LYS:HD2   | 2.14                     | 0.47              |
| 1:G:122:VAL:C    | 1:G:123:VAL:HG23 | 2.39                     | 0.47              |
| 1:G:397:ASP:O    | 1:G:398:PHE:C    | 2.57                     | 0.47              |
| 1:G:489:LEU:C    | 1:G:489:LEU:HD12 | 2.40                     | 0.47              |
| 2:H:10:GLU:HA    | 2:H:13:GLU:CG    | 2.43                     | 0.47              |
| 2:H:139:ASN:OD1  | 2:H:142:GLU:HG2  | 2.14                     | 0.47              |
| 2:H:143:LEU:O    | 2:H:147:VAL:HG22 | 2.15                     | 0.47              |
| 1:A:64:ASN:C     | 1:A:66:LYS:N     | 2.72                     | 0.47              |
| 1:A:330:GLU:O    | 1:A:331:MET:C    | 2.57                     | 0.47              |
| 1:A:746:PHE:CZ   | 2:H:13:GLU:OE1   | 2.68                     | 0.47              |
| 1:A:814:LYS:C    | 1:A:816:GLN:N    | 2.72                     | 0.47              |
| 2:B:76:ILE:O     | 2:B:77:ALA:C     | 2.57                     | 0.47              |
| 2:B:131:HIS:NE2  | 2:B:146:MET:HE3  | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:44:PHE:CD2   | 1:C:98:ALA:HA    | 2.50                     | 0.47              |
| 1:C:134:SER:O    | 1:C:135:GLU:C    | 2.57                     | 0.47              |
| 2:D:85:PHE:HA    | 2:D:89:VAL:HG13  | 1.95                     | 0.47              |
| 1:E:134:SER:O    | 1:E:135:GLU:C    | 2.55                     | 0.47              |
| 1:E:180:GLY:C    | 1:E:182:GLY:H    | 2.21                     | 0.47              |
| 1:E:272:LEU:C    | 1:E:272:LEU:CD1  | 2.80                     | 0.47              |
| 1:E:342:MET:HE3  | 1:E:342:MET:C    | 2.39                     | 0.47              |
| 1:E:354:ARG:HG3  | 1:E:355:VAL:N    | 2.29                     | 0.47              |
| 1:E:391:MET:HB3  | 1:E:393:ILE:HG12 | 1.96                     | 0.47              |
| 1:E:578:LYS:C    | 1:E:579:THR:HG1  | 2.22                     | 0.47              |
| 1:E:815:ARG:NE   | 1:E:818:GLN:NE2  | 2.62                     | 0.47              |
| 1:G:370:GLU:O    | 1:G:374:ASP:CA   | 2.62                     | 0.47              |
| 1:G:409:VAL:HG13 | 1:G:634:LEU:HD11 | 1.97                     | 0.47              |
| 1:G:513:ASN:O    | 1:G:515:ILE:HD12 | 2.14                     | 0.47              |
| 1:G:618:ASP:HB3  | 1:G:621:VAL:HG23 | 1.97                     | 0.47              |
| 1:G:711:LEU:HD22 | 1:G:711:LEU:H    | 1.79                     | 0.47              |
| 1:G:716:ILE:HA   | 1:G:719:GLN:HB2  | 1.96                     | 0.47              |
| 1:A:362:LEU:HD12 | 1:A:387:VAL:HG13 | 1.96                     | 0.47              |
| 1:A:513:ASN:O    | 1:A:515:ILE:HD12 | 2.14                     | 0.47              |
| 1:C:22:ASN:HA    | 1:C:23:PRO:HD3   | 1.77                     | 0.47              |
| 1:C:89:MET:HA    | 1:C:92:LEU:HD12  | 1.97                     | 0.47              |
| 1:C:100:VAL:HG21 | 1:C:711:LEU:CD1  | 2.44                     | 0.47              |
| 1:C:183:LYS:HE2  | 5:C:998:ADP:O1B  | 2.14                     | 0.47              |
| 1:C:424:ASP:O    | 1:C:426:ALA:N    | 2.47                     | 0.47              |
| 1:C:747:MET:HE3  | 1:C:752:ALA:CA   | 2.38                     | 0.47              |
| 1:E:424:ASP:C    | 1:E:426:ALA:H    | 2.22                     | 0.47              |
| 2:F:69:PHE:HA    | 2:F:72:MET:HE3   | 1.96                     | 0.47              |
| 2:F:131:HIS:NE2  | 2:F:146:MET:HE3  | 2.29                     | 0.47              |
| 1:G:149:MET:HB3  | 1:G:150:PRO:HD2  | 1.95                     | 0.47              |
| 1:G:235:GLY:HA3  | 1:G:248:PHE:CE1  | 2.50                     | 0.47              |
| 1:G:513:ASN:O    | 1:G:513:ASN:ND2  | 2.44                     | 0.47              |
| 1:G:556:VAL:O    | 1:G:560:ILE:HG12 | 2.15                     | 0.47              |
| 2:H:76:ILE:O     | 2:H:77:ALA:C     | 2.57                     | 0.47              |
| 2:H:92:LEU:C     | 2:H:94:VAL:H     | 2.23                     | 0.47              |
| 1:A:13:LEU:HG    | 1:A:132:ILE:HG21 | 1.96                     | 0.47              |
| 1:A:261:TYR:CD1  | 1:A:261:TYR:N    | 2.82                     | 0.47              |
| 1:A:333:GLN:O    | 1:A:337:GLU:HG3  | 2.15                     | 0.47              |
| 1:A:424:ASP:O    | 1:A:426:ALA:N    | 2.48                     | 0.47              |
| 1:A:728:GLN:NE2  | 1:A:728:GLN:O    | 2.47                     | 0.47              |
| 2:B:105:GLY:O    | 2:B:109:ARG:NH1  | 2.47                     | 0.47              |
| 1:C:12:PHE:CD2   | 1:C:131:PRO:CD   | 2.98                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:149:MET:HB3  | 1:C:150:PRO:HD2  | 1.96                     | 0.47              |
| 1:C:449:ALA:C    | 1:C:451:ASP:N    | 2.70                     | 0.47              |
| 1:C:545:CYS:O    | 1:C:602:MET:HE1  | 2.14                     | 0.47              |
| 1:C:711:LEU:H    | 1:C:711:LEU:CD2  | 2.27                     | 0.47              |
| 2:D:140:TYR:O    | 2:D:142:GLU:N    | 2.47                     | 0.47              |
| 1:E:370:GLU:O    | 1:E:374:ASP:CA   | 2.62                     | 0.47              |
| 2:F:36:ARG:O     | 2:F:39:GLY:N     | 2.44                     | 0.47              |
| 1:G:33:LYS:HB2   | 1:G:48:SER:OG    | 2.14                     | 0.47              |
| 1:G:321:VAL:HG13 | 1:G:322:PRO:HD2  | 1.95                     | 0.47              |
| 1:G:407:ILE:CD1  | 1:G:409:VAL:N    | 2.78                     | 0.47              |
| 1:G:747:MET:CG   | 1:G:751:GLN:NE2  | 2.78                     | 0.47              |
| 1:G:768:ARG:HD3  | 1:G:768:ARG:HA   | 1.61                     | 0.47              |
| 2:H:69:PHE:CZ    | 2:H:73:MET:HG2   | 2.49                     | 0.47              |
| 1:A:77:LYS:H     | 1:A:77:LYS:HD2   | 1.79                     | 0.47              |
| 1:A:407:ILE:CD1  | 1:A:409:VAL:N    | 2.76                     | 0.47              |
| 1:A:424:ASP:C    | 1:A:426:ALA:H    | 2.22                     | 0.47              |
| 1:A:569:PHE:CD2  | 1:A:570:GLN:N    | 2.83                     | 0.47              |
| 1:A:711:LEU:CD2  | 1:A:711:LEU:N    | 2.78                     | 0.47              |
| 1:E:107:ARG:HB3  | 1:E:112:LEU:HD12 | 1.96                     | 0.47              |
| 1:E:152:HIS:CE1  | 1:E:154:TYR:CD2  | 3.02                     | 0.47              |
| 1:E:606:ASN:OD1  | 1:E:608:ASN:HB2  | 2.15                     | 0.47              |
| 1:E:613:LEU:C    | 1:E:615:GLN:N    | 2.71                     | 0.47              |
| 2:F:55:LYS:H     | 2:F:58:GLU:CG    | 2.27                     | 0.47              |
| 1:G:174:LEU:HD12 | 1:G:681:PHE:CE1  | 2.50                     | 0.47              |
| 1:G:193:TYR:CZ   | 1:G:197:VAL:HG21 | 2.50                     | 0.47              |
| 1:G:416:LYS:NZ   | 1:G:417:ALA:O    | 2.42                     | 0.47              |
| 1:A:79:ASN:OD1   | 1:A:94:CYS:HB2   | 2.15                     | 0.47              |
| 1:A:271:LEU:HD21 | 1:A:663:TYR:CZ   | 2.49                     | 0.47              |
| 1:A:310:PHE:O    | 1:A:311:ASN:HB2  | 2.15                     | 0.47              |
| 1:A:397:ASP:O    | 1:A:398:PHE:C    | 2.57                     | 0.47              |
| 1:A:489:LEU:C    | 1:A:489:LEU:HD12 | 2.40                     | 0.47              |
| 1:A:543:GLU:C    | 1:A:545:CYS:N    | 2.69                     | 0.47              |
| 1:A:613:LEU:C    | 1:A:615:GLN:N    | 2.72                     | 0.47              |
| 1:A:745:GLY:HA3  | 1:G:819:LEU:HD21 | 1.96                     | 0.47              |
| 1:A:814:LYS:O    | 1:A:818:GLN:OE1  | 2.32                     | 0.47              |
| 1:C:9:ASP:O      | 1:C:12:PHE:HB2   | 2.15                     | 0.47              |
| 1:C:287:PHE:O    | 1:C:288:HIS:C    | 2.58                     | 0.47              |
| 1:C:330:GLU:O    | 1:C:331:MET:C    | 2.57                     | 0.47              |
| 1:C:345:THR:HG22 | 1:C:346:GLU:HG2  | 1.97                     | 0.47              |
| 1:C:349:GLN:O    | 1:C:350:THR:C    | 2.57                     | 0.47              |
| 1:C:565:ASN:CG   | 1:C:565:ASN:O    | 2.58                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:683:ARG:H    | 1:C:683:ARG:HG2  | 1.39                     | 0.47              |
| 1:C:806:TYR:CG   | 2:D:147:VAL:HG12 | 2.50                     | 0.47              |
| 1:E:31:ALA:C     | 1:E:33:LYS:N     | 2.72                     | 0.47              |
| 1:E:80:PRO:HD2   | 1:E:83:PHE:CE2   | 2.50                     | 0.47              |
| 1:E:226:GLN:HG2  | 1:E:341:ILE:HB   | 1.95                     | 0.47              |
| 1:E:355:VAL:HG21 | 1:E:620:PHE:CE2  | 2.49                     | 0.47              |
| 1:E:420:LYS:HD2  | 1:E:421:GLU:OE2  | 2.13                     | 0.47              |
| 1:E:607:ASP:C    | 1:E:610:THR:HB   | 2.40                     | 0.47              |
| 1:E:802:GLN:NE2  | 2:F:88:TYR:OH    | 2.42                     | 0.47              |
| 1:E:806:TYR:CB   | 2:F:147:VAL:HG12 | 2.44                     | 0.47              |
| 1:E:806:TYR:HB3  | 2:F:147:VAL:HG12 | 1.97                     | 0.47              |
| 1:E:814:LYS:O    | 1:E:818:GLN:OE1  | 2.32                     | 0.47              |
| 2:F:54:PRO:HB2   | 2:F:59:MET:HG2   | 1.96                     | 0.47              |
| 1:G:164:MET:HG2  | 1:G:165:LEU:N    | 2.29                     | 0.47              |
| 1:G:267:ILE:HB   | 1:G:447:ASN:HD21 | 1.80                     | 0.47              |
| 1:G:405:PRO:HG2  | 1:G:416:LYS:HG3  | 1.96                     | 0.47              |
| 1:G:479:GLN:OE1  | 1:G:479:GLN:N    | 2.48                     | 0.47              |
| 1:G:575:LEU:C    | 1:G:577:ASP:N    | 2.71                     | 0.47              |
| 1:G:763:ASP:C    | 1:G:765:ASN:H    | 2.22                     | 0.47              |
| 2:H:69:PHE:HA    | 2:H:72:MET:HE3   | 1.97                     | 0.47              |
| 2:H:76:ILE:O     | 2:H:78:LYS:N     | 2.47                     | 0.47              |
| 2:H:95:PHE:CZ    | 2:H:111:VAL:HG21 | 2.49                     | 0.47              |
| 1:A:79:ASN:OD1   | 1:A:92:LEU:HB3   | 2.15                     | 0.47              |
| 1:C:87:GLU:OE1   | 1:C:107:ARG:NH2  | 2.48                     | 0.47              |
| 2:D:69:PHE:CZ    | 2:D:73:MET:HG2   | 2.49                     | 0.47              |
| 1:E:89:MET:HA    | 1:E:92:LEU:HD12  | 1.96                     | 0.47              |
| 1:E:306:LEU:HD22 | 1:E:386:LYS:HD3  | 1.97                     | 0.47              |
| 1:E:308:GLU:OE1  | 1:E:312:ASN:HB3  | 2.14                     | 0.47              |
| 1:E:382:THR:OG1  | 1:E:383:ALA:N    | 2.48                     | 0.47              |
| 2:F:105:GLY:O    | 2:F:109:ARG:NH1  | 2.47                     | 0.47              |
| 1:G:86:VAL:HG12  | 1:G:103:ASN:ND2  | 2.29                     | 0.47              |
| 1:G:172:SER:HA   | 1:G:462:GLY:O    | 2.15                     | 0.47              |
| 1:G:228:ASN:N    | 1:G:229:PRO:CD   | 2.78                     | 0.47              |
| 1:G:278:ILE:HG22 | 1:G:315:PHE:CE1  | 2.50                     | 0.47              |
| 1:G:326:GLN:HG3  | 1:G:331:MET:HE3  | 1.97                     | 0.47              |
| 1:G:569:PHE:CD2  | 1:G:570:GLN:N    | 2.83                     | 0.47              |
| 2:H:20:ARG:HE    | 2:H:20:ARG:HB2   | 1.45                     | 0.47              |
| 1:A:106:GLU:O    | 1:A:107:ARG:C    | 2.57                     | 0.47              |
| 1:A:244:ASN:O    | 1:A:244:ASN:CG   | 2.58                     | 0.47              |
| 1:A:311:ASN:HD22 | 1:A:311:ASN:N    | 2.12                     | 0.47              |
| 1:A:355:VAL:HG21 | 1:A:620:PHE:CE2  | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:521:LEU:O    | 1:A:522:GLN:C    | 2.58                     | 0.47              |
| 1:A:573:LYS:N    | 1:A:573:LYS:HD2  | 2.29                     | 0.47              |
| 2:B:104:MET:C    | 2:B:106:ALA:N    | 2.72                     | 0.47              |
| 1:C:152:HIS:CE1  | 1:C:154:TYR:CG   | 3.03                     | 0.47              |
| 1:C:182:GLY:HA2  | 5:C:998:ADP:PA   | 2.55                     | 0.47              |
| 1:C:294:ILE:HB   | 1:C:310:PHE:CZ   | 2.50                     | 0.47              |
| 1:C:369:LYS:HG3  | 1:C:370:GLU:H    | 1.79                     | 0.47              |
| 1:C:397:ASP:O    | 1:C:398:PHE:C    | 2.57                     | 0.47              |
| 1:E:253:ARG:O    | 1:E:265:ALA:HA   | 2.14                     | 0.47              |
| 1:E:409:VAL:HG13 | 1:E:634:LEU:HD11 | 1.96                     | 0.47              |
| 1:E:521:LEU:O    | 1:E:522:GLN:C    | 2.58                     | 0.47              |
| 1:E:556:VAL:O    | 1:E:560:ILE:HG12 | 2.14                     | 0.47              |
| 1:E:607:ASP:OD1  | 1:E:607:ASP:N    | 2.33                     | 0.47              |
| 2:F:105:GLY:O    | 2:F:109:ARG:HB2  | 2.15                     | 0.47              |
| 1:G:106:GLU:O    | 1:G:107:ARG:C    | 2.57                     | 0.47              |
| 1:G:193:TYR:CE1  | 1:G:197:VAL:HG21 | 2.49                     | 0.47              |
| 1:G:382:THR:OG1  | 1:G:383:ALA:N    | 2.47                     | 0.47              |
| 1:G:558:LYS:O    | 1:G:561:GLN:N    | 2.48                     | 0.47              |
| 1:G:662:LEU:HD12 | 1:G:662:LEU:HA   | 1.73                     | 0.47              |
| 1:G:742:ILE:CD1  | 1:G:756:MET:HE3  | 2.44                     | 0.47              |
| 1:A:36:TRP:NE1   | 1:A:78:MET:HA    | 2.30                     | 0.47              |
| 1:A:235:GLY:HA3  | 1:A:248:PHE:HE2  | 1.79                     | 0.47              |
| 1:C:106:GLU:O    | 1:C:107:ARG:C    | 2.57                     | 0.47              |
| 1:C:189:LYS:O    | 1:C:192:GLN:HB3  | 2.15                     | 0.47              |
| 1:C:746:PHE:O    | 1:C:747:MET:HB2  | 2.14                     | 0.47              |
| 1:C:785:GLU:CD   | 1:C:788:ARG:HH21 | 2.22                     | 0.47              |
| 2:D:69:PHE:HA    | 2:D:72:MET:HE3   | 1.97                     | 0.47              |
| 1:E:318:ASN:O    | 1:E:319:GLY:C    | 2.58                     | 0.47              |
| 2:F:104:MET:O    | 2:F:106:ALA:N    | 2.48                     | 0.47              |
| 1:G:199:SER:HB2  | 1:G:221:GLU:OE2  | 2.14                     | 0.47              |
| 1:G:342:MET:HE3  | 1:G:342:MET:C    | 2.39                     | 0.47              |
| 1:A:354:ARG:HG3  | 1:A:355:VAL:N    | 2.30                     | 0.46              |
| 1:A:416:LYS:NZ   | 1:A:417:ALA:O    | 2.40                     | 0.46              |
| 1:A:769:ILE:CD1  | 1:A:774:ILE:HG12 | 2.45                     | 0.46              |
| 2:B:69:PHE:HA    | 2:B:72:MET:HE3   | 1.97                     | 0.46              |
| 1:C:183:LYS:HE2  | 1:C:183:LYS:HB2  | 1.69                     | 0.46              |
| 1:C:597:TRP:O    | 1:C:601:ASN:HB2  | 2.15                     | 0.46              |
| 1:E:87:GLU:OE1   | 1:E:107:ARG:NH2  | 2.48                     | 0.46              |
| 2:F:135:ASN:HB2  | 2:F:137:CYS:SG   | 2.56                     | 0.46              |
| 1:G:64:ASN:C     | 1:G:66:LYS:N     | 2.73                     | 0.46              |
| 1:G:250:LYS:HD2  | 1:G:252:ILE:HD11 | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:272:LEU:C    | 1:G:272:LEU:CD1  | 2.81                     | 0.46              |
| 1:G:287:PHE:O    | 1:G:288:HIS:C    | 2.58                     | 0.46              |
| 1:G:330:GLU:O    | 1:G:331:MET:C    | 2.58                     | 0.46              |
| 1:A:446:VAL:HG12 | 1:A:447:ASN:N    | 2.29                     | 0.46              |
| 1:A:540:LEU:C    | 1:A:542:ASP:H    | 2.24                     | 0.46              |
| 1:A:721:PHE:CE2  | 1:A:768:ARG:HG2  | 2.50                     | 0.46              |
| 1:A:726:VAL:HA   | 1:A:773:LYS:HA   | 1.97                     | 0.46              |
| 1:A:756:MET:O    | 1:A:760:LEU:HG   | 2.15                     | 0.46              |
| 2:B:139:ASN:HD21 | 2:B:141:GLU:HG3  | 1.79                     | 0.46              |
| 1:C:733:ARG:HG2  | 1:C:734:TYR:CE1  | 2.50                     | 0.46              |
| 1:E:769:ILE:HD13 | 1:E:774:ILE:HG12 | 1.96                     | 0.46              |
| 1:G:196:VAL:CG1  | 1:G:197:VAL:N    | 2.78                     | 0.46              |
| 1:G:726:VAL:HA   | 1:G:773:LYS:HA   | 1.96                     | 0.46              |
| 2:H:97:LYS:HG2   | 2:H:98:GLU:HG3   | 1.97                     | 0.46              |
| 1:A:199:SER:HB2  | 1:A:221:GLU:OE2  | 2.15                     | 0.46              |
| 1:A:211:GLN:HG3  | 1:A:214:SER:HB2  | 1.97                     | 0.46              |
| 1:A:607:ASP:O    | 1:A:610:THR:HB   | 2.16                     | 0.46              |
| 1:C:31:ALA:C     | 1:C:33:LYS:N     | 2.73                     | 0.46              |
| 1:C:235:GLY:HA3  | 1:C:248:PHE:HE1  | 1.80                     | 0.46              |
| 2:D:104:MET:O    | 2:D:106:ALA:N    | 2.48                     | 0.46              |
| 2:D:140:TYR:CE1  | 2:D:141:GLU:HG2  | 2.50                     | 0.46              |
| 1:E:133:TYR:HB3  | 1:E:154:TYR:OH   | 2.16                     | 0.46              |
| 1:E:545:CYS:HA   | 1:E:598:LEU:HD22 | 1.97                     | 0.46              |
| 1:E:763:ASP:C    | 1:E:765:ASN:H    | 2.23                     | 0.46              |
| 1:G:9:ASP:O      | 1:G:12:PHE:HB2   | 2.15                     | 0.46              |
| 1:G:189:LYS:O    | 1:G:192:GLN:HB3  | 2.15                     | 0.46              |
| 1:G:313:TYR:N    | 1:G:313:TYR:CD1  | 2.83                     | 0.46              |
| 1:G:508:GLU:HG3  | 1:G:775:PHE:HE1  | 1.80                     | 0.46              |
| 1:A:100:VAL:HG21 | 1:A:711:LEU:HD11 | 1.96                     | 0.46              |
| 1:A:237:ALA:HA   | 1:A:288:HIS:CD2  | 2.50                     | 0.46              |
| 1:A:294:ILE:HB   | 1:A:310:PHE:CZ   | 2.50                     | 0.46              |
| 1:A:420:LYS:HD2  | 1:A:421:GLU:OE2  | 2.15                     | 0.46              |
| 1:A:474:ILE:H    | 1:A:474:ILE:HG13 | 1.48                     | 0.46              |
| 1:A:768:ARG:HD3  | 1:A:768:ARG:HA   | 1.63                     | 0.46              |
| 1:C:280:GLN:OE1  | 1:C:316:LEU:HA   | 2.15                     | 0.46              |
| 1:C:327:GLN:HG2  | 1:C:330:GLU:HG2  | 1.96                     | 0.46              |
| 1:C:425:PHE:CD1  | 1:C:425:PHE:O    | 2.68                     | 0.46              |
| 1:C:508:GLU:HG3  | 1:C:775:PHE:HE1  | 1.80                     | 0.46              |
| 1:C:541:LEU:CD2  | 1:C:601:ASN:HD22 | 2.14                     | 0.46              |
| 1:E:342:MET:HE3  | 1:E:342:MET:O    | 2.14                     | 0.46              |
| 1:E:416:LYS:NZ   | 1:E:417:ALA:O    | 2.41                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:437:ARG:HD2  | 1:E:624:LEU:O    | 2.14                     | 0.46              |
| 1:E:747:MET:HG2  | 1:E:751:GLN:NE2  | 2.30                     | 0.46              |
| 1:E:763:ASP:HB3  | 1:E:766:LEU:CD1  | 2.44                     | 0.46              |
| 1:G:31:ALA:C     | 1:G:33:LYS:N     | 2.74                     | 0.46              |
| 1:G:253:ARG:O    | 1:G:265:ALA:HA   | 2.14                     | 0.46              |
| 1:G:402:ILE:HG22 | 1:G:403:LEU:HG   | 1.96                     | 0.46              |
| 1:G:763:ASP:N    | 1:G:766:LEU:HD12 | 2.31                     | 0.46              |
| 2:H:108:ILE:HG22 | 2:H:109:ARG:N    | 2.31                     | 0.46              |
| 1:A:80:PRO:HD2   | 1:A:83:PHE:HD2   | 1.81                     | 0.46              |
| 1:A:280:GLN:OE1  | 1:A:316:LEU:HA   | 2.15                     | 0.46              |
| 1:A:718:ARG:HG3  | 1:A:719:GLN:N    | 2.30                     | 0.46              |
| 1:C:296:GLY:HA3  | 1:C:332:PHE:CG   | 2.50                     | 0.46              |
| 1:C:522:GLN:OE1  | 1:C:525:ILE:HD12 | 2.15                     | 0.46              |
| 1:C:545:CYS:HA   | 1:C:598:LEU:HD22 | 1.96                     | 0.46              |
| 2:D:70:LEU:HG    | 2:D:74:GLN:HE21  | 1.81                     | 0.46              |
| 1:E:177:GLY:O    | 1:E:183:LYS:NZ   | 2.48                     | 0.46              |
| 1:E:449:ALA:C    | 1:E:451:ASP:N    | 2.69                     | 0.46              |
| 1:E:544:GLU:OE1  | 1:E:550:ALA:HB1  | 2.14                     | 0.46              |
| 2:F:4:SER:N      | 2:F:7:GLN:NE2    | 2.61                     | 0.46              |
| 1:G:13:LEU:HD21  | 1:G:132:ILE:HD12 | 1.97                     | 0.46              |
| 1:G:61:LEU:C     | 1:G:63:GLU:N     | 2.64                     | 0.46              |
| 1:A:806:TYR:CB   | 2:B:147:VAL:HG12 | 2.45                     | 0.46              |
| 1:C:32:LYS:C     | 1:C:34:LEU:N     | 2.74                     | 0.46              |
| 1:C:60:GLU:OE1   | 1:C:67:LYS:HD2   | 2.16                     | 0.46              |
| 1:C:226:GLN:HG2  | 1:C:341:ILE:HB   | 1.98                     | 0.46              |
| 1:C:234:PHE:HD1  | 1:C:289:ILE:CG2  | 2.25                     | 0.46              |
| 1:C:308:GLU:OE1  | 1:C:312:ASN:HB3  | 2.15                     | 0.46              |
| 1:C:337:GLU:O    | 1:C:340:THR:OG1  | 2.28                     | 0.46              |
| 1:C:416:LYS:NZ   | 1:C:417:ALA:O    | 2.41                     | 0.46              |
| 2:D:104:MET:C    | 2:D:106:ALA:N    | 2.74                     | 0.46              |
| 2:D:116:GLY:O    | 2:D:118:LYS:N    | 2.47                     | 0.46              |
| 2:D:143:LEU:O    | 2:D:147:VAL:HG22 | 2.15                     | 0.46              |
| 1:E:235:GLY:HA3  | 1:E:248:PHE:HE1  | 1.81                     | 0.46              |
| 1:E:271:LEU:HD21 | 1:E:663:TYR:CZ   | 2.49                     | 0.46              |
| 1:E:275:SER:C    | 1:E:277:ALA:H    | 2.23                     | 0.46              |
| 1:E:293:LEU:HA   | 1:E:332:PHE:HE1  | 1.79                     | 0.46              |
| 1:E:520:ASP:OD1  | 1:E:523:PRO:HD2  | 2.15                     | 0.46              |
| 1:E:763:ASP:N    | 1:E:766:LEU:HD12 | 2.31                     | 0.46              |
| 1:G:231:LEU:HD23 | 1:G:231:LEU:N    | 2.30                     | 0.46              |
| 1:G:308:GLU:OE1  | 1:G:312:ASN:HB3  | 2.16                     | 0.46              |
| 1:G:361:GLN:CG   | 1:G:387:VAL:HG23 | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:551:THR:O    | 1:A:554:SER:N    | 2.48                     | 0.46              |
| 1:A:763:ASP:OD1  | 1:A:765:ASN:N    | 2.48                     | 0.46              |
| 1:C:280:GLN:CD   | 1:C:280:GLN:N    | 2.74                     | 0.46              |
| 1:C:306:LEU:HD22 | 1:C:386:LYS:CD   | 2.46                     | 0.46              |
| 1:C:480:LEU:HD11 | 1:C:528:ILE:CD1  | 2.46                     | 0.46              |
| 1:C:489:LEU:C    | 1:C:489:LEU:HD12 | 2.41                     | 0.46              |
| 1:C:712:GLU:OE1  | 1:C:712:GLU:N    | 2.38                     | 0.46              |
| 2:D:74:GLN:O     | 2:D:78:LYS:HD2   | 2.16                     | 0.46              |
| 2:D:124:VAL:HG23 | 2:D:125:GLU:N    | 2.31                     | 0.46              |
| 1:E:106:GLU:O    | 1:E:107:ARG:C    | 2.57                     | 0.46              |
| 1:E:395:VAL:O    | 1:E:396:THR:C    | 2.58                     | 0.46              |
| 1:E:479:GLN:OE1  | 1:E:479:GLN:N    | 2.49                     | 0.46              |
| 1:E:487:GLU:OE1  | 1:E:585:HIS:HA   | 2.16                     | 0.46              |
| 1:E:575:LEU:C    | 1:E:577:ASP:N    | 2.74                     | 0.46              |
| 1:E:767:TYR:CD1  | 1:E:767:TYR:C    | 2.94                     | 0.46              |
| 2:F:43:THR:HG23  | 2:F:46:GLU:OE1   | 2.16                     | 0.46              |
| 2:F:70:LEU:HG    | 2:F:74:GLN:HE21  | 1.81                     | 0.46              |
| 1:G:280:GLN:OE1  | 1:G:316:LEU:HA   | 2.16                     | 0.46              |
| 1:G:551:THR:O    | 1:G:554:SER:N    | 2.49                     | 0.46              |
| 1:A:141:TYR:CE1  | 1:A:149:MET:HB3  | 2.51                     | 0.46              |
| 1:A:267:ILE:CD1  | 1:A:450:LEU:HD12 | 2.45                     | 0.46              |
| 1:A:275:SER:C    | 1:A:277:ALA:H    | 2.24                     | 0.46              |
| 1:A:469:PHE:N    | 1:A:486:ASN:OD1  | 2.46                     | 0.46              |
| 1:A:532:THR:C    | 1:A:533:ASN:O    | 2.57                     | 0.46              |
| 2:B:43:THR:HG23  | 2:B:46:GLU:OE1   | 2.16                     | 0.46              |
| 1:C:235:GLY:HA3  | 1:C:248:PHE:CE1  | 2.51                     | 0.46              |
| 1:C:370:GLU:O    | 1:C:374:ASP:CA   | 2.64                     | 0.46              |
| 1:C:699:HIS:HA   | 1:C:702:LEU:HB2  | 1.96                     | 0.46              |
| 1:E:39:SER:OG    | 1:E:42:HIS:HB2   | 2.16                     | 0.46              |
| 1:E:100:VAL:HG21 | 1:E:711:LEU:HD11 | 1.98                     | 0.46              |
| 1:E:172:SER:HA   | 1:E:462:GLY:O    | 2.15                     | 0.46              |
| 1:E:330:GLU:O    | 1:E:331:MET:C    | 2.58                     | 0.46              |
| 1:E:513:ASN:O    | 1:E:515:ILE:HD12 | 2.15                     | 0.46              |
| 1:E:553:THR:HA   | 1:E:579:THR:HG21 | 1.97                     | 0.46              |
| 1:G:104:LEU:CD1  | 1:G:705:LEU:HD11 | 2.45                     | 0.46              |
| 1:G:256:PHE:HE1  | 1:G:262:ILE:HG13 | 1.81                     | 0.46              |
| 1:G:408:LYS:HG2  | 1:G:412:ASP:O    | 2.16                     | 0.46              |
| 1:G:804:ARG:O    | 1:G:808:ALA:HB2  | 2.15                     | 0.46              |
| 2:H:70:LEU:HG    | 2:H:74:GLN:HE21  | 1.80                     | 0.46              |
| 1:A:226:GLN:HG2  | 1:A:341:ILE:HB   | 1.97                     | 0.46              |
| 1:A:504:GLU:O    | 1:A:504:GLU:HG3  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:763:ASP:C    | 1:A:765:ASN:H    | 2.24                     | 0.46              |
| 2:B:74:GLN:O     | 2:B:78:LYS:HD2   | 2.16                     | 0.46              |
| 1:C:77:LYS:H     | 1:C:77:LYS:HD2   | 1.80                     | 0.46              |
| 1:C:318:ASN:O    | 1:C:319:GLY:C    | 2.57                     | 0.46              |
| 1:C:382:THR:OG1  | 1:C:383:ALA:N    | 2.49                     | 0.46              |
| 1:C:468:GLY:O    | 1:C:469:PHE:C    | 2.58                     | 0.46              |
| 1:C:475:ASN:HB2  | 1:C:592:TYR:HA   | 1.98                     | 0.46              |
| 1:C:619:LYS:HA   | 1:C:622:ALA:HB3  | 1.97                     | 0.46              |
| 1:C:726:VAL:HA   | 1:C:773:LYS:HA   | 1.98                     | 0.46              |
| 1:C:814:LYS:C    | 1:C:816:GLN:N    | 2.73                     | 0.46              |
| 2:D:111:VAL:HG12 | 2:D:112:LEU:HD23 | 1.97                     | 0.46              |
| 1:E:267:ILE:CD1  | 1:E:450:LEU:HD12 | 2.46                     | 0.46              |
| 1:E:604:PRO:O    | 1:E:605:LEU:HB2  | 2.16                     | 0.46              |
| 1:G:22:ASN:O     | 1:G:22:ASN:ND2   | 2.49                     | 0.46              |
| 1:G:161:TYR:CE1  | 1:G:165:LEU:HD11 | 2.51                     | 0.46              |
| 1:G:235:GLY:HA3  | 1:G:248:PHE:HE1  | 1.81                     | 0.46              |
| 1:G:280:GLN:N    | 1:G:280:GLN:CD   | 2.74                     | 0.46              |
| 1:G:355:VAL:HG21 | 1:G:620:PHE:CE2  | 2.51                     | 0.46              |
| 1:G:407:ILE:HD12 | 1:G:409:VAL:H    | 1.80                     | 0.46              |
| 1:G:527:LEU:HD12 | 1:G:566:HIS:CD2  | 2.50                     | 0.46              |
| 1:G:611:SER:HA   | 1:G:614:ASN:HB2  | 1.97                     | 0.46              |
| 1:G:699:HIS:HA   | 1:G:702:LEU:HB2  | 1.98                     | 0.46              |
| 1:G:763:ASP:HB3  | 1:G:766:LEU:CD1  | 2.46                     | 0.46              |
| 1:G:814:LYS:C    | 1:G:816:GLN:N    | 2.74                     | 0.46              |
| 1:A:13:LEU:HD11  | 1:A:132:ILE:CB   | 2.35                     | 0.46              |
| 1:A:31:ALA:C     | 1:A:33:LYS:N     | 2.73                     | 0.46              |
| 1:A:147:HIS:C    | 1:A:149:MET:N    | 2.74                     | 0.46              |
| 1:A:306:LEU:HD22 | 1:A:386:LYS:HD3  | 1.98                     | 0.46              |
| 1:C:342:MET:O    | 1:C:342:MET:HE3  | 2.16                     | 0.46              |
| 1:C:438:LEU:HD12 | 1:C:438:LEU:HA   | 1.77                     | 0.46              |
| 1:C:682:VAL:O    | 1:C:682:VAL:HG12 | 2.15                     | 0.46              |
| 1:C:724:ARG:HE   | 1:C:724:ARG:HB3  | 1.62                     | 0.46              |
| 2:D:86:GLU:CD    | 2:D:86:GLU:H     | 2.24                     | 0.46              |
| 1:E:280:GLN:OE1  | 1:E:316:LEU:HA   | 2.15                     | 0.46              |
| 1:E:425:PHE:O    | 1:E:425:PHE:CD1  | 2.69                     | 0.46              |
| 1:E:682:VAL:O    | 1:E:682:VAL:HG12 | 2.16                     | 0.46              |
| 1:E:711:LEU:N    | 1:E:711:LEU:CD2  | 2.76                     | 0.46              |
| 1:G:177:GLY:O    | 1:G:183:LYS:NZ   | 2.49                     | 0.46              |
| 1:G:275:SER:C    | 1:G:277:ALA:H    | 2.22                     | 0.46              |
| 1:G:345:THR:HG22 | 1:G:346:GLU:HG2  | 1.97                     | 0.46              |
| 1:G:573:LYS:HD2  | 1:G:573:LYS:N    | 2.31                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:742:ILE:HG23 | 1:G:747:MET:HE2  | 1.97                     | 0.46              |
| 2:H:121:GLU:CD   | 2:H:121:GLU:H    | 2.23                     | 0.46              |
| 2:H:135:ASN:N    | 2:H:135:ASN:ND2  | 2.64                     | 0.46              |
| 1:A:133:TYR:HB3  | 1:A:154:TYR:OH   | 2.15                     | 0.45              |
| 1:A:478:GLU:H    | 1:A:478:GLU:CD   | 2.18                     | 0.45              |
| 1:A:621:VAL:HG12 | 1:A:625:TRP:HD1  | 1.80                     | 0.45              |
| 2:B:110:HIS:O    | 2:B:111:VAL:C    | 2.58                     | 0.45              |
| 2:B:133:ASP:OD1  | 2:B:135:ASN:N    | 2.49                     | 0.45              |
| 1:C:122:VAL:C    | 1:C:123:VAL:HG23 | 2.41                     | 0.45              |
| 1:C:465:ASP:O    | 1:C:465:ASP:CG   | 2.60                     | 0.45              |
| 1:C:513:ASN:O    | 1:C:513:ASN:ND2  | 2.46                     | 0.45              |
| 1:C:581:PHE:CZ   | 1:C:597:TRP:CH2  | 3.03                     | 0.45              |
| 1:C:623:ASP:OD1  | 1:C:623:ASP:N    | 2.49                     | 0.45              |
| 1:C:716:ILE:HA   | 1:C:719:GLN:HB2  | 1.98                     | 0.45              |
| 2:D:43:THR:HG23  | 2:D:46:GLU:OE1   | 2.16                     | 0.45              |
| 2:D:110:HIS:O    | 2:D:111:VAL:C    | 2.59                     | 0.45              |
| 1:E:275:SER:O    | 1:E:278:ILE:HG12 | 2.16                     | 0.45              |
| 1:E:424:ASP:O    | 1:E:426:ALA:N    | 2.49                     | 0.45              |
| 2:F:74:GLN:O     | 2:F:78:LYS:HD2   | 2.16                     | 0.45              |
| 1:G:747:MET:HG2  | 1:G:751:GLN:NE2  | 2.31                     | 0.45              |
| 2:H:111:VAL:HA   | 2:H:115:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:88:ASP:HB3   | 1:A:91:GLU:CD    | 2.41                     | 0.45              |
| 1:A:132:ILE:HD12 | 1:A:152:HIS:HD2  | 1.82                     | 0.45              |
| 1:A:236:ASN:HD22 | 1:A:245:SER:C    | 2.24                     | 0.45              |
| 1:A:508:GLU:HG3  | 1:A:775:PHE:HE1  | 1.80                     | 0.45              |
| 1:A:547:PHE:C    | 1:A:547:PHE:CD1  | 2.94                     | 0.45              |
| 1:A:566:HIS:CE1  | 1:A:568:LYS:HB2  | 2.50                     | 0.45              |
| 2:B:10:GLU:HG3   | 2:B:13:GLU:CD    | 2.41                     | 0.45              |
| 2:B:97:LYS:HG2   | 2:B:98:GLU:HG3   | 1.97                     | 0.45              |
| 1:C:250:LYS:HD2  | 1:C:252:ILE:HD11 | 1.98                     | 0.45              |
| 1:C:275:SER:C    | 1:C:277:ALA:H    | 2.24                     | 0.45              |
| 1:C:362:LEU:CD2  | 1:C:427:ILE:HG13 | 2.45                     | 0.45              |
| 1:C:575:LEU:HD23 | 1:C:577:ASP:OD1  | 2.17                     | 0.45              |
| 1:E:9:ASP:O      | 1:E:12:PHE:HB2   | 2.16                     | 0.45              |
| 1:E:278:ILE:HG22 | 1:E:315:PHE:CE1  | 2.51                     | 0.45              |
| 1:E:407:ILE:CD1  | 1:E:409:VAL:N    | 2.76                     | 0.45              |
| 1:E:446:VAL:HG12 | 1:E:447:ASN:N    | 2.31                     | 0.45              |
| 1:E:475:ASN:HB2  | 1:E:592:TYR:HA   | 1.98                     | 0.45              |
| 1:E:530:ARG:HG3  | 1:E:531:PRO:N    | 2.31                     | 0.45              |
| 1:E:581:PHE:CZ   | 1:E:597:TRP:CH2  | 3.05                     | 0.45              |
| 1:E:613:LEU:C    | 1:E:615:GLN:H    | 2.24                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:623:ASP:OD1  | 1:E:623:ASP:N    | 2.48                     | 0.45              |
| 1:G:100:VAL:HG21 | 1:G:711:LEU:HD11 | 1.97                     | 0.45              |
| 1:G:145:LYS:HE3  | 1:G:145:LYS:HB2  | 1.57                     | 0.45              |
| 1:G:161:TYR:O    | 1:G:161:TYR:CG   | 2.68                     | 0.45              |
| 1:G:530:ARG:HA   | 1:G:531:PRO:HD3  | 1.79                     | 0.45              |
| 1:G:683:ARG:H    | 1:G:683:ARG:HG2  | 1.35                     | 0.45              |
| 1:G:769:ILE:HD13 | 1:G:774:ILE:HG23 | 1.98                     | 0.45              |
| 2:H:74:GLN:O     | 2:H:78:LYS:HD2   | 2.16                     | 0.45              |
| 1:A:465:ASP:CG   | 1:A:465:ASP:O    | 2.59                     | 0.45              |
| 1:A:527:LEU:HD12 | 1:A:566:HIS:CD2  | 2.51                     | 0.45              |
| 1:A:747:MET:CG   | 1:A:751:GLN:NE2  | 2.79                     | 0.45              |
| 2:D:35:MET:CE    | 2:D:73:MET:HA    | 2.47                     | 0.45              |
| 1:E:33:LYS:O     | 1:E:48:SER:HA    | 2.16                     | 0.45              |
| 1:E:53:LYS:HD2   | 1:E:58:THR:HG23  | 1.98                     | 0.45              |
| 1:E:763:ASP:OD1  | 1:E:765:ASN:N    | 2.49                     | 0.45              |
| 1:E:769:ILE:CD1  | 1:E:774:ILE:HG12 | 2.47                     | 0.45              |
| 2:F:85:PHE:CA    | 2:F:89:VAL:HG13  | 2.40                     | 0.45              |
| 1:G:294:ILE:HB   | 1:G:310:PHE:CZ   | 2.50                     | 0.45              |
| 1:G:391:MET:HB3  | 1:G:393:ILE:HG12 | 1.98                     | 0.45              |
| 1:G:420:LYS:HD2  | 1:G:421:GLU:OE2  | 2.16                     | 0.45              |
| 1:G:432:LYS:HE2  | 1:G:432:LYS:HB2  | 1.80                     | 0.45              |
| 1:G:508:GLU:HG3  | 1:G:775:PHE:CE1  | 2.52                     | 0.45              |
| 1:G:767:TYR:CD1  | 1:G:767:TYR:C    | 2.95                     | 0.45              |
| 2:H:43:THR:HG23  | 2:H:46:GLU:OE1   | 2.16                     | 0.45              |
| 1:A:223:GLN:C    | 1:A:225:LEU:N    | 2.73                     | 0.45              |
| 1:A:682:VAL:O    | 1:A:682:VAL:HG12 | 2.16                     | 0.45              |
| 1:A:763:ASP:N    | 1:A:766:LEU:HD12 | 2.32                     | 0.45              |
| 1:C:13:LEU:HD21  | 1:C:132:ILE:HD13 | 1.97                     | 0.45              |
| 1:C:153:ILE:CG2  | 1:C:154:TYR:N    | 2.79                     | 0.45              |
| 1:C:293:LEU:HA   | 1:C:332:PHE:HE1  | 1.80                     | 0.45              |
| 1:C:474:ILE:H    | 1:C:474:ILE:HG13 | 1.48                     | 0.45              |
| 1:C:611:SER:O    | 1:C:615:GLN:NE2  | 2.49                     | 0.45              |
| 1:C:776:PHE:CD2  | 1:C:781:LEU:HD22 | 2.51                     | 0.45              |
| 1:C:806:TYR:HB3  | 2:D:147:VAL:HG12 | 1.97                     | 0.45              |
| 2:F:44:ASN:ND2   | 2:F:117:GLU:HB3  | 2.29                     | 0.45              |
| 1:G:293:LEU:HA   | 1:G:332:PHE:HE1  | 1.81                     | 0.45              |
| 1:G:352:ILE:HG21 | 1:G:442:ILE:CD1  | 2.41                     | 0.45              |
| 2:H:10:GLU:HG3   | 2:H:13:GLU:CD    | 2.42                     | 0.45              |
| 1:A:508:GLU:HG3  | 1:A:775:PHE:CE1  | 2.51                     | 0.45              |
| 1:A:662:LEU:HD12 | 1:A:662:LEU:HA   | 1.74                     | 0.45              |
| 2:B:70:LEU:HG    | 2:B:74:GLN:HE21  | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:475:ASN:ND2  | 1:C:590:VAL:CG1  | 2.79                     | 0.45              |
| 1:C:607:ASP:O    | 1:C:610:THR:HB   | 2.17                     | 0.45              |
| 2:D:16:GLN:C     | 2:D:18:PHE:H     | 2.24                     | 0.45              |
| 2:D:26:ILE:HG22  | 2:D:26:ILE:O     | 2.16                     | 0.45              |
| 1:E:223:GLN:C    | 1:E:225:LEU:N    | 2.73                     | 0.45              |
| 1:E:611:SER:HA   | 1:E:614:ASN:HB2  | 1.99                     | 0.45              |
| 1:E:699:HIS:HA   | 1:E:702:LEU:HB2  | 1.98                     | 0.45              |
| 1:E:746:PHE:O    | 1:E:747:MET:HB2  | 2.17                     | 0.45              |
| 1:G:39:SER:OG    | 1:G:42:HIS:HB2   | 2.17                     | 0.45              |
| 1:G:145:LYS:HG3  | 1:G:146:ARG:NE   | 2.32                     | 0.45              |
| 1:A:43:GLY:HA2   | 1:A:699:HIS:CE1  | 2.51                     | 0.45              |
| 1:A:226:GLN:O    | 1:A:230:ILE:HD12 | 2.17                     | 0.45              |
| 1:A:278:ILE:C    | 1:A:279:ARG:HG3  | 2.40                     | 0.45              |
| 1:A:607:ASP:C    | 1:A:610:THR:HB   | 2.42                     | 0.45              |
| 1:A:625:TRP:O    | 1:A:626:LYS:C    | 2.60                     | 0.45              |
| 1:A:719:GLN:HA   | 1:A:719:GLN:HE21 | 1.81                     | 0.45              |
| 1:C:89:MET:O     | 1:C:91:GLU:N     | 2.49                     | 0.45              |
| 1:C:116:TYR:HD1  | 1:C:121:CYS:HB2  | 1.80                     | 0.45              |
| 1:C:196:VAL:CG1  | 1:C:197:VAL:N    | 2.79                     | 0.45              |
| 1:C:282:LYS:O    | 1:C:283:ASP:HB2  | 2.17                     | 0.45              |
| 1:C:409:VAL:O    | 1:C:410:GLY:C    | 2.60                     | 0.45              |
| 1:C:420:LYS:HD2  | 1:C:421:GLU:OE2  | 2.17                     | 0.45              |
| 1:C:742:ILE:HD13 | 1:C:756:MET:HE3  | 1.98                     | 0.45              |
| 1:E:797:ILE:CG1  | 2:F:117:GLU:HG2  | 2.46                     | 0.45              |
| 1:G:8:ASP:HA     | 1:G:11:LYS:CD    | 2.21                     | 0.45              |
| 1:G:39:SER:C     | 1:G:41:LYS:H     | 2.25                     | 0.45              |
| 1:G:362:LEU:HD12 | 1:G:387:VAL:HG13 | 1.97                     | 0.45              |
| 1:G:521:LEU:O    | 1:G:522:GLN:C    | 2.59                     | 0.45              |
| 2:H:71:PRO:HA    | 2:H:74:GLN:NE2   | 2.32                     | 0.45              |
| 1:A:17:LYS:HE2   | 1:A:17:LYS:HB3   | 1.66                     | 0.45              |
| 1:A:272:LEU:C    | 1:A:272:LEU:CD1  | 2.83                     | 0.45              |
| 1:A:395:VAL:O    | 1:A:396:THR:C    | 2.59                     | 0.45              |
| 1:A:699:HIS:HA   | 1:A:702:LEU:HB2  | 1.98                     | 0.45              |
| 1:A:806:TYR:CG   | 2:B:147:VAL:HG12 | 2.52                     | 0.45              |
| 2:B:35:MET:CE    | 2:B:73:MET:HA    | 2.47                     | 0.45              |
| 2:B:71:PRO:HA    | 2:B:74:GLN:NE2   | 2.32                     | 0.45              |
| 2:B:85:PHE:CD1   | 2:B:144:VAL:HG11 | 2.52                     | 0.45              |
| 2:B:140:TYR:O    | 2:B:142:GLU:N    | 2.50                     | 0.45              |
| 2:B:140:TYR:CE1  | 2:B:141:GLU:HG2  | 2.51                     | 0.45              |
| 1:C:30:SER:C     | 1:C:32:LYS:N     | 2.65                     | 0.45              |
| 1:C:132:ILE:HD12 | 1:C:152:HIS:HD2  | 1.82                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:236:ASN:ND2  | 1:C:246:SER:CA   | 2.76                     | 0.45              |
| 1:C:348:GLU:O    | 1:C:352:ILE:HG13 | 2.16                     | 0.45              |
| 1:C:504:GLU:O    | 1:C:504:GLU:HG3  | 2.15                     | 0.45              |
| 1:C:557:GLU:O    | 1:C:560:ILE:HG12 | 2.16                     | 0.45              |
| 1:C:728:GLN:NE2  | 1:C:728:GLN:O    | 2.50                     | 0.45              |
| 1:E:310:PHE:O    | 1:E:311:ASN:HB2  | 2.16                     | 0.45              |
| 1:E:344:PHE:HE1  | 1:E:445:ARG:HB3  | 1.78                     | 0.45              |
| 1:E:352:ILE:O    | 1:E:356:VAL:HG23 | 2.16                     | 0.45              |
| 1:E:543:GLU:HG2  | 1:E:544:GLU:N    | 2.31                     | 0.45              |
| 1:E:575:LEU:HD23 | 1:E:577:ASP:OD1  | 2.17                     | 0.45              |
| 1:E:747:MET:CG   | 1:E:751:GLN:NE2  | 2.80                     | 0.45              |
| 1:G:267:ILE:CD1  | 1:G:450:LEU:HD12 | 2.45                     | 0.45              |
| 1:G:395:VAL:O    | 1:G:396:THR:C    | 2.59                     | 0.45              |
| 1:G:425:PHE:CD1  | 1:G:425:PHE:C    | 2.95                     | 0.45              |
| 1:G:522:GLN:OE1  | 1:G:525:ILE:HD12 | 2.17                     | 0.45              |
| 2:H:132:GLU:H    | 2:H:132:GLU:HG2  | 1.49                     | 0.45              |
| 1:A:265:ALA:N    | 1:A:450:LEU:O    | 2.49                     | 0.45              |
| 1:A:308:GLU:OE1  | 1:A:312:ASN:HB3  | 2.16                     | 0.45              |
| 1:A:342:MET:O    | 1:A:342:MET:HE3  | 2.16                     | 0.45              |
| 1:A:409:VAL:HB   | 1:A:414:VAL:CG2  | 2.46                     | 0.45              |
| 1:A:776:PHE:CD2  | 1:A:781:LEU:HD22 | 2.51                     | 0.45              |
| 2:B:16:GLN:C     | 2:B:18:PHE:H     | 2.25                     | 0.45              |
| 1:C:39:SER:C     | 1:C:41:LYS:H     | 2.24                     | 0.45              |
| 1:C:145:LYS:HB2  | 1:C:145:LYS:HE3  | 1.57                     | 0.45              |
| 1:C:239:THR:C    | 1:C:241:LYS:N    | 2.73                     | 0.45              |
| 1:C:566:HIS:CE1  | 1:C:568:LYS:HB2  | 2.52                     | 0.45              |
| 2:D:95:PHE:CZ    | 2:D:111:VAL:HG21 | 2.50                     | 0.45              |
| 2:D:114:THR:O    | 2:D:115:LEU:HD12 | 2.16                     | 0.45              |
| 1:E:267:ILE:N    | 1:E:447:ASN:HD21 | 2.15                     | 0.45              |
| 4:E:999:ALF:F4   | 5:E:998:ADP:PB   | 2.65                     | 0.45              |
| 2:F:35:MET:CE    | 2:F:73:MET:HA    | 2.47                     | 0.45              |
| 1:G:239:THR:C    | 1:G:241:LYS:N    | 2.75                     | 0.45              |
| 1:G:762:LEU:HD13 | 1:G:766:LEU:HD13 | 1.98                     | 0.45              |
| 2:H:26:ILE:O     | 2:H:26:ILE:HG22  | 2.17                     | 0.45              |
| 1:A:149:MET:HB3  | 1:A:150:PRO:HD2  | 1.99                     | 0.45              |
| 1:A:280:GLN:CD   | 1:A:286:THR:HG23 | 2.42                     | 0.45              |
| 1:A:378:MET:HA   | 1:A:378:MET:CE   | 2.45                     | 0.45              |
| 1:A:425:PHE:O    | 1:A:425:PHE:CD1  | 2.69                     | 0.45              |
| 1:A:611:SER:HA   | 1:A:614:ASN:HB2  | 1.98                     | 0.45              |
| 1:A:762:LEU:HD13 | 1:A:766:LEU:CD1  | 2.47                     | 0.45              |
| 4:A:999:ALF:F4   | 5:A:998:ADP:PB   | 2.64                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:92:LEU:HD13 | 2:B:108:ILE:HD11 | 1.98                     | 0.45              |
| 1:C:428:GLU:C   | 1:C:430:LEU:N    | 2.73                     | 0.45              |
| 1:C:522:GLN:O   | 1:C:525:ILE:HG13 | 2.16                     | 0.45              |
| 1:C:802:GLN:HG3 | 2:D:88:TYR:OH    | 2.17                     | 0.45              |
| 4:C:999:ALF:F4  | 5:C:998:ADP:PB   | 2.65                     | 0.45              |
| 2:D:131:HIS:NE2 | 2:D:146:MET:HE3  | 2.32                     | 0.45              |
| 1:E:183:LYS:HE2 | 5:E:998:ADP:O1B  | 2.17                     | 0.45              |
| 1:E:267:ILE:H   | 1:E:447:ASN:HD21 | 1.64                     | 0.45              |
| 1:E:437:ARG:NH2 | 1:E:625:TRP:CE3  | 2.85                     | 0.45              |
| 1:E:552:ASP:CG  | 1:E:596:ALA:H    | 2.25                     | 0.45              |
| 2:F:80:LYS:H    | 2:F:80:LYS:CD    | 2.29                     | 0.45              |
| 1:G:32:LYS:C    | 1:G:34:LEU:N     | 2.73                     | 0.45              |
| 1:G:53:LYS:HD2  | 1:G:58:THR:HG23  | 1.98                     | 0.45              |
| 1:G:376:ALA:CB  | 1:G:420:LYS:HB2  | 2.42                     | 0.45              |
| 2:H:66:PHE:C    | 2:H:66:PHE:CD1   | 2.95                     | 0.45              |
| 2:H:133:ASP:OD1 | 2:H:135:ASN:N    | 2.50                     | 0.45              |
| 1:A:53:LYS:HD2  | 1:A:58:THR:HG23  | 1.99                     | 0.45              |
| 1:A:177:GLY:O   | 1:A:183:LYS:NZ   | 2.49                     | 0.45              |
| 2:B:121:GLU:H   | 2:B:121:GLU:CD   | 2.25                     | 0.45              |
| 1:C:80:PRO:HD2  | 1:C:83:PHE:HD2   | 1.81                     | 0.45              |
| 1:C:146:ARG:NH1 | 1:C:159:THR:HG23 | 2.32                     | 0.45              |
| 1:C:211:GLN:HG3 | 1:C:214:SER:HB2  | 1.97                     | 0.45              |
| 1:C:256:PHE:HE1 | 1:C:262:ILE:HG13 | 1.81                     | 0.45              |
| 1:C:748:ASP:O   | 1:C:749:GLY:C    | 2.60                     | 0.45              |
| 1:C:765:ASN:O   | 1:C:777:ARG:NH2  | 2.47                     | 0.45              |
| 2:D:105:GLY:O   | 2:D:109:ARG:HB2  | 2.16                     | 0.45              |
| 1:E:148:GLU:C   | 1:E:149:MET:HG2  | 2.42                     | 0.45              |
| 1:E:288:HIS:O   | 1:E:289:ILE:C    | 2.60                     | 0.45              |
| 1:E:326:GLN:HG3 | 1:E:331:MET:HE3  | 1.99                     | 0.45              |
| 2:F:128:VAL:O   | 2:F:129:ALA:C    | 2.60                     | 0.45              |
| 1:G:288:HIS:O   | 1:G:289:ILE:C    | 2.60                     | 0.45              |
| 1:G:344:PHE:N   | 1:G:344:PHE:CD1  | 2.83                     | 0.45              |
| 1:G:540:LEU:C   | 1:G:542:ASP:H    | 2.25                     | 0.45              |
| 1:G:683:ARG:HE  | 1:G:683:ARG:HB3  | 1.53                     | 0.45              |
| 1:G:748:ASP:O   | 1:G:749:GLY:C    | 2.60                     | 0.45              |
| 1:G:806:TYR:CG  | 2:H:147:VAL:HG12 | 2.51                     | 0.45              |
| 1:A:88:ASP:O    | 1:A:91:GLU:N     | 2.50                     | 0.44              |
| 1:A:228:ASN:N   | 1:A:229:PRO:CD   | 2.80                     | 0.44              |
| 1:A:342:MET:HE3 | 1:A:342:MET:C    | 2.42                     | 0.44              |
| 1:A:663:TYR:CZ  | 1:A:667:LEU:HD13 | 2.52                     | 0.44              |
| 2:B:86:GLU:CD   | 2:B:86:GLU:N     | 2.71                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:352:ILE:O    | 1:C:356:VAL:HG23 | 2.17                     | 0.44              |
| 1:C:375:GLN:HG3  | 1:C:418:GLN:O    | 2.18                     | 0.44              |
| 1:C:419:THR:O    | 1:C:422:GLN:N    | 2.51                     | 0.44              |
| 1:C:504:GLU:OE2  | 1:C:508:GLU:HG2  | 2.17                     | 0.44              |
| 1:C:535:PRO:CB   | 1:C:540:LEU:HD21 | 2.46                     | 0.44              |
| 1:C:540:LEU:C    | 1:C:542:ASP:N    | 2.75                     | 0.44              |
| 1:C:547:PHE:CD1  | 1:C:547:PHE:C    | 2.94                     | 0.44              |
| 2:D:10:GLU:HG3   | 2:D:13:GLU:CD    | 2.42                     | 0.44              |
| 2:D:144:VAL:O    | 2:D:147:VAL:HG23 | 2.17                     | 0.44              |
| 1:E:153:ILE:CG2  | 1:E:154:TYR:N    | 2.80                     | 0.44              |
| 1:E:522:GLN:O    | 1:E:525:ILE:HG13 | 2.17                     | 0.44              |
| 1:E:569:PHE:CD2  | 1:E:570:GLN:N    | 2.84                     | 0.44              |
| 1:E:573:LYS:HD2  | 1:E:573:LYS:N    | 2.31                     | 0.44              |
| 1:E:719:GLN:NE2  | 1:E:719:GLN:CA   | 2.78                     | 0.44              |
| 2:F:10:GLU:HG3   | 2:F:13:GLU:CD    | 2.41                     | 0.44              |
| 1:G:46:ALA:HB1   | 1:G:62:GLN:HG2   | 1.99                     | 0.44              |
| 1:G:480:LEU:HA   | 1:G:592:TYR:CE1  | 2.52                     | 0.44              |
| 1:G:613:LEU:C    | 1:G:615:GLN:H    | 2.25                     | 0.44              |
| 1:A:402:ILE:HG22 | 1:A:403:LEU:HG   | 1.99                     | 0.44              |
| 1:A:525:ILE:O    | 1:A:529:GLU:HB3  | 2.18                     | 0.44              |
| 1:A:619:LYS:HA   | 1:A:622:ALA:HB3  | 1.99                     | 0.44              |
| 1:A:720:GLY:C    | 1:A:721:PHE:CD1  | 2.95                     | 0.44              |
| 2:B:26:ILE:O     | 2:B:26:ILE:HG22  | 2.17                     | 0.44              |
| 1:C:152:HIS:ND1  | 1:C:154:TYR:N    | 2.62                     | 0.44              |
| 1:C:310:PHE:O    | 1:C:311:ASN:HB2  | 2.17                     | 0.44              |
| 1:C:355:VAL:HG21 | 1:C:620:PHE:CE2  | 2.52                     | 0.44              |
| 1:C:437:ARG:HD2  | 1:C:624:LEU:O    | 2.17                     | 0.44              |
| 1:C:508:GLU:HG3  | 1:C:775:PHE:CE1  | 2.53                     | 0.44              |
| 1:C:719:GLN:HE21 | 1:C:719:GLN:CA   | 2.30                     | 0.44              |
| 2:D:135:ASN:HB2  | 2:D:137:CYS:SG   | 2.57                     | 0.44              |
| 1:E:103:ASN:HD21 | 1:E:107:ARG:HD2  | 1.81                     | 0.44              |
| 1:E:120:PHE:CD1  | 1:E:120:PHE:N    | 2.73                     | 0.44              |
| 1:E:365:ILE:HD11 | 1:E:384:ALA:HB2  | 1.98                     | 0.44              |
| 1:E:726:VAL:HA   | 1:E:773:LYS:HA   | 1.98                     | 0.44              |
| 2:F:16:GLN:C     | 2:F:18:PHE:H     | 2.25                     | 0.44              |
| 2:F:87:ASP:O     | 2:F:88:TYR:C     | 2.60                     | 0.44              |
| 1:G:102:HIS:O    | 1:G:105:ARG:N    | 2.50                     | 0.44              |
| 1:G:132:ILE:HD12 | 1:G:152:HIS:HD2  | 1.80                     | 0.44              |
| 1:G:225:LEU:HD12 | 1:G:225:LEU:HA   | 1.86                     | 0.44              |
| 1:G:296:GLY:HA3  | 1:G:332:PHE:CG   | 2.52                     | 0.44              |
| 1:G:553:THR:HG22 | 1:G:557:GLU:OE2  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:104:MET:C    | 2:H:106:ALA:N    | 2.75                     | 0.44              |
| 1:A:145:LYS:HB2  | 1:A:145:LYS:HE3  | 1.56                     | 0.44              |
| 1:A:152:HIS:CE1  | 1:A:153:ILE:HG22 | 2.53                     | 0.44              |
| 1:A:266:ASN:HD22 | 1:A:267:ILE:H    | 1.65                     | 0.44              |
| 1:A:735:GLU:HA   | 1:A:756:MET:HE1  | 1.98                     | 0.44              |
| 2:B:9:ALA:HA     | 2:B:12:LYS:CE    | 2.48                     | 0.44              |
| 1:C:7:SER:N      | 1:C:10:GLU:OE1   | 2.45                     | 0.44              |
| 1:C:342:MET:HE3  | 1:C:342:MET:C    | 2.42                     | 0.44              |
| 1:C:763:ASP:N    | 1:C:766:LEU:HD12 | 2.32                     | 0.44              |
| 1:E:236:ASN:HD22 | 1:E:245:SER:C    | 2.26                     | 0.44              |
| 1:E:306:LEU:HD22 | 1:E:386:LYS:CD   | 2.47                     | 0.44              |
| 1:E:321:VAL:HG13 | 1:E:322:PRO:HD2  | 1.98                     | 0.44              |
| 1:E:338:ALA:O    | 1:E:339:MET:C    | 2.60                     | 0.44              |
| 1:E:369:LYS:HG3  | 1:E:370:GLU:H    | 1.82                     | 0.44              |
| 1:E:399:THR:C    | 1:E:403:LEU:HD12 | 2.42                     | 0.44              |
| 1:E:428:GLU:C    | 1:E:430:LEU:N    | 2.72                     | 0.44              |
| 1:E:527:LEU:HD12 | 1:E:566:HIS:CD2  | 2.52                     | 0.44              |
| 1:E:541:LEU:HD11 | 1:E:597:TRP:HB3  | 2.00                     | 0.44              |
| 1:E:718:ARG:HG3  | 1:E:719:GLN:N    | 2.33                     | 0.44              |
| 1:E:814:LYS:C    | 1:E:816:GLN:N    | 2.72                     | 0.44              |
| 1:G:33:LYS:O     | 1:G:48:SER:HA    | 2.17                     | 0.44              |
| 1:G:162:ARG:O    | 1:G:163:SER:C    | 2.60                     | 0.44              |
| 1:G:256:PHE:HA   | 1:G:261:TYR:O    | 2.18                     | 0.44              |
| 1:G:272:LEU:O    | 1:G:274:LYS:N    | 2.47                     | 0.44              |
| 1:G:465:ASP:O    | 1:G:465:ASP:CG   | 2.59                     | 0.44              |
| 4:G:999:ALF:F4   | 5:G:998:ADP:PB   | 2.64                     | 0.44              |
| 2:H:76:ILE:O     | 2:H:79:ASN:CG    | 2.60                     | 0.44              |
| 1:A:103:ASN:HD21 | 1:A:107:ARG:HD2  | 1.82                     | 0.44              |
| 1:A:145:LYS:CG   | 1:A:146:ARG:N    | 2.78                     | 0.44              |
| 1:A:189:LYS:O    | 1:A:192:GLN:HB3  | 2.17                     | 0.44              |
| 1:A:345:THR:O    | 1:A:346:GLU:C    | 2.61                     | 0.44              |
| 1:A:491:GLN:OE1  | 1:A:521:LEU:HG   | 2.16                     | 0.44              |
| 1:A:575:LEU:HD23 | 1:A:577:ASP:OD1  | 2.17                     | 0.44              |
| 1:A:745:GLY:H    | 1:G:819:LEU:CD2  | 2.31                     | 0.44              |
| 2:B:133:ASP:OD1  | 2:B:133:ASP:C    | 2.59                     | 0.44              |
| 1:C:102:HIS:O    | 1:C:103:ASN:C    | 2.59                     | 0.44              |
| 1:C:395:VAL:O    | 1:C:398:PHE:N    | 2.50                     | 0.44              |
| 1:C:540:LEU:C    | 1:C:542:ASP:H    | 2.26                     | 0.44              |
| 1:C:700:LEU:HD23 | 1:C:700:LEU:O    | 2.17                     | 0.44              |
| 1:E:3:GLN:O      | 1:E:4:LYS:O      | 2.36                     | 0.44              |
| 1:E:38:PRO:HG2   | 1:E:70:LEU:HD13  | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:145:LYS:HG3  | 1:E:146:ARG:NE   | 2.32                     | 0.44              |
| 1:E:409:VAL:HB   | 1:E:414:VAL:CG2  | 2.48                     | 0.44              |
| 1:E:553:THR:HG22 | 1:E:557:GLU:OE2  | 2.18                     | 0.44              |
| 1:E:663:TYR:CZ   | 1:E:667:LEU:HD13 | 2.52                     | 0.44              |
| 1:E:716:ILE:HA   | 1:E:719:GLN:HB2  | 1.98                     | 0.44              |
| 2:F:71:PRO:HA    | 2:F:74:GLN:NE2   | 2.32                     | 0.44              |
| 2:F:104:MET:H    | 2:F:104:MET:HG3  | 1.51                     | 0.44              |
| 1:G:101:LEU:O    | 1:G:102:HIS:C    | 2.61                     | 0.44              |
| 1:G:197:VAL:O    | 1:G:197:VAL:HG12 | 2.17                     | 0.44              |
| 1:G:257:ASP:C    | 1:G:257:ASP:OD1  | 2.60                     | 0.44              |
| 1:G:437:ARG:NE   | 1:G:625:TRP:HA   | 2.26                     | 0.44              |
| 1:A:22:ASN:O     | 1:A:22:ASN:ND2   | 2.51                     | 0.44              |
| 1:A:42:HIS:C     | 1:A:44:PHE:N     | 2.75                     | 0.44              |
| 1:A:146:ARG:NH1  | 1:A:159:THR:HG23 | 2.31                     | 0.44              |
| 1:A:171:GLN:HA   | 1:A:678:ASN:H    | 1.83                     | 0.44              |
| 1:A:234:PHE:CE1  | 1:A:289:ILE:HG12 | 2.53                     | 0.44              |
| 1:A:300:GLN:C    | 1:A:302:ARG:N    | 2.75                     | 0.44              |
| 1:A:391:MET:HB3  | 1:A:393:ILE:HG12 | 2.00                     | 0.44              |
| 1:A:466:ILE:HD12 | 1:A:467:ALA:O    | 2.16                     | 0.44              |
| 2:B:66:PHE:CD1   | 2:B:66:PHE:C     | 2.95                     | 0.44              |
| 1:C:53:LYS:HD2   | 1:C:58:THR:HG23  | 1.99                     | 0.44              |
| 1:C:145:LYS:HG3  | 1:C:146:ARG:NE   | 2.33                     | 0.44              |
| 1:C:153:ILE:C    | 1:C:155:ALA:N    | 2.74                     | 0.44              |
| 1:C:162:ARG:O    | 1:C:163:SER:C    | 2.61                     | 0.44              |
| 1:C:402:ILE:HG22 | 1:C:403:LEU:HG   | 1.99                     | 0.44              |
| 1:C:556:VAL:O    | 1:C:560:ILE:HG12 | 2.17                     | 0.44              |
| 1:C:613:LEU:C    | 1:C:615:GLN:H    | 2.25                     | 0.44              |
| 1:C:769:ILE:HD13 | 1:C:774:ILE:HG23 | 2.00                     | 0.44              |
| 2:D:71:PRO:HA    | 2:D:74:GLN:NE2   | 2.32                     | 0.44              |
| 1:E:153:ILE:C    | 1:E:155:ALA:N    | 2.75                     | 0.44              |
| 1:E:742:ILE:HG23 | 1:E:747:MET:HE2  | 1.99                     | 0.44              |
| 2:F:84:CYS:O     | 2:F:86:GLU:N     | 2.50                     | 0.44              |
| 1:G:610:THR:CG2  | 1:G:631:ILE:HG13 | 2.34                     | 0.44              |
| 2:H:4:SER:N      | 2:H:7:GLN:NE2    | 2.61                     | 0.44              |
| 2:H:85:PHE:CE1   | 2:H:144:VAL:HG12 | 2.52                     | 0.44              |
| 2:H:140:TYR:O    | 2:H:142:GLU:N    | 2.50                     | 0.44              |
| 1:A:12:PHE:CD1   | 1:A:111:GLY:HA3  | 2.53                     | 0.44              |
| 1:A:23:PRO:O     | 1:A:27:ALA:CB    | 2.66                     | 0.44              |
| 1:A:32:LYS:C     | 1:A:34:LEU:N     | 2.75                     | 0.44              |
| 1:A:152:HIS:ND1  | 1:A:154:TYR:N    | 2.62                     | 0.44              |
| 1:A:172:SER:OG   | 1:A:679:PRO:HA   | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:369:LYS:HG3  | 1:A:370:GLU:H    | 1.81                     | 0.44              |
| 1:A:408:LYS:HG2  | 1:A:412:ASP:O    | 2.17                     | 0.44              |
| 1:A:477:PHE:O    | 1:A:480:LEU:N    | 2.46                     | 0.44              |
| 1:A:565:ASN:O    | 1:A:565:ASN:CG   | 2.60                     | 0.44              |
| 2:B:55:LYS:H     | 2:B:58:GLU:HG2   | 1.83                     | 0.44              |
| 1:C:13:LEU:HD11  | 1:C:132:ILE:CB   | 2.32                     | 0.44              |
| 1:C:38:PRO:HG2   | 1:C:70:LEU:HD13  | 1.99                     | 0.44              |
| 1:C:228:ASN:N    | 1:C:229:PRO:CD   | 2.81                     | 0.44              |
| 1:C:253:ARG:O    | 1:C:265:ALA:HA   | 2.18                     | 0.44              |
| 2:D:128:VAL:O    | 2:D:129:ALA:C    | 2.60                     | 0.44              |
| 1:E:32:LYS:C     | 1:E:34:LEU:N     | 2.75                     | 0.44              |
| 1:E:361:GLN:CG   | 1:E:387:VAL:HG23 | 2.47                     | 0.44              |
| 1:E:425:PHE:CD1  | 1:E:425:PHE:C    | 2.96                     | 0.44              |
| 2:F:26:ILE:O     | 2:F:26:ILE:HG22  | 2.17                     | 0.44              |
| 2:F:27:LEU:C     | 2:F:29:SER:N     | 2.76                     | 0.44              |
| 1:G:116:TYR:HD1  | 1:G:121:CYS:HB2  | 1.82                     | 0.44              |
| 1:G:153:ILE:C    | 1:G:155:ALA:N    | 2.75                     | 0.44              |
| 1:G:270:TYR:OH   | 1:G:670:LEU:HD22 | 2.17                     | 0.44              |
| 1:G:582:CYS:HA   | 1:G:590:VAL:O    | 2.18                     | 0.44              |
| 1:A:257:ASP:C    | 1:A:257:ASP:OD1  | 2.57                     | 0.44              |
| 1:A:404:THR:OG1  | 1:A:404:THR:O    | 2.31                     | 0.44              |
| 1:A:405:PRO:C    | 1:A:407:ILE:N    | 2.76                     | 0.44              |
| 1:A:475:ASN:HB2  | 1:A:592:TYR:HA   | 1.99                     | 0.44              |
| 2:B:20:ARG:HE    | 2:B:20:ARG:HB2   | 1.47                     | 0.44              |
| 1:C:88:ASP:HB3   | 1:C:91:GLU:CD    | 2.42                     | 0.44              |
| 1:C:305:LEU:HB2  | 1:C:307:LEU:HG   | 1.98                     | 0.44              |
| 1:C:359:VAL:O    | 1:C:359:VAL:CG1  | 2.66                     | 0.44              |
| 1:C:521:LEU:O    | 1:C:522:GLN:C    | 2.60                     | 0.44              |
| 1:C:604:PRO:O    | 1:C:605:LEU:HB2  | 2.17                     | 0.44              |
| 2:D:9:ALA:HA     | 2:D:12:LYS:CE    | 2.47                     | 0.44              |
| 2:D:50:VAL:O     | 2:D:51:LEU:HD23  | 2.18                     | 0.44              |
| 1:E:44:PHE:CD2   | 1:E:98:ALA:HA    | 2.53                     | 0.44              |
| 1:E:141:TYR:CE1  | 1:E:149:MET:HB3  | 2.53                     | 0.44              |
| 1:E:419:THR:O    | 1:E:422:GLN:N    | 2.51                     | 0.44              |
| 1:E:610:THR:CG2  | 1:E:631:ILE:HG13 | 2.33                     | 0.44              |
| 2:F:25:LYS:HE3   | 2:F:65:LYS:HE2   | 2.00                     | 0.44              |
| 2:F:86:GLU:H     | 2:F:86:GLU:CD    | 2.25                     | 0.44              |
| 2:F:104:MET:C    | 2:F:106:ALA:N    | 2.74                     | 0.44              |
| 2:F:128:VAL:HG23 | 2:F:129:ALA:N    | 2.33                     | 0.44              |
| 1:G:37:VAL:CB    | 1:G:38:PRO:HD2   | 2.47                     | 0.44              |
| 1:G:51:GLU:HB3   | 1:G:53:LYS:HD2   | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:153:ILE:CG2  | 1:G:154:TYR:N    | 2.81                     | 0.44              |
| 1:G:261:TYR:CD1  | 1:G:261:TYR:N    | 2.86                     | 0.44              |
| 1:G:375:GLN:HG3  | 1:G:418:GLN:O    | 2.18                     | 0.44              |
| 1:G:405:PRO:C    | 1:G:407:ILE:N    | 2.75                     | 0.44              |
| 1:G:407:ILE:CD1  | 1:G:409:VAL:H    | 2.30                     | 0.44              |
| 1:G:575:LEU:HD23 | 1:G:577:ASP:OD1  | 2.18                     | 0.44              |
| 2:H:98:GLU:O     | 2:H:100:ASN:OD1  | 2.36                     | 0.44              |
| 1:A:116:TYR:HD1  | 1:A:121:CYS:HB2  | 1.82                     | 0.44              |
| 1:A:326:GLN:CG   | 1:A:331:MET:HE3  | 2.48                     | 0.44              |
| 1:A:540:LEU:C    | 1:A:542:ASP:N    | 2.74                     | 0.44              |
| 1:A:746:PHE:O    | 1:G:816:GLN:CD   | 2.60                     | 0.44              |
| 1:A:799:PHE:O    | 1:A:800:GLN:C    | 2.60                     | 0.44              |
| 2:B:98:GLU:O     | 2:B:100:ASN:OD1  | 2.36                     | 0.44              |
| 1:C:88:ASP:O     | 1:C:91:GLU:HB2   | 2.18                     | 0.44              |
| 1:C:267:ILE:CD1  | 1:C:450:LEU:HD12 | 2.48                     | 0.44              |
| 1:C:280:GLN:NE2  | 1:C:280:GLN:N    | 2.66                     | 0.44              |
| 1:C:354:ARG:HG3  | 1:C:355:VAL:N    | 2.32                     | 0.44              |
| 2:D:14:ALA:HB3   | 2:D:38:LEU:HD21  | 2.00                     | 0.44              |
| 1:E:566:HIS:CE1  | 1:E:568:LYS:HB2  | 2.52                     | 0.44              |
| 1:E:767:TYR:O    | 1:E:768:ARG:HD3  | 2.18                     | 0.44              |
| 2:F:9:ALA:HA     | 2:F:12:LYS:CE    | 2.47                     | 0.44              |
| 2:F:125:GLU:O    | 2:F:129:ALA:CB   | 2.66                     | 0.44              |
| 1:G:138:ILE:HG21 | 1:G:196:VAL:HG11 | 1.99                     | 0.44              |
| 1:G:226:GLN:HG2  | 1:G:341:ILE:HB   | 1.99                     | 0.44              |
| 1:G:278:ILE:C    | 1:G:279:ARG:HG3  | 2.43                     | 0.44              |
| 1:G:365:ILE:HD11 | 1:G:384:ALA:HB2  | 2.00                     | 0.44              |
| 1:G:395:VAL:O    | 1:G:398:PHE:N    | 2.51                     | 0.44              |
| 2:H:35:MET:CE    | 2:H:73:MET:HA    | 2.47                     | 0.44              |
| 2:H:120:THR:HG23 | 2:H:123:GLU:CG   | 2.48                     | 0.44              |
| 1:A:742:ILE:HD13 | 1:A:756:MET:HE3  | 2.00                     | 0.44              |
| 1:C:42:HIS:C     | 1:C:44:PHE:N     | 2.75                     | 0.44              |
| 1:C:45:GLU:OE2   | 1:C:61:LEU:HB3   | 2.18                     | 0.44              |
| 1:C:88:ASP:O     | 1:C:89:MET:C     | 2.61                     | 0.44              |
| 1:C:236:ASN:HD22 | 1:C:245:SER:C    | 2.26                     | 0.44              |
| 1:C:275:SER:O    | 1:C:278:ILE:HG12 | 2.18                     | 0.44              |
| 1:C:288:HIS:O    | 1:C:289:ILE:C    | 2.60                     | 0.44              |
| 1:C:370:GLU:OE1  | 1:C:372:ASN:HB2  | 2.18                     | 0.44              |
| 1:C:388:CYS:SG   | 1:C:393:ILE:HD11 | 2.57                     | 0.44              |
| 1:E:51:GLU:HB3   | 1:E:53:LYS:HD2   | 2.00                     | 0.44              |
| 1:E:128:LYS:HG2  | 1:E:129:GLN:N    | 2.32                     | 0.44              |
| 1:E:280:GLN:CD   | 1:E:280:GLN:N    | 2.76                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:285:ARG:HG2  | 1:E:291:TYR:CZ   | 2.52                     | 0.44              |
| 1:E:294:ILE:HB   | 1:E:310:PHE:CZ   | 2.53                     | 0.44              |
| 1:E:619:LYS:O    | 1:E:622:ALA:CB   | 2.63                     | 0.44              |
| 1:G:33:LYS:O     | 1:G:49:ILE:HG13  | 2.18                     | 0.44              |
| 1:G:236:ASN:HD22 | 1:G:245:SER:C    | 2.25                     | 0.44              |
| 1:G:306:LEU:HD22 | 1:G:386:LYS:HD3  | 1.99                     | 0.44              |
| 1:G:352:ILE:HG22 | 1:G:438:LEU:HD21 | 2.00                     | 0.44              |
| 1:G:369:LYS:HG3  | 1:G:370:GLU:H    | 1.82                     | 0.44              |
| 1:G:409:VAL:HB   | 1:G:414:VAL:CG2  | 2.48                     | 0.44              |
| 1:G:606:ASN:OD1  | 1:G:608:ASN:HB2  | 2.17                     | 0.44              |
| 1:G:728:GLN:O    | 1:G:728:GLN:NE2  | 2.51                     | 0.44              |
| 2:H:9:ALA:HA     | 2:H:12:LYS:CE    | 2.48                     | 0.44              |
| 2:H:86:GLU:N     | 2:H:86:GLU:CD    | 2.75                     | 0.44              |
| 1:A:3:GLN:O      | 1:A:4:LYS:O      | 2.36                     | 0.43              |
| 1:A:33:LYS:CG    | 1:A:49:ILE:HB    | 2.48                     | 0.43              |
| 1:A:87:GLU:OE1   | 1:A:107:ARG:NH2  | 2.51                     | 0.43              |
| 1:A:172:SER:HA   | 1:A:462:GLY:O    | 2.17                     | 0.43              |
| 1:A:251:PHE:CD1  | 1:A:251:PHE:O    | 2.71                     | 0.43              |
| 1:A:610:THR:HG22 | 1:A:628:VAL:HG11 | 2.00                     | 0.43              |
| 1:A:743:PRO:HB2  | 1:G:816:GLN:CG   | 2.47                     | 0.43              |
| 1:C:172:SER:HA   | 1:C:462:GLY:O    | 2.18                     | 0.43              |
| 1:C:367:PHE:CE1  | 1:C:378:MET:SD   | 3.11                     | 0.43              |
| 1:C:575:LEU:HA   | 1:C:577:ASP:OD2  | 2.17                     | 0.43              |
| 1:C:576:LYS:C    | 1:C:579:THR:H    | 2.26                     | 0.43              |
| 1:C:771:GLN:O    | 1:C:771:GLN:NE2  | 2.49                     | 0.43              |
| 1:E:138:ILE:HG21 | 1:E:196:VAL:HG11 | 2.00                     | 0.43              |
| 1:E:362:LEU:HD12 | 1:E:387:VAL:HG13 | 2.00                     | 0.43              |
| 1:E:620:PHE:O    | 1:E:624:LEU:HB2  | 2.18                     | 0.43              |
| 1:G:88:ASP:HB3   | 1:G:91:GLU:CD    | 2.42                     | 0.43              |
| 1:G:176:THR:O    | 1:G:183:LYS:HD2  | 2.18                     | 0.43              |
| 1:G:485:THR:HA   | 1:G:488:LYS:HB2  | 2.00                     | 0.43              |
| 1:G:545:CYS:HA   | 1:G:598:LEU:HD22 | 2.01                     | 0.43              |
| 1:G:621:VAL:HG12 | 1:G:625:TRP:CD1  | 2.53                     | 0.43              |
| 2:H:50:VAL:O     | 2:H:51:LEU:HD23  | 2.18                     | 0.43              |
| 2:H:140:TYR:CE1  | 2:H:141:GLU:HG2  | 2.53                     | 0.43              |
| 2:H:144:VAL:O    | 2:H:147:VAL:HG23 | 2.18                     | 0.43              |
| 1:A:121:CYS:SG   | 1:A:156:ILE:HD11 | 2.58                     | 0.43              |
| 1:A:256:PHE:HA   | 1:A:261:TYR:O    | 2.19                     | 0.43              |
| 1:A:256:PHE:CE1  | 1:A:262:ILE:HG13 | 2.52                     | 0.43              |
| 1:A:375:GLN:O    | 1:A:376:ALA:C    | 2.61                     | 0.43              |
| 1:A:399:THR:C    | 1:A:403:LEU:HD12 | 2.43                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:442:ILE:O    | 1:A:445:ARG:N    | 2.43                     | 0.43              |
| 1:A:487:GLU:OE1  | 1:A:585:HIS:HA   | 2.18                     | 0.43              |
| 1:A:728:GLN:CA   | 1:A:728:GLN:NE2  | 2.80                     | 0.43              |
| 1:C:407:ILE:HD12 | 1:C:408:LYS:C    | 2.42                     | 0.43              |
| 2:D:66:PHE:CD1   | 2:D:66:PHE:C     | 2.95                     | 0.43              |
| 2:D:128:VAL:HG23 | 2:D:129:ALA:N    | 2.33                     | 0.43              |
| 1:E:98:ALA:O     | 1:E:101:LEU:HB3  | 2.18                     | 0.43              |
| 1:E:362:LEU:CD2  | 1:E:427:ILE:HG13 | 2.48                     | 0.43              |
| 1:E:532:THR:C    | 1:E:533:ASN:O    | 2.59                     | 0.43              |
| 2:F:111:VAL:HA   | 2:F:115:LEU:HD13 | 1.99                     | 0.43              |
| 2:F:143:LEU:O    | 2:F:147:VAL:HG22 | 2.18                     | 0.43              |
| 1:G:42:HIS:C     | 1:G:44:PHE:N     | 2.76                     | 0.43              |
| 1:G:158:ASP:HB2  | 1:G:193:TYR:CZ   | 2.54                     | 0.43              |
| 1:G:762:LEU:HD13 | 1:G:766:LEU:HD12 | 2.00                     | 0.43              |
| 2:H:84:CYS:N     | 2:H:88:TYR:CE2   | 2.86                     | 0.43              |
| 1:A:45:GLU:OE2   | 1:A:61:LEU:HB3   | 2.19                     | 0.43              |
| 1:A:407:ILE:CG1  | 1:A:414:VAL:O    | 2.63                     | 0.43              |
| 1:A:606:ASN:OD1  | 1:A:608:ASN:HB2  | 2.18                     | 0.43              |
| 1:C:33:LYS:O     | 1:C:49:ILE:HG13  | 2.18                     | 0.43              |
| 1:C:265:ALA:O    | 1:C:450:LEU:HB2  | 2.18                     | 0.43              |
| 1:C:405:PRO:O    | 1:C:407:ILE:HG23 | 2.19                     | 0.43              |
| 1:C:425:PHE:CD1  | 1:C:425:PHE:C    | 2.97                     | 0.43              |
| 1:C:573:LYS:N    | 1:C:573:LYS:HD2  | 2.32                     | 0.43              |
| 1:C:610:THR:HG21 | 1:C:628:VAL:HG13 | 2.00                     | 0.43              |
| 2:D:18:PHE:CD2   | 2:D:34:VAL:HG22  | 2.53                     | 0.43              |
| 1:E:45:GLU:OE2   | 1:E:61:LEU:HB3   | 2.18                     | 0.43              |
| 1:E:405:PRO:C    | 1:E:407:ILE:N    | 2.76                     | 0.43              |
| 1:E:785:GLU:CD   | 1:E:788:ARG:HH21 | 2.26                     | 0.43              |
| 1:G:270:TYR:CZ   | 1:G:670:LEU:HD22 | 2.53                     | 0.43              |
| 1:G:388:CYS:SG   | 1:G:393:ILE:HD11 | 2.58                     | 0.43              |
| 1:G:547:PHE:C    | 1:G:547:PHE:CD1  | 2.94                     | 0.43              |
| 2:H:27:LEU:C     | 2:H:29:SER:N     | 2.76                     | 0.43              |
| 1:A:9:ASP:O      | 1:A:12:PHE:HB2   | 2.18                     | 0.43              |
| 1:A:239:THR:C    | 1:A:241:LYS:N    | 2.75                     | 0.43              |
| 1:A:323:ILE:HG23 | 1:A:323:ILE:O    | 2.18                     | 0.43              |
| 1:A:344:PHE:N    | 1:A:344:PHE:CD1  | 2.86                     | 0.43              |
| 1:A:373:THR:O    | 1:A:374:ASP:HB2  | 2.19                     | 0.43              |
| 1:A:413:VAL:O    | 1:A:415:GLN:N    | 2.51                     | 0.43              |
| 1:A:419:THR:O    | 1:A:422:GLN:N    | 2.51                     | 0.43              |
| 1:A:468:GLY:O    | 1:A:469:PHE:C    | 2.61                     | 0.43              |
| 1:A:767:TYR:CD1  | 1:A:767:TYR:C    | 2.96                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:85:PHE:CZ    | 2:B:145:ARG:NH1  | 2.86                     | 0.43              |
| 2:B:96:ASP:O     | 2:B:98:GLU:N     | 2.52                     | 0.43              |
| 1:C:148:GLU:C    | 1:C:149:MET:HG2  | 2.42                     | 0.43              |
| 1:C:405:PRO:CD   | 1:C:416:LYS:O    | 2.66                     | 0.43              |
| 1:E:302:ARG:CZ   | 1:E:303:ASN:HA   | 2.49                     | 0.43              |
| 1:E:345:THR:O    | 1:E:346:GLU:C    | 2.61                     | 0.43              |
| 1:E:437:ARG:NH2  | 1:E:625:TRP:HE3  | 2.16                     | 0.43              |
| 2:F:66:PHE:CD1   | 2:F:66:PHE:C     | 2.95                     | 0.43              |
| 2:F:111:VAL:HG12 | 2:F:112:LEU:HD23 | 2.00                     | 0.43              |
| 1:G:83:PHE:CZ    | 1:G:92:LEU:HA    | 2.54                     | 0.43              |
| 1:G:625:TRP:C    | 1:G:627:ASP:N    | 2.76                     | 0.43              |
| 2:H:16:GLN:C     | 2:H:18:PHE:H     | 2.25                     | 0.43              |
| 2:H:104:MET:H    | 2:H:104:MET:HG3  | 1.48                     | 0.43              |
| 2:H:109:ARG:NH2  | 2:H:132:GLU:OE2  | 2.50                     | 0.43              |
| 1:A:33:LYS:O     | 1:A:49:ILE:HG13  | 2.18                     | 0.43              |
| 1:A:46:ALA:HB1   | 1:A:62:GLN:HG2   | 2.00                     | 0.43              |
| 1:A:60:GLU:OE1   | 1:A:67:LYS:HD2   | 2.17                     | 0.43              |
| 1:A:607:ASP:OD1  | 1:A:607:ASP:N    | 2.34                     | 0.43              |
| 2:B:27:LEU:C     | 2:B:29:SER:N     | 2.76                     | 0.43              |
| 2:B:96:ASP:C     | 2:B:96:ASP:OD1   | 2.62                     | 0.43              |
| 2:B:124:VAL:HG23 | 2:B:125:GLU:N    | 2.33                     | 0.43              |
| 1:C:87:GLU:OE1   | 1:C:87:GLU:HA    | 2.18                     | 0.43              |
| 1:C:101:LEU:O    | 1:C:102:HIS:C    | 2.62                     | 0.43              |
| 1:C:104:LEU:CD1  | 1:C:705:LEU:HD11 | 2.48                     | 0.43              |
| 1:C:347:GLU:H    | 1:C:347:GLU:HG3  | 1.55                     | 0.43              |
| 1:C:365:ILE:HD13 | 1:C:427:ILE:CD1  | 2.47                     | 0.43              |
| 1:C:558:LYS:O    | 1:C:561:GLN:N    | 2.51                     | 0.43              |
| 1:C:606:ASN:OD1  | 1:C:608:ASN:HB2  | 2.17                     | 0.43              |
| 1:E:80:PRO:CD    | 1:E:83:PHE:CD2   | 2.99                     | 0.43              |
| 1:E:88:ASP:HB3   | 1:E:91:GLU:CD    | 2.44                     | 0.43              |
| 1:E:132:ILE:HD12 | 1:E:152:HIS:HD2  | 1.83                     | 0.43              |
| 1:E:326:GLN:CG   | 1:E:331:MET:HE3  | 2.48                     | 0.43              |
| 1:E:409:VAL:HG13 | 1:E:634:LEU:HD12 | 2.00                     | 0.43              |
| 1:E:504:GLU:OE2  | 1:E:508:GLU:HG2  | 2.18                     | 0.43              |
| 1:E:553:THR:HG23 | 1:E:579:THR:CG2  | 2.49                     | 0.43              |
| 1:E:806:TYR:C    | 1:E:808:ALA:N    | 2.76                     | 0.43              |
| 1:G:311:ASN:C    | 1:G:312:ASN:HD22 | 2.26                     | 0.43              |
| 1:G:349:GLN:HA   | 1:G:352:ILE:HG13 | 2.00                     | 0.43              |
| 1:A:288:HIS:O    | 1:A:289:ILE:C    | 2.61                     | 0.43              |
| 1:A:349:GLN:HA   | 1:A:352:ILE:HG13 | 2.01                     | 0.43              |
| 1:A:375:GLN:HG3  | 1:A:418:GLN:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:686:ILE:HG22 | 1:A:686:ILE:O    | 2.17                     | 0.43              |
| 1:C:39:SER:OG    | 1:C:42:HIS:HB2   | 2.19                     | 0.43              |
| 1:C:329:ASP:OD1  | 1:C:329:ASP:N    | 2.42                     | 0.43              |
| 1:C:814:LYS:CE   | 1:C:818:GLN:HE22 | 2.22                     | 0.43              |
| 1:E:37:VAL:CB    | 1:E:38:PRO:HD2   | 2.48                     | 0.43              |
| 1:E:88:ASP:O     | 1:E:89:MET:C     | 2.61                     | 0.43              |
| 1:E:152:HIS:ND1  | 1:E:154:TYR:N    | 2.63                     | 0.43              |
| 1:E:298:SER:O    | 1:E:299:GLU:C    | 2.61                     | 0.43              |
| 1:E:323:ILE:HG23 | 1:E:323:ILE:O    | 2.19                     | 0.43              |
| 1:E:582:CYS:HA   | 1:E:590:VAL:O    | 2.19                     | 0.43              |
| 1:E:619:LYS:HA   | 1:E:622:ALA:CB   | 2.48                     | 0.43              |
| 2:F:3:PHE:C      | 2:F:7:GLN:HE21   | 2.26                     | 0.43              |
| 1:G:102:HIS:O    | 1:G:103:ASN:C    | 2.61                     | 0.43              |
| 1:G:514:PHE:CG   | 1:G:515:ILE:N    | 2.86                     | 0.43              |
| 2:H:14:ALA:HB3   | 2:H:38:LEU:HD21  | 2.00                     | 0.43              |
| 2:H:25:LYS:HE3   | 2:H:65:LYS:HE2   | 2.00                     | 0.43              |
| 2:H:114:THR:O    | 2:H:115:LEU:HD12 | 2.18                     | 0.43              |
| 1:A:102:HIS:O    | 1:A:105:ARG:N    | 2.52                     | 0.43              |
| 1:A:376:ALA:CB   | 1:A:420:LYS:HB2  | 2.44                     | 0.43              |
| 1:A:391:MET:HG3  | 1:A:434:LYS:HZ2  | 1.84                     | 0.43              |
| 1:A:492:LEU:O    | 1:A:496:THR:OG1  | 2.37                     | 0.43              |
| 1:A:530:ARG:HA   | 1:A:531:PRO:HD3  | 1.79                     | 0.43              |
| 1:A:797:ILE:CG1  | 2:B:117:GLU:HG2  | 2.49                     | 0.43              |
| 2:B:50:VAL:O     | 2:B:51:LEU:HD23  | 2.18                     | 0.43              |
| 2:B:111:VAL:HA   | 2:B:115:LEU:HD13 | 2.00                     | 0.43              |
| 1:C:182:GLY:HA2  | 5:C:998:ADP:O1A  | 2.19                     | 0.43              |
| 1:C:278:ILE:C    | 1:C:279:ARG:HG3  | 2.44                     | 0.43              |
| 1:C:298:SER:O    | 1:C:299:GLU:C    | 2.61                     | 0.43              |
| 1:C:361:GLN:CG   | 1:C:387:VAL:HG23 | 2.48                     | 0.43              |
| 1:C:373:THR:O    | 1:C:374:ASP:HB2  | 2.19                     | 0.43              |
| 1:C:382:THR:CA   | 1:C:385:GLN:HB3  | 2.49                     | 0.43              |
| 1:C:394:ASN:OD1  | 1:C:397:ASP:OD2  | 2.37                     | 0.43              |
| 1:C:407:ILE:HD12 | 1:C:408:LYS:CA   | 2.48                     | 0.43              |
| 1:C:619:LYS:HA   | 1:C:622:ALA:CB   | 2.49                     | 0.43              |
| 1:E:145:LYS:CG   | 1:E:146:ARG:N    | 2.81                     | 0.43              |
| 1:E:231:LEU:HD23 | 1:E:231:LEU:N    | 2.33                     | 0.43              |
| 1:E:239:THR:C    | 1:E:241:LYS:N    | 2.77                     | 0.43              |
| 1:E:247:ARG:HH22 | 1:E:470:GLU:CD   | 2.26                     | 0.43              |
| 1:E:540:LEU:C    | 1:E:542:ASP:N    | 2.77                     | 0.43              |
| 1:G:293:LEU:O    | 1:G:297:ALA:HB2  | 2.19                     | 0.43              |
| 1:G:465:ASP:OD1  | 1:G:465:ASP:C    | 2.61                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:474:ILE:H    | 1:G:474:ILE:HG13 | 1.47                     | 0.43              |
| 1:G:525:ILE:O    | 1:G:529:GLU:HB3  | 2.18                     | 0.43              |
| 1:G:711:LEU:N    | 1:G:711:LEU:CD2  | 2.81                     | 0.43              |
| 2:H:122:GLU:O    | 2:H:123:GLU:C    | 2.62                     | 0.43              |
| 1:A:250:LYS:CE   | 1:A:465:ASP:OD2  | 2.66                     | 0.43              |
| 1:A:395:VAL:O    | 1:A:398:PHE:N    | 2.52                     | 0.43              |
| 1:A:409:VAL:HG13 | 1:A:634:LEU:HD11 | 1.99                     | 0.43              |
| 1:A:522:GLN:OE1  | 1:A:525:ILE:HD12 | 2.19                     | 0.43              |
| 1:A:582:CYS:HA   | 1:A:590:VAL:O    | 2.19                     | 0.43              |
| 1:A:613:LEU:C    | 1:A:615:GLN:H    | 2.27                     | 0.43              |
| 2:B:25:LYS:HE3   | 2:B:65:LYS:HE2   | 2.00                     | 0.43              |
| 1:C:195:ALA:O    | 1:C:199:SER:HB3  | 2.18                     | 0.43              |
| 1:C:541:LEU:HD22 | 1:C:597:TRP:HE3  | 1.84                     | 0.43              |
| 1:C:543:GLU:HG2  | 1:C:544:GLU:N    | 2.30                     | 0.43              |
| 1:C:572:SER:HB2  | 1:C:580:GLU:HG3  | 2.01                     | 0.43              |
| 1:C:582:CYS:HA   | 1:C:590:VAL:O    | 2.19                     | 0.43              |
| 1:C:607:ASP:C    | 1:C:610:THR:HB   | 2.44                     | 0.43              |
| 1:C:696:LEU:C    | 1:C:696:LEU:HD12 | 2.43                     | 0.43              |
| 2:D:55:LYS:H     | 2:D:58:GLU:HG2   | 1.82                     | 0.43              |
| 1:E:42:HIS:C     | 1:E:44:PHE:N     | 2.76                     | 0.43              |
| 1:E:235:GLY:HA3  | 1:E:248:PHE:CE1  | 2.54                     | 0.43              |
| 1:E:280:GLN:N    | 1:E:280:GLN:NE2  | 2.67                     | 0.43              |
| 1:E:280:GLN:NE2  | 1:E:315:PHE:O    | 2.46                     | 0.43              |
| 1:E:327:GLN:HB3  | 1:E:330:GLU:CG   | 2.49                     | 0.43              |
| 1:E:344:PHE:N    | 1:E:344:PHE:CD1  | 2.85                     | 0.43              |
| 1:E:415:GLN:OE1  | 1:E:416:LYS:N    | 2.51                     | 0.43              |
| 2:F:139:ASN:OD1  | 2:F:142:GLU:HG2  | 2.18                     | 0.43              |
| 1:G:164:MET:CE   | 1:G:256:PHE:CE2  | 2.87                     | 0.43              |
| 1:G:195:ALA:O    | 1:G:199:SER:HB3  | 2.18                     | 0.43              |
| 1:G:532:THR:C    | 1:G:533:ASN:O    | 2.59                     | 0.43              |
| 2:H:104:MET:O    | 2:H:106:ALA:N    | 2.51                     | 0.43              |
| 1:A:318:ASN:O    | 1:A:319:GLY:C    | 2.59                     | 0.43              |
| 1:A:425:PHE:CD1  | 1:A:425:PHE:C    | 2.96                     | 0.43              |
| 1:A:748:ASP:O    | 1:A:749:GLY:C    | 2.59                     | 0.43              |
| 1:A:750:LYS:O    | 1:A:751:GLN:C    | 2.61                     | 0.43              |
| 1:A:806:TYR:HB3  | 2:B:147:VAL:HG12 | 2.01                     | 0.43              |
| 1:C:171:GLN:HA   | 1:C:678:ASN:H    | 1.84                     | 0.43              |
| 1:C:730:PHE:C    | 1:C:732:GLN:H    | 2.26                     | 0.43              |
| 1:C:763:ASP:C    | 1:C:765:ASN:H    | 2.26                     | 0.43              |
| 2:D:41:ASN:N     | 2:D:42:PRO:CD    | 2.82                     | 0.43              |
| 2:D:87:ASP:O     | 2:D:88:TYR:C     | 2.61                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:111:VAL:HA   | 2:D:115:LEU:HD13 | 2.00                     | 0.43              |
| 1:E:404:THR:OG1  | 1:E:404:THR:O    | 2.30                     | 0.43              |
| 1:E:575:LEU:C    | 1:E:577:ASP:H    | 2.26                     | 0.43              |
| 1:E:817:GLN:HG2  | 1:E:818:GLN:OE1  | 2.19                     | 0.43              |
| 1:G:88:ASP:O     | 1:G:91:GLU:HB2   | 2.19                     | 0.43              |
| 1:G:298:SER:O    | 1:G:299:GLU:C    | 2.62                     | 0.43              |
| 1:G:323:ILE:HG23 | 1:G:323:ILE:O    | 2.18                     | 0.43              |
| 1:G:540:LEU:C    | 1:G:542:ASP:N    | 2.75                     | 0.43              |
| 2:H:133:ASP:OD1  | 2:H:133:ASP:C    | 2.61                     | 0.43              |
| 1:A:26:GLN:C     | 1:A:26:GLN:HE21  | 2.27                     | 0.43              |
| 1:A:361:GLN:CG   | 1:A:387:VAL:HG23 | 2.49                     | 0.43              |
| 1:A:480:LEU:HA   | 1:A:592:TYR:CE1  | 2.54                     | 0.43              |
| 1:C:76:GLN:OE1   | 1:C:96:ASN:HB3   | 2.18                     | 0.43              |
| 1:C:96:ASN:C     | 1:C:98:ALA:N     | 2.75                     | 0.43              |
| 1:C:161:TYR:O    | 1:C:161:TYR:CG   | 2.71                     | 0.43              |
| 1:C:409:VAL:HG13 | 1:C:634:LEU:HD12 | 1.99                     | 0.43              |
| 1:C:467:ALA:O    | 1:C:486:ASN:ND2  | 2.44                     | 0.43              |
| 1:C:514:PHE:CG   | 1:C:515:ILE:N    | 2.86                     | 0.43              |
| 1:C:532:THR:C    | 1:C:533:ASN:O    | 2.60                     | 0.43              |
| 2:D:98:GLU:O     | 2:D:100:ASN:OD1  | 2.37                     | 0.43              |
| 1:E:172:SER:OG   | 1:E:679:PRO:HA   | 2.19                     | 0.43              |
| 1:E:371:ARG:H    | 1:E:371:ARG:HG3  | 1.42                     | 0.43              |
| 1:E:475:ASN:ND2  | 1:E:590:VAL:CG1  | 2.82                     | 0.43              |
| 1:E:741:ALA:O    | 1:E:755:LEU:HD23 | 2.19                     | 0.43              |
| 1:E:799:PHE:O    | 1:E:800:GLN:C    | 2.62                     | 0.43              |
| 1:E:804:ARG:NH1  | 1:E:804:ARG:CG   | 2.77                     | 0.43              |
| 2:F:50:VAL:O     | 2:F:51:LEU:HD23  | 2.18                     | 0.43              |
| 2:F:76:ILE:O     | 2:F:79:ASN:CG    | 2.62                     | 0.43              |
| 1:G:180:GLY:C    | 1:G:182:GLY:H    | 2.27                     | 0.43              |
| 1:G:275:SER:O    | 1:G:278:ILE:HG12 | 2.19                     | 0.43              |
| 1:G:409:VAL:HG13 | 1:G:634:LEU:HD12 | 2.00                     | 0.43              |
| 1:G:466:ILE:HD12 | 1:G:467:ALA:O    | 2.18                     | 0.43              |
| 1:G:704:GLN:O    | 1:G:708:ASN:HB2  | 2.19                     | 0.43              |
| 2:H:3:PHE:C      | 2:H:7:GLN:HE21   | 2.27                     | 0.43              |
| 1:A:13:LEU:HG    | 1:A:132:ILE:CG2  | 2.49                     | 0.42              |
| 1:A:39:SER:OG    | 1:A:42:HIS:HB2   | 2.19                     | 0.42              |
| 1:A:225:LEU:HD12 | 1:A:225:LEU:HA   | 1.89                     | 0.42              |
| 1:A:356:VAL:O    | 1:A:360:LEU:HD12 | 2.19                     | 0.42              |
| 1:A:407:ILE:CD1  | 1:A:409:VAL:H    | 2.30                     | 0.42              |
| 1:A:541:LEU:HD11 | 1:A:597:TRP:HB3  | 2.00                     | 0.42              |
| 1:A:742:ILE:HG23 | 1:A:747:MET:HE2  | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:769:ILE:HD13 | 1:A:769:ILE:HA   | 1.78                     | 0.42              |
| 2:B:76:ILE:O     | 2:B:79:ASN:CG    | 2.62                     | 0.42              |
| 1:C:89:MET:HG2   | 1:C:116:TYR:O    | 2.18                     | 0.42              |
| 1:C:174:LEU:HD12 | 1:C:681:PHE:CE1  | 2.53                     | 0.42              |
| 1:C:180:GLY:C    | 1:C:182:GLY:H    | 2.26                     | 0.42              |
| 1:C:345:THR:O    | 1:C:346:GLU:C    | 2.62                     | 0.42              |
| 1:C:465:ASP:OD1  | 1:C:465:ASP:C    | 2.62                     | 0.42              |
| 1:C:762:LEU:HD13 | 1:C:766:LEU:HD13 | 2.01                     | 0.42              |
| 1:E:37:VAL:HG13  | 1:E:75:ILE:HG22  | 2.01                     | 0.42              |
| 1:E:51:GLU:CG    | 1:E:53:LYS:HE3   | 2.48                     | 0.42              |
| 1:E:80:PRO:CD    | 1:E:83:PHE:HD2   | 2.32                     | 0.42              |
| 1:E:183:LYS:HE2  | 1:E:183:LYS:HB2  | 1.65                     | 0.42              |
| 1:E:375:GLN:HG3  | 1:E:418:GLN:O    | 2.19                     | 0.42              |
| 1:E:491:GLN:OE1  | 1:E:521:LEU:HG   | 2.19                     | 0.42              |
| 1:E:619:LYS:HA   | 1:E:622:ALA:HB3  | 2.01                     | 0.42              |
| 1:E:623:ASP:HA   | 1:E:626:LYS:HB3  | 2.01                     | 0.42              |
| 1:E:696:LEU:HD12 | 1:E:696:LEU:C    | 2.44                     | 0.42              |
| 1:E:748:ASP:O    | 1:E:749:GLY:C    | 2.62                     | 0.42              |
| 2:F:41:ASN:N     | 2:F:42:PRO:CD    | 2.82                     | 0.42              |
| 2:F:98:GLU:O     | 2:F:100:ASN:OD1  | 2.37                     | 0.42              |
| 1:G:33:LYS:CG    | 1:G:49:ILE:HB    | 2.48                     | 0.42              |
| 1:G:146:ARG:NH1  | 1:G:159:THR:HG23 | 2.34                     | 0.42              |
| 1:G:164:MET:SD   | 1:G:256:PHE:HD2  | 2.41                     | 0.42              |
| 1:G:419:THR:O    | 1:G:421:GLU:N    | 2.51                     | 0.42              |
| 1:G:619:LYS:HA   | 1:G:622:ALA:HB3  | 2.00                     | 0.42              |
| 2:H:41:ASN:N     | 2:H:42:PRO:CD    | 2.82                     | 0.42              |
| 2:H:98:GLU:C     | 2:H:100:ASN:N    | 2.77                     | 0.42              |
| 1:A:71:SER:HB3   | 1:A:73:ASP:OD2   | 2.19                     | 0.42              |
| 1:A:405:PRO:HB2  | 1:A:407:ILE:HG22 | 1.98                     | 0.42              |
| 1:C:349:GLN:HA   | 1:C:352:ILE:HG13 | 2.00                     | 0.42              |
| 1:C:359:VAL:O    | 1:C:359:VAL:HG12 | 2.19                     | 0.42              |
| 1:C:478:GLU:OE1  | 1:C:478:GLU:N    | 2.26                     | 0.42              |
| 2:D:135:ASN:ND2  | 2:D:135:ASN:N    | 2.67                     | 0.42              |
| 1:E:154:TYR:OH   | 1:E:192:GLN:NE2  | 2.53                     | 0.42              |
| 1:E:243:ASP:CB   | 1:E:323:ILE:HD11 | 2.46                     | 0.42              |
| 1:E:382:THR:HA   | 1:E:385:GLN:CD   | 2.44                     | 0.42              |
| 1:E:540:LEU:C    | 1:E:542:ASP:H    | 2.27                     | 0.42              |
| 1:E:545:CYS:SG   | 1:E:602:MET:SD   | 3.17                     | 0.42              |
| 1:E:730:PHE:C    | 1:E:732:GLN:H    | 2.25                     | 0.42              |
| 1:E:814:LYS:C    | 1:E:816:GLN:H    | 2.26                     | 0.42              |
| 2:F:95:PHE:CZ    | 2:F:111:VAL:HG21 | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:240:VAL:HG22 | 1:G:472:PHE:CE1  | 2.54                     | 0.42              |
| 1:G:382:THR:CA   | 1:G:385:GLN:HB3  | 2.49                     | 0.42              |
| 1:G:426:ALA:C    | 1:G:428:GLU:N    | 2.77                     | 0.42              |
| 1:G:702:LEU:HD12 | 1:G:702:LEU:HA   | 1.82                     | 0.42              |
| 1:G:763:ASP:H    | 1:G:766:LEU:CD1  | 2.31                     | 0.42              |
| 1:A:49:ILE:HG23  | 1:A:57:VAL:CG1   | 2.49                     | 0.42              |
| 1:A:178:GLU:O    | 1:A:183:LYS:NZ   | 2.53                     | 0.42              |
| 1:A:196:VAL:CG1  | 1:A:197:VAL:N    | 2.81                     | 0.42              |
| 1:A:275:SER:O    | 1:A:278:ILE:HG12 | 2.19                     | 0.42              |
| 1:A:715:ARG:HH21 | 1:A:719:GLN:CD   | 2.28                     | 0.42              |
| 2:B:18:PHE:CD2   | 2:B:34:VAL:HG22  | 2.54                     | 0.42              |
| 1:C:173:ILE:HD12 | 1:C:461:LEU:HD21 | 2.01                     | 0.42              |
| 1:C:413:VAL:O    | 1:C:415:GLN:N    | 2.53                     | 0.42              |
| 2:D:3:PHE:C      | 2:D:7:GLN:HE21   | 2.27                     | 0.42              |
| 2:D:27:LEU:C     | 2:D:29:SER:N     | 2.76                     | 0.42              |
| 1:E:60:GLU:OE1   | 1:E:67:LYS:HD2   | 2.18                     | 0.42              |
| 1:E:116:TYR:HD1  | 1:E:121:CYS:HB2  | 1.84                     | 0.42              |
| 1:E:135:GLU:CD   | 1:E:215:PHE:CB   | 2.89                     | 0.42              |
| 1:E:147:HIS:C    | 1:E:149:MET:N    | 2.77                     | 0.42              |
| 1:E:291:TYR:HD2  | 1:E:310:PHE:HE2  | 1.67                     | 0.42              |
| 1:E:469:PHE:CD2  | 1:E:587:ALA:HB3  | 2.54                     | 0.42              |
| 1:E:551:THR:O    | 1:E:554:SER:N    | 2.52                     | 0.42              |
| 2:F:127:LEU:HD11 | 2:F:147:VAL:HG13 | 2.02                     | 0.42              |
| 2:F:142:GLU:O    | 2:F:143:LEU:C    | 2.62                     | 0.42              |
| 1:G:37:VAL:HG13  | 1:G:75:ILE:HA    | 2.01                     | 0.42              |
| 1:G:121:CYS:SG   | 1:G:156:ILE:HD11 | 2.59                     | 0.42              |
| 1:G:133:TYR:HB3  | 1:G:154:TYR:OH   | 2.19                     | 0.42              |
| 1:G:138:ILE:HD11 | 1:G:154:TYR:CZ   | 2.54                     | 0.42              |
| 1:G:172:SER:OG   | 1:G:679:PRO:HA   | 2.20                     | 0.42              |
| 1:G:306:LEU:HD22 | 1:G:386:LYS:CD   | 2.49                     | 0.42              |
| 1:G:352:ILE:O    | 1:G:356:VAL:HG23 | 2.19                     | 0.42              |
| 1:G:522:GLN:N    | 1:G:523:PRO:CD   | 2.82                     | 0.42              |
| 2:H:18:PHE:CD2   | 2:H:34:VAL:HG22  | 2.54                     | 0.42              |
| 1:A:24:LEU:N     | 1:A:24:LEU:HD23  | 2.34                     | 0.42              |
| 1:A:176:THR:O    | 1:A:183:LYS:HD2  | 2.20                     | 0.42              |
| 1:A:527:LEU:HD23 | 1:A:527:LEU:C    | 2.41                     | 0.42              |
| 2:B:128:VAL:O    | 2:B:129:ALA:C    | 2.63                     | 0.42              |
| 1:C:302:ARG:CZ   | 1:C:303:ASN:HA   | 2.49                     | 0.42              |
| 1:E:102:HIS:O    | 1:E:103:ASN:C    | 2.62                     | 0.42              |
| 1:E:228:ASN:N    | 1:E:229:PRO:CD   | 2.82                     | 0.42              |
| 1:E:305:LEU:HB2  | 1:E:307:LEU:HG   | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:468:GLY:O    | 1:E:469:PHE:C    | 2.62                     | 0.42              |
| 1:E:480:LEU:HA   | 1:E:592:TYR:CE1  | 2.54                     | 0.42              |
| 1:E:535:PRO:CB   | 1:E:540:LEU:HD21 | 2.48                     | 0.42              |
| 1:E:728:GLN:CA   | 1:E:728:GLN:NE2  | 2.81                     | 0.42              |
| 2:F:14:ALA:HB3   | 2:F:38:LEU:HD21  | 2.00                     | 0.42              |
| 1:G:23:PRO:O     | 1:G:27:ALA:CB    | 2.67                     | 0.42              |
| 1:G:382:THR:HA   | 1:G:385:GLN:CD   | 2.45                     | 0.42              |
| 2:H:38:LEU:CD1   | 2:H:73:MET:HE2   | 2.48                     | 0.42              |
| 1:A:33:LYS:O     | 1:A:48:SER:HA    | 2.19                     | 0.42              |
| 1:A:83:PHE:CB    | 1:A:92:LEU:HD23  | 2.43                     | 0.42              |
| 1:A:236:ASN:ND2  | 1:A:246:SER:CA   | 2.73                     | 0.42              |
| 1:A:572:SER:HB2  | 1:A:580:GLU:HG3  | 2.01                     | 0.42              |
| 1:A:683:ARG:HE   | 1:A:683:ARG:HB3  | 1.50                     | 0.42              |
| 2:B:92:LEU:C     | 2:B:94:VAL:H     | 2.26                     | 0.42              |
| 1:C:178:GLU:O    | 1:C:183:LYS:NZ   | 2.52                     | 0.42              |
| 1:C:494:ASN:N    | 1:C:494:ASN:ND2  | 2.58                     | 0.42              |
| 1:C:763:ASP:H    | 1:C:766:LEU:CD1  | 2.32                     | 0.42              |
| 1:C:767:TYR:O    | 1:C:768:ARG:HD3  | 2.19                     | 0.42              |
| 1:E:236:ASN:ND2  | 1:E:246:SER:CA   | 2.73                     | 0.42              |
| 1:E:375:GLN:O    | 1:E:376:ALA:C    | 2.63                     | 0.42              |
| 1:E:466:ILE:HD12 | 1:E:467:ALA:O    | 2.20                     | 0.42              |
| 2:F:55:LYS:H     | 2:F:58:GLU:HG2   | 1.83                     | 0.42              |
| 1:G:291:TYR:O    | 1:G:292:TYR:C    | 2.61                     | 0.42              |
| 1:G:320:HIS:ND1  | 1:G:320:HIS:O    | 2.42                     | 0.42              |
| 1:G:506:GLN:O    | 1:G:509:GLY:N    | 2.53                     | 0.42              |
| 1:G:541:LEU:HD11 | 1:G:597:TRP:HB3  | 2.00                     | 0.42              |
| 1:G:576:LYS:C    | 1:G:579:THR:H    | 2.28                     | 0.42              |
| 1:G:812:PHE:O    | 1:G:814:LYS:N    | 2.52                     | 0.42              |
| 1:A:43:GLY:HA2   | 1:A:699:HIS:NE2  | 2.34                     | 0.42              |
| 1:A:51:GLU:CG    | 1:A:53:LYS:HE3   | 2.50                     | 0.42              |
| 1:A:162:ARG:O    | 1:A:163:SER:C    | 2.62                     | 0.42              |
| 1:A:195:ALA:O    | 1:A:199:SER:HB3  | 2.19                     | 0.42              |
| 1:A:298:SER:O    | 1:A:299:GLU:C    | 2.62                     | 0.42              |
| 1:A:513:ASN:O    | 1:A:513:ASN:ND2  | 2.41                     | 0.42              |
| 1:A:576:LYS:C    | 1:A:579:THR:H    | 2.27                     | 0.42              |
| 1:A:619:LYS:HA   | 1:A:622:ALA:CB   | 2.49                     | 0.42              |
| 1:A:817:GLN:HG2  | 1:A:818:GLN:OE1  | 2.19                     | 0.42              |
| 1:C:17:LYS:HB3   | 1:C:17:LYS:HE2   | 1.67                     | 0.42              |
| 1:C:37:VAL:CB    | 1:C:38:PRO:HD2   | 2.49                     | 0.42              |
| 1:C:89:MET:HG2   | 1:C:89:MET:H     | 1.51                     | 0.42              |
| 1:C:97:GLU:HG2   | 1:C:702:LEU:HD11 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:154:TYR:OH   | 1:C:192:GLN:NE2  | 2.53                     | 0.42              |
| 1:C:272:LEU:HD12 | 1:C:273:GLU:N    | 2.34                     | 0.42              |
| 1:C:326:GLN:CG   | 1:C:331:MET:HE3  | 2.50                     | 0.42              |
| 1:C:344:PHE:N    | 1:C:344:PHE:CD1  | 2.88                     | 0.42              |
| 1:C:485:THR:HA   | 1:C:488:LYS:HB2  | 2.01                     | 0.42              |
| 1:E:685:ILE:HD11 | 1:E:705:LEU:HD23 | 2.02                     | 0.42              |
| 2:F:10:GLU:CA    | 2:F:13:GLU:HG3   | 2.45                     | 0.42              |
| 2:F:121:GLU:CD   | 2:F:121:GLU:H    | 2.27                     | 0.42              |
| 1:G:557:GLU:O    | 1:G:560:ILE:HG12 | 2.19                     | 0.42              |
| 1:G:572:SER:HB2  | 1:G:580:GLU:HG3  | 2.01                     | 0.42              |
| 1:G:718:ARG:HG3  | 1:G:719:GLN:N    | 2.34                     | 0.42              |
| 1:G:814:LYS:CE   | 1:G:818:GLN:HE22 | 2.22                     | 0.42              |
| 1:A:352:ILE:HG21 | 1:A:442:ILE:CD1  | 2.41                     | 0.42              |
| 1:A:407:ILE:HD12 | 1:A:409:VAL:H    | 1.80                     | 0.42              |
| 1:A:530:ARG:HG3  | 1:A:531:PRO:N    | 2.35                     | 0.42              |
| 2:B:14:ALA:HB3   | 2:B:38:LEU:HD21  | 2.00                     | 0.42              |
| 2:B:41:ASN:N     | 2:B:42:PRO:CD    | 2.82                     | 0.42              |
| 1:C:24:LEU:HD23  | 1:C:24:LEU:N     | 2.35                     | 0.42              |
| 1:C:138:ILE:HG21 | 1:C:196:VAL:CG1  | 2.49                     | 0.42              |
| 1:C:183:LYS:NZ   | 1:C:468:GLY:HA3  | 2.35                     | 0.42              |
| 1:C:703:GLU:O    | 1:C:704:GLN:C    | 2.63                     | 0.42              |
| 1:E:171:GLN:HA   | 1:E:678:ASN:H    | 1.85                     | 0.42              |
| 1:E:362:LEU:HD23 | 1:E:427:ILE:O    | 2.20                     | 0.42              |
| 1:E:405:PRO:HB2  | 1:E:407:ILE:HG22 | 2.00                     | 0.42              |
| 1:E:547:PHE:CD1  | 1:E:547:PHE:C    | 2.95                     | 0.42              |
| 1:E:661:GLN:HE21 | 1:E:661:GLN:HB2  | 1.59                     | 0.42              |
| 1:E:819:LEU:C    | 1:E:821:SER:H    | 2.28                     | 0.42              |
| 2:F:18:PHE:CD2   | 2:F:34:VAL:HG22  | 2.54                     | 0.42              |
| 2:F:38:LEU:CD1   | 2:F:73:MET:HE2   | 2.48                     | 0.42              |
| 2:F:124:VAL:HG23 | 2:F:125:GLU:N    | 2.34                     | 0.42              |
| 1:G:49:ILE:HG23  | 1:G:57:VAL:CG1   | 2.50                     | 0.42              |
| 1:G:492:LEU:O    | 1:G:492:LEU:HD12 | 2.19                     | 0.42              |
| 1:G:543:GLU:HG2  | 1:G:544:GLU:N    | 2.32                     | 0.42              |
| 1:G:607:ASP:O    | 1:G:610:THR:HB   | 2.20                     | 0.42              |
| 1:A:104:LEU:CD1  | 1:A:705:LEU:HD11 | 2.48                     | 0.42              |
| 1:A:107:ARG:CB   | 1:A:112:LEU:HD12 | 2.48                     | 0.42              |
| 1:A:235:GLY:HA3  | 1:A:248:PHE:CE2  | 2.54                     | 0.42              |
| 1:A:663:TYR:O    | 1:A:666:GLN:N    | 2.53                     | 0.42              |
| 1:A:769:ILE:HD13 | 1:A:774:ILE:HG12 | 2.00                     | 0.42              |
| 1:A:800:GLN:O    | 1:A:803:CYS:HB2  | 2.20                     | 0.42              |
| 2:B:71:PRO:HA    | 2:B:74:GLN:OE1   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:51:GLU:HB3   | 1:C:53:LYS:HD2   | 2.02                     | 0.42              |
| 1:C:179:SER:HA   | 1:C:183:LYS:HZ1  | 1.84                     | 0.42              |
| 1:C:353:LEU:HA   | 1:C:356:VAL:HG23 | 2.02                     | 0.42              |
| 1:C:702:LEU:HD12 | 1:C:702:LEU:HA   | 1.83                     | 0.42              |
| 1:C:799:PHE:O    | 1:C:800:GLN:C    | 2.63                     | 0.42              |
| 2:D:148:LEU:C    | 2:D:150:GLY:N    | 2.77                     | 0.42              |
| 1:E:49:ILE:HG23  | 1:E:57:VAL:CG1   | 2.49                     | 0.42              |
| 1:E:104:LEU:CD1  | 1:E:705:LEU:HD11 | 2.49                     | 0.42              |
| 1:E:365:ILE:HG13 | 1:E:383:ALA:HB1  | 2.01                     | 0.42              |
| 1:E:725:ILE:HD13 | 1:E:730:PHE:HB2  | 2.02                     | 0.42              |
| 1:G:31:ALA:O     | 1:G:32:LYS:C     | 2.62                     | 0.42              |
| 1:G:120:PHE:HE1  | 1:G:713:GLY:O    | 2.03                     | 0.42              |
| 1:G:170:ASP:C    | 1:G:171:GLN:HG2  | 2.44                     | 0.42              |
| 1:G:547:PHE:HA   | 1:G:548:PRO:HD2  | 1.76                     | 0.42              |
| 1:G:625:TRP:C    | 1:G:627:ASP:H    | 2.27                     | 0.42              |
| 1:G:628:VAL:HG22 | 1:G:631:ILE:HD11 | 2.02                     | 0.42              |
| 2:H:55:LYS:H     | 2:H:58:GLU:HG2   | 1.84                     | 0.42              |
| 2:H:115:LEU:HD12 | 2:H:115:LEU:N    | 2.35                     | 0.42              |
| 2:H:128:VAL:O    | 2:H:129:ALA:C    | 2.62                     | 0.42              |
| 1:A:63:GLU:CD    | 1:A:63:GLU:C     | 2.88                     | 0.42              |
| 1:A:77:LYS:H     | 1:A:77:LYS:CD    | 2.33                     | 0.42              |
| 1:A:294:ILE:O    | 1:A:294:ILE:HG22 | 2.20                     | 0.42              |
| 1:A:558:LYS:O    | 1:A:561:GLN:N    | 2.53                     | 0.42              |
| 1:A:619:LYS:O    | 1:A:622:ALA:N    | 2.52                     | 0.42              |
| 2:B:10:GLU:HA    | 2:B:13:GLU:CG    | 2.42                     | 0.42              |
| 2:B:140:TYR:HE1  | 2:B:141:GLU:OE2  | 2.03                     | 0.42              |
| 1:C:278:ILE:HG22 | 1:C:315:PHE:CE1  | 2.54                     | 0.42              |
| 1:C:378:MET:HA   | 1:C:378:MET:CE   | 2.45                     | 0.42              |
| 1:C:405:PRO:C    | 1:C:407:ILE:N    | 2.77                     | 0.42              |
| 1:C:525:ILE:O    | 1:C:529:GLU:HB3  | 2.20                     | 0.42              |
| 1:C:553:THR:HG22 | 1:C:557:GLU:OE2  | 2.18                     | 0.42              |
| 1:C:683:ARG:HE   | 1:C:683:ARG:HB3  | 1.54                     | 0.42              |
| 1:E:59:VAL:HG12  | 1:E:60:GLU:N     | 2.35                     | 0.42              |
| 1:G:236:ASN:HD21 | 1:G:246:SER:HA   | 1.77                     | 0.42              |
| 1:G:719:GLN:HE21 | 1:G:719:GLN:CA   | 2.32                     | 0.42              |
| 1:G:819:LEU:C    | 1:G:821:SER:H    | 2.28                     | 0.42              |
| 1:A:37:VAL:CB    | 1:A:38:PRO:HD2   | 2.50                     | 0.42              |
| 1:A:274:LYS:HD2  | 1:A:274:LYS:C    | 2.44                     | 0.42              |
| 1:A:347:GLU:H    | 1:A:347:GLU:HG3  | 1.55                     | 0.42              |
| 1:A:352:ILE:O    | 1:A:356:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:405:PRO:CD   | 1:A:416:LYS:O    | 2.68                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:59:VAL:HG12  | 1:C:60:GLU:N     | 2.34                     | 0.42              |
| 1:C:469:PHE:N    | 1:C:486:ASN:OD1  | 2.47                     | 0.42              |
| 2:D:57:ASP:OD1   | 2:D:57:ASP:N     | 2.49                     | 0.42              |
| 2:D:96:ASP:O     | 2:D:98:GLU:N     | 2.53                     | 0.42              |
| 2:D:133:ASP:OD1  | 2:D:133:ASP:C    | 2.63                     | 0.42              |
| 1:E:46:ALA:HB1   | 1:E:62:GLN:HG2   | 2.01                     | 0.42              |
| 1:E:91:GLU:O     | 1:E:92:LEU:C     | 2.63                     | 0.42              |
| 1:E:164:MET:HG2  | 1:E:165:LEU:N    | 2.31                     | 0.42              |
| 1:E:613:LEU:O    | 1:E:616:SER:N    | 2.25                     | 0.42              |
| 1:G:33:LYS:HB3   | 1:G:49:ILE:CA    | 2.50                     | 0.42              |
| 1:G:148:GLU:C    | 1:G:149:MET:HG2  | 2.43                     | 0.42              |
| 1:G:154:TYR:OH   | 1:G:192:GLN:NE2  | 2.53                     | 0.42              |
| 1:G:378:MET:HA   | 1:G:378:MET:CE   | 2.48                     | 0.42              |
| 1:G:747:MET:CB   | 1:G:752:ALA:HB2  | 2.45                     | 0.42              |
| 1:G:800:GLN:O    | 1:G:803:CYS:HB2  | 2.20                     | 0.42              |
| 2:H:92:LEU:C     | 2:H:94:VAL:N     | 2.77                     | 0.42              |
| 1:A:33:LYS:N     | 1:A:33:LYS:HE2   | 2.35                     | 0.41              |
| 1:A:38:PRO:HG2   | 1:A:70:LEU:HD13  | 2.02                     | 0.41              |
| 1:A:293:LEU:HA   | 1:A:332:PHE:HE1  | 1.81                     | 0.41              |
| 2:B:128:VAL:HG23 | 2:B:129:ALA:N    | 2.35                     | 0.41              |
| 2:B:141:GLU:HG2  | 2:B:141:GLU:H    | 1.73                     | 0.41              |
| 1:C:72:LYS:HG2   | 1:C:72:LYS:O     | 2.20                     | 0.41              |
| 1:C:103:ASN:HD21 | 1:C:107:ARG:HD2  | 1.85                     | 0.41              |
| 1:C:121:CYS:SG   | 1:C:156:ILE:HD11 | 2.60                     | 0.41              |
| 1:C:530:ARG:HA   | 1:C:531:PRO:HD3  | 1.78                     | 0.41              |
| 1:C:730:PHE:CE2  | 1:C:776:PHE:CZ   | 3.08                     | 0.41              |
| 2:D:10:GLU:O     | 2:D:11:PHE:C     | 2.62                     | 0.41              |
| 2:D:25:LYS:HE3   | 2:D:65:LYS:HE2   | 2.00                     | 0.41              |
| 2:D:142:GLU:O    | 2:D:143:LEU:C    | 2.63                     | 0.41              |
| 1:E:120:PHE:HE1  | 1:E:713:GLY:O    | 2.02                     | 0.41              |
| 1:E:152:HIS:CE1  | 1:E:154:TYR:CG   | 3.08                     | 0.41              |
| 1:E:179:SER:HA   | 1:E:183:LYS:HZ1  | 1.85                     | 0.41              |
| 1:E:270:TYR:OH   | 1:E:670:LEU:HD22 | 2.20                     | 0.41              |
| 1:E:376:ALA:CB   | 1:E:420:LYS:HB2  | 2.44                     | 0.41              |
| 1:E:388:CYS:SG   | 1:E:393:ILE:HD11 | 2.60                     | 0.41              |
| 1:E:474:ILE:H    | 1:E:474:ILE:HG13 | 1.48                     | 0.41              |
| 1:E:558:LYS:O    | 1:E:561:GLN:N    | 2.53                     | 0.41              |
| 1:E:630:ARG:O    | 1:E:631:ILE:C    | 2.63                     | 0.41              |
| 2:F:10:GLU:O     | 2:F:11:PHE:C     | 2.62                     | 0.41              |
| 2:F:71:PRO:HA    | 2:F:74:GLN:OE1   | 2.20                     | 0.41              |
| 2:F:103:VAL:CG2  | 2:F:140:TYR:HD2  | 2.33                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:140:TYR:CE1  | 2:F:141:GLU:HG2  | 2.54                     | 0.41              |
| 1:G:161:TYR:O    | 1:G:165:LEU:CD1  | 2.62                     | 0.41              |
| 1:G:274:LYS:HD2  | 1:G:274:LYS:C    | 2.45                     | 0.41              |
| 1:G:658:THR:HG23 | 1:G:661:GLN:CB   | 2.50                     | 0.41              |
| 1:G:817:GLN:HG2  | 1:G:818:GLN:OE1  | 2.20                     | 0.41              |
| 2:H:10:GLU:O     | 2:H:11:PHE:C     | 2.62                     | 0.41              |
| 1:A:133:TYR:HB3  | 1:A:154:TYR:HH   | 1.85                     | 0.41              |
| 1:A:306:LEU:HD22 | 1:A:386:LYS:CD   | 2.50                     | 0.41              |
| 2:B:46:GLU:O     | 2:B:50:VAL:HG23  | 2.20                     | 0.41              |
| 1:C:43:GLY:HA2   | 1:C:699:HIS:NE2  | 2.34                     | 0.41              |
| 1:C:274:LYS:HD2  | 1:C:274:LYS:C    | 2.46                     | 0.41              |
| 1:C:300:GLN:C    | 1:C:302:ARG:N    | 2.77                     | 0.41              |
| 1:C:479:GLN:OE1  | 1:C:479:GLN:N    | 2.54                     | 0.41              |
| 1:C:720:GLY:C    | 1:C:721:PHE:CD1  | 2.98                     | 0.41              |
| 1:C:751:GLN:HE21 | 1:C:751:GLN:HB3  | 1.65                     | 0.41              |
| 1:C:768:ARG:HD3  | 1:C:768:ARG:HA   | 1.62                     | 0.41              |
| 2:D:120:THR:HG23 | 2:D:123:GLU:CG   | 2.49                     | 0.41              |
| 2:D:132:GLU:H    | 2:D:132:GLU:HG2  | 1.48                     | 0.41              |
| 1:E:33:LYS:O     | 1:E:49:ILE:HG13  | 2.19                     | 0.41              |
| 1:E:395:VAL:O    | 1:E:398:PHE:N    | 2.53                     | 0.41              |
| 1:E:630:ARG:O    | 1:E:631:ILE:O    | 2.37                     | 0.41              |
| 1:E:743:PRO:HD2  | 1:E:747:MET:HE1  | 2.02                     | 0.41              |
| 2:F:112:LEU:HD22 | 2:F:112:LEU:HA   | 1.87                     | 0.41              |
| 1:G:138:ILE:HG21 | 1:G:196:VAL:CG1  | 2.50                     | 0.41              |
| 1:G:358:SER:C    | 1:G:360:LEU:H    | 2.28                     | 0.41              |
| 1:G:555:PHE:CE1  | 1:G:559:LEU:HD13 | 2.55                     | 0.41              |
| 1:G:566:HIS:C    | 1:G:568:LYS:N    | 2.77                     | 0.41              |
| 1:G:799:PHE:CZ   | 1:G:803:CYS:SG   | 3.13                     | 0.41              |
| 2:H:120:THR:O    | 2:H:124:VAL:HG22 | 2.20                     | 0.41              |
| 1:A:156:ILE:HD13 | 1:A:682:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:299:GLU:O    | 1:A:302:ARG:HB3  | 2.21                     | 0.41              |
| 1:A:305:LEU:HB2  | 1:A:307:LEU:HG   | 2.01                     | 0.41              |
| 1:A:349:GLN:C    | 1:A:351:SER:N    | 2.78                     | 0.41              |
| 1:A:358:SER:C    | 1:A:360:LEU:H    | 2.28                     | 0.41              |
| 1:A:610:THR:HG21 | 1:A:628:VAL:HG13 | 2.02                     | 0.41              |
| 2:B:125:GLU:O    | 2:B:129:ALA:CB   | 2.68                     | 0.41              |
| 1:C:91:GLU:O     | 1:C:92:LEU:C     | 2.64                     | 0.41              |
| 1:C:150:PRO:O    | 1:C:151:PRO:C    | 2.64                     | 0.41              |
| 1:C:223:GLN:C    | 1:C:225:LEU:N    | 2.75                     | 0.41              |
| 1:C:247:ARG:HH22 | 1:C:470:GLU:CD   | 2.29                     | 0.41              |
| 1:C:661:GLN:HE21 | 1:C:661:GLN:HB2  | 1.57                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:33:LYS:N     | 1:E:33:LYS:HE2   | 2.36                     | 0.41              |
| 1:E:71:SER:C     | 1:E:73:ASP:N     | 2.78                     | 0.41              |
| 1:E:162:ARG:O    | 1:E:163:SER:C    | 2.63                     | 0.41              |
| 1:E:299:GLU:O    | 1:E:302:ARG:HB3  | 2.20                     | 0.41              |
| 1:E:311:ASN:C    | 1:E:312:ASN:HD22 | 2.28                     | 0.41              |
| 1:E:352:ILE:HG22 | 1:E:438:LEU:HD21 | 2.02                     | 0.41              |
| 1:E:405:PRO:O    | 1:E:407:ILE:HG23 | 2.19                     | 0.41              |
| 1:E:525:ILE:O    | 1:E:529:GLU:HB3  | 2.20                     | 0.41              |
| 1:E:560:ILE:HG12 | 1:E:560:ILE:H    | 1.59                     | 0.41              |
| 2:F:92:LEU:C     | 2:F:94:VAL:N     | 2.77                     | 0.41              |
| 2:F:120:THR:HG23 | 2:F:123:GLU:CG   | 2.50                     | 0.41              |
| 1:G:280:GLN:OE1  | 1:G:317:SER:N    | 2.52                     | 0.41              |
| 1:G:409:VAL:O    | 1:G:410:GLY:C    | 2.61                     | 0.41              |
| 1:G:581:PHE:CZ   | 1:G:597:TRP:CH2  | 3.06                     | 0.41              |
| 1:A:153:ILE:C    | 1:A:155:ALA:N    | 2.75                     | 0.41              |
| 1:A:265:ALA:O    | 1:A:450:LEU:HB2  | 2.20                     | 0.41              |
| 1:A:409:VAL:O    | 1:A:410:GLY:C    | 2.63                     | 0.41              |
| 1:A:426:ALA:C    | 1:A:428:GLU:N    | 2.78                     | 0.41              |
| 1:A:514:PHE:CG   | 1:A:515:ILE:N    | 2.88                     | 0.41              |
| 1:A:545:CYS:SG   | 1:A:602:MET:SD   | 3.19                     | 0.41              |
| 1:A:696:LEU:C    | 1:A:696:LEU:HD12 | 2.46                     | 0.41              |
| 1:A:719:GLN:HE21 | 1:A:719:GLN:CA   | 2.33                     | 0.41              |
| 1:A:746:PHE:O    | 1:A:747:MET:HB2  | 2.20                     | 0.41              |
| 1:A:812:PHE:CD2  | 1:A:813:ALA:N    | 2.89                     | 0.41              |
| 2:B:104:MET:H    | 2:B:104:MET:HG3  | 1.47                     | 0.41              |
| 2:B:142:GLU:O    | 2:B:143:LEU:C    | 2.63                     | 0.41              |
| 2:B:148:LEU:C    | 2:B:150:GLY:N    | 2.78                     | 0.41              |
| 1:C:22:ASN:ND2   | 1:C:22:ASN:O     | 2.54                     | 0.41              |
| 2:D:71:PRO:HA    | 2:D:74:GLN:OE1   | 2.20                     | 0.41              |
| 1:E:80:PRO:HG2   | 1:E:83:PHE:CD2   | 2.54                     | 0.41              |
| 1:E:348:GLU:O    | 1:E:352:ILE:HG13 | 2.20                     | 0.41              |
| 1:E:382:THR:CA   | 1:E:385:GLN:HB3  | 2.50                     | 0.41              |
| 1:E:409:VAL:O    | 1:E:410:GLY:C    | 2.62                     | 0.41              |
| 1:E:513:ASN:O    | 1:E:513:ASN:ND2  | 2.44                     | 0.41              |
| 1:G:59:VAL:HG12  | 1:G:60:GLU:N     | 2.35                     | 0.41              |
| 1:G:122:VAL:O    | 1:G:123:VAL:CG2  | 2.69                     | 0.41              |
| 1:G:152:HIS:CE1  | 1:G:153:ILE:HG22 | 2.55                     | 0.41              |
| 1:G:438:LEU:HA   | 1:G:438:LEU:HD12 | 1.74                     | 0.41              |
| 1:G:621:VAL:HG12 | 1:G:625:TRP:HD1  | 1.85                     | 0.41              |
| 1:G:747:MET:HB3  | 1:G:752:ALA:CB   | 2.46                     | 0.41              |
| 2:H:46:GLU:O     | 2:H:50:VAL:HG23  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:125:GLU:O    | 2:H:129:ALA:CB   | 2.68                     | 0.41              |
| 1:A:140:MET:C    | 1:A:149:MET:HE3  | 2.46                     | 0.41              |
| 1:A:348:GLU:O    | 1:A:352:ILE:HG13 | 2.20                     | 0.41              |
| 1:A:606:ASN:OD1  | 1:A:606:ASN:O    | 2.39                     | 0.41              |
| 1:A:712:GLU:C    | 1:A:714:ILE:N    | 2.78                     | 0.41              |
| 1:A:771:GLN:O    | 1:A:771:GLN:NE2  | 2.53                     | 0.41              |
| 2:B:3:PHE:C      | 2:B:7:GLN:HE21   | 2.27                     | 0.41              |
| 2:B:38:LEU:CD1   | 2:B:73:MET:HE2   | 2.48                     | 0.41              |
| 2:B:95:PHE:CZ    | 2:B:111:VAL:HG21 | 2.55                     | 0.41              |
| 2:B:132:GLU:H    | 2:B:132:GLU:HG2  | 1.46                     | 0.41              |
| 1:C:299:GLU:O    | 1:C:302:ARG:HB3  | 2.21                     | 0.41              |
| 1:C:399:THR:O    | 1:C:400:ARG:C    | 2.61                     | 0.41              |
| 1:C:492:LEU:HD12 | 1:C:492:LEU:O    | 2.21                     | 0.41              |
| 1:C:817:GLN:HG2  | 1:C:818:GLN:OE1  | 2.20                     | 0.41              |
| 1:E:122:VAL:C    | 1:E:123:VAL:HG23 | 2.45                     | 0.41              |
| 1:E:393:ILE:HD12 | 1:E:612:LEU:HD21 | 2.01                     | 0.41              |
| 1:G:265:ALA:O    | 1:G:450:LEU:HB2  | 2.20                     | 0.41              |
| 1:G:302:ARG:CZ   | 1:G:303:ASN:HA   | 2.50                     | 0.41              |
| 1:G:415:GLN:OE1  | 1:G:416:LYS:N    | 2.53                     | 0.41              |
| 1:G:419:THR:O    | 1:G:422:GLN:N    | 2.54                     | 0.41              |
| 2:H:10:GLU:O     | 2:H:13:GLU:N     | 2.53                     | 0.41              |
| 1:A:87:GLU:OE1   | 1:A:87:GLU:HA    | 2.20                     | 0.41              |
| 1:A:138:ILE:HG21 | 1:A:196:VAL:HG11 | 2.01                     | 0.41              |
| 1:A:407:ILE:HD12 | 1:A:408:LYS:C    | 2.45                     | 0.41              |
| 1:A:506:GLN:O    | 1:A:509:GLY:N    | 2.53                     | 0.41              |
| 1:C:33:LYS:CG    | 1:C:49:ILE:HB    | 2.50                     | 0.41              |
| 1:C:107:ARG:CB   | 1:C:112:LEU:HD12 | 2.51                     | 0.41              |
| 1:C:152:HIS:CE1  | 1:C:154:TYR:H    | 2.38                     | 0.41              |
| 1:C:611:SER:HA   | 1:C:614:ASN:HB2  | 2.02                     | 0.41              |
| 1:C:750:LYS:O    | 1:C:751:GLN:C    | 2.63                     | 0.41              |
| 1:C:802:GLN:NE2  | 2:D:88:TYR:CE2   | 2.88                     | 0.41              |
| 2:D:10:GLU:CA    | 2:D:13:GLU:HG3   | 2.44                     | 0.41              |
| 2:D:85:PHE:C     | 2:D:87:ASP:N     | 2.75                     | 0.41              |
| 2:D:92:LEU:C     | 2:D:94:VAL:N     | 2.78                     | 0.41              |
| 2:D:125:GLU:O    | 2:D:129:ALA:CB   | 2.66                     | 0.41              |
| 1:E:72:LYS:O     | 1:E:72:LYS:HG2   | 2.21                     | 0.41              |
| 1:E:101:LEU:O    | 1:E:102:HIS:C    | 2.64                     | 0.41              |
| 1:E:114:TYR:HE2  | 1:E:153:ILE:HB   | 1.77                     | 0.41              |
| 1:E:256:PHE:HA   | 1:E:261:TYR:O    | 2.20                     | 0.41              |
| 1:E:274:LYS:HD2  | 1:E:274:LYS:C    | 2.45                     | 0.41              |
| 1:E:373:THR:O    | 1:E:374:ASP:HB2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:384:ALA:HA   | 1:E:387:VAL:HB   | 2.02                     | 0.41              |
| 1:E:413:VAL:O    | 1:E:415:GLN:N    | 2.54                     | 0.41              |
| 1:E:438:LEU:O    | 1:E:439:PHE:C    | 2.62                     | 0.41              |
| 1:E:514:PHE:CG   | 1:E:515:ILE:N    | 2.88                     | 0.41              |
| 1:E:730:PHE:C    | 1:E:732:GLN:N    | 2.78                     | 0.41              |
| 1:G:147:HIS:C    | 1:G:149:MET:N    | 2.77                     | 0.41              |
| 1:G:299:GLU:O    | 1:G:302:ARG:HB3  | 2.21                     | 0.41              |
| 1:G:347:GLU:H    | 1:G:347:GLU:HG3  | 1.54                     | 0.41              |
| 1:G:575:LEU:HA   | 1:G:577:ASP:OD2  | 2.20                     | 0.41              |
| 1:G:712:GLU:C    | 1:G:714:ILE:N    | 2.78                     | 0.41              |
| 1:G:751:GLN:HE21 | 1:G:751:GLN:HB3  | 1.65                     | 0.41              |
| 2:H:71:PRO:HA    | 2:H:74:GLN:OE1   | 2.20                     | 0.41              |
| 2:H:124:VAL:HG23 | 2:H:125:GLU:N    | 2.36                     | 0.41              |
| 1:A:36:TRP:C     | 1:A:37:VAL:HG22  | 2.45                     | 0.41              |
| 1:A:179:SER:HA   | 1:A:183:LYS:HZ1  | 1.85                     | 0.41              |
| 1:A:352:ILE:HG23 | 1:A:438:LEU:HD11 | 2.02                     | 0.41              |
| 1:A:437:ARG:NE   | 1:A:625:TRP:HA   | 2.25                     | 0.41              |
| 2:B:139:ASN:OD1  | 2:B:142:GLU:HG2  | 2.20                     | 0.41              |
| 1:C:31:ALA:O     | 1:C:32:LYS:C     | 2.64                     | 0.41              |
| 1:C:164:MET:HG2  | 1:C:165:LEU:N    | 2.34                     | 0.41              |
| 1:C:362:LEU:HD12 | 1:C:387:VAL:CG1  | 2.51                     | 0.41              |
| 1:C:365:ILE:HD11 | 1:C:384:ALA:HB2  | 2.03                     | 0.41              |
| 1:C:428:GLU:OE1  | 1:C:429:ALA:N    | 2.53                     | 0.41              |
| 1:C:522:GLN:N    | 1:C:523:PRO:CD   | 2.82                     | 0.41              |
| 2:D:98:GLU:C     | 2:D:100:ASN:N    | 2.78                     | 0.41              |
| 2:D:124:VAL:O    | 2:D:128:VAL:HG22 | 2.21                     | 0.41              |
| 1:E:31:ALA:O     | 1:E:34:LEU:N     | 2.54                     | 0.41              |
| 1:E:418:GLN:H    | 1:E:418:GLN:HG3  | 1.73                     | 0.41              |
| 1:E:619:LYS:O    | 1:E:622:ALA:N    | 2.54                     | 0.41              |
| 1:E:763:ASP:H    | 1:E:766:LEU:CD1  | 2.32                     | 0.41              |
| 1:E:765:ASN:O    | 1:E:777:ARG:NH2  | 2.47                     | 0.41              |
| 2:F:46:GLU:O     | 2:F:50:VAL:HG23  | 2.21                     | 0.41              |
| 1:G:243:ASP:O    | 1:G:323:ILE:CD1  | 2.68                     | 0.41              |
| 1:G:299:GLU:O    | 1:G:302:ARG:HB2  | 2.21                     | 0.41              |
| 1:G:338:ALA:O    | 1:G:339:MET:C    | 2.63                     | 0.41              |
| 1:G:362:LEU:CD2  | 1:G:427:ILE:HG13 | 2.48                     | 0.41              |
| 1:G:405:PRO:HB2  | 1:G:407:ILE:HG22 | 1.99                     | 0.41              |
| 1:G:586:TYR:CD1  | 1:G:586:TYR:N    | 2.87                     | 0.41              |
| 2:H:111:VAL:HG12 | 2:H:112:LEU:HD23 | 2.02                     | 0.41              |
| 1:A:72:LYS:O     | 1:A:72:LYS:HG2   | 2.20                     | 0.41              |
| 1:A:140:MET:HB3  | 1:A:149:MET:CE   | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:302:ARG:CZ   | 1:A:303:ASN:HA   | 2.50                     | 0.41              |
| 1:A:338:ALA:O    | 1:A:339:MET:C    | 2.64                     | 0.41              |
| 1:A:384:ALA:HA   | 1:A:387:VAL:HB   | 2.02                     | 0.41              |
| 1:A:619:LYS:O    | 1:A:622:ALA:CB   | 2.66                     | 0.41              |
| 1:A:809:ARG:HD2  | 2:B:36:ARG:O     | 2.21                     | 0.41              |
| 1:A:819:LEU:C    | 1:A:821:SER:H    | 2.29                     | 0.41              |
| 2:B:10:GLU:O     | 2:B:11:PHE:C     | 2.62                     | 0.41              |
| 2:B:81:ASP:O     | 2:B:82:GLN:HB2   | 2.20                     | 0.41              |
| 1:C:31:ALA:O     | 1:C:34:LEU:N     | 2.54                     | 0.41              |
| 1:C:134:SER:OG   | 1:C:136:LYS:HB3  | 2.21                     | 0.41              |
| 1:C:172:SER:OG   | 1:C:679:PRO:HA   | 2.21                     | 0.41              |
| 1:C:487:GLU:OE1  | 1:C:585:HIS:HA   | 2.19                     | 0.41              |
| 1:C:630:ARG:O    | 1:C:631:ILE:C    | 2.63                     | 0.41              |
| 1:C:804:ARG:O    | 1:C:808:ALA:HB2  | 2.21                     | 0.41              |
| 1:E:407:ILE:CG1  | 1:E:414:VAL:O    | 2.61                     | 0.41              |
| 1:E:469:PHE:N    | 1:E:486:ASN:OD1  | 2.52                     | 0.41              |
| 1:E:555:PHE:CE1  | 1:E:559:LEU:HD13 | 2.56                     | 0.41              |
| 1:E:660:GLY:O    | 1:E:664:LYS:HB2  | 2.21                     | 0.41              |
| 1:E:724:ARG:HE   | 1:E:724:ARG:HB3  | 1.63                     | 0.41              |
| 1:E:760:LEU:HB2  | 1:E:762:LEU:HD23 | 2.03                     | 0.41              |
| 1:E:806:TYR:CG   | 2:F:147:VAL:HA   | 2.54                     | 0.41              |
| 2:F:70:LEU:N     | 2:F:71:PRO:CD    | 2.83                     | 0.41              |
| 2:F:96:ASP:O     | 2:F:98:GLU:N     | 2.54                     | 0.41              |
| 1:G:13:LEU:CD1   | 1:G:132:ILE:HB   | 2.48                     | 0.41              |
| 1:G:240:VAL:CG2  | 1:G:472:PHE:CD1  | 3.03                     | 0.41              |
| 1:G:399:THR:C    | 1:G:403:LEU:HD12 | 2.46                     | 0.41              |
| 1:G:500:LEU:HD23 | 1:G:500:LEU:HA   | 1.86                     | 0.41              |
| 1:G:522:GLN:O    | 1:G:525:ILE:HG13 | 2.20                     | 0.41              |
| 1:A:22:ASN:HA    | 1:A:23:PRO:HD3   | 1.82                     | 0.41              |
| 1:A:23:PRO:O     | 1:A:27:ALA:HB2   | 2.21                     | 0.41              |
| 1:A:153:ILE:CG2  | 1:A:154:TYR:N    | 2.82                     | 0.41              |
| 1:A:311:ASN:C    | 1:A:312:ASN:HD22 | 2.28                     | 0.41              |
| 1:A:329:ASP:OD1  | 1:A:329:ASP:N    | 2.43                     | 0.41              |
| 1:A:520:ASP:OD1  | 1:A:522:GLN:N    | 2.49                     | 0.41              |
| 1:A:610:THR:HG23 | 1:A:628:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:785:GLU:CD   | 1:A:788:ARG:HH21 | 2.28                     | 0.41              |
| 2:B:37:ALA:C     | 2:B:39:GLY:H     | 2.29                     | 0.41              |
| 2:B:65:LYS:O     | 2:B:66:PHE:C     | 2.64                     | 0.41              |
| 2:B:110:HIS:O    | 2:B:113:VAL:N    | 2.37                     | 0.41              |
| 1:C:52:GLU:HA    | 1:C:57:VAL:HG22  | 2.03                     | 0.41              |
| 1:C:240:VAL:HG22 | 1:C:472:PHE:CE1  | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:337:GLU:O    | 1:C:341:ILE:HG12 | 2.20                     | 0.41              |
| 1:C:371:ARG:H    | 1:C:371:ARG:HG3  | 1.44                     | 0.41              |
| 1:C:485:THR:HG23 | 1:C:667:LEU:HD11 | 2.03                     | 0.41              |
| 1:C:569:PHE:CZ   | 1:C:581:PHE:HB2  | 2.56                     | 0.41              |
| 1:C:735:GLU:O    | 1:C:735:GLU:HG3  | 2.21                     | 0.41              |
| 1:C:762:LEU:HD13 | 1:C:766:LEU:HD12 | 2.02                     | 0.41              |
| 1:C:814:LYS:C    | 1:C:816:GLN:H    | 2.27                     | 0.41              |
| 2:D:121:GLU:H    | 2:D:121:GLU:CD   | 2.28                     | 0.41              |
| 1:E:164:MET:HE3  | 1:E:461:LEU:HD12 | 2.01                     | 0.41              |
| 1:E:278:ILE:C    | 1:E:279:ARG:HG3  | 2.46                     | 0.41              |
| 1:E:370:GLU:OE1  | 1:E:372:ASN:HB2  | 2.20                     | 0.41              |
| 1:E:541:LEU:HD13 | 1:E:555:PHE:CE2  | 2.56                     | 0.41              |
| 1:E:576:LYS:CD   | 1:E:576:LYS:H    | 2.32                     | 0.41              |
| 1:E:622:ALA:O    | 1:E:626:LYS:N    | 2.54                     | 0.41              |
| 1:E:814:LYS:CE   | 1:E:818:GLN:HE22 | 2.23                     | 0.41              |
| 2:F:12:LYS:HG3   | 2:F:12:LYS:H     | 1.58                     | 0.41              |
| 2:F:37:ALA:C     | 2:F:39:GLY:H     | 2.29                     | 0.41              |
| 2:F:144:VAL:O    | 2:F:147:VAL:HG23 | 2.21                     | 0.41              |
| 1:G:7:SER:N      | 1:G:10:GLU:OE1   | 2.42                     | 0.41              |
| 1:G:88:ASP:O     | 1:G:89:MET:C     | 2.64                     | 0.41              |
| 1:G:96:ASN:C     | 1:G:98:ALA:N     | 2.78                     | 0.41              |
| 1:G:164:MET:HE1  | 1:G:256:PHE:CD2  | 2.50                     | 0.41              |
| 1:G:183:LYS:HB2  | 1:G:183:LYS:HE2  | 1.68                     | 0.41              |
| 1:G:293:LEU:C    | 1:G:295:ALA:N    | 2.79                     | 0.41              |
| 1:G:370:GLU:OE1  | 1:G:372:ASN:HB2  | 2.20                     | 0.41              |
| 1:G:475:ASN:ND2  | 1:G:590:VAL:CG1  | 2.84                     | 0.41              |
| 1:G:541:LEU:HD13 | 1:G:555:PHE:CE2  | 2.56                     | 0.41              |
| 1:G:553:THR:O    | 1:G:557:GLU:OE2  | 2.39                     | 0.41              |
| 2:H:81:ASP:HB3   | 2:H:82:GLN:H     | 1.59                     | 0.41              |
| 1:A:165:LEU:HD21 | 1:A:260:GLY:CA   | 2.51                     | 0.41              |
| 1:A:183:LYS:HE2  | 1:A:183:LYS:HB2  | 1.61                     | 0.41              |
| 1:A:606:ASN:OD1  | 1:A:606:ASN:C    | 2.63                     | 0.41              |
| 1:A:704:GLN:O    | 1:A:708:ASN:HB2  | 2.21                     | 0.41              |
| 1:A:747:MET:HG2  | 1:A:751:GLN:NE2  | 2.36                     | 0.41              |
| 2:B:87:ASP:O     | 2:B:88:TYR:C     | 2.64                     | 0.41              |
| 2:B:144:VAL:O    | 2:B:147:VAL:HG23 | 2.21                     | 0.41              |
| 1:C:269:THR:HG23 | 1:C:440:ARG:CZ   | 2.51                     | 0.41              |
| 1:C:409:VAL:HB   | 1:C:414:VAL:CG2  | 2.49                     | 0.41              |
| 1:C:445:ARG:HD2  | 1:C:445:ARG:HA   | 1.64                     | 0.41              |
| 1:C:471:ILE:HD13 | 1:C:471:ILE:HG21 | 1.83                     | 0.41              |
| 1:C:718:ARG:HG3  | 1:C:719:GLN:N    | 2.36                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:71:PRO:HA    | 2:D:74:GLN:CD    | 2.46                     | 0.41              |
| 2:D:76:ILE:O     | 2:D:79:ASN:CG    | 2.64                     | 0.41              |
| 2:D:127:LEU:HD11 | 2:D:147:VAL:HG13 | 2.03                     | 0.41              |
| 1:E:378:MET:HA   | 1:E:378:MET:CE   | 2.45                     | 0.41              |
| 1:E:393:ILE:HG22 | 1:E:616:SER:HB2  | 2.03                     | 0.41              |
| 2:F:10:GLU:HA    | 2:F:13:GLU:CG    | 2.42                     | 0.41              |
| 1:G:17:LYS:HB3   | 1:G:17:LYS:HE2   | 1.68                     | 0.41              |
| 1:G:77:LYS:H     | 1:G:77:LYS:CD    | 2.28                     | 0.41              |
| 1:G:196:VAL:HG13 | 1:G:197:VAL:N    | 2.36                     | 0.41              |
| 1:G:354:ARG:C    | 1:G:356:VAL:N    | 2.79                     | 0.41              |
| 2:H:65:LYS:O     | 2:H:66:PHE:C     | 2.64                     | 0.41              |
| 2:H:80:LYS:H     | 2:H:80:LYS:CD    | 2.31                     | 0.41              |
| 2:H:92:LEU:N     | 2:H:92:LEU:HD23  | 2.35                     | 0.41              |
| 1:A:52:GLU:HA    | 1:A:57:VAL:HG22  | 2.03                     | 0.40              |
| 1:A:164:MET:HE3  | 1:A:461:LEU:HD12 | 2.03                     | 0.40              |
| 1:A:345:THR:N    | 1:A:348:GLU:HB3  | 2.35                     | 0.40              |
| 1:A:362:LEU:HD12 | 1:A:387:VAL:CG1  | 2.51                     | 0.40              |
| 1:A:365:ILE:HD11 | 1:A:384:ALA:HB2  | 2.03                     | 0.40              |
| 1:A:366:VAL:O    | 1:A:378:MET:HE1  | 2.21                     | 0.40              |
| 1:C:3:GLN:O      | 1:C:4:LYS:O      | 2.39                     | 0.40              |
| 1:C:49:ILE:HG23  | 1:C:57:VAL:CG1   | 2.51                     | 0.40              |
| 1:C:240:VAL:CG2  | 1:C:472:PHE:HD1  | 2.34                     | 0.40              |
| 1:C:311:ASN:C    | 1:C:312:ASN:HD22 | 2.28                     | 0.40              |
| 1:C:375:GLN:O    | 1:C:376:ALA:C    | 2.64                     | 0.40              |
| 1:C:399:THR:C    | 1:C:403:LEU:HD12 | 2.46                     | 0.40              |
| 1:C:527:LEU:HD23 | 1:C:527:LEU:C    | 2.40                     | 0.40              |
| 1:C:530:ARG:HG3  | 1:C:531:PRO:N    | 2.33                     | 0.40              |
| 1:C:730:PHE:C    | 1:C:732:GLN:N    | 2.79                     | 0.40              |
| 1:C:769:ILE:HD13 | 1:C:774:ILE:HG12 | 2.04                     | 0.40              |
| 1:C:806:TYR:C    | 1:C:808:ALA:N    | 2.79                     | 0.40              |
| 1:E:23:PRO:O     | 1:E:27:ALA:CB    | 2.69                     | 0.40              |
| 1:E:270:TYR:CZ   | 1:E:670:LEU:HD22 | 2.56                     | 0.40              |
| 1:E:275:SER:C    | 1:E:277:ALA:N    | 2.80                     | 0.40              |
| 1:E:304:ASP:C    | 1:E:305:LEU:HD23 | 2.46                     | 0.40              |
| 1:E:355:VAL:O    | 1:E:355:VAL:HG12 | 2.21                     | 0.40              |
| 1:E:367:PHE:CE1  | 1:E:378:MET:SD   | 3.14                     | 0.40              |
| 1:E:407:ILE:HD12 | 1:E:408:LYS:C    | 2.46                     | 0.40              |
| 1:E:489:LEU:O    | 1:E:489:LEU:HD12 | 2.21                     | 0.40              |
| 1:E:500:LEU:HA   | 1:E:500:LEU:HD23 | 1.88                     | 0.40              |
| 2:F:71:PRO:HA    | 2:F:74:GLN:CD    | 2.46                     | 0.40              |
| 2:F:110:HIS:O    | 2:F:111:VAL:C    | 2.64                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:148:LEU:C    | 2:F:150:GLY:N    | 2.79                     | 0.40              |
| 1:G:26:GLN:HE21  | 1:G:26:GLN:C     | 2.30                     | 0.40              |
| 1:G:38:PRO:HG2   | 1:G:70:LEU:HD13  | 2.02                     | 0.40              |
| 1:G:45:GLU:OE2   | 1:G:61:LEU:HB3   | 2.20                     | 0.40              |
| 1:G:91:GLU:O     | 1:G:92:LEU:C     | 2.64                     | 0.40              |
| 1:G:98:ALA:O     | 1:G:101:LEU:HB3  | 2.21                     | 0.40              |
| 1:G:305:LEU:HB2  | 1:G:307:LEU:HG   | 2.03                     | 0.40              |
| 1:G:326:GLN:CG   | 1:G:331:MET:HE3  | 2.51                     | 0.40              |
| 1:G:801:ALA:HA   | 1:G:804:ARG:HD2  | 2.04                     | 0.40              |
| 1:A:8:ASP:OD1    | 1:A:8:ASP:N      | 2.53                     | 0.40              |
| 1:A:201:HIS:C    | 1:A:203:GLY:H    | 2.30                     | 0.40              |
| 1:A:275:SER:C    | 1:A:277:ALA:N    | 2.80                     | 0.40              |
| 1:A:299:GLU:O    | 1:A:302:ARG:HB2  | 2.22                     | 0.40              |
| 1:A:438:LEU:O    | 1:A:441:TRP:HB3  | 2.21                     | 0.40              |
| 1:A:581:PHE:CZ   | 1:A:597:TRP:CH2  | 3.09                     | 0.40              |
| 1:C:201:HIS:C    | 1:C:203:GLY:H    | 2.29                     | 0.40              |
| 1:C:291:TYR:HD2  | 1:C:310:PHE:HE2  | 1.69                     | 0.40              |
| 1:C:424:ASP:O    | 1:C:425:PHE:C    | 2.64                     | 0.40              |
| 1:C:480:LEU:HA   | 1:C:592:TYR:CE1  | 2.56                     | 0.40              |
| 1:C:769:ILE:HD13 | 1:C:769:ILE:HA   | 1.86                     | 0.40              |
| 2:D:25:LYS:CE    | 2:D:65:LYS:HE2   | 2.52                     | 0.40              |
| 2:D:119:MET:HB3  | 2:D:123:GLU:OE1  | 2.21                     | 0.40              |
| 2:D:120:THR:HG23 | 2:D:123:GLU:OE1  | 2.22                     | 0.40              |
| 2:D:133:ASP:OD1  | 2:D:135:ASN:N    | 2.55                     | 0.40              |
| 1:E:89:MET:HG2   | 1:E:116:TYR:O    | 2.21                     | 0.40              |
| 1:E:138:ILE:HG21 | 1:E:196:VAL:CG1  | 2.51                     | 0.40              |
| 1:E:250:LYS:NZ   | 1:E:465:ASP:OD2  | 2.54                     | 0.40              |
| 1:E:358:SER:C    | 1:E:360:LEU:H    | 2.29                     | 0.40              |
| 1:E:437:ARG:CD   | 1:E:624:LEU:O    | 2.70                     | 0.40              |
| 1:E:614:ASN:C    | 1:E:615:GLN:HG3  | 2.46                     | 0.40              |
| 1:E:621:VAL:HG12 | 1:E:625:TRP:HD1  | 1.87                     | 0.40              |
| 2:F:10:GLU:O     | 2:F:13:GLU:N     | 2.54                     | 0.40              |
| 2:F:115:LEU:HD12 | 2:F:115:LEU:N    | 2.36                     | 0.40              |
| 2:F:120:THR:O    | 2:F:124:VAL:HG22 | 2.21                     | 0.40              |
| 1:G:57:VAL:HG23  | 1:G:72:LYS:HB2   | 2.03                     | 0.40              |
| 1:G:77:LYS:HD2   | 1:G:96:ASN:HD21  | 1.87                     | 0.40              |
| 1:G:468:GLY:O    | 1:G:469:PHE:C    | 2.63                     | 0.40              |
| 1:G:607:ASP:C    | 1:G:610:THR:HB   | 2.46                     | 0.40              |
| 1:G:742:ILE:HD13 | 1:G:756:MET:HE3  | 2.02                     | 0.40              |
| 1:G:771:GLN:CA   | 1:G:771:GLN:NE2  | 2.84                     | 0.40              |
| 1:A:304:ASP:C    | 1:A:305:LEU:HD23 | 2.46                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:445:ARG:HA   | 1:A:445:ARG:HD2  | 1.65                     | 0.40              |
| 1:A:522:GLN:N    | 1:A:523:PRO:CD   | 2.79                     | 0.40              |
| 1:A:685:ILE:HD11 | 1:A:705:LEU:HD23 | 2.02                     | 0.40              |
| 1:A:716:ILE:HA   | 1:A:719:GLN:HB2  | 2.02                     | 0.40              |
| 2:B:120:THR:O    | 2:B:124:VAL:HG22 | 2.21                     | 0.40              |
| 1:C:71:SER:C     | 1:C:73:ASP:N     | 2.78                     | 0.40              |
| 1:C:541:LEU:CD2  | 1:C:597:TRP:HB3  | 2.45                     | 0.40              |
| 1:C:742:ILE:HG23 | 1:C:747:MET:HE2  | 2.04                     | 0.40              |
| 2:D:46:GLU:O     | 2:D:50:VAL:HG23  | 2.20                     | 0.40              |
| 1:E:13:LEU:HD23  | 1:E:13:LEU:HA    | 1.99                     | 0.40              |
| 1:E:31:ALA:O     | 1:E:32:LYS:C     | 2.63                     | 0.40              |
| 1:E:265:ALA:O    | 1:E:450:LEU:HB2  | 2.21                     | 0.40              |
| 1:E:349:GLN:C    | 1:E:351:SER:N    | 2.76                     | 0.40              |
| 1:E:465:ASP:OD1  | 1:E:465:ASP:C    | 2.64                     | 0.40              |
| 1:E:522:GLN:N    | 1:E:523:PRO:CD   | 2.84                     | 0.40              |
| 1:E:727:PHE:CE2  | 1:E:750:LYS:HB2  | 2.57                     | 0.40              |
| 1:E:735:GLU:O    | 1:E:735:GLU:HG3  | 2.20                     | 0.40              |
| 1:E:750:LYS:O    | 1:E:751:GLN:C    | 2.63                     | 0.40              |
| 1:E:762:LEU:HD13 | 1:E:766:LEU:HD12 | 2.03                     | 0.40              |
| 1:G:22:ASN:HA    | 1:G:23:PRO:HD3   | 1.77                     | 0.40              |
| 1:G:37:VAL:O     | 1:G:44:PHE:HA    | 2.21                     | 0.40              |
| 1:G:300:GLN:C    | 1:G:302:ARG:N    | 2.77                     | 0.40              |
| 1:G:492:LEU:HD12 | 1:G:492:LEU:C    | 2.47                     | 0.40              |
| 1:G:530:ARG:HG3  | 1:G:531:PRO:N    | 2.33                     | 0.40              |
| 1:G:619:LYS:HA   | 1:G:622:ALA:CB   | 2.51                     | 0.40              |
| 1:G:663:TYR:O    | 1:G:666:GLN:N    | 2.53                     | 0.40              |
| 2:H:71:PRO:HA    | 2:H:74:GLN:CD    | 2.46                     | 0.40              |
| 1:A:51:GLU:HB3   | 1:A:53:LYS:HD2   | 2.03                     | 0.40              |
| 1:A:86:VAL:HG12  | 1:A:103:ASN:CG   | 2.47                     | 0.40              |
| 1:A:152:HIS:O    | 1:A:155:ALA:HB3  | 2.22                     | 0.40              |
| 1:A:230:ILE:C    | 1:A:232:GLU:N    | 2.80                     | 0.40              |
| 1:A:231:LEU:HD23 | 1:A:231:LEU:N    | 2.37                     | 0.40              |
| 1:A:394:ASN:OD1  | 1:A:397:ASP:OD1  | 2.39                     | 0.40              |
| 1:A:806:TYR:C    | 1:A:808:ALA:N    | 2.78                     | 0.40              |
| 2:B:98:GLU:C     | 2:B:100:ASN:N    | 2.79                     | 0.40              |
| 1:C:240:VAL:CG2  | 1:C:472:PHE:CD1  | 3.05                     | 0.40              |
| 1:C:280:GLN:OE1  | 1:C:317:SER:N    | 2.53                     | 0.40              |
| 1:C:338:ALA:O    | 1:C:339:MET:C    | 2.64                     | 0.40              |
| 1:C:771:GLN:CA   | 1:C:771:GLN:NE2  | 2.82                     | 0.40              |
| 1:E:226:GLN:HG2  | 1:E:341:ILE:CB   | 2.52                     | 0.40              |
| 1:E:294:ILE:O    | 1:E:294:ILE:HG22 | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:349:GLN:O    | 1:E:352:ILE:N    | 2.55                     | 0.40              |
| 1:E:475:ASN:HB2  | 1:E:591:THR:O    | 2.21                     | 0.40              |
| 1:E:527:LEU:HD23 | 1:E:527:LEU:C    | 2.42                     | 0.40              |
| 1:G:31:ALA:O     | 1:G:34:LEU:N     | 2.54                     | 0.40              |
| 1:G:72:LYS:O     | 1:G:72:LYS:HG2   | 2.21                     | 0.40              |
| 1:G:201:HIS:C    | 1:G:203:GLY:H    | 2.30                     | 0.40              |
| 1:G:223:GLN:O    | 1:G:224:LEU:C    | 2.65                     | 0.40              |
| 1:G:345:THR:N    | 1:G:348:GLU:HB3  | 2.36                     | 0.40              |
| 1:G:365:ILE:HD13 | 1:G:427:ILE:CD1  | 2.44                     | 0.40              |
| 1:G:373:THR:O    | 1:G:374:ASP:HB2  | 2.22                     | 0.40              |
| 1:G:613:LEU:O    | 1:G:614:ASN:C    | 2.65                     | 0.40              |
| 1:G:763:ASP:OD1  | 1:G:765:ASN:N    | 2.54                     | 0.40              |
| 2:H:86:GLU:CD    | 2:H:86:GLU:H     | 2.26                     | 0.40              |
| 1:A:31:ALA:O     | 1:A:32:LYS:C     | 2.64                     | 0.40              |
| 1:A:333:GLN:HA   | 1:A:336:LEU:HB2  | 2.03                     | 0.40              |
| 1:A:370:GLU:OE1  | 1:A:372:ASN:HB2  | 2.21                     | 0.40              |
| 1:A:382:THR:CA   | 1:A:385:GLN:HB3  | 2.51                     | 0.40              |
| 1:A:409:VAL:HG13 | 1:A:634:LEU:HD12 | 2.03                     | 0.40              |
| 1:A:531:PRO:O    | 1:A:535:PRO:HA   | 2.21                     | 0.40              |
| 1:C:77:LYS:H     | 1:C:77:LYS:CD    | 2.33                     | 0.40              |
| 1:C:485:THR:CG2  | 1:C:667:LEU:HD11 | 2.52                     | 0.40              |
| 1:C:541:LEU:HD13 | 1:C:555:PHE:CE2  | 2.57                     | 0.40              |
| 1:C:704:GLN:O    | 1:C:708:ASN:HB2  | 2.22                     | 0.40              |
| 2:D:38:LEU:CD1   | 2:D:73:MET:HE2   | 2.48                     | 0.40              |
| 2:D:65:LYS:O     | 2:D:66:PHE:C     | 2.64                     | 0.40              |
| 2:D:84:CYS:SG    | 2:D:86:GLU:HB2   | 2.61                     | 0.40              |
| 2:D:140:TYR:HE1  | 2:D:141:GLU:OE2  | 2.04                     | 0.40              |
| 1:E:122:VAL:CG1  | 1:E:685:ILE:HG13 | 2.52                     | 0.40              |
| 1:E:257:ASP:OD1  | 1:E:260:GLY:N    | 2.55                     | 0.40              |
| 1:E:366:VAL:O    | 1:E:378:MET:HE1  | 2.21                     | 0.40              |
| 1:E:485:THR:HG23 | 1:E:667:LEU:HD11 | 2.04                     | 0.40              |
| 1:E:540:LEU:H    | 1:E:540:LEU:HG   | 1.54                     | 0.40              |
| 1:E:731:ARG:HD2  | 1:E:731:ARG:O    | 2.22                     | 0.40              |
| 2:F:124:VAL:O    | 2:F:128:VAL:HG22 | 2.22                     | 0.40              |
| 1:G:145:LYS:HB3  | 1:G:148:GLU:HG2  | 2.02                     | 0.40              |
| 1:G:240:VAL:CG2  | 1:G:472:PHE:HD1  | 2.34                     | 0.40              |
| 1:G:344:PHE:HA   | 1:G:348:GLU:OE2  | 2.21                     | 0.40              |
| 1:G:526:GLU:C    | 1:G:528:ILE:N    | 2.79                     | 0.40              |
| 1:G:806:TYR:C    | 1:G:808:ALA:N    | 2.79                     | 0.40              |
| 2:H:42:PRO:HA    | 2:H:46:GLU:OE1   | 2.21                     | 0.40              |
| 2:H:96:ASP:O     | 2:H:97:LYS:C     | 2.64                     | 0.40              |

All (17) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:E:19:PHE:CE1  | 1:G:786:GLU:OE2[1_556] | 1.59                     | 0.61              |
| 1:E:19:PHE:CD1  | 1:G:786:GLU:OE2[1_556] | 1.66                     | 0.54              |
| 2:D:23:ASP:N    | 1:G:371:ARG:NH2[1_545] | 1.81                     | 0.39              |
| 2:D:22:GLY:N    | 1:G:371:ARG:CZ[1_545]  | 1.88                     | 0.32              |
| 1:A:371:ARG:NH1 | 2:F:22:GLY:N[1_544]    | 1.91                     | 0.29              |
| 1:E:19:PHE:CE1  | 1:G:786:GLU:CD[1_556]  | 1.91                     | 0.29              |
| 2:D:22:GLY:CA   | 1:G:371:ARG:NE[1_545]  | 1.96                     | 0.24              |
| 2:D:22:GLY:N    | 1:G:371:ARG:NH1[1_545] | 1.96                     | 0.24              |
| 2:D:22:GLY:C    | 1:G:371:ARG:NE[1_545]  | 2.07                     | 0.13              |
| 1:A:371:ARG:NE  | 2:F:22:GLY:CA[1_544]   | 2.09                     | 0.11              |
| 2:D:21:THR:OG1  | 1:G:371:ARG:NH1[1_545] | 2.11                     | 0.09              |
| 2:D:23:ASP:CG   | 1:G:371:ARG:NH2[1_545] | 2.11                     | 0.09              |
| 1:A:371:ARG:NE  | 2:F:22:GLY:C[1_544]    | 2.13                     | 0.07              |
| 2:D:22:GLY:N    | 1:G:371:ARG:NE[1_545]  | 2.14                     | 0.06              |
| 1:E:19:PHE:CD1  | 1:G:786:GLU:CD[1_556]  | 2.15                     | 0.05              |
| 1:A:371:ARG:NE  | 2:F:22:GLY:O[1_544]    | 2.18                     | 0.02              |
| 1:A:371:ARG:CZ  | 2:F:22:GLY:CA[1_544]   | 2.19                     | 0.01              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed   | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|-----------|----------|-------------|---|
| 1   | A     | 779/820 (95%) | 549 (70%) | 172 (22%) | 58 (7%)  | 1           | 9 |
| 1   | C     | 779/820 (95%) | 553 (71%) | 163 (21%) | 63 (8%)  | 1           | 8 |
| 1   | E     | 779/820 (95%) | 547 (70%) | 173 (22%) | 59 (8%)  | 1           | 8 |
| 1   | G     | 779/820 (95%) | 552 (71%) | 165 (21%) | 62 (8%)  | 1           | 8 |
| 2   | B     | 146/150 (97%) | 102 (70%) | 30 (20%)  | 14 (10%) | 0           | 6 |
| 2   | D     | 146/150 (97%) | 104 (71%) | 28 (19%)  | 14 (10%) | 0           | 6 |
| 2   | F     | 146/150 (97%) | 101 (69%) | 33 (23%)  | 12 (8%)  | 0           | 8 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|-----------|----------|-------------|---|
| 2   | H     | 146/150 (97%)   | 104 (71%)  | 28 (19%)  | 14 (10%) | 0           | 6 |
| All | All   | 3700/3880 (95%) | 2612 (71%) | 792 (21%) | 296 (8%) | 1           | 8 |

All (296) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 145 | LYS  |
| 1   | A     | 170 | ASP  |
| 1   | A     | 383 | ALA  |
| 1   | A     | 395 | VAL  |
| 1   | A     | 414 | VAL  |
| 1   | A     | 531 | PRO  |
| 1   | A     | 614 | ASN  |
| 1   | A     | 626 | LYS  |
| 1   | A     | 664 | LYS  |
| 1   | A     | 683 | ARG  |
| 2   | B     | 97  | LYS  |
| 1   | C     | 145 | LYS  |
| 1   | C     | 170 | ASP  |
| 1   | C     | 383 | ALA  |
| 1   | C     | 395 | VAL  |
| 1   | C     | 414 | VAL  |
| 1   | C     | 531 | PRO  |
| 1   | C     | 614 | ASN  |
| 1   | C     | 664 | LYS  |
| 1   | C     | 683 | ARG  |
| 2   | D     | 97  | LYS  |
| 1   | E     | 145 | LYS  |
| 1   | E     | 170 | ASP  |
| 1   | E     | 276 | ARG  |
| 1   | E     | 383 | ALA  |
| 1   | E     | 395 | VAL  |
| 1   | E     | 414 | VAL  |
| 1   | E     | 531 | PRO  |
| 1   | E     | 614 | ASN  |
| 1   | E     | 631 | ILE  |
| 1   | E     | 664 | LYS  |
| 1   | E     | 683 | ARG  |
| 2   | F     | 97  | LYS  |
| 1   | G     | 145 | LYS  |
| 1   | G     | 276 | ARG  |
| 1   | G     | 383 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 395 | VAL  |
| 1   | G     | 414 | VAL  |
| 1   | G     | 531 | PRO  |
| 1   | G     | 614 | ASN  |
| 1   | G     | 626 | LYS  |
| 1   | G     | 664 | LYS  |
| 1   | G     | 683 | ARG  |
| 2   | H     | 97  | LYS  |
| 1   | A     | 32  | LYS  |
| 1   | A     | 38  | PRO  |
| 1   | A     | 123 | VAL  |
| 1   | A     | 181 | ALA  |
| 1   | A     | 273 | GLU  |
| 1   | A     | 276 | ARG  |
| 1   | A     | 362 | LEU  |
| 1   | A     | 376 | ALA  |
| 1   | A     | 420 | LYS  |
| 1   | A     | 541 | LEU  |
| 1   | A     | 564 | GLY  |
| 1   | A     | 572 | SER  |
| 1   | A     | 606 | ASN  |
| 1   | A     | 750 | LYS  |
| 2   | B     | 56  | SER  |
| 2   | B     | 77  | ALA  |
| 2   | B     | 99  | GLY  |
| 2   | B     | 105 | GLY  |
| 2   | B     | 117 | GLU  |
| 1   | C     | 32  | LYS  |
| 1   | C     | 38  | PRO  |
| 1   | C     | 123 | VAL  |
| 1   | C     | 181 | ALA  |
| 1   | C     | 273 | GLU  |
| 1   | C     | 276 | ARG  |
| 1   | C     | 281 | ALA  |
| 1   | C     | 362 | LEU  |
| 1   | C     | 420 | LYS  |
| 1   | C     | 476 | SER  |
| 1   | C     | 564 | GLY  |
| 1   | C     | 572 | SER  |
| 1   | C     | 750 | LYS  |
| 2   | D     | 56  | SER  |
| 2   | D     | 77  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 99  | GLY  |
| 2   | D     | 105 | GLY  |
| 2   | D     | 117 | GLU  |
| 2   | D     | 148 | LEU  |
| 1   | E     | 32  | LYS  |
| 1   | E     | 38  | PRO  |
| 1   | E     | 90  | ALA  |
| 1   | E     | 181 | ALA  |
| 1   | E     | 273 | GLU  |
| 1   | E     | 281 | ALA  |
| 1   | E     | 304 | ASP  |
| 1   | E     | 376 | ALA  |
| 1   | E     | 420 | LYS  |
| 1   | E     | 541 | LEU  |
| 1   | E     | 564 | GLY  |
| 1   | E     | 572 | SER  |
| 1   | E     | 727 | PHE  |
| 1   | E     | 750 | LYS  |
| 2   | F     | 56  | SER  |
| 2   | F     | 77  | ALA  |
| 2   | F     | 99  | GLY  |
| 2   | F     | 105 | GLY  |
| 2   | F     | 117 | GLU  |
| 2   | F     | 148 | LEU  |
| 1   | G     | 32  | LYS  |
| 1   | G     | 38  | PRO  |
| 1   | G     | 123 | VAL  |
| 1   | G     | 168 | ARG  |
| 1   | G     | 181 | ALA  |
| 1   | G     | 273 | GLU  |
| 1   | G     | 362 | LEU  |
| 1   | G     | 420 | LYS  |
| 1   | G     | 476 | SER  |
| 1   | G     | 564 | GLY  |
| 1   | G     | 572 | SER  |
| 1   | G     | 606 | ASN  |
| 1   | G     | 750 | LYS  |
| 2   | H     | 56  | SER  |
| 2   | H     | 77  | ALA  |
| 2   | H     | 99  | GLY  |
| 2   | H     | 117 | GLU  |
| 2   | H     | 148 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 131 | PRO  |
| 1   | A     | 288 | HIS  |
| 1   | A     | 304 | ASP  |
| 1   | A     | 348 | GLU  |
| 1   | A     | 533 | ASN  |
| 1   | A     | 562 | GLU  |
| 1   | A     | 727 | PHE  |
| 2   | B     | 82  | GLN  |
| 2   | B     | 148 | LEU  |
| 1   | C     | 90  | ALA  |
| 1   | C     | 131 | PRO  |
| 1   | C     | 288 | HIS  |
| 1   | C     | 304 | ASP  |
| 1   | C     | 348 | GLU  |
| 1   | C     | 376 | ALA  |
| 1   | C     | 533 | ASN  |
| 1   | C     | 541 | LEU  |
| 1   | C     | 562 | GLU  |
| 1   | C     | 606 | ASN  |
| 1   | C     | 727 | PHE  |
| 1   | C     | 807 | LEU  |
| 2   | D     | 22  | GLY  |
| 2   | D     | 82  | GLN  |
| 2   | D     | 86  | GLU  |
| 1   | E     | 123 | VAL  |
| 1   | E     | 131 | PRO  |
| 1   | E     | 288 | HIS  |
| 1   | E     | 362 | LEU  |
| 1   | E     | 382 | THR  |
| 1   | E     | 476 | SER  |
| 1   | E     | 533 | ASN  |
| 1   | E     | 562 | GLU  |
| 1   | E     | 606 | ASN  |
| 2   | F     | 82  | GLN  |
| 1   | G     | 90  | ALA  |
| 1   | G     | 131 | PRO  |
| 1   | G     | 288 | HIS  |
| 1   | G     | 304 | ASP  |
| 1   | G     | 376 | ALA  |
| 1   | G     | 533 | ASN  |
| 1   | G     | 541 | LEU  |
| 1   | G     | 562 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 82  | GLN  |
| 2   | H     | 105 | GLY  |
| 1   | A     | 72  | LYS  |
| 1   | A     | 90  | ALA  |
| 1   | A     | 106 | GLU  |
| 1   | A     | 382 | THR  |
| 1   | A     | 407 | ILE  |
| 1   | A     | 476 | SER  |
| 1   | A     | 563 | GLN  |
| 1   | A     | 579 | THR  |
| 1   | A     | 610 | THR  |
| 2   | B     | 22  | GLY  |
| 2   | B     | 86  | GLU  |
| 2   | B     | 141 | GLU  |
| 1   | C     | 33  | LYS  |
| 1   | C     | 72  | LYS  |
| 1   | C     | 271 | LEU  |
| 1   | C     | 382 | THR  |
| 1   | C     | 407 | ILE  |
| 1   | C     | 425 | PHE  |
| 1   | C     | 563 | GLN  |
| 1   | C     | 579 | THR  |
| 1   | C     | 610 | THR  |
| 1   | C     | 631 | ILE  |
| 2   | D     | 141 | GLU  |
| 2   | D     | 149 | SER  |
| 1   | E     | 33  | LYS  |
| 1   | E     | 72  | LYS  |
| 1   | E     | 233 | ALA  |
| 1   | E     | 271 | LEU  |
| 1   | E     | 348 | GLU  |
| 1   | E     | 407 | ILE  |
| 1   | E     | 563 | GLN  |
| 1   | E     | 610 | THR  |
| 1   | E     | 807 | LEU  |
| 2   | F     | 149 | SER  |
| 1   | G     | 33  | LYS  |
| 1   | G     | 72  | LYS  |
| 1   | G     | 233 | ALA  |
| 1   | G     | 289 | ILE  |
| 1   | G     | 348 | GLU  |
| 1   | G     | 382 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 407 | ILE  |
| 1   | G     | 425 | PHE  |
| 1   | G     | 563 | GLN  |
| 1   | G     | 579 | THR  |
| 1   | G     | 610 | THR  |
| 1   | G     | 727 | PHE  |
| 2   | H     | 22  | GLY  |
| 2   | H     | 141 | GLU  |
| 1   | A     | 4   | LYS  |
| 1   | A     | 89  | MET  |
| 1   | A     | 168 | ARG  |
| 1   | A     | 233 | ALA  |
| 1   | A     | 300 | GLN  |
| 1   | A     | 534 | PRO  |
| 1   | A     | 631 | ILE  |
| 2   | B     | 149 | SER  |
| 1   | C     | 106 | GLU  |
| 1   | C     | 126 | PRO  |
| 1   | C     | 168 | ARG  |
| 1   | C     | 233 | ALA  |
| 1   | C     | 300 | GLN  |
| 1   | C     | 511 | GLU  |
| 1   | C     | 534 | PRO  |
| 1   | C     | 663 | TYR  |
| 1   | E     | 4   | LYS  |
| 1   | E     | 106 | GLU  |
| 1   | E     | 126 | PRO  |
| 1   | E     | 168 | ARG  |
| 1   | E     | 215 | PHE  |
| 1   | E     | 300 | GLN  |
| 1   | E     | 534 | PRO  |
| 1   | E     | 663 | TYR  |
| 1   | G     | 106 | GLU  |
| 1   | G     | 271 | LEU  |
| 1   | G     | 300 | GLN  |
| 1   | G     | 524 | CYS  |
| 1   | G     | 534 | PRO  |
| 1   | G     | 585 | HIS  |
| 1   | G     | 663 | TYR  |
| 2   | H     | 85  | PHE  |
| 2   | H     | 111 | VAL  |
| 2   | H     | 149 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 126 | PRO  |
| 1   | A     | 148 | GLU  |
| 1   | A     | 215 | PHE  |
| 1   | A     | 289 | ILE  |
| 1   | A     | 663 | TYR  |
| 1   | A     | 764 | PRO  |
| 2   | B     | 54  | PRO  |
| 2   | B     | 111 | VAL  |
| 1   | C     | 240 | VAL  |
| 1   | C     | 289 | ILE  |
| 1   | C     | 352 | ILE  |
| 1   | C     | 369 | LYS  |
| 1   | C     | 396 | THR  |
| 1   | C     | 585 | HIS  |
| 1   | C     | 764 | PRO  |
| 2   | D     | 111 | VAL  |
| 1   | E     | 289 | ILE  |
| 1   | E     | 764 | PRO  |
| 2   | F     | 54  | PRO  |
| 1   | G     | 89  | MET  |
| 1   | G     | 126 | PRO  |
| 1   | G     | 369 | LYS  |
| 1   | G     | 396 | THR  |
| 1   | G     | 764 | PRO  |
| 1   | A     | 240 | VAL  |
| 1   | A     | 352 | ILE  |
| 1   | C     | 4   | LYS  |
| 1   | C     | 410 | GLY  |
| 2   | D     | 54  | PRO  |
| 1   | E     | 352 | ILE  |
| 2   | F     | 22  | GLY  |
| 1   | G     | 352 | ILE  |
| 1   | G     | 523 | PRO  |
| 1   | G     | 631 | ILE  |
| 2   | H     | 54  | PRO  |
| 1   | A     | 410 | GLY  |
| 1   | A     | 523 | PRO  |
| 1   | E     | 410 | GLY  |
| 2   | F     | 111 | VAL  |
| 1   | G     | 4   | LYS  |
| 1   | G     | 240 | VAL  |
| 1   | G     | 410 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 523 | PRO  |
| 1   | E     | 523 | PRO  |
| 1   | G     | 235 | GLY  |
| 1   | A     | 235 | GLY  |
| 1   | C     | 235 | GLY  |
| 1   | E     | 499 | ILE  |
| 1   | E     | 235 | GLY  |
| 1   | E     | 240 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |   |
|-----|-------|-----------------|------------|------------|-------------|---|
| 1   | A     | 689/718 (96%)   | 433 (63%)  | 256 (37%)  | 0           | 1 |
| 1   | C     | 689/718 (96%)   | 431 (63%)  | 258 (37%)  | 0           | 1 |
| 1   | E     | 689/718 (96%)   | 430 (62%)  | 259 (38%)  | 0           | 1 |
| 1   | G     | 689/718 (96%)   | 431 (63%)  | 258 (37%)  | 0           | 1 |
| 2   | B     | 127/129 (98%)   | 77 (61%)   | 50 (39%)   | 0           | 1 |
| 2   | D     | 127/129 (98%)   | 77 (61%)   | 50 (39%)   | 0           | 1 |
| 2   | F     | 127/129 (98%)   | 77 (61%)   | 50 (39%)   | 0           | 1 |
| 2   | H     | 127/129 (98%)   | 77 (61%)   | 50 (39%)   | 0           | 1 |
| All | All   | 3264/3388 (96%) | 2033 (62%) | 1231 (38%) | 0           | 1 |

All (1231) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | SER  |
| 1   | A     | 8   | ASP  |
| 1   | A     | 11  | LYS  |
| 1   | A     | 15  | VAL  |
| 1   | A     | 17  | LYS  |
| 1   | A     | 18  | ASN  |
| 1   | A     | 21  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 22  | ASN  |
| 1   | A     | 24  | LEU  |
| 1   | A     | 26  | GLN  |
| 1   | A     | 33  | LYS  |
| 1   | A     | 37  | VAL  |
| 1   | A     | 41  | LYS  |
| 1   | A     | 52  | GLU  |
| 1   | A     | 53  | LYS  |
| 1   | A     | 61  | LEU  |
| 1   | A     | 62  | GLN  |
| 1   | A     | 66  | LYS  |
| 1   | A     | 71  | SER  |
| 1   | A     | 72  | LYS  |
| 1   | A     | 73  | ASP  |
| 1   | A     | 77  | LYS  |
| 1   | A     | 79  | ASN  |
| 1   | A     | 82  | LYS  |
| 1   | A     | 84  | SER  |
| 1   | A     | 86  | VAL  |
| 1   | A     | 89  | MET  |
| 1   | A     | 91  | GLU  |
| 1   | A     | 92  | LEU  |
| 1   | A     | 93  | THR  |
| 1   | A     | 95  | LEU  |
| 1   | A     | 99  | SER  |
| 1   | A     | 101 | LEU  |
| 1   | A     | 106 | GLU  |
| 1   | A     | 107 | ARG  |
| 1   | A     | 112 | LEU  |
| 1   | A     | 113 | ILE  |
| 1   | A     | 117 | SER  |
| 1   | A     | 121 | CYS  |
| 1   | A     | 127 | TYR  |
| 1   | A     | 134 | SER  |
| 1   | A     | 135 | GLU  |
| 1   | A     | 137 | ILE  |
| 1   | A     | 144 | LYS  |
| 1   | A     | 145 | LYS  |
| 1   | A     | 146 | ARG  |
| 1   | A     | 148 | GLU  |
| 1   | A     | 162 | ARG  |
| 1   | A     | 163 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 164 | MET  |
| 1   | A     | 165 | LEU  |
| 1   | A     | 169 | GLU  |
| 1   | A     | 171 | GLN  |
| 1   | A     | 178 | GLU  |
| 1   | A     | 183 | LYS  |
| 1   | A     | 189 | LYS  |
| 1   | A     | 194 | LEU  |
| 1   | A     | 201 | HIS  |
| 1   | A     | 211 | GLN  |
| 1   | A     | 216 | SER  |
| 1   | A     | 222 | LYS  |
| 1   | A     | 225 | LEU  |
| 1   | A     | 226 | GLN  |
| 1   | A     | 228 | ASN  |
| 1   | A     | 230 | ILE  |
| 1   | A     | 234 | PHE  |
| 1   | A     | 238 | LYS  |
| 1   | A     | 239 | THR  |
| 1   | A     | 247 | ARG  |
| 1   | A     | 250 | LYS  |
| 1   | A     | 254 | ILE  |
| 1   | A     | 258 | VAL  |
| 1   | A     | 259 | THR  |
| 1   | A     | 262 | ILE  |
| 1   | A     | 263 | VAL  |
| 1   | A     | 266 | ASN  |
| 1   | A     | 269 | THR  |
| 1   | A     | 271 | LEU  |
| 1   | A     | 272 | LEU  |
| 1   | A     | 274 | LYS  |
| 1   | A     | 282 | LYS  |
| 1   | A     | 286 | THR  |
| 1   | A     | 298 | SER  |
| 1   | A     | 299 | GLU  |
| 1   | A     | 302 | ARG  |
| 1   | A     | 308 | GLU  |
| 1   | A     | 312 | ASN  |
| 1   | A     | 313 | TYR  |
| 1   | A     | 314 | THR  |
| 1   | A     | 316 | LEU  |
| 1   | A     | 317 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 320 | HIS  |
| 1   | A     | 323 | ILE  |
| 1   | A     | 329 | ASP  |
| 1   | A     | 331 | MET  |
| 1   | A     | 335 | THR  |
| 1   | A     | 336 | LEU  |
| 1   | A     | 346 | GLU  |
| 1   | A     | 347 | GLU  |
| 1   | A     | 351 | SER  |
| 1   | A     | 352 | ILE  |
| 1   | A     | 357 | SER  |
| 1   | A     | 358 | SER  |
| 1   | A     | 360 | LEU  |
| 1   | A     | 362 | LEU  |
| 1   | A     | 365 | ILE  |
| 1   | A     | 366 | VAL  |
| 1   | A     | 368 | LYS  |
| 1   | A     | 369 | LYS  |
| 1   | A     | 370 | GLU  |
| 1   | A     | 371 | ARG  |
| 1   | A     | 372 | ASN  |
| 1   | A     | 378 | MET  |
| 1   | A     | 382 | THR  |
| 1   | A     | 391 | MET  |
| 1   | A     | 395 | VAL  |
| 1   | A     | 399 | THR  |
| 1   | A     | 401 | SER  |
| 1   | A     | 402 | ILE  |
| 1   | A     | 406 | ARG  |
| 1   | A     | 407 | ILE  |
| 1   | A     | 408 | LYS  |
| 1   | A     | 411 | ARG  |
| 1   | A     | 412 | ASP  |
| 1   | A     | 415 | GLN  |
| 1   | A     | 416 | LYS  |
| 1   | A     | 418 | GLN  |
| 1   | A     | 419 | THR  |
| 1   | A     | 420 | LYS  |
| 1   | A     | 427 | ILE  |
| 1   | A     | 428 | GLU  |
| 1   | A     | 432 | LYS  |
| 1   | A     | 437 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 443 | LEU  |
| 1   | A     | 444 | THR  |
| 1   | A     | 445 | ARG  |
| 1   | A     | 446 | VAL  |
| 1   | A     | 447 | ASN  |
| 1   | A     | 448 | LYS  |
| 1   | A     | 450 | LEU  |
| 1   | A     | 451 | ASP  |
| 1   | A     | 459 | SER  |
| 1   | A     | 461 | LEU  |
| 1   | A     | 465 | ASP  |
| 1   | A     | 471 | ILE  |
| 1   | A     | 473 | GLU  |
| 1   | A     | 474 | ILE  |
| 1   | A     | 479 | GLN  |
| 1   | A     | 481 | CYS  |
| 1   | A     | 482 | ILE  |
| 1   | A     | 485 | THR  |
| 1   | A     | 488 | LYS  |
| 1   | A     | 489 | LEU  |
| 1   | A     | 492 | LEU  |
| 1   | A     | 494 | ASN  |
| 1   | A     | 496 | THR  |
| 1   | A     | 497 | MET  |
| 1   | A     | 502 | GLN  |
| 1   | A     | 503 | GLU  |
| 1   | A     | 504 | GLU  |
| 1   | A     | 506 | GLN  |
| 1   | A     | 513 | ASN  |
| 1   | A     | 515 | ILE  |
| 1   | A     | 521 | LEU  |
| 1   | A     | 522 | GLN  |
| 1   | A     | 525 | ILE  |
| 1   | A     | 526 | GLU  |
| 1   | A     | 530 | ARG  |
| 1   | A     | 543 | GLU  |
| 1   | A     | 545 | CYS  |
| 1   | A     | 549 | LYS  |
| 1   | A     | 553 | THR  |
| 1   | A     | 560 | ILE  |
| 1   | A     | 561 | GLN  |
| 1   | A     | 563 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 565 | ASN  |
| 1   | A     | 568 | LYS  |
| 1   | A     | 573 | LYS  |
| 1   | A     | 575 | LEU  |
| 1   | A     | 576 | LYS  |
| 1   | A     | 577 | ASP  |
| 1   | A     | 578 | LYS  |
| 1   | A     | 579 | THR  |
| 1   | A     | 580 | GLU  |
| 1   | A     | 583 | ILE  |
| 1   | A     | 586 | TYR  |
| 1   | A     | 591 | THR  |
| 1   | A     | 595 | SER  |
| 1   | A     | 599 | THR  |
| 1   | A     | 603 | ASP  |
| 1   | A     | 607 | ASP  |
| 1   | A     | 608 | ASN  |
| 1   | A     | 610 | THR  |
| 1   | A     | 611 | SER  |
| 1   | A     | 613 | LEU  |
| 1   | A     | 615 | GLN  |
| 1   | A     | 616 | SER  |
| 1   | A     | 617 | SER  |
| 1   | A     | 619 | LYS  |
| 1   | A     | 621 | VAL  |
| 1   | A     | 623 | ASP  |
| 1   | A     | 624 | LEU  |
| 1   | A     | 626 | LYS  |
| 1   | A     | 628 | VAL  |
| 1   | A     | 630 | ARG  |
| 1   | A     | 657 | ARG  |
| 1   | A     | 659 | VAL  |
| 1   | A     | 661 | GLN  |
| 1   | A     | 662 | LEU  |
| 1   | A     | 664 | LYS  |
| 1   | A     | 665 | GLU  |
| 1   | A     | 668 | THR  |
| 1   | A     | 673 | THR  |
| 1   | A     | 683 | ARG  |
| 1   | A     | 685 | ILE  |
| 1   | A     | 686 | ILE  |
| 1   | A     | 690 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 701 | VAL  |
| 1   | A     | 702 | LEU  |
| 1   | A     | 704 | GLN  |
| 1   | A     | 718 | ARG  |
| 1   | A     | 721 | PHE  |
| 1   | A     | 724 | ARG  |
| 1   | A     | 725 | ILE  |
| 1   | A     | 728 | GLN  |
| 1   | A     | 729 | GLU  |
| 1   | A     | 731 | ARG  |
| 1   | A     | 735 | GLU  |
| 1   | A     | 740 | ASN  |
| 1   | A     | 744 | LYS  |
| 1   | A     | 750 | LYS  |
| 1   | A     | 751 | GLN  |
| 1   | A     | 753 | CYS  |
| 1   | A     | 755 | LEU  |
| 1   | A     | 762 | LEU  |
| 1   | A     | 768 | ARG  |
| 1   | A     | 771 | GLN  |
| 1   | A     | 773 | LYS  |
| 1   | A     | 777 | ARG  |
| 1   | A     | 778 | THR  |
| 1   | A     | 781 | LEU  |
| 1   | A     | 784 | LEU  |
| 1   | A     | 790 | LEU  |
| 1   | A     | 791 | LYS  |
| 1   | A     | 792 | ILE  |
| 1   | A     | 793 | THR  |
| 1   | A     | 794 | ASP  |
| 1   | A     | 795 | VAL  |
| 1   | A     | 797 | ILE  |
| 1   | A     | 800 | GLN  |
| 1   | A     | 809 | ARG  |
| 1   | A     | 812 | PHE  |
| 1   | A     | 814 | LYS  |
| 1   | A     | 815 | ARG  |
| 1   | A     | 818 | GLN  |
| 1   | A     | 819 | LEU  |
| 2   | B     | 10  | GLU  |
| 2   | B     | 20  | ARG  |
| 2   | B     | 21  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 23  | ASP  |
| 2   | B     | 25  | LYS  |
| 2   | B     | 26  | ILE  |
| 2   | B     | 38  | LEU  |
| 2   | B     | 40  | GLN  |
| 2   | B     | 43  | THR  |
| 2   | B     | 47  | VAL  |
| 2   | B     | 49  | LYS  |
| 2   | B     | 50  | VAL  |
| 2   | B     | 51  | LEU  |
| 2   | B     | 53  | ASN  |
| 2   | B     | 55  | LYS  |
| 2   | B     | 57  | ASP  |
| 2   | B     | 59  | MET  |
| 2   | B     | 60  | ASN  |
| 2   | B     | 64  | LEU  |
| 2   | B     | 67  | GLU  |
| 2   | B     | 68  | GLN  |
| 2   | B     | 70  | LEU  |
| 2   | B     | 73  | MET  |
| 2   | B     | 74  | GLN  |
| 2   | B     | 75  | THR  |
| 2   | B     | 76  | ILE  |
| 2   | B     | 78  | LYS  |
| 2   | B     | 80  | LYS  |
| 2   | B     | 82  | GLN  |
| 2   | B     | 88  | TYR  |
| 2   | B     | 89  | VAL  |
| 2   | B     | 90  | GLU  |
| 2   | B     | 98  | GLU  |
| 2   | B     | 100 | ASN  |
| 2   | B     | 103 | VAL  |
| 2   | B     | 104 | MET  |
| 2   | B     | 107 | GLU  |
| 2   | B     | 108 | ILE  |
| 2   | B     | 109 | ARG  |
| 2   | B     | 112 | LEU  |
| 2   | B     | 114 | THR  |
| 2   | B     | 119 | MET  |
| 2   | B     | 120 | THR  |
| 2   | B     | 121 | GLU  |
| 2   | B     | 132 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 134 | SER  |
| 2   | B     | 135 | ASN  |
| 2   | B     | 144 | VAL  |
| 2   | B     | 146 | MET  |
| 2   | B     | 147 | VAL  |
| 1   | C     | 7   | SER  |
| 1   | C     | 8   | ASP  |
| 1   | C     | 11  | LYS  |
| 1   | C     | 15  | VAL  |
| 1   | C     | 17  | LYS  |
| 1   | C     | 18  | ASN  |
| 1   | C     | 21  | ASN  |
| 1   | C     | 22  | ASN  |
| 1   | C     | 24  | LEU  |
| 1   | C     | 26  | GLN  |
| 1   | C     | 33  | LYS  |
| 1   | C     | 37  | VAL  |
| 1   | C     | 41  | LYS  |
| 1   | C     | 52  | GLU  |
| 1   | C     | 53  | LYS  |
| 1   | C     | 61  | LEU  |
| 1   | C     | 62  | GLN  |
| 1   | C     | 66  | LYS  |
| 1   | C     | 71  | SER  |
| 1   | C     | 72  | LYS  |
| 1   | C     | 73  | ASP  |
| 1   | C     | 77  | LYS  |
| 1   | C     | 79  | ASN  |
| 1   | C     | 82  | LYS  |
| 1   | C     | 84  | SER  |
| 1   | C     | 86  | VAL  |
| 1   | C     | 89  | MET  |
| 1   | C     | 91  | GLU  |
| 1   | C     | 92  | LEU  |
| 1   | C     | 93  | THR  |
| 1   | C     | 95  | LEU  |
| 1   | C     | 99  | SER  |
| 1   | C     | 101 | LEU  |
| 1   | C     | 106 | GLU  |
| 1   | C     | 107 | ARG  |
| 1   | C     | 112 | LEU  |
| 1   | C     | 113 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 117 | SER  |
| 1   | C     | 121 | CYS  |
| 1   | C     | 134 | SER  |
| 1   | C     | 135 | GLU  |
| 1   | C     | 137 | ILE  |
| 1   | C     | 144 | LYS  |
| 1   | C     | 145 | LYS  |
| 1   | C     | 146 | ARG  |
| 1   | C     | 148 | GLU  |
| 1   | C     | 162 | ARG  |
| 1   | C     | 163 | SER  |
| 1   | C     | 164 | MET  |
| 1   | C     | 165 | LEU  |
| 1   | C     | 169 | GLU  |
| 1   | C     | 171 | GLN  |
| 1   | C     | 178 | GLU  |
| 1   | C     | 183 | LYS  |
| 1   | C     | 189 | LYS  |
| 1   | C     | 194 | LEU  |
| 1   | C     | 201 | HIS  |
| 1   | C     | 211 | GLN  |
| 1   | C     | 216 | SER  |
| 1   | C     | 222 | LYS  |
| 1   | C     | 225 | LEU  |
| 1   | C     | 226 | GLN  |
| 1   | C     | 228 | ASN  |
| 1   | C     | 230 | ILE  |
| 1   | C     | 234 | PHE  |
| 1   | C     | 238 | LYS  |
| 1   | C     | 239 | THR  |
| 1   | C     | 247 | ARG  |
| 1   | C     | 250 | LYS  |
| 1   | C     | 254 | ILE  |
| 1   | C     | 258 | VAL  |
| 1   | C     | 259 | THR  |
| 1   | C     | 262 | ILE  |
| 1   | C     | 263 | VAL  |
| 1   | C     | 266 | ASN  |
| 1   | C     | 269 | THR  |
| 1   | C     | 271 | LEU  |
| 1   | C     | 272 | LEU  |
| 1   | C     | 274 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 282 | LYS  |
| 1   | C     | 286 | THR  |
| 1   | C     | 298 | SER  |
| 1   | C     | 299 | GLU  |
| 1   | C     | 302 | ARG  |
| 1   | C     | 308 | GLU  |
| 1   | C     | 312 | ASN  |
| 1   | C     | 313 | TYR  |
| 1   | C     | 314 | THR  |
| 1   | C     | 316 | LEU  |
| 1   | C     | 317 | SER  |
| 1   | C     | 320 | HIS  |
| 1   | C     | 321 | VAL  |
| 1   | C     | 323 | ILE  |
| 1   | C     | 329 | ASP  |
| 1   | C     | 331 | MET  |
| 1   | C     | 335 | THR  |
| 1   | C     | 336 | LEU  |
| 1   | C     | 346 | GLU  |
| 1   | C     | 347 | GLU  |
| 1   | C     | 351 | SER  |
| 1   | C     | 352 | ILE  |
| 1   | C     | 357 | SER  |
| 1   | C     | 358 | SER  |
| 1   | C     | 360 | LEU  |
| 1   | C     | 362 | LEU  |
| 1   | C     | 365 | ILE  |
| 1   | C     | 366 | VAL  |
| 1   | C     | 368 | LYS  |
| 1   | C     | 369 | LYS  |
| 1   | C     | 370 | GLU  |
| 1   | C     | 371 | ARG  |
| 1   | C     | 372 | ASN  |
| 1   | C     | 378 | MET  |
| 1   | C     | 382 | THR  |
| 1   | C     | 391 | MET  |
| 1   | C     | 395 | VAL  |
| 1   | C     | 399 | THR  |
| 1   | C     | 401 | SER  |
| 1   | C     | 402 | ILE  |
| 1   | C     | 406 | ARG  |
| 1   | C     | 407 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 408 | LYS  |
| 1   | C     | 411 | ARG  |
| 1   | C     | 412 | ASP  |
| 1   | C     | 415 | GLN  |
| 1   | C     | 416 | LYS  |
| 1   | C     | 418 | GLN  |
| 1   | C     | 419 | THR  |
| 1   | C     | 420 | LYS  |
| 1   | C     | 427 | ILE  |
| 1   | C     | 428 | GLU  |
| 1   | C     | 432 | LYS  |
| 1   | C     | 437 | ARG  |
| 1   | C     | 443 | LEU  |
| 1   | C     | 444 | THR  |
| 1   | C     | 445 | ARG  |
| 1   | C     | 446 | VAL  |
| 1   | C     | 447 | ASN  |
| 1   | C     | 448 | LYS  |
| 1   | C     | 450 | LEU  |
| 1   | C     | 451 | ASP  |
| 1   | C     | 459 | SER  |
| 1   | C     | 461 | LEU  |
| 1   | C     | 465 | ASP  |
| 1   | C     | 471 | ILE  |
| 1   | C     | 473 | GLU  |
| 1   | C     | 474 | ILE  |
| 1   | C     | 479 | GLN  |
| 1   | C     | 481 | CYS  |
| 1   | C     | 482 | ILE  |
| 1   | C     | 485 | THR  |
| 1   | C     | 488 | LYS  |
| 1   | C     | 489 | LEU  |
| 1   | C     | 492 | LEU  |
| 1   | C     | 494 | ASN  |
| 1   | C     | 496 | THR  |
| 1   | C     | 497 | MET  |
| 1   | C     | 502 | GLN  |
| 1   | C     | 503 | GLU  |
| 1   | C     | 504 | GLU  |
| 1   | C     | 506 | GLN  |
| 1   | C     | 513 | ASN  |
| 1   | C     | 515 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 521 | LEU  |
| 1   | C     | 522 | GLN  |
| 1   | C     | 525 | ILE  |
| 1   | C     | 526 | GLU  |
| 1   | C     | 530 | ARG  |
| 1   | C     | 543 | GLU  |
| 1   | C     | 545 | CYS  |
| 1   | C     | 549 | LYS  |
| 1   | C     | 553 | THR  |
| 1   | C     | 560 | ILE  |
| 1   | C     | 561 | GLN  |
| 1   | C     | 563 | GLN  |
| 1   | C     | 565 | ASN  |
| 1   | C     | 568 | LYS  |
| 1   | C     | 573 | LYS  |
| 1   | C     | 575 | LEU  |
| 1   | C     | 576 | LYS  |
| 1   | C     | 577 | ASP  |
| 1   | C     | 578 | LYS  |
| 1   | C     | 579 | THR  |
| 1   | C     | 580 | GLU  |
| 1   | C     | 583 | ILE  |
| 1   | C     | 586 | TYR  |
| 1   | C     | 591 | THR  |
| 1   | C     | 595 | SER  |
| 1   | C     | 599 | THR  |
| 1   | C     | 603 | ASP  |
| 1   | C     | 607 | ASP  |
| 1   | C     | 608 | ASN  |
| 1   | C     | 610 | THR  |
| 1   | C     | 611 | SER  |
| 1   | C     | 613 | LEU  |
| 1   | C     | 615 | GLN  |
| 1   | C     | 616 | SER  |
| 1   | C     | 617 | SER  |
| 1   | C     | 619 | LYS  |
| 1   | C     | 621 | VAL  |
| 1   | C     | 623 | ASP  |
| 1   | C     | 624 | LEU  |
| 1   | C     | 626 | LYS  |
| 1   | C     | 628 | VAL  |
| 1   | C     | 630 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 657 | ARG  |
| 1   | C     | 659 | VAL  |
| 1   | C     | 661 | GLN  |
| 1   | C     | 662 | LEU  |
| 1   | C     | 664 | LYS  |
| 1   | C     | 665 | GLU  |
| 1   | C     | 668 | THR  |
| 1   | C     | 673 | THR  |
| 1   | C     | 683 | ARG  |
| 1   | C     | 685 | ILE  |
| 1   | C     | 686 | ILE  |
| 1   | C     | 690 | GLU  |
| 1   | C     | 696 | LEU  |
| 1   | C     | 701 | VAL  |
| 1   | C     | 702 | LEU  |
| 1   | C     | 704 | GLN  |
| 1   | C     | 718 | ARG  |
| 1   | C     | 721 | PHE  |
| 1   | C     | 724 | ARG  |
| 1   | C     | 725 | ILE  |
| 1   | C     | 728 | GLN  |
| 1   | C     | 729 | GLU  |
| 1   | C     | 731 | ARG  |
| 1   | C     | 735 | GLU  |
| 1   | C     | 740 | ASN  |
| 1   | C     | 744 | LYS  |
| 1   | C     | 751 | GLN  |
| 1   | C     | 753 | CYS  |
| 1   | C     | 754 | ILE  |
| 1   | C     | 755 | LEU  |
| 1   | C     | 757 | ILE  |
| 1   | C     | 762 | LEU  |
| 1   | C     | 768 | ARG  |
| 1   | C     | 771 | GLN  |
| 1   | C     | 773 | LYS  |
| 1   | C     | 777 | ARG  |
| 1   | C     | 778 | THR  |
| 1   | C     | 781 | LEU  |
| 1   | C     | 784 | LEU  |
| 1   | C     | 790 | LEU  |
| 1   | C     | 791 | LYS  |
| 1   | C     | 792 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 793 | THR  |
| 1   | C     | 794 | ASP  |
| 1   | C     | 795 | VAL  |
| 1   | C     | 797 | ILE  |
| 1   | C     | 800 | GLN  |
| 1   | C     | 809 | ARG  |
| 1   | C     | 812 | PHE  |
| 1   | C     | 814 | LYS  |
| 1   | C     | 815 | ARG  |
| 1   | C     | 818 | GLN  |
| 1   | C     | 819 | LEU  |
| 2   | D     | 10  | GLU  |
| 2   | D     | 20  | ARG  |
| 2   | D     | 21  | THR  |
| 2   | D     | 23  | ASP  |
| 2   | D     | 25  | LYS  |
| 2   | D     | 26  | ILE  |
| 2   | D     | 38  | LEU  |
| 2   | D     | 40  | GLN  |
| 2   | D     | 43  | THR  |
| 2   | D     | 47  | VAL  |
| 2   | D     | 49  | LYS  |
| 2   | D     | 50  | VAL  |
| 2   | D     | 51  | LEU  |
| 2   | D     | 53  | ASN  |
| 2   | D     | 55  | LYS  |
| 2   | D     | 57  | ASP  |
| 2   | D     | 59  | MET  |
| 2   | D     | 60  | ASN  |
| 2   | D     | 64  | LEU  |
| 2   | D     | 67  | GLU  |
| 2   | D     | 68  | GLN  |
| 2   | D     | 70  | LEU  |
| 2   | D     | 73  | MET  |
| 2   | D     | 74  | GLN  |
| 2   | D     | 75  | THR  |
| 2   | D     | 76  | ILE  |
| 2   | D     | 78  | LYS  |
| 2   | D     | 80  | LYS  |
| 2   | D     | 82  | GLN  |
| 2   | D     | 88  | TYR  |
| 2   | D     | 89  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 90  | GLU  |
| 2   | D     | 98  | GLU  |
| 2   | D     | 100 | ASN  |
| 2   | D     | 103 | VAL  |
| 2   | D     | 104 | MET  |
| 2   | D     | 107 | GLU  |
| 2   | D     | 108 | ILE  |
| 2   | D     | 109 | ARG  |
| 2   | D     | 112 | LEU  |
| 2   | D     | 114 | THR  |
| 2   | D     | 119 | MET  |
| 2   | D     | 120 | THR  |
| 2   | D     | 121 | GLU  |
| 2   | D     | 132 | GLU  |
| 2   | D     | 134 | SER  |
| 2   | D     | 135 | ASN  |
| 2   | D     | 144 | VAL  |
| 2   | D     | 146 | MET  |
| 2   | D     | 147 | VAL  |
| 1   | E     | 7   | SER  |
| 1   | E     | 8   | ASP  |
| 1   | E     | 11  | LYS  |
| 1   | E     | 15  | VAL  |
| 1   | E     | 17  | LYS  |
| 1   | E     | 18  | ASN  |
| 1   | E     | 21  | ASN  |
| 1   | E     | 22  | ASN  |
| 1   | E     | 24  | LEU  |
| 1   | E     | 26  | GLN  |
| 1   | E     | 33  | LYS  |
| 1   | E     | 37  | VAL  |
| 1   | E     | 41  | LYS  |
| 1   | E     | 45  | GLU  |
| 1   | E     | 52  | GLU  |
| 1   | E     | 53  | LYS  |
| 1   | E     | 61  | LEU  |
| 1   | E     | 62  | GLN  |
| 1   | E     | 66  | LYS  |
| 1   | E     | 71  | SER  |
| 1   | E     | 72  | LYS  |
| 1   | E     | 73  | ASP  |
| 1   | E     | 77  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 79  | ASN  |
| 1   | E     | 82  | LYS  |
| 1   | E     | 84  | SER  |
| 1   | E     | 86  | VAL  |
| 1   | E     | 91  | GLU  |
| 1   | E     | 92  | LEU  |
| 1   | E     | 93  | THR  |
| 1   | E     | 95  | LEU  |
| 1   | E     | 99  | SER  |
| 1   | E     | 101 | LEU  |
| 1   | E     | 107 | ARG  |
| 1   | E     | 112 | LEU  |
| 1   | E     | 113 | ILE  |
| 1   | E     | 117 | SER  |
| 1   | E     | 121 | CYS  |
| 1   | E     | 127 | TYR  |
| 1   | E     | 134 | SER  |
| 1   | E     | 135 | GLU  |
| 1   | E     | 137 | ILE  |
| 1   | E     | 144 | LYS  |
| 1   | E     | 145 | LYS  |
| 1   | E     | 146 | ARG  |
| 1   | E     | 148 | GLU  |
| 1   | E     | 162 | ARG  |
| 1   | E     | 163 | SER  |
| 1   | E     | 164 | MET  |
| 1   | E     | 165 | LEU  |
| 1   | E     | 169 | GLU  |
| 1   | E     | 171 | GLN  |
| 1   | E     | 178 | GLU  |
| 1   | E     | 183 | LYS  |
| 1   | E     | 189 | LYS  |
| 1   | E     | 194 | LEU  |
| 1   | E     | 200 | SER  |
| 1   | E     | 201 | HIS  |
| 1   | E     | 211 | GLN  |
| 1   | E     | 216 | SER  |
| 1   | E     | 222 | LYS  |
| 1   | E     | 226 | GLN  |
| 1   | E     | 228 | ASN  |
| 1   | E     | 230 | ILE  |
| 1   | E     | 234 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 238 | LYS  |
| 1   | E     | 239 | THR  |
| 1   | E     | 247 | ARG  |
| 1   | E     | 250 | LYS  |
| 1   | E     | 254 | ILE  |
| 1   | E     | 258 | VAL  |
| 1   | E     | 259 | THR  |
| 1   | E     | 262 | ILE  |
| 1   | E     | 263 | VAL  |
| 1   | E     | 266 | ASN  |
| 1   | E     | 269 | THR  |
| 1   | E     | 271 | LEU  |
| 1   | E     | 272 | LEU  |
| 1   | E     | 274 | LYS  |
| 1   | E     | 282 | LYS  |
| 1   | E     | 286 | THR  |
| 1   | E     | 298 | SER  |
| 1   | E     | 299 | GLU  |
| 1   | E     | 302 | ARG  |
| 1   | E     | 308 | GLU  |
| 1   | E     | 312 | ASN  |
| 1   | E     | 313 | TYR  |
| 1   | E     | 314 | THR  |
| 1   | E     | 316 | LEU  |
| 1   | E     | 317 | SER  |
| 1   | E     | 320 | HIS  |
| 1   | E     | 323 | ILE  |
| 1   | E     | 329 | ASP  |
| 1   | E     | 331 | MET  |
| 1   | E     | 334 | GLU  |
| 1   | E     | 335 | THR  |
| 1   | E     | 336 | LEU  |
| 1   | E     | 346 | GLU  |
| 1   | E     | 347 | GLU  |
| 1   | E     | 351 | SER  |
| 1   | E     | 352 | ILE  |
| 1   | E     | 357 | SER  |
| 1   | E     | 358 | SER  |
| 1   | E     | 360 | LEU  |
| 1   | E     | 362 | LEU  |
| 1   | E     | 365 | ILE  |
| 1   | E     | 366 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 368 | LYS  |
| 1   | E     | 369 | LYS  |
| 1   | E     | 370 | GLU  |
| 1   | E     | 371 | ARG  |
| 1   | E     | 372 | ASN  |
| 1   | E     | 378 | MET  |
| 1   | E     | 382 | THR  |
| 1   | E     | 391 | MET  |
| 1   | E     | 395 | VAL  |
| 1   | E     | 399 | THR  |
| 1   | E     | 401 | SER  |
| 1   | E     | 402 | ILE  |
| 1   | E     | 406 | ARG  |
| 1   | E     | 407 | ILE  |
| 1   | E     | 408 | LYS  |
| 1   | E     | 411 | ARG  |
| 1   | E     | 412 | ASP  |
| 1   | E     | 415 | GLN  |
| 1   | E     | 416 | LYS  |
| 1   | E     | 418 | GLN  |
| 1   | E     | 419 | THR  |
| 1   | E     | 420 | LYS  |
| 1   | E     | 427 | ILE  |
| 1   | E     | 428 | GLU  |
| 1   | E     | 432 | LYS  |
| 1   | E     | 437 | ARG  |
| 1   | E     | 443 | LEU  |
| 1   | E     | 444 | THR  |
| 1   | E     | 445 | ARG  |
| 1   | E     | 446 | VAL  |
| 1   | E     | 447 | ASN  |
| 1   | E     | 448 | LYS  |
| 1   | E     | 450 | LEU  |
| 1   | E     | 451 | ASP  |
| 1   | E     | 459 | SER  |
| 1   | E     | 461 | LEU  |
| 1   | E     | 465 | ASP  |
| 1   | E     | 466 | ILE  |
| 1   | E     | 471 | ILE  |
| 1   | E     | 473 | GLU  |
| 1   | E     | 474 | ILE  |
| 1   | E     | 479 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 481 | CYS  |
| 1   | E     | 482 | ILE  |
| 1   | E     | 485 | THR  |
| 1   | E     | 488 | LYS  |
| 1   | E     | 489 | LEU  |
| 1   | E     | 492 | LEU  |
| 1   | E     | 494 | ASN  |
| 1   | E     | 496 | THR  |
| 1   | E     | 502 | GLN  |
| 1   | E     | 503 | GLU  |
| 1   | E     | 504 | GLU  |
| 1   | E     | 506 | GLN  |
| 1   | E     | 513 | ASN  |
| 1   | E     | 515 | ILE  |
| 1   | E     | 521 | LEU  |
| 1   | E     | 522 | GLN  |
| 1   | E     | 525 | ILE  |
| 1   | E     | 526 | GLU  |
| 1   | E     | 530 | ARG  |
| 1   | E     | 543 | GLU  |
| 1   | E     | 545 | CYS  |
| 1   | E     | 549 | LYS  |
| 1   | E     | 553 | THR  |
| 1   | E     | 560 | ILE  |
| 1   | E     | 561 | GLN  |
| 1   | E     | 563 | GLN  |
| 1   | E     | 565 | ASN  |
| 1   | E     | 568 | LYS  |
| 1   | E     | 573 | LYS  |
| 1   | E     | 575 | LEU  |
| 1   | E     | 576 | LYS  |
| 1   | E     | 577 | ASP  |
| 1   | E     | 578 | LYS  |
| 1   | E     | 579 | THR  |
| 1   | E     | 580 | GLU  |
| 1   | E     | 583 | ILE  |
| 1   | E     | 586 | TYR  |
| 1   | E     | 591 | THR  |
| 1   | E     | 595 | SER  |
| 1   | E     | 599 | THR  |
| 1   | E     | 603 | ASP  |
| 1   | E     | 607 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 608 | ASN  |
| 1   | E     | 610 | THR  |
| 1   | E     | 611 | SER  |
| 1   | E     | 613 | LEU  |
| 1   | E     | 615 | GLN  |
| 1   | E     | 616 | SER  |
| 1   | E     | 617 | SER  |
| 1   | E     | 619 | LYS  |
| 1   | E     | 621 | VAL  |
| 1   | E     | 623 | ASP  |
| 1   | E     | 624 | LEU  |
| 1   | E     | 626 | LYS  |
| 1   | E     | 628 | VAL  |
| 1   | E     | 630 | ARG  |
| 1   | E     | 657 | ARG  |
| 1   | E     | 659 | VAL  |
| 1   | E     | 661 | GLN  |
| 1   | E     | 662 | LEU  |
| 1   | E     | 664 | LYS  |
| 1   | E     | 665 | GLU  |
| 1   | E     | 668 | THR  |
| 1   | E     | 673 | THR  |
| 1   | E     | 683 | ARG  |
| 1   | E     | 685 | ILE  |
| 1   | E     | 686 | ILE  |
| 1   | E     | 690 | GLU  |
| 1   | E     | 701 | VAL  |
| 1   | E     | 702 | LEU  |
| 1   | E     | 704 | GLN  |
| 1   | E     | 718 | ARG  |
| 1   | E     | 721 | PHE  |
| 1   | E     | 724 | ARG  |
| 1   | E     | 725 | ILE  |
| 1   | E     | 728 | GLN  |
| 1   | E     | 729 | GLU  |
| 1   | E     | 731 | ARG  |
| 1   | E     | 735 | GLU  |
| 1   | E     | 740 | ASN  |
| 1   | E     | 744 | LYS  |
| 1   | E     | 750 | LYS  |
| 1   | E     | 751 | GLN  |
| 1   | E     | 753 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 754 | ILE  |
| 1   | E     | 755 | LEU  |
| 1   | E     | 757 | ILE  |
| 1   | E     | 762 | LEU  |
| 1   | E     | 768 | ARG  |
| 1   | E     | 771 | GLN  |
| 1   | E     | 773 | LYS  |
| 1   | E     | 777 | ARG  |
| 1   | E     | 778 | THR  |
| 1   | E     | 781 | LEU  |
| 1   | E     | 784 | LEU  |
| 1   | E     | 790 | LEU  |
| 1   | E     | 791 | LYS  |
| 1   | E     | 792 | ILE  |
| 1   | E     | 793 | THR  |
| 1   | E     | 794 | ASP  |
| 1   | E     | 795 | VAL  |
| 1   | E     | 797 | ILE  |
| 1   | E     | 800 | GLN  |
| 1   | E     | 804 | ARG  |
| 1   | E     | 809 | ARG  |
| 1   | E     | 812 | PHE  |
| 1   | E     | 814 | LYS  |
| 1   | E     | 815 | ARG  |
| 1   | E     | 818 | GLN  |
| 1   | E     | 819 | LEU  |
| 2   | F     | 10  | GLU  |
| 2   | F     | 20  | ARG  |
| 2   | F     | 21  | THR  |
| 2   | F     | 23  | ASP  |
| 2   | F     | 25  | LYS  |
| 2   | F     | 26  | ILE  |
| 2   | F     | 38  | LEU  |
| 2   | F     | 40  | GLN  |
| 2   | F     | 43  | THR  |
| 2   | F     | 47  | VAL  |
| 2   | F     | 49  | LYS  |
| 2   | F     | 50  | VAL  |
| 2   | F     | 51  | LEU  |
| 2   | F     | 53  | ASN  |
| 2   | F     | 55  | LYS  |
| 2   | F     | 57  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 59  | MET  |
| 2   | F     | 60  | ASN  |
| 2   | F     | 64  | LEU  |
| 2   | F     | 67  | GLU  |
| 2   | F     | 68  | GLN  |
| 2   | F     | 70  | LEU  |
| 2   | F     | 73  | MET  |
| 2   | F     | 74  | GLN  |
| 2   | F     | 75  | THR  |
| 2   | F     | 76  | ILE  |
| 2   | F     | 78  | LYS  |
| 2   | F     | 80  | LYS  |
| 2   | F     | 82  | GLN  |
| 2   | F     | 88  | TYR  |
| 2   | F     | 89  | VAL  |
| 2   | F     | 90  | GLU  |
| 2   | F     | 98  | GLU  |
| 2   | F     | 100 | ASN  |
| 2   | F     | 103 | VAL  |
| 2   | F     | 104 | MET  |
| 2   | F     | 107 | GLU  |
| 2   | F     | 108 | ILE  |
| 2   | F     | 109 | ARG  |
| 2   | F     | 112 | LEU  |
| 2   | F     | 114 | THR  |
| 2   | F     | 119 | MET  |
| 2   | F     | 120 | THR  |
| 2   | F     | 121 | GLU  |
| 2   | F     | 132 | GLU  |
| 2   | F     | 134 | SER  |
| 2   | F     | 135 | ASN  |
| 2   | F     | 144 | VAL  |
| 2   | F     | 146 | MET  |
| 2   | F     | 147 | VAL  |
| 1   | G     | 7   | SER  |
| 1   | G     | 8   | ASP  |
| 1   | G     | 11  | LYS  |
| 1   | G     | 15  | VAL  |
| 1   | G     | 17  | LYS  |
| 1   | G     | 21  | ASN  |
| 1   | G     | 22  | ASN  |
| 1   | G     | 24  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 26  | GLN  |
| 1   | G     | 33  | LYS  |
| 1   | G     | 37  | VAL  |
| 1   | G     | 41  | LYS  |
| 1   | G     | 52  | GLU  |
| 1   | G     | 53  | LYS  |
| 1   | G     | 61  | LEU  |
| 1   | G     | 62  | GLN  |
| 1   | G     | 66  | LYS  |
| 1   | G     | 71  | SER  |
| 1   | G     | 72  | LYS  |
| 1   | G     | 73  | ASP  |
| 1   | G     | 77  | LYS  |
| 1   | G     | 79  | ASN  |
| 1   | G     | 82  | LYS  |
| 1   | G     | 84  | SER  |
| 1   | G     | 86  | VAL  |
| 1   | G     | 89  | MET  |
| 1   | G     | 91  | GLU  |
| 1   | G     | 92  | LEU  |
| 1   | G     | 93  | THR  |
| 1   | G     | 95  | LEU  |
| 1   | G     | 99  | SER  |
| 1   | G     | 101 | LEU  |
| 1   | G     | 106 | GLU  |
| 1   | G     | 107 | ARG  |
| 1   | G     | 112 | LEU  |
| 1   | G     | 113 | ILE  |
| 1   | G     | 115 | THR  |
| 1   | G     | 117 | SER  |
| 1   | G     | 120 | PHE  |
| 1   | G     | 121 | CYS  |
| 1   | G     | 127 | TYR  |
| 1   | G     | 134 | SER  |
| 1   | G     | 135 | GLU  |
| 1   | G     | 137 | ILE  |
| 1   | G     | 144 | LYS  |
| 1   | G     | 145 | LYS  |
| 1   | G     | 146 | ARG  |
| 1   | G     | 148 | GLU  |
| 1   | G     | 162 | ARG  |
| 1   | G     | 163 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 164 | MET  |
| 1   | G     | 178 | GLU  |
| 1   | G     | 183 | LYS  |
| 1   | G     | 189 | LYS  |
| 1   | G     | 194 | LEU  |
| 1   | G     | 201 | HIS  |
| 1   | G     | 211 | GLN  |
| 1   | G     | 216 | SER  |
| 1   | G     | 222 | LYS  |
| 1   | G     | 225 | LEU  |
| 1   | G     | 226 | GLN  |
| 1   | G     | 228 | ASN  |
| 1   | G     | 230 | ILE  |
| 1   | G     | 231 | LEU  |
| 1   | G     | 234 | PHE  |
| 1   | G     | 238 | LYS  |
| 1   | G     | 239 | THR  |
| 1   | G     | 247 | ARG  |
| 1   | G     | 250 | LYS  |
| 1   | G     | 254 | ILE  |
| 1   | G     | 258 | VAL  |
| 1   | G     | 259 | THR  |
| 1   | G     | 262 | ILE  |
| 1   | G     | 263 | VAL  |
| 1   | G     | 266 | ASN  |
| 1   | G     | 269 | THR  |
| 1   | G     | 271 | LEU  |
| 1   | G     | 272 | LEU  |
| 1   | G     | 274 | LYS  |
| 1   | G     | 282 | LYS  |
| 1   | G     | 286 | THR  |
| 1   | G     | 298 | SER  |
| 1   | G     | 299 | GLU  |
| 1   | G     | 302 | ARG  |
| 1   | G     | 308 | GLU  |
| 1   | G     | 312 | ASN  |
| 1   | G     | 313 | TYR  |
| 1   | G     | 314 | THR  |
| 1   | G     | 316 | LEU  |
| 1   | G     | 317 | SER  |
| 1   | G     | 320 | HIS  |
| 1   | G     | 323 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 329 | ASP  |
| 1   | G     | 331 | MET  |
| 1   | G     | 335 | THR  |
| 1   | G     | 336 | LEU  |
| 1   | G     | 346 | GLU  |
| 1   | G     | 347 | GLU  |
| 1   | G     | 351 | SER  |
| 1   | G     | 352 | ILE  |
| 1   | G     | 357 | SER  |
| 1   | G     | 358 | SER  |
| 1   | G     | 360 | LEU  |
| 1   | G     | 362 | LEU  |
| 1   | G     | 365 | ILE  |
| 1   | G     | 366 | VAL  |
| 1   | G     | 368 | LYS  |
| 1   | G     | 369 | LYS  |
| 1   | G     | 370 | GLU  |
| 1   | G     | 371 | ARG  |
| 1   | G     | 372 | ASN  |
| 1   | G     | 378 | MET  |
| 1   | G     | 382 | THR  |
| 1   | G     | 391 | MET  |
| 1   | G     | 395 | VAL  |
| 1   | G     | 399 | THR  |
| 1   | G     | 401 | SER  |
| 1   | G     | 402 | ILE  |
| 1   | G     | 406 | ARG  |
| 1   | G     | 407 | ILE  |
| 1   | G     | 408 | LYS  |
| 1   | G     | 411 | ARG  |
| 1   | G     | 412 | ASP  |
| 1   | G     | 415 | GLN  |
| 1   | G     | 416 | LYS  |
| 1   | G     | 418 | GLN  |
| 1   | G     | 419 | THR  |
| 1   | G     | 420 | LYS  |
| 1   | G     | 427 | ILE  |
| 1   | G     | 428 | GLU  |
| 1   | G     | 432 | LYS  |
| 1   | G     | 437 | ARG  |
| 1   | G     | 443 | LEU  |
| 1   | G     | 444 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 445 | ARG  |
| 1   | G     | 446 | VAL  |
| 1   | G     | 447 | ASN  |
| 1   | G     | 448 | LYS  |
| 1   | G     | 450 | LEU  |
| 1   | G     | 451 | ASP  |
| 1   | G     | 459 | SER  |
| 1   | G     | 461 | LEU  |
| 1   | G     | 465 | ASP  |
| 1   | G     | 471 | ILE  |
| 1   | G     | 473 | GLU  |
| 1   | G     | 474 | ILE  |
| 1   | G     | 479 | GLN  |
| 1   | G     | 481 | CYS  |
| 1   | G     | 482 | ILE  |
| 1   | G     | 485 | THR  |
| 1   | G     | 488 | LYS  |
| 1   | G     | 489 | LEU  |
| 1   | G     | 492 | LEU  |
| 1   | G     | 494 | ASN  |
| 1   | G     | 496 | THR  |
| 1   | G     | 502 | GLN  |
| 1   | G     | 503 | GLU  |
| 1   | G     | 504 | GLU  |
| 1   | G     | 506 | GLN  |
| 1   | G     | 513 | ASN  |
| 1   | G     | 515 | ILE  |
| 1   | G     | 521 | LEU  |
| 1   | G     | 522 | GLN  |
| 1   | G     | 525 | ILE  |
| 1   | G     | 526 | GLU  |
| 1   | G     | 530 | ARG  |
| 1   | G     | 543 | GLU  |
| 1   | G     | 545 | CYS  |
| 1   | G     | 549 | LYS  |
| 1   | G     | 553 | THR  |
| 1   | G     | 560 | ILE  |
| 1   | G     | 561 | GLN  |
| 1   | G     | 563 | GLN  |
| 1   | G     | 565 | ASN  |
| 1   | G     | 568 | LYS  |
| 1   | G     | 573 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 575 | LEU  |
| 1   | G     | 576 | LYS  |
| 1   | G     | 577 | ASP  |
| 1   | G     | 578 | LYS  |
| 1   | G     | 579 | THR  |
| 1   | G     | 580 | GLU  |
| 1   | G     | 583 | ILE  |
| 1   | G     | 586 | TYR  |
| 1   | G     | 591 | THR  |
| 1   | G     | 595 | SER  |
| 1   | G     | 599 | THR  |
| 1   | G     | 603 | ASP  |
| 1   | G     | 607 | ASP  |
| 1   | G     | 608 | ASN  |
| 1   | G     | 610 | THR  |
| 1   | G     | 611 | SER  |
| 1   | G     | 613 | LEU  |
| 1   | G     | 615 | GLN  |
| 1   | G     | 616 | SER  |
| 1   | G     | 617 | SER  |
| 1   | G     | 619 | LYS  |
| 1   | G     | 621 | VAL  |
| 1   | G     | 623 | ASP  |
| 1   | G     | 624 | LEU  |
| 1   | G     | 626 | LYS  |
| 1   | G     | 628 | VAL  |
| 1   | G     | 630 | ARG  |
| 1   | G     | 657 | ARG  |
| 1   | G     | 659 | VAL  |
| 1   | G     | 661 | GLN  |
| 1   | G     | 662 | LEU  |
| 1   | G     | 664 | LYS  |
| 1   | G     | 665 | GLU  |
| 1   | G     | 668 | THR  |
| 1   | G     | 673 | THR  |
| 1   | G     | 683 | ARG  |
| 1   | G     | 685 | ILE  |
| 1   | G     | 686 | ILE  |
| 1   | G     | 690 | GLU  |
| 1   | G     | 701 | VAL  |
| 1   | G     | 702 | LEU  |
| 1   | G     | 704 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 718 | ARG  |
| 1   | G     | 721 | PHE  |
| 1   | G     | 724 | ARG  |
| 1   | G     | 725 | ILE  |
| 1   | G     | 728 | GLN  |
| 1   | G     | 729 | GLU  |
| 1   | G     | 731 | ARG  |
| 1   | G     | 735 | GLU  |
| 1   | G     | 740 | ASN  |
| 1   | G     | 744 | LYS  |
| 1   | G     | 750 | LYS  |
| 1   | G     | 751 | GLN  |
| 1   | G     | 753 | CYS  |
| 1   | G     | 754 | ILE  |
| 1   | G     | 755 | LEU  |
| 1   | G     | 757 | ILE  |
| 1   | G     | 762 | LEU  |
| 1   | G     | 766 | LEU  |
| 1   | G     | 768 | ARG  |
| 1   | G     | 771 | GLN  |
| 1   | G     | 773 | LYS  |
| 1   | G     | 777 | ARG  |
| 1   | G     | 778 | THR  |
| 1   | G     | 781 | LEU  |
| 1   | G     | 784 | LEU  |
| 1   | G     | 790 | LEU  |
| 1   | G     | 791 | LYS  |
| 1   | G     | 792 | ILE  |
| 1   | G     | 793 | THR  |
| 1   | G     | 794 | ASP  |
| 1   | G     | 795 | VAL  |
| 1   | G     | 797 | ILE  |
| 1   | G     | 800 | GLN  |
| 1   | G     | 804 | ARG  |
| 1   | G     | 809 | ARG  |
| 1   | G     | 812 | PHE  |
| 1   | G     | 814 | LYS  |
| 1   | G     | 815 | ARG  |
| 1   | G     | 818 | GLN  |
| 1   | G     | 819 | LEU  |
| 2   | H     | 10  | GLU  |
| 2   | H     | 20  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 21  | THR  |
| 2   | H     | 23  | ASP  |
| 2   | H     | 25  | LYS  |
| 2   | H     | 26  | ILE  |
| 2   | H     | 38  | LEU  |
| 2   | H     | 40  | GLN  |
| 2   | H     | 43  | THR  |
| 2   | H     | 47  | VAL  |
| 2   | H     | 49  | LYS  |
| 2   | H     | 50  | VAL  |
| 2   | H     | 51  | LEU  |
| 2   | H     | 53  | ASN  |
| 2   | H     | 55  | LYS  |
| 2   | H     | 57  | ASP  |
| 2   | H     | 59  | MET  |
| 2   | H     | 60  | ASN  |
| 2   | H     | 67  | GLU  |
| 2   | H     | 68  | GLN  |
| 2   | H     | 70  | LEU  |
| 2   | H     | 73  | MET  |
| 2   | H     | 74  | GLN  |
| 2   | H     | 75  | THR  |
| 2   | H     | 76  | ILE  |
| 2   | H     | 78  | LYS  |
| 2   | H     | 80  | LYS  |
| 2   | H     | 82  | GLN  |
| 2   | H     | 86  | GLU  |
| 2   | H     | 88  | TYR  |
| 2   | H     | 89  | VAL  |
| 2   | H     | 90  | GLU  |
| 2   | H     | 98  | GLU  |
| 2   | H     | 100 | ASN  |
| 2   | H     | 103 | VAL  |
| 2   | H     | 104 | MET  |
| 2   | H     | 107 | GLU  |
| 2   | H     | 108 | ILE  |
| 2   | H     | 109 | ARG  |
| 2   | H     | 112 | LEU  |
| 2   | H     | 114 | THR  |
| 2   | H     | 119 | MET  |
| 2   | H     | 120 | THR  |
| 2   | H     | 121 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 132 | GLU  |
| 2   | H     | 134 | SER  |
| 2   | H     | 135 | ASN  |
| 2   | H     | 144 | VAL  |
| 2   | H     | 146 | MET  |
| 2   | H     | 147 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | GLN  |
| 1   | A     | 26  | GLN  |
| 1   | A     | 96  | ASN  |
| 1   | A     | 166 | GLN  |
| 1   | A     | 186 | ASN  |
| 1   | A     | 201 | HIS  |
| 1   | A     | 226 | GLN  |
| 1   | A     | 244 | ASN  |
| 1   | A     | 266 | ASN  |
| 1   | A     | 288 | HIS  |
| 1   | A     | 311 | ASN  |
| 1   | A     | 312 | ASN  |
| 1   | A     | 326 | GLN  |
| 1   | A     | 361 | GLN  |
| 1   | A     | 422 | GLN  |
| 1   | A     | 447 | ASN  |
| 1   | A     | 494 | ASN  |
| 1   | A     | 495 | HIS  |
| 1   | A     | 533 | ASN  |
| 1   | A     | 565 | ASN  |
| 1   | A     | 601 | ASN  |
| 1   | A     | 661 | GLN  |
| 1   | A     | 678 | ASN  |
| 1   | A     | 728 | GLN  |
| 1   | A     | 771 | GLN  |
| 1   | A     | 783 | HIS  |
| 2   | B     | 7   | GLN  |
| 2   | B     | 30  | GLN  |
| 2   | B     | 53  | ASN  |
| 2   | B     | 60  | ASN  |
| 2   | B     | 110 | HIS  |
| 2   | B     | 139 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 3   | GLN  |
| 1   | C     | 26  | GLN  |
| 1   | C     | 79  | ASN  |
| 1   | C     | 96  | ASN  |
| 1   | C     | 102 | HIS  |
| 1   | C     | 103 | ASN  |
| 1   | C     | 166 | GLN  |
| 1   | C     | 186 | ASN  |
| 1   | C     | 226 | GLN  |
| 1   | C     | 228 | ASN  |
| 1   | C     | 244 | ASN  |
| 1   | C     | 266 | ASN  |
| 1   | C     | 288 | HIS  |
| 1   | C     | 311 | ASN  |
| 1   | C     | 312 | ASN  |
| 1   | C     | 361 | GLN  |
| 1   | C     | 375 | GLN  |
| 1   | C     | 422 | GLN  |
| 1   | C     | 494 | ASN  |
| 1   | C     | 495 | HIS  |
| 1   | C     | 533 | ASN  |
| 1   | C     | 601 | ASN  |
| 1   | C     | 614 | ASN  |
| 1   | C     | 615 | GLN  |
| 1   | C     | 661 | GLN  |
| 1   | C     | 678 | ASN  |
| 1   | C     | 728 | GLN  |
| 1   | C     | 751 | GLN  |
| 1   | C     | 771 | GLN  |
| 2   | D     | 7   | GLN  |
| 2   | D     | 30  | GLN  |
| 2   | D     | 60  | ASN  |
| 2   | D     | 79  | ASN  |
| 2   | D     | 110 | HIS  |
| 2   | D     | 135 | ASN  |
| 2   | D     | 139 | ASN  |
| 1   | E     | 3   | GLN  |
| 1   | E     | 26  | GLN  |
| 1   | E     | 79  | ASN  |
| 1   | E     | 96  | ASN  |
| 1   | E     | 103 | ASN  |
| 1   | E     | 166 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 186 | ASN  |
| 1   | E     | 226 | GLN  |
| 1   | E     | 228 | ASN  |
| 1   | E     | 266 | ASN  |
| 1   | E     | 311 | ASN  |
| 1   | E     | 312 | ASN  |
| 1   | E     | 361 | GLN  |
| 1   | E     | 364 | ASN  |
| 1   | E     | 375 | GLN  |
| 1   | E     | 422 | GLN  |
| 1   | E     | 447 | ASN  |
| 1   | E     | 494 | ASN  |
| 1   | E     | 495 | HIS  |
| 1   | E     | 533 | ASN  |
| 1   | E     | 565 | ASN  |
| 1   | E     | 601 | ASN  |
| 1   | E     | 614 | ASN  |
| 1   | E     | 661 | GLN  |
| 1   | E     | 678 | ASN  |
| 1   | E     | 728 | GLN  |
| 1   | E     | 751 | GLN  |
| 1   | E     | 771 | GLN  |
| 1   | E     | 783 | HIS  |
| 2   | F     | 7   | GLN  |
| 2   | F     | 30  | GLN  |
| 2   | F     | 44  | ASN  |
| 2   | F     | 60  | ASN  |
| 2   | F     | 110 | HIS  |
| 1   | G     | 3   | GLN  |
| 1   | G     | 26  | GLN  |
| 1   | G     | 96  | ASN  |
| 1   | G     | 166 | GLN  |
| 1   | G     | 186 | ASN  |
| 1   | G     | 228 | ASN  |
| 1   | G     | 244 | ASN  |
| 1   | G     | 266 | ASN  |
| 1   | G     | 288 | HIS  |
| 1   | G     | 311 | ASN  |
| 1   | G     | 312 | ASN  |
| 1   | G     | 361 | GLN  |
| 1   | G     | 422 | GLN  |
| 1   | G     | 475 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 490 | GLN  |
| 1   | G     | 494 | ASN  |
| 1   | G     | 495 | HIS  |
| 1   | G     | 533 | ASN  |
| 1   | G     | 601 | ASN  |
| 1   | G     | 661 | GLN  |
| 1   | G     | 678 | ASN  |
| 1   | G     | 728 | GLN  |
| 1   | G     | 751 | GLN  |
| 1   | G     | 771 | GLN  |
| 1   | G     | 816 | GLN  |
| 2   | H     | 7   | GLN  |
| 2   | H     | 30  | GLN  |
| 2   | H     | 44  | ASN  |
| 2   | H     | 60  | ASN  |
| 2   | H     | 110 | HIS  |
| 2   | H     | 135 | ASN  |
| 2   | H     | 139 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link    | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|---------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |         | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | ALF  | C     | 999 | 5,6,1,3 | 4,4,4        | 1.47 | 0           | -           |      |             |
| 5   | ADP  | G     | 998 | 4,3     | 28,29,29     | 0.91 | 0           | 43,45,45    | 0.88 | 2 (4%)      |
| 4   | ALF  | E     | 999 | 5,6,1,3 | 4,4,4        | 1.47 | 0           | -           |      |             |
| 5   | ADP  | A     | 998 | 4,3     | 28,29,29     | 0.91 | 0           | 43,45,45    | 0.88 | 2 (4%)      |
| 4   | ALF  | G     | 999 | 5,6,1,3 | 4,4,4        | 1.47 | 0           | -           |      |             |
| 5   | ADP  | C     | 998 | 4,3     | 28,29,29     | 0.91 | 0           | 43,45,45    | 0.88 | 2 (4%)      |
| 4   | ALF  | A     | 999 | 5,6,1,3 | 4,4,4        | 1.47 | 0           | -           |      |             |
| 5   | ADP  | E     | 998 | 4,3     | 28,29,29     | 0.90 | 0           | 43,45,45    | 0.88 | 2 (4%)      |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | ADP  | G     | 998 | 4,3  | -       | 5/16/32/32 | 0/3/3/3 |
| 5   | ADP  | E     | 998 | 4,3  | -       | 5/16/32/32 | 0/3/3/3 |
| 5   | ADP  | C     | 998 | 4,3  | -       | 5/16/32/32 | 0/3/3/3 |
| 5   | ADP  | A     | 998 | 4,3  | -       | 5/16/32/32 | 0/3/3/3 |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 5   | E     | 998 | ADP  | O3'-C3'-C2' | 2.50 | 119.84      | 111.82   |
| 5   | A     | 998 | ADP  | O3'-C3'-C2' | 2.49 | 119.79      | 111.82   |
| 5   | G     | 998 | ADP  | O3'-C3'-C2' | 2.49 | 119.79      | 111.82   |
| 5   | C     | 998 | ADP  | O3'-C3'-C2' | 2.48 | 119.77      | 111.82   |
| 5   | C     | 998 | ADP  | O2B-PB-O3A  | 2.27 | 112.24      | 104.64   |
| 5   | A     | 998 | ADP  | O2B-PB-O3A  | 2.26 | 112.20      | 104.64   |
| 5   | E     | 998 | ADP  | O2B-PB-O3A  | 2.25 | 112.18      | 104.64   |
| 5   | G     | 998 | ADP  | O2B-PB-O3A  | 2.25 | 112.18      | 104.64   |

There are no chirality outliers.

All (20) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | A     | 998 | ADP  | C5'-O5'-PA-O1A  |
| 5   | A     | 998 | ADP  | C5'-O5'-PA-O2A  |
| 5   | A     | 998 | ADP  | C5'-O5'-PA-O3A  |
| 5   | C     | 998 | ADP  | C5'-O5'-PA-O1A  |
| 5   | C     | 998 | ADP  | C5'-O5'-PA-O2A  |
| 5   | C     | 998 | ADP  | C5'-O5'-PA-O3A  |
| 5   | E     | 998 | ADP  | C5'-O5'-PA-O1A  |
| 5   | E     | 998 | ADP  | C5'-O5'-PA-O2A  |
| 5   | E     | 998 | ADP  | C5'-O5'-PA-O3A  |
| 5   | G     | 998 | ADP  | C5'-O5'-PA-O1A  |
| 5   | G     | 998 | ADP  | C5'-O5'-PA-O2A  |
| 5   | G     | 998 | ADP  | C5'-O5'-PA-O3A  |
| 5   | A     | 998 | ADP  | O4'-C4'-C5'-O5' |
| 5   | C     | 998 | ADP  | O4'-C4'-C5'-O5' |
| 5   | E     | 998 | ADP  | O4'-C4'-C5'-O5' |
| 5   | G     | 998 | ADP  | O4'-C4'-C5'-O5' |
| 5   | A     | 998 | ADP  | C3'-C4'-C5'-O5' |
| 5   | C     | 998 | ADP  | C3'-C4'-C5'-O5' |
| 5   | E     | 998 | ADP  | C3'-C4'-C5'-O5' |
| 5   | G     | 998 | ADP  | C3'-C4'-C5'-O5' |

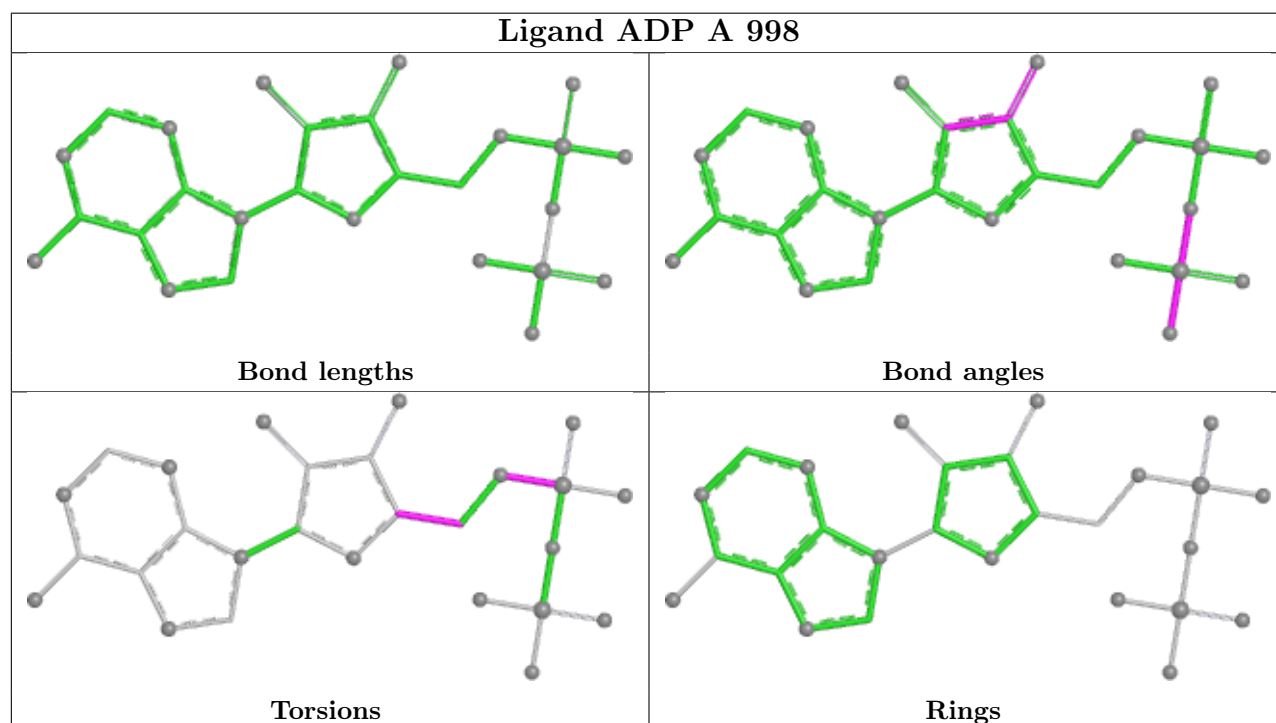
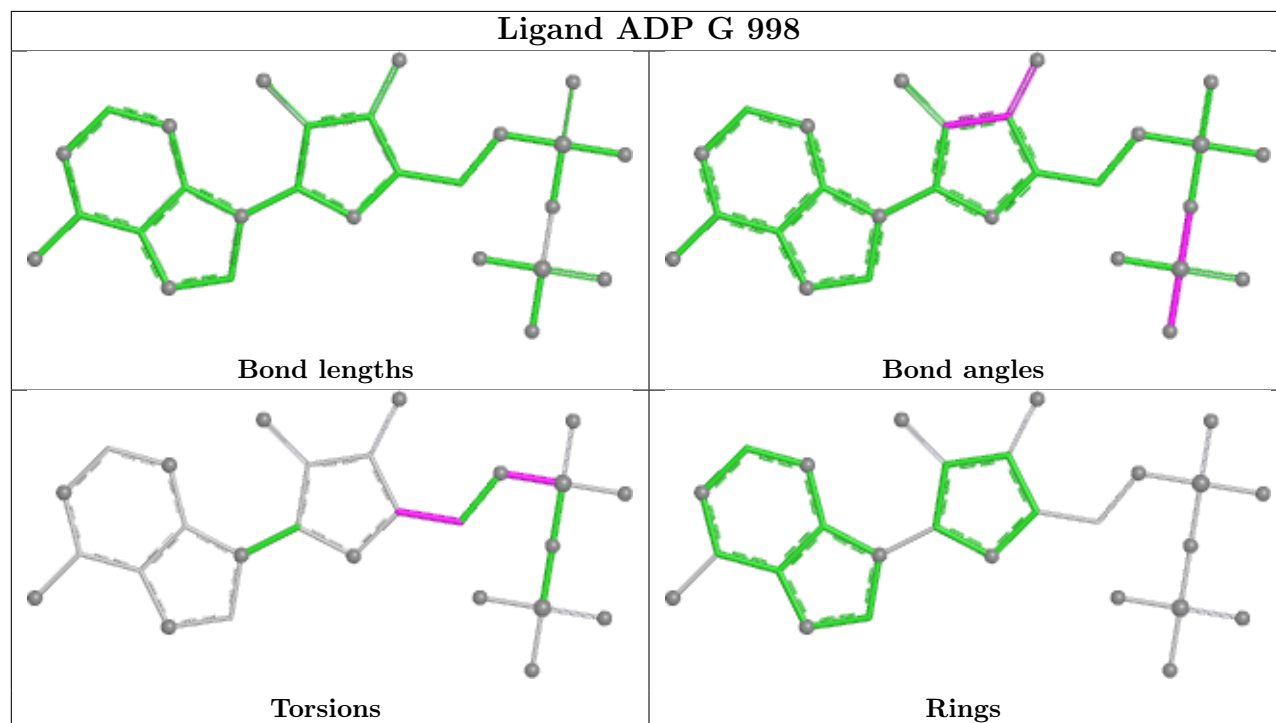
There are no ring outliers.

8 monomers are involved in 12 short contacts:

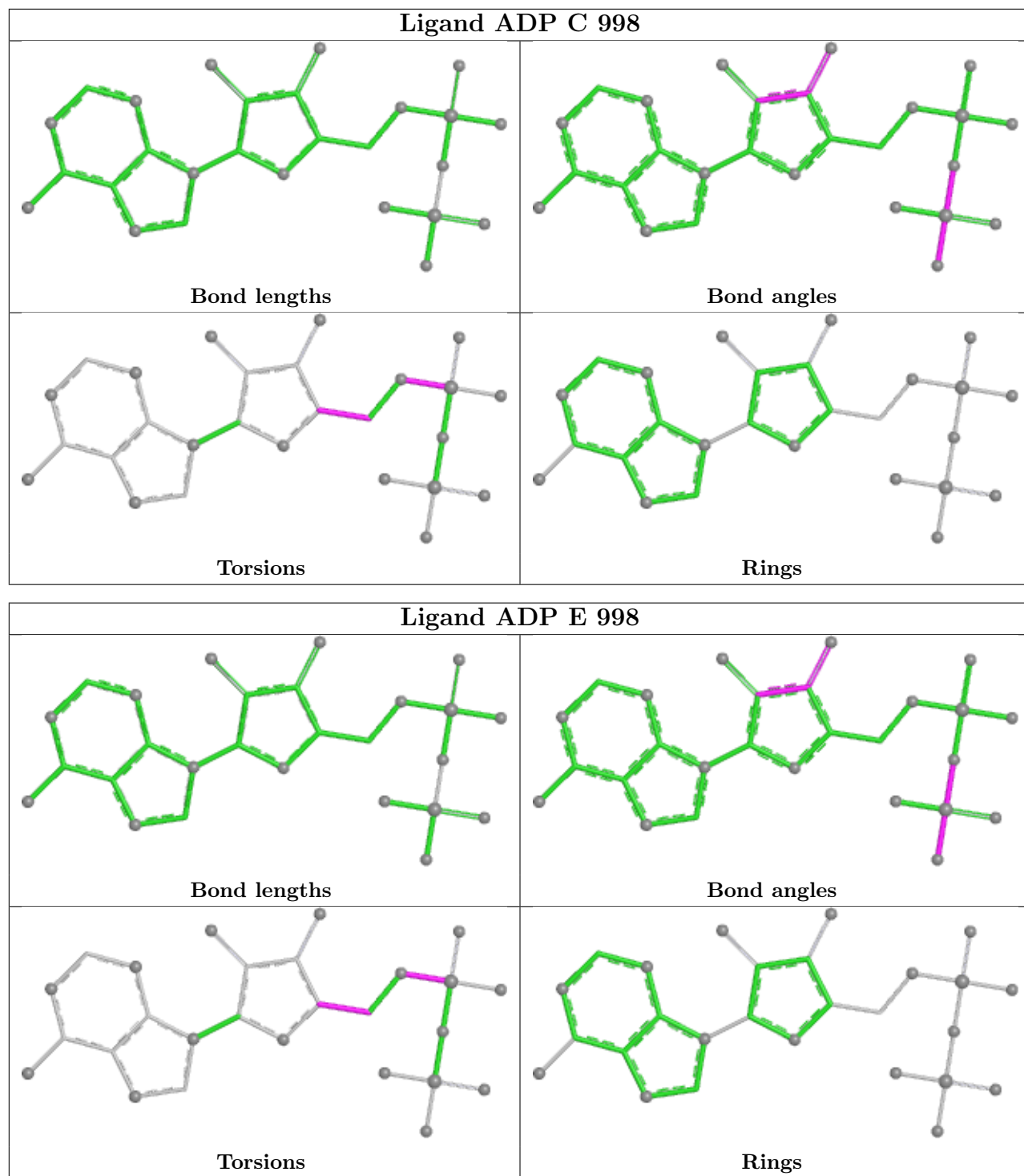
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | C     | 999 | ALF  | 1       | 0            |
| 5   | G     | 998 | ADP  | 3       | 0            |
| 4   | E     | 999 | ALF  | 1       | 0            |
| 5   | A     | 998 | ADP  | 1       | 0            |
| 4   | G     | 999 | ALF  | 1       | 0            |
| 5   | C     | 998 | ADP  | 4       | 0            |
| 4   | A     | 999 | ALF  | 1       | 0            |
| 5   | E     | 998 | ADP  | 4       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.