



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:46 am BST

PDB ID : 3AOI  
Title : RNA polymerase-Gfh1 complex (Crystal type 2)  
Authors : Tagami, S.; Sekine, S.; Kumarevel, T.; Yamamoto, M.; Yokoyama, S.; RIKEN  
Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2010-09-30  
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

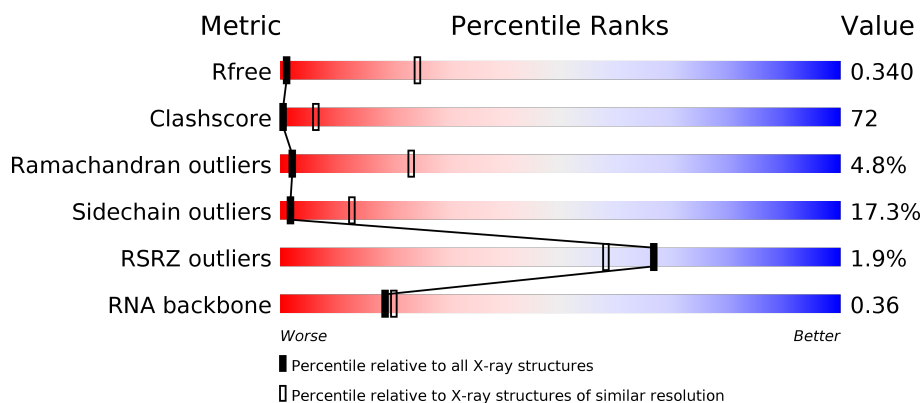
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.30 Å.

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





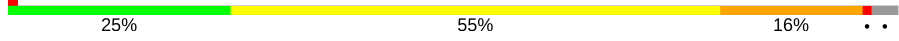
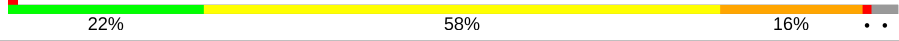
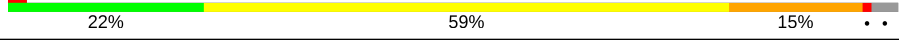
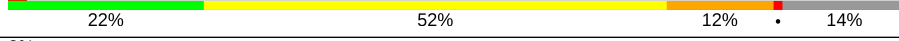
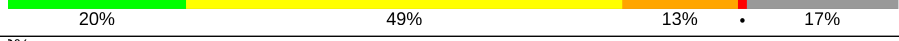
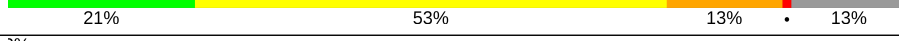
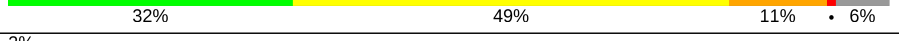
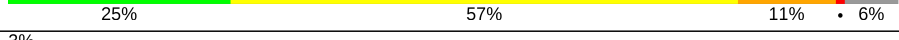
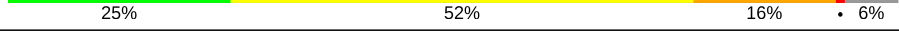



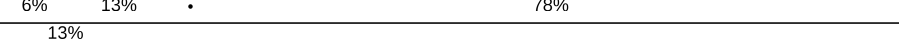

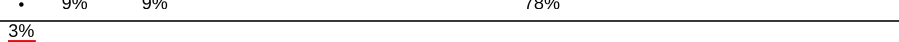
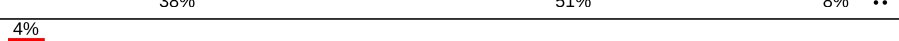
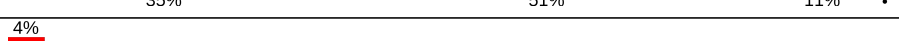

| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1014 (4.80-3.80)                                      |
| Clashscore            | 141614                      | 1077 (4.80-3.80)                                      |
| Ramachandran outliers | 138981                      | 1029 (4.80-3.80)                                      |
| Sidechain outliers    | 138945                      | 1012 (4.80-3.80)                                      |
| RSRZ outliers         | 127900                      | 1075 (4.90-3.70)                                      |
| RNA backbone          | 3102                        | 1058 (5.60-3.00)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 315    |                  |
| 1   | B     | 315    |                  |
| 1   | F     | 315    |                  |
| 1   | G     | 315    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | K     | 315    |    |
| 1   | L     | 315    |    |
| 2   | C     | 1119   |    |
| 2   | H     | 1119   |    |
| 2   | M     | 1119   |    |
| 3   | D     | 1524   |    |
| 3   | I     | 1524   |    |
| 3   | N     | 1524   |    |
| 4   | E     | 99     |    |
| 4   | J     | 99     |    |
| 4   | O     | 99     |    |
| 5   | P     | 27     |   |
| 5   | R     | 27     |  |
| 5   | T     | 27     |  |
| 6   | Q     | 32     |  |
| 6   | S     | 32     |  |
| 6   | U     | 32     |  |
| 7   | X     | 156    |  |
| 7   | Y     | 156    |  |
| 7   | Z     | 156    |  |

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 73646 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 DNA-directed RNA polymerase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1759  | 1123 | 306 | 328 | 2 |         |         |       |
| 1   | B     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1759  | 1123 | 306 | 328 | 2 |         |         |       |
| 1   | F     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1759  | 1123 | 306 | 328 | 2 |         |         |       |
| 1   | G     | 224      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1764  | 1126 | 307 | 329 | 2 |         |         |       |
| 1   | K     | 225      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1769  | 1129 | 308 | 330 | 2 |         |         |       |
| 1   | L     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1759  | 1123 | 306 | 328 | 2 |         |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | C     | 1083     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8550  | 5413 | 1525 | 1588 | 24 |         |         |       |
| 2   | H     | 1080     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8524  | 5395 | 1521 | 1584 | 24 |         |         |       |
| 2   | M     | 1084     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8555  | 5413 | 1528 | 1590 | 24 |         |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | D     | 1316     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10384 | 6574 | 1840 | 1941 | 29 |         |         |       |
| 3   | I     | 1262     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9965  | 6314 | 1765 | 1858 | 28 |         |         |       |
| 3   | N     | 1327     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10475 | 6634 | 1852 | 1961 | 28 |         |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | E     | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 754   | 481 | 131 | 138 | 4 |         |         |       |
| 4   | J     | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 754   | 481 | 131 | 138 | 4 |         |         |       |
| 4   | O     | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 754   | 481 | 131 | 138 | 4 |         |         |       |

- Molecule 5 is a DNA chain called DNA (5'-D(\*GP\*GP\*TP\*CP\*TP\*GP\*TP\*AP\*TP\*CP\*AP\*CP\*GP\*AP\*GP\*CP\*CP\*A\*CP\*CP\*GP\*CP\*CP\*GP\*CP\*AP\*T)-3').

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 5   | P     | 7        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 136   | 65 | 25 | 40 | 6 |         |         |       |
| 5   | R     | 6        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 119   | 57 | 24 | 33 | 5 |         |         |       |
| 5   | T     | 5        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 98    | 47 | 19 | 28 | 4 |         |         |       |

- Molecule 6 is a RNA chain called RNA (5'-R(\*CP\*CP\*CP\*GP\*GP\*AP\*AP\*GP\*AP\*UP\*CP\*AP\*UP\*CP\*UP\*UP\*CP\*CP\*GP\*GP\*GP\*GP\*GP\*AP\*U\*GP\*CP\*GP\*GP\*CP\*GP\*G)-3').

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 6   | Q     | 7        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 152   | 68 | 31 | 47 | 6 |         |         |       |
| 6   | S     | 8        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 172   | 77 | 33 | 55 | 7 |         |         |       |
| 6   | U     | 7        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 152   | 68 | 31 | 47 | 6 |         |         |       |

- Molecule 7 is a protein called Anti-cleavage anti-GreA transcription factor Gfh1.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | X     | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1189  | 730 | 212 | 243 | 4 |         |         |       |
| 7   | Y     | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1169  | 719 | 207 | 239 | 4 |         |         |       |
| 7   | Z     | 152      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1169  | 719 | 207 | 239 | 4 |         |         |       |

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 8   | I     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 8   | D     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 8   | N     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

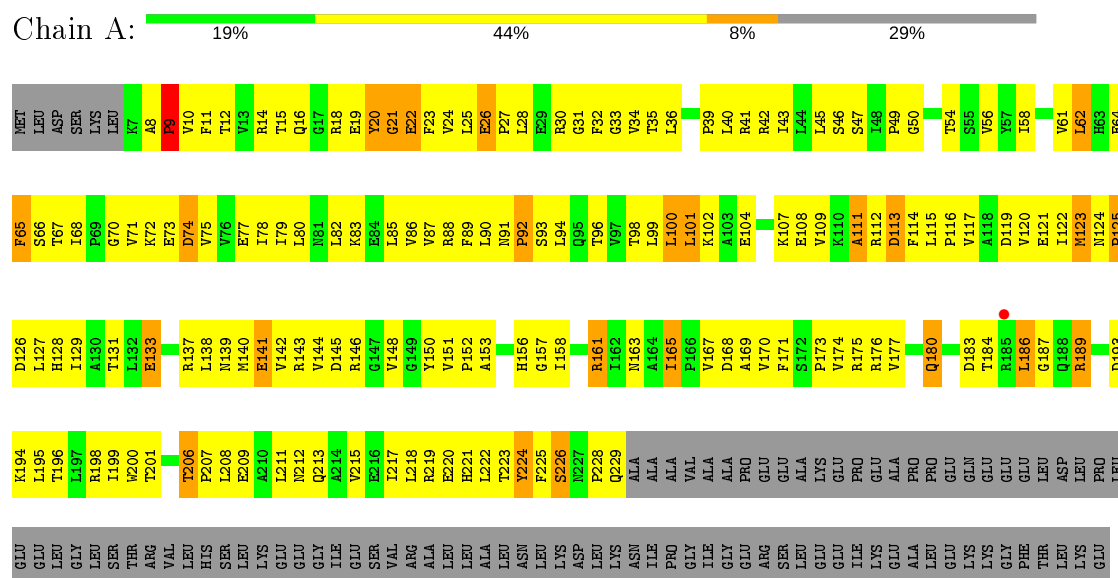
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 9   | D     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 9   | S     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 9   | N     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

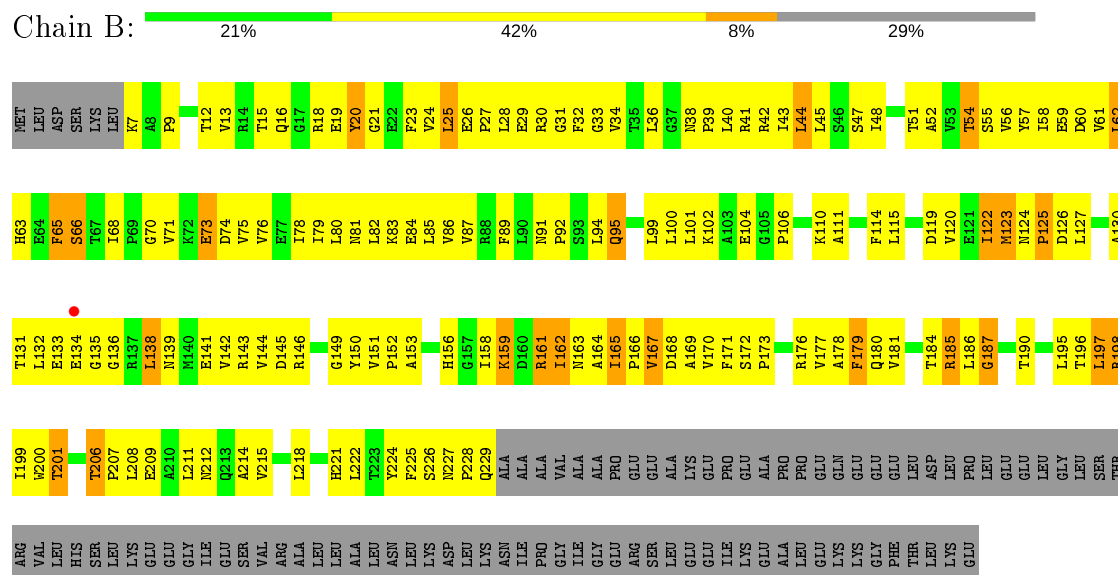
### 3 Residue-property plots

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

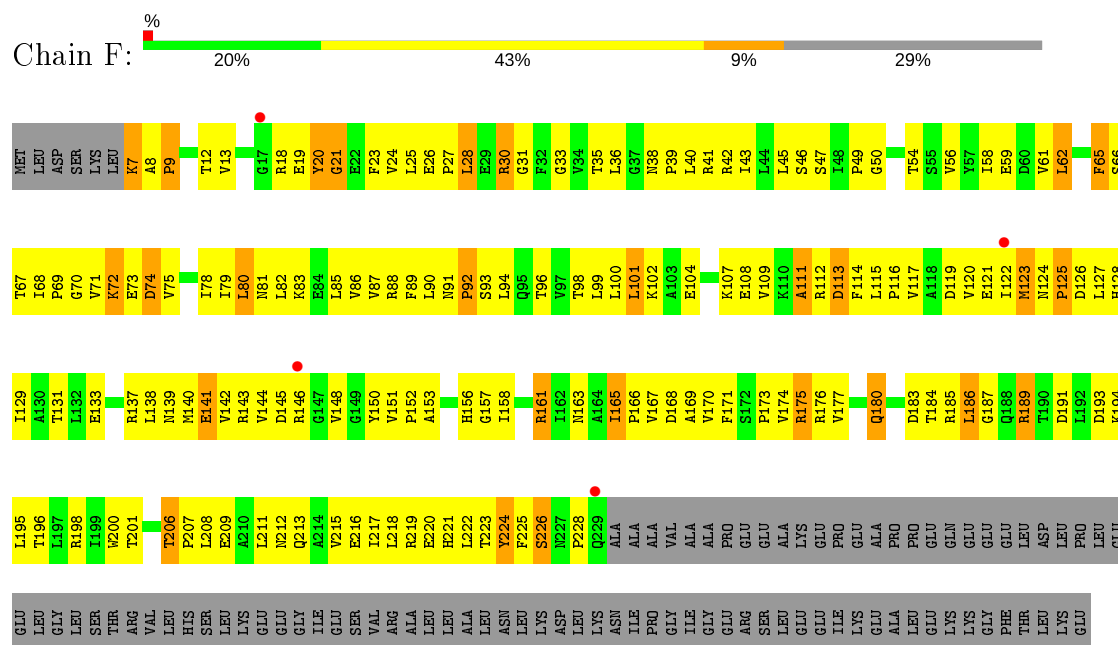
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



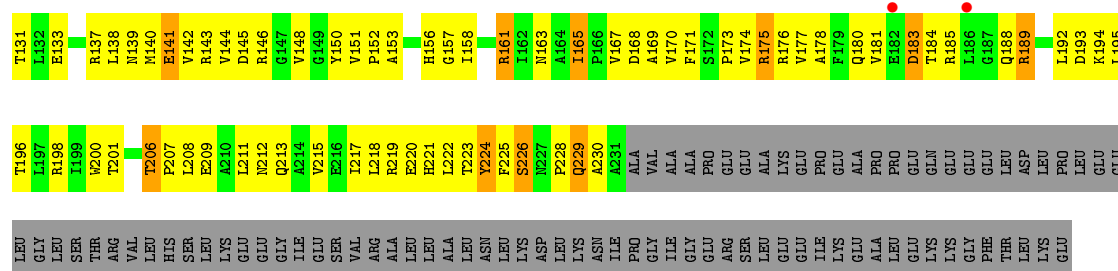
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



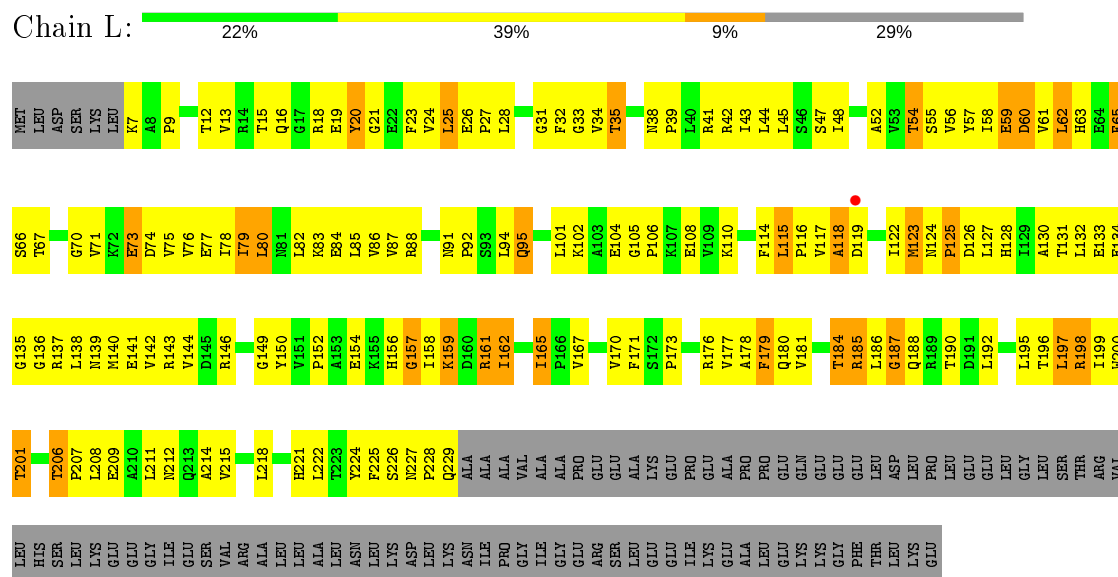
• Molecule 1: DNA-directed RNA polymerase subunit alpha



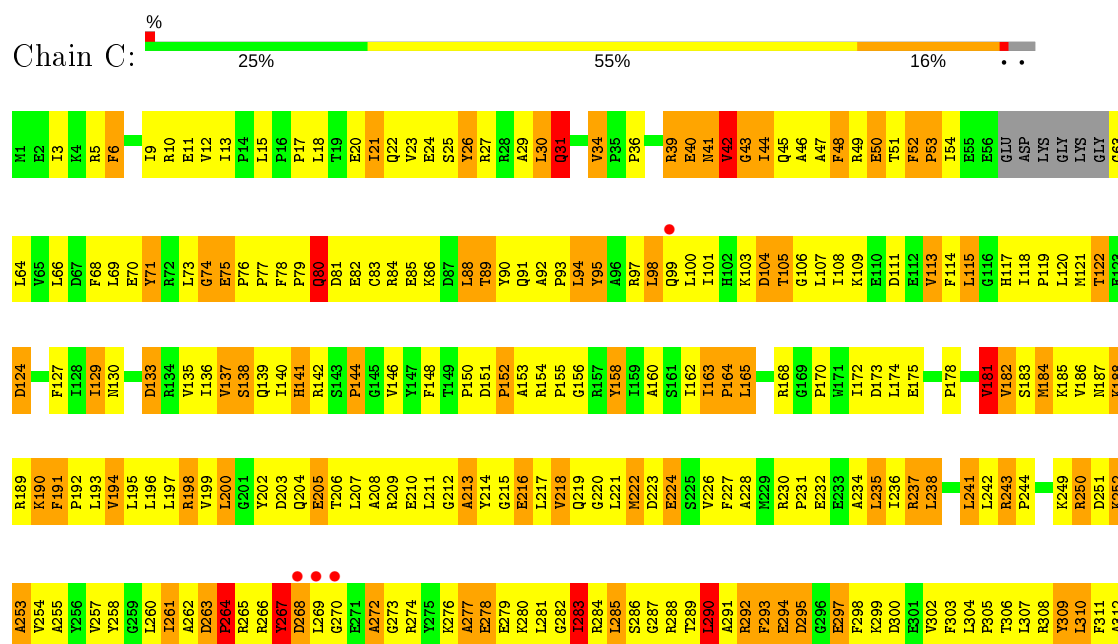


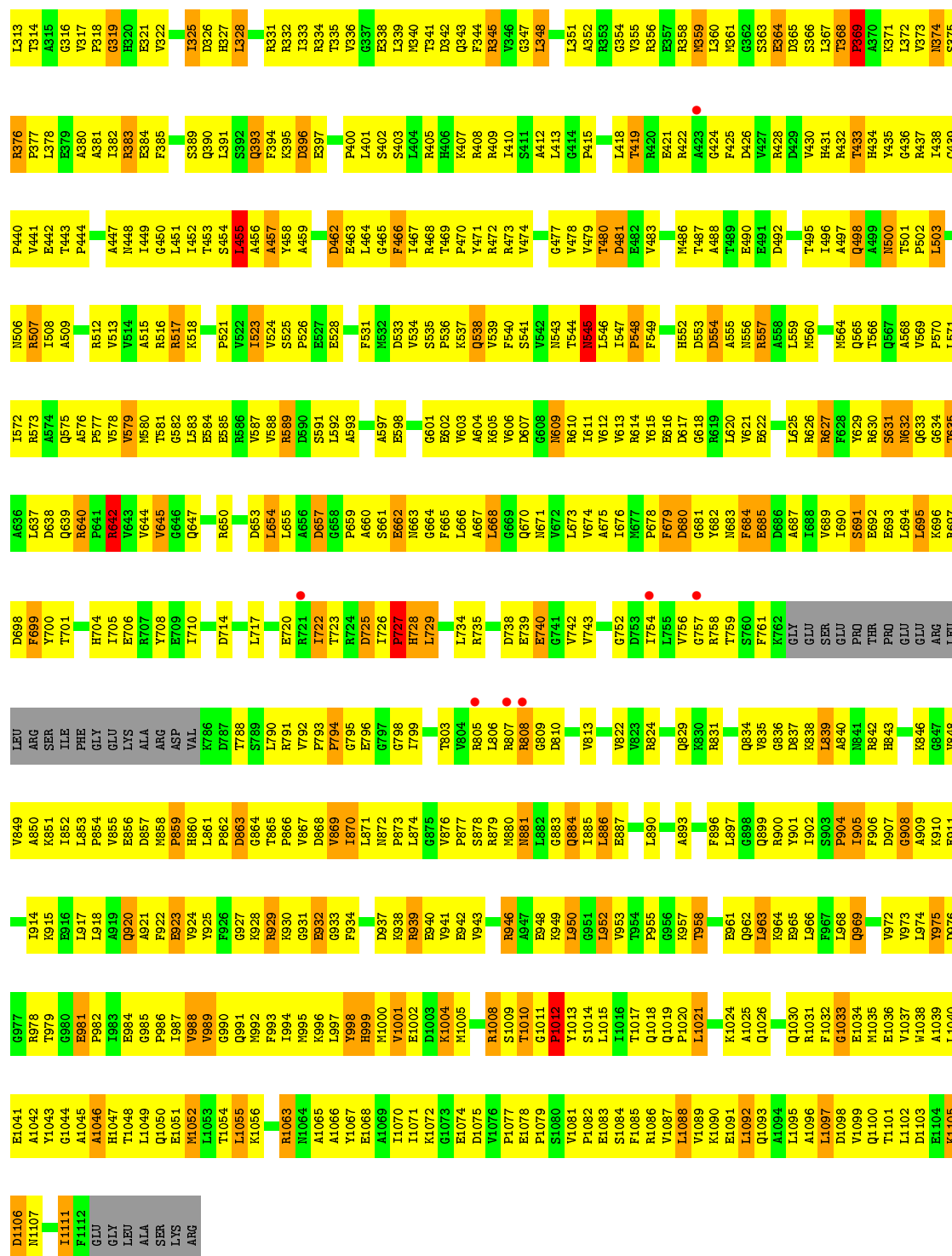


• Molecule 1: DNA-directed RNA polymerase subunit alpha

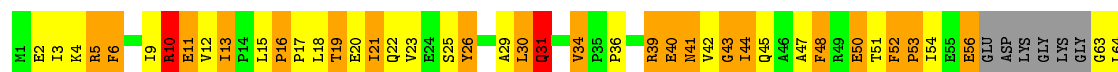


• Molecule 2: DNA-directed RNA polymerase subunit beta

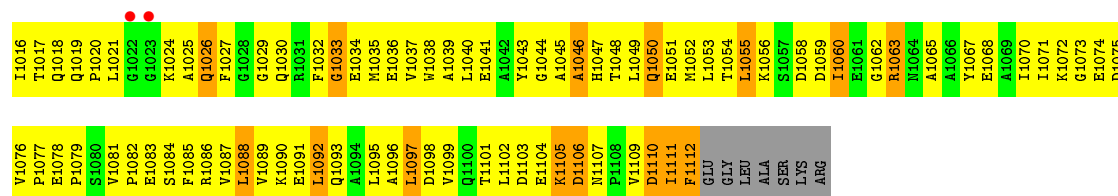




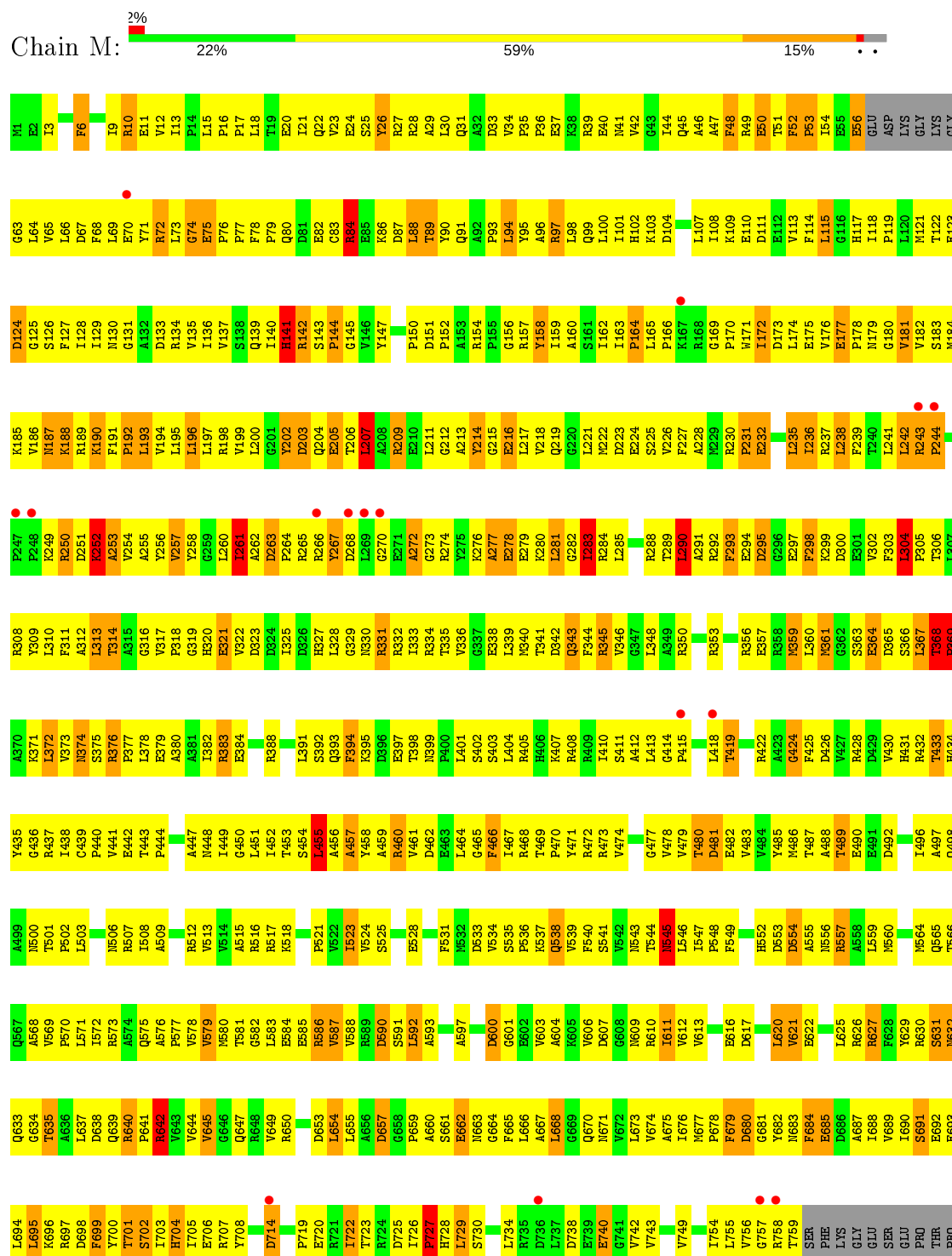
### • Molecule 2: DNA-directed RNA polymerase subunit beta

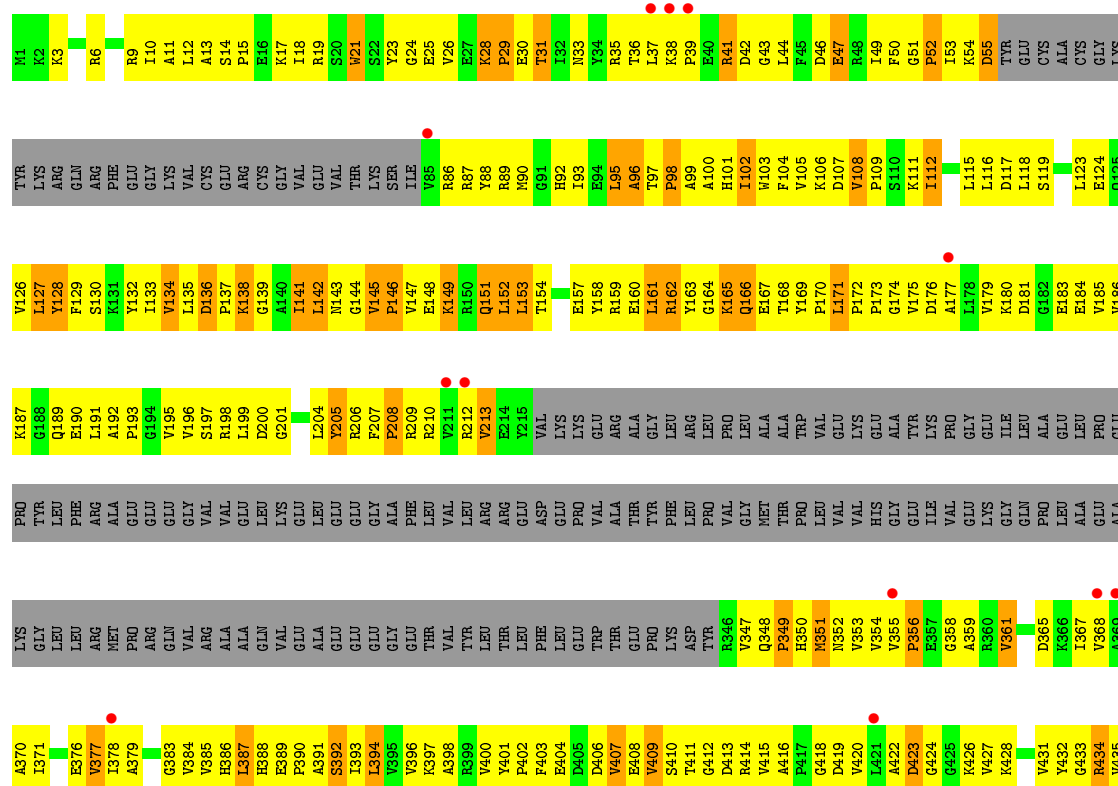




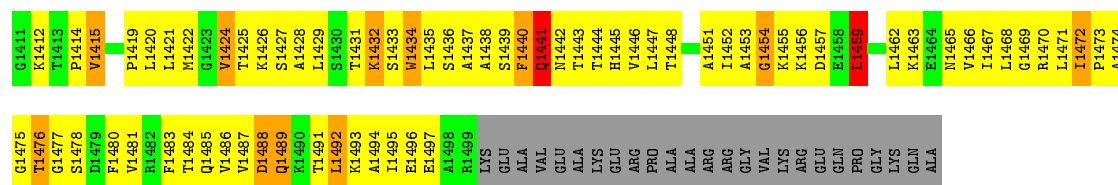


### • Molecule 2: DNA-directed RNA polymerase subunit beta

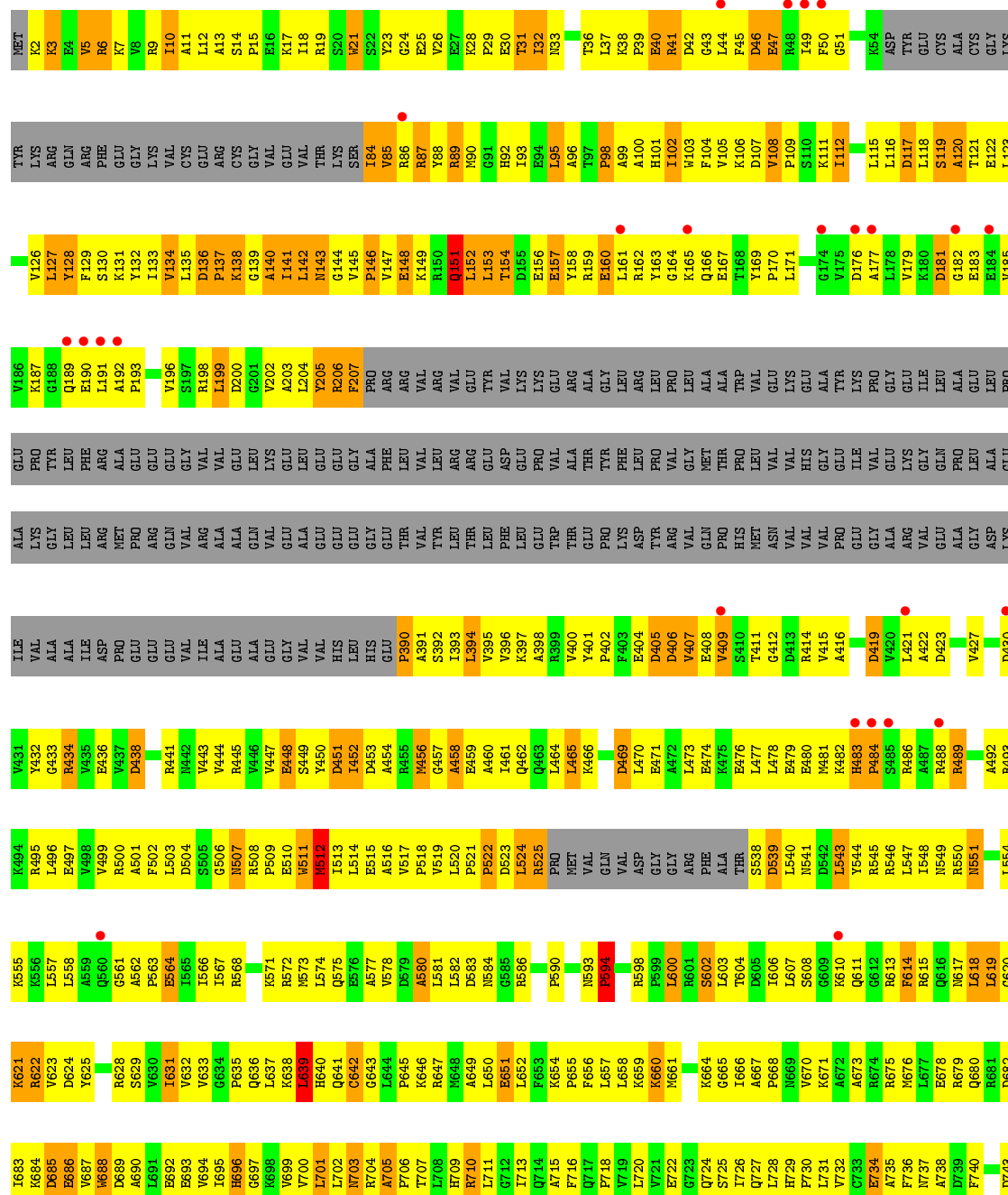
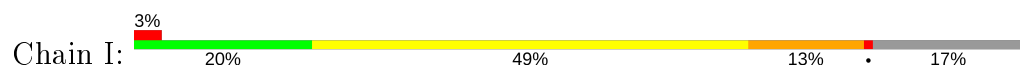








### • Molecule 3: DNA-directed RNA polymerase subunit beta'

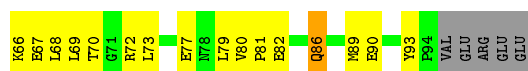




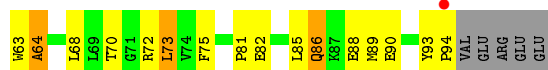




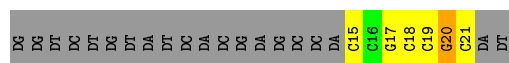




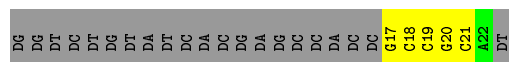
- Molecule 4: DNA-directed RNA polymerase subunit omega



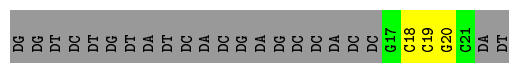
- Molecule 5: DNA (5'-D(\*GP\*GP\*TP\*CP\*TP\*GP\*TP\*AP\*TP\*CP\*AP\*CP\*GP\*AP\*GP\*CP\*CP\*A\*CP\*CP\*GP\*CP\*CP\*GP\*CP\*AP\*T)-3')



- Molecule 5: DNA (5'-D(\*GP\*GP\*TP\*CP\*TP\*GP\*TP\*AP\*TP\*CP\*AP\*CP\*GP\*AP\*GP\*CP\*CP\*A\*CP\*CP\*GP\*CP\*CP\*GP\*CP\*AP\*T)-3')



- Molecule 5: DNA (5'-D(\*GP\*GP\*TP\*CP\*TP\*GP\*TP\*AP\*TP\*CP\*AP\*CP\*GP\*AP\*GP\*CP\*CP\*A\*CP\*CP\*GP\*CP\*CP\*GP\*CP\*AP\*T)-3')



- Molecule 6: RNA (5'-R(\*CP\*CP\*CP\*GP\*GP\*AP\*AP\*GP\*AP\*UP\*CP\*AP\*UP\*CP\*UP\*UP\*CP\*CP\*GP\*GP\*GP\*GP\*AP\*U\*GP\*CP\*GP\*GP\*CP\*GP\*G)-3')



- Molecule 6: RNA (5'-R(\*CP\*CP\*CP\*GP\*GP\*AP\*AP\*GP\*AP\*UP\*CP\*AP\*UP\*CP\*UP\*UP\*CP\*CP\*GP\*GP\*GP\*GP\*AP\*U\*GP\*CP\*GP\*GP\*CP\*GP\*G)-3')

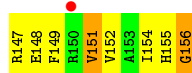
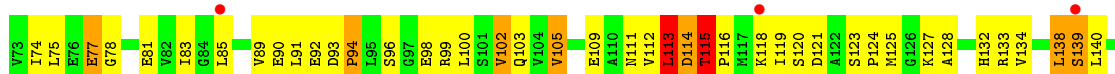
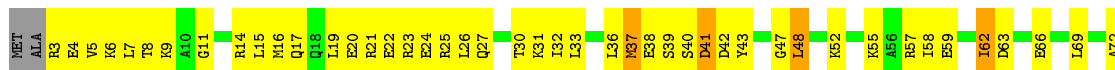




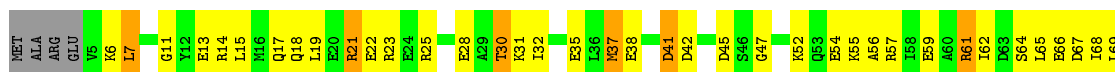
- Molecule 6: RNA (5'-R(\*CP\*CP\*CP\*GP\*GP\*AP\*AP\*GP\*AP\*UP\*CP\*AP\*UP\*CP\*UP\*UP\*CP\*CP\*GP\*GP\*GP\*GP\*AP\*U\*GP\*CP\*GP\*GP\*CP\*GP\*G)-3')



- Molecule 7: Anti-cleavage anti-GreA transcription factor Gfh1



- Molecule 7: Anti-cleavage anti-GreA transcription factor Gfh1



- Molecule 7: Anti-cleavage anti-GreA transcription factor Gfh1



|      |
|------|
| F149 |
| R150 |
| V151 |
| V152 |
| A153 |
| I154 |
| H155 |
| G156 |

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 189.23Å 264.51Å 193.93Å<br>90.00° 116.68° 90.00°            | Depositor        |
| Resolution (Å)  | 47.57 – 4.30<br>47.57 – 4.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.6 (47.57-4.30)<br>97.7 (47.57-4.30)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.68 (at 4.29Å)   | Xtriage          |
| Refinement program  | CNS 1.2   | Depositor        |
| R, $R_{free}$   | 0.317 , 0.338<br>0.320 , 0.340                              | Depositor<br>DCC |
| $R_{free}$ test set   | 3392 reflections (3.01%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 128.7   | Xtriage          |
| Anisotropy  | 0.299   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 107.0  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$ | Xtriage          |
| Estimated twinning fraction   | 0.054 for l,-k,h  | Xtriage          |
| $F_o, F_c$ correlation  | 0.81  | EDS              |
| Total number of atoms   | 73646   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 160.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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     | 0.48         | 0/1791         | 0.76        | 0/2436           |
| 1   | B     | 0.47         | 0/1791         | 0.71        | 1/2436 (0.0%)    |
| 1   | F     | 0.48         | 0/1791         | 0.75        | 0/2436           |
| 1   | G     | 0.47         | 0/1796         | 0.70        | 1/2443 (0.0%)    |
| 1   | K     | 0.50         | 0/1801         | 0.76        | 0/2450           |
| 1   | L     | 0.48         | 0/1791         | 0.70        | 1/2436 (0.0%)    |
| 2   | C     | 0.49         | 0/8713         | 0.78        | 5/11785 (0.0%)   |
| 2   | H     | 0.51         | 0/8686         | 0.78        | 3/11750 (0.0%)   |
| 2   | M     | 0.51         | 0/8717         | 0.81        | 6/11792 (0.1%)   |
| 3   | D     | 0.50         | 0/10559        | 0.77        | 5/14272 (0.0%)   |
| 3   | I     | 0.50         | 0/10131        | 0.79        | 6/13685 (0.0%)   |
| 3   | N     | 0.49         | 0/10653        | 0.79        | 8/14403 (0.1%)   |
| 4   | E     | 0.47         | 0/768          | 0.72        | 1/1035 (0.1%)    |
| 4   | J     | 0.47         | 0/768          | 0.73        | 1/1035 (0.1%)    |
| 4   | O     | 0.49         | 0/768          | 0.77        | 1/1035 (0.1%)    |
| 5   | P     | 0.89         | 0/151          | 1.70        | 3/230 (1.3%)     |
| 5   | R     | 0.81         | 0/133          | 1.04        | 0/203            |
| 5   | T     | 0.84         | 0/109          | 0.89        | 0/166            |
| 6   | Q     | 1.05         | 0/170          | 1.04        | 0/265            |
| 6   | S     | 1.02         | 0/192          | 0.92        | 0/299            |
| 6   | U     | 0.94         | 0/170          | 0.97        | 2/265 (0.8%)     |
| 7   | X     | 0.56         | 1/1198 (0.1%)  | 0.70        | 1/1608 (0.1%)    |
| 7   | Y     | 0.64         | 1/1178 (0.1%)  | 0.66        | 0/1582           |
| 7   | Z     | 0.65         | 1/1178 (0.1%)  | 0.68        | 1/1582 (0.1%)    |
| All | All   | 0.51         | 3/75003 (0.0%) | 0.78        | 46/101629 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | C     | 0                   | 5                   |
| 2   | H     | 0                   | 1                   |
| 2   | M     | 0                   | 3                   |
| 3   | D     | 0                   | 2                   |
| 3   | I     | 0                   | 4                   |
| 3   | N     | 0                   | 5                   |
| 6   | Q     | 0                   | 1                   |
| 6   | S     | 0                   | 1                   |
| All | All   | 0                   | 22                  |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7   | Z     | 156 | GLY  | C-OXT | 16.27 | 1.54        | 1.23     |
| 7   | Y     | 156 | GLY  | C-OXT | 16.19 | 1.54        | 1.23     |
| 7   | X     | 156 | GLY  | C-OXT | 11.06 | 1.44        | 1.23     |

All (46) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | P     | 20   | DG   | N9-C1'-C2'  | 9.98  | 131.56      | 112.60   |
| 5   | P     | 20   | DG   | O4'-C1'-C2' | 8.43  | 112.64      | 105.90   |
| 3   | I     | 1209 | LEU  | N-CA-C      | -8.04 | 89.28       | 111.00   |
| 3   | N     | 1209 | LEU  | N-CA-C      | -7.97 | 89.49       | 111.00   |
| 3   | N     | 142  | LEU  | CA-CB-CG    | 7.29  | 132.07      | 115.30   |
| 2   | C     | 163  | ILE  | C-N-CD      | -6.96 | 105.28      | 120.60   |
| 3   | N     | 1314 | LYS  | CD-CE-NZ    | -6.86 | 95.93       | 111.70   |
| 3   | I     | 1314 | LYS  | CD-CE-NZ    | -6.85 | 95.94       | 111.70   |
| 3   | D     | 1314 | LYS  | CD-CE-NZ    | -6.81 | 96.03       | 111.70   |
| 3   | D     | 28   | LYS  | C-N-CD      | -6.61 | 106.06      | 120.60   |
| 5   | P     | 19   | DC   | O4'-C1'-N1  | 6.48  | 112.54      | 108.00   |
| 2   | M     | 795  | GLY  | N-CA-C      | -6.31 | 97.32       | 113.10   |
| 3   | N     | 143  | ASN  | N-CA-C      | -6.28 | 94.06       | 111.00   |
| 2   | M     | 243  | ARG  | C-N-CD      | -6.26 | 106.82      | 120.60   |
| 2   | C     | 455  | LEU  | CA-CB-CG    | 6.15  | 129.46      | 115.30   |
| 7   | Z     | 113  | LEU  | CA-CB-CG    | 6.14  | 129.43      | 115.30   |
| 7   | X     | 113  | LEU  | CA-CB-CG    | 6.14  | 129.42      | 115.30   |
| 2   | H     | 455  | LEU  | CA-CB-CG    | 6.10  | 129.32      | 115.30   |
| 2   | M     | 455  | LEU  | CA-CB-CG    | 6.10  | 129.33      | 115.30   |
| 3   | N     | 211  | VAL  | CB-CA-C     | -5.91 | 100.18      | 111.40   |
| 2   | C     | 795  | GLY  | N-CA-C      | -5.88 | 98.41       | 113.10   |
| 4   | J     | 49   | GLN  | N-CA-C      | 5.84  | 126.77      | 111.00   |
| 2   | M     | 372  | LEU  | CA-CB-CG    | 5.84  | 128.72      | 115.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | H     | 795  | GLY  | N-CA-C      | -5.83 | 98.53       | 113.10   |
| 3   | N     | 1110 | ALA  | N-CA-C      | -5.82 | 95.29       | 111.00   |
| 3   | I     | 46   | ASP  | O-C-N       | -5.69 | 113.60      | 122.70   |
| 3   | D     | 1110 | ALA  | N-CA-C      | -5.63 | 95.81       | 111.00   |
| 2   | M     | 304  | LEU  | CA-CB-CG    | 5.48  | 127.89      | 115.30   |
| 6   | U     | 15   | G    | N9-C1'-C2'  | -5.47 | 105.98      | 112.00   |
| 4   | E     | 49   | GLN  | N-CA-C      | 5.39  | 125.56      | 111.00   |
| 3   | I     | 1110 | ALA  | N-CA-C      | -5.32 | 96.63       | 111.00   |
| 4   | O     | 49   | GLN  | N-CA-C      | 5.31  | 125.35      | 111.00   |
| 3   | D     | 166  | GLN  | N-CA-C      | -5.30 | 96.69       | 111.00   |
| 3   | N     | 166  | GLN  | N-CA-C      | -5.27 | 96.78       | 111.00   |
| 2   | C     | 319  | GLY  | N-CA-C      | -5.24 | 100.00      | 113.10   |
| 3   | D     | 851  | LEU  | CA-CB-CG    | -5.23 | 103.28      | 115.30   |
| 3   | N     | 851  | LEU  | CA-CB-CG    | -5.22 | 103.30      | 115.30   |
| 3   | I     | 543  | LEU  | CA-CB-CG    | -5.19 | 103.36      | 115.30   |
| 1   | B     | 135  | GLY  | N-CA-C      | -5.18 | 100.16      | 113.10   |
| 1   | G     | 135  | GLY  | N-CA-C      | -5.17 | 100.18      | 113.10   |
| 3   | I     | 851  | LEU  | CA-CB-CG    | -5.17 | 103.42      | 115.30   |
| 1   | L     | 135  | GLY  | N-CA-C      | -5.16 | 100.19      | 113.10   |
| 2   | H     | 322  | VAL  | N-CA-C      | -5.08 | 97.28       | 111.00   |
| 6   | U     | 16   | G    | C2'-C3'-O3' | 5.08  | 121.83      | 113.70   |
| 2   | C     | 886  | LEU  | CA-CB-CG    | -5.06 | 103.66      | 115.30   |
| 2   | M     | 886  | LEU  | CA-CB-CG    | -5.01 | 103.78      | 115.30   |

There are no chirality outliers.

All (22) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 2   | C     | 267  | TYR  | Sidechain |
| 2   | C     | 589  | ARG  | Sidechain |
| 2   | C     | 642  | ARG  | Sidechain |
| 2   | C     | 71   | TYR  | Sidechain |
| 2   | C     | 735  | ARG  | Sidechain |
| 3   | D     | 1058 | ARG  | Sidechain |
| 3   | D     | 1327 | ARG  | Sidechain |
| 2   | H     | 642  | ARG  | Sidechain |
| 3   | I     | 1029 | ARG  | Sidechain |
| 3   | I     | 1058 | ARG  | Sidechain |
| 3   | I     | 1327 | ARG  | Sidechain |
| 3   | I     | 783  | ARG  | Sidechain |
| 2   | M     | 202  | TYR  | Sidechain |
| 2   | M     | 642  | ARG  | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 2   | M     | 84   | ARG  | Sidechain |
| 3   | N     | 1058 | ARG  | Sidechain |
| 3   | N     | 1327 | ARG  | Sidechain |
| 3   | N     | 215  | TYR  | Sidechain |
| 3   | N     | 56   | TYR  | Sidechain |
| 3   | N     | 783  | ARG  | Sidechain |
| 6   | Q     | 12   | G    | Sidechain |
| 6   | S     | 9    | U    | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1759  | 0        | 1805     | 209     | 3            |
| 1   | B     | 1759  | 0        | 1805     | 263     | 2            |
| 1   | F     | 1759  | 0        | 1805     | 195     | 3            |
| 1   | G     | 1764  | 0        | 1810     | 253     | 3            |
| 1   | K     | 1769  | 0        | 1815     | 202     | 0            |
| 1   | L     | 1759  | 0        | 1805     | 220     | 0            |
| 2   | C     | 8550  | 0        | 8654     | 1412    | 1            |
| 2   | H     | 8524  | 0        | 8626     | 1521    | 0            |
| 2   | M     | 8555  | 0        | 8658     | 1519    | 1            |
| 3   | D     | 10384 | 0        | 10615    | 1752    | 3            |
| 3   | I     | 9965  | 0        | 10206    | 1707    | 1            |
| 3   | N     | 10475 | 0        | 10699    | 1791    | 3            |
| 4   | E     | 754   | 0        | 769      | 94      | 0            |
| 4   | J     | 754   | 0        | 769      | 116     | 0            |
| 4   | O     | 754   | 0        | 769      | 111     | 0            |
| 5   | P     | 136   | 0        | 79       | 3       | 0            |
| 5   | R     | 119   | 0        | 68       | 12      | 0            |
| 5   | T     | 98    | 0        | 57       | 8       | 0            |
| 6   | Q     | 152   | 0        | 78       | 10      | 0            |
| 6   | S     | 172   | 0        | 88       | 12      | 0            |
| 6   | U     | 152   | 0        | 79       | 12      | 0            |
| 7   | X     | 1189  | 0        | 1205     | 141     | 0            |
| 7   | Y     | 1169  | 0        | 1186     | 151     | 0            |
| 7   | Z     | 1169  | 0        | 1186     | 146     | 0            |
| 8   | D     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8   | I     | 1     | 0        | 0        | 0       | 0            |
| 8   | N     | 1     | 0        | 0        | 0       | 0            |
| 9   | D     | 1     | 0        | 0        | 0       | 0            |
| 9   | N     | 1     | 0        | 0        | 0       | 0            |
| 9   | S     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 73646 | 0        | 74636    | 10729   | 10           |

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 (10729) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:50:PHE:CD2   | 3:N:522:PRO:HD3  | 1.20                     | 1.62              |
| 2:H:182:VAL:HG11 | 2:H:193:LEU:CD2  | 1.09                     | 1.56              |
| 2:H:1090:LYS:HE3 | 3:I:90:MET:SD    | 1.45                     | 1.55              |
| 2:H:182:VAL:CG1  | 2:H:193:LEU:HD21 | 1.13                     | 1.55              |
| 3:I:783:ARG:NH1  | 7:Y:41:ASP:CB    | 1.67                     | 1.53              |
| 2:C:193:LEU:CD2  | 2:C:307:LEU:HD22 | 1.36                     | 1.52              |
| 3:I:131:LYS:HG3  | 3:I:568:ARG:CD   | 1.35                     | 1.51              |
| 3:N:50:PHE:CD2   | 3:N:522:PRO:CD   | 1.92                     | 1.50              |
| 2:H:1019:GLN:NE2 | 3:I:621:LYS:CG   | 1.71                     | 1.47              |
| 2:H:1019:GLN:CD  | 3:I:621:LYS:HG3  | 1.35                     | 1.46              |
| 3:I:131:LYS:CG   | 3:I:568:ARG:HD3  | 1.43                     | 1.44              |
| 3:I:50:PHE:O     | 3:I:89:ARG:CD    | 1.65                     | 1.44              |
| 2:C:1004:LYS:HD2 | 3:D:744:GLN:NE2  | 1.29                     | 1.42              |
| 3:I:783:ARG:NH1  | 7:Y:41:ASP:HB3   | 1.20                     | 1.42              |
| 3:N:970:LYS:NZ   | 7:Z:113:LEU:HD23 | 1.11                     | 1.41              |
| 1:B:187:GLY:HA3  | 3:D:685:ASP:CB   | 1.50                     | 1.40              |
| 1:G:185:ARG:CZ   | 3:I:692:GLU:HG2  | 1.49                     | 1.40              |
| 3:N:970:LYS:NZ   | 7:Z:113:LEU:CD2  | 1.84                     | 1.39              |
| 2:M:39:ARG:HE    | 2:M:45:GLN:NE2   | 1.13                     | 1.38              |
| 3:N:783:ARG:CD   | 7:Z:41:ASP:OD2   | 1.71                     | 1.38              |
| 3:D:136:ASP:CG   | 3:D:137:PRO:HD3  | 1.43                     | 1.38              |
| 3:D:127:LEU:O    | 3:D:457:GLY:HA2  | 1.20                     | 1.36              |
| 3:N:783:ARG:HH11 | 7:Z:41:ASP:CB    | 1.35                     | 1.36              |
| 2:H:1090:LYS:CE  | 3:I:90:MET:SD    | 2.12                     | 1.35              |
| 3:D:87:ARG:HB3   | 3:D:523:ASP:CB   | 1.58                     | 1.33              |
| 2:H:1086:ARG:NH1 | 3:I:88:TYR:CE2   | 1.96                     | 1.33              |
| 2:M:911:GLU:OE1  | 3:N:951:ILE:CD1  | 1.76                     | 1.32              |
| 2:M:911:GLU:OE1  | 3:N:951:ILE:HD11 | 1.14                     | 1.31              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:87:ARG:CB     | 3:D:523:ASP:HB2  | 1.61                     | 1.30              |
| 3:D:50:PHE:CD2    | 3:D:522:PRO:HD3  | 1.64                     | 1.30              |
| 3:N:783:ARG:NH1   | 7:Z:41:ASP:CB    | 1.90                     | 1.30              |
| 3:I:131:LYS:CG    | 3:I:568:ARG:CD   | 2.02                     | 1.29              |
| 2:M:39:ARG:HG2    | 2:M:45:GLN:CD    | 1.52                     | 1.29              |
| 1:G:185:ARG:NE    | 3:I:692:GLU:HG2  | 1.46                     | 1.29              |
| 2:H:1004:LYS:HD2  | 3:I:744:GLN:NE2  | 1.45                     | 1.29              |
| 2:H:122:THR:CG2   | 2:H:124:ASP:OD1  | 1.81                     | 1.29              |
| 2:M:1090:LYS:HE3  | 3:N:90:MET:CG    | 1.63                     | 1.29              |
| 3:N:783:ARG:NH1   | 7:Z:41:ASP:HB2   | 1.41                     | 1.29              |
| 3:N:50:PHE:CG     | 3:N:522:PRO:HG2  | 1.68                     | 1.28              |
| 2:M:39:ARG:CG     | 2:M:45:GLN:OE1   | 1.80                     | 1.28              |
| 2:C:685:GLU:HG3   | 7:X:41:ASP:OD1   | 1.20                     | 1.28              |
| 3:N:970:LYS:CE    | 7:Z:113:LEU:HD23 | 1.60                     | 1.28              |
| 3:I:12:LEU:HD21   | 3:I:104:PHE:CE1  | 1.70                     | 1.27              |
| 2:M:122:THR:CG2   | 2:M:124:ASP:OD1  | 1.81                     | 1.26              |
| 2:C:185:LYS:CD    | 2:C:190:LYS:HG2  | 1.64                     | 1.26              |
| 3:N:50:PHE:CG     | 3:N:522:PRO:CG   | 2.17                     | 1.25              |
| 2:M:41:ASN:O      | 2:M:46:ALA:HB2   | 1.12                     | 1.25              |
| 3:N:675:ARG:O     | 3:N:679:ARG:HB2  | 1.37                     | 1.24              |
| 2:M:84:ARG:NH2    | 2:M:133:ASP:OD2  | 1.71                     | 1.23              |
| 2:H:309:TYR:O     | 2:H:313:LEU:HD13 | 1.36                     | 1.23              |
| 2:M:39:ARG:NE     | 2:M:45:GLN:NE2   | 1.85                     | 1.23              |
| 2:H:1103:ASP:OD2  | 3:I:2:LYS:HA     | 1.33                     | 1.22              |
| 3:I:131:LYS:CB    | 3:I:568:ARG:HD2  | 1.69                     | 1.22              |
| 3:N:86:ARG:CG     | 3:N:523:ASP:OD2  | 1.86                     | 1.22              |
| 3:D:124:GLU:HG3   | 3:D:128:TYR:CE1  | 1.75                     | 1.21              |
| 2:M:30:LEU:HD12   | 2:M:30:LEU:O     | 1.40                     | 1.21              |
| 2:H:1086:ARG:CZ   | 3:I:88:TYR:CE2   | 2.23                     | 1.21              |
| 2:C:879:ARG:NH2   | 7:X:42:ASP:OD1   | 1.73                     | 1.21              |
| 2:M:217:LEU:HB2   | 2:M:311:PHE:CE1  | 1.74                     | 1.21              |
| 3:N:86:ARG:HG2    | 3:N:523:ASP:OD2  | 1.34                     | 1.21              |
| 2:M:1093:GLN:HB3  | 3:N:21:TRP:CZ3   | 1.76                     | 1.20              |
| 2:H:1019:GLN:CD   | 3:I:621:LYS:CD   | 2.09                     | 1.20              |
| 2:M:140:ILE:CD1   | 2:M:331:ARG:HH21 | 1.54                     | 1.20              |
| 2:C:1097:LEU:HD11 | 3:D:1451:ALA:CB  | 1.71                     | 1.20              |
| 2:H:1019:GLN:CD   | 3:I:621:LYS:CG   | 1.98                     | 1.20              |
| 2:H:122:THR:HG22  | 2:H:124:ASP:OD1  | 1.42                     | 1.20              |
| 3:N:970:LYS:HZ1   | 7:Z:113:LEU:CG   | 1.54                     | 1.20              |
| 2:M:432:ARG:NH2   | 3:N:1047:LYS:HD3 | 1.56                     | 1.20              |
| 2:H:1030:GLN:NE2  | 3:I:628:ARG:HD3  | 1.57                     | 1.19              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:970:LYS:HZ3   | 7:Z:113:LEU:CD2   | 1.43                     | 1.19              |
| 3:D:157:GLU:O     | 3:D:161:LEU:CD1   | 1.89                     | 1.19              |
| 2:M:1030:GLN:NE2  | 3:N:628:ARG:HD3   | 1.56                     | 1.19              |
| 2:H:1019:GLN:NE2  | 3:I:621:LYS:HG3   | 0.87                     | 1.19              |
| 3:N:452:ILE:HD13  | 3:N:452:ILE:O     | 1.39                     | 1.19              |
| 3:I:131:LYS:HB2   | 3:I:568:ARG:CD    | 1.72                     | 1.18              |
| 3:I:131:LYS:CB    | 3:I:568:ARG:CD    | 2.19                     | 1.18              |
| 2:H:1019:GLN:CD   | 3:I:621:LYS:HD2   | 1.63                     | 1.18              |
| 3:N:131:LYS:HG3   | 3:N:568:ARG:HD3   | 1.25                     | 1.18              |
| 2:H:185:LYS:HD2   | 2:H:190:LYS:HG2   | 1.24                     | 1.18              |
| 1:L:185:ARG:CZ    | 3:N:692:GLU:HG2   | 1.72                     | 1.18              |
| 3:N:432:TYR:CD2   | 3:N:450:TYR:CD2   | 2.31                     | 1.17              |
| 2:C:224:GLU:CB    | 2:C:228:ALA:HB2   | 1.73                     | 1.17              |
| 2:M:122:THR:HG22  | 2:M:124:ASP:OD1   | 1.41                     | 1.17              |
| 2:C:685:GLU:CG    | 7:X:41:ASP:OD1    | 1.92                     | 1.16              |
| 3:N:50:PHE:CD2    | 3:N:522:PRO:CG    | 2.28                     | 1.16              |
| 1:B:187:GLY:CA    | 3:D:685:ASP:HA    | 1.75                     | 1.16              |
| 2:H:182:VAL:HB    | 2:H:193:LEU:HD13  | 1.27                     | 1.16              |
| 3:D:136:ASP:OD2   | 3:D:137:PRO:HD3   | 1.45                     | 1.16              |
| 1:G:76:VAL:HB     | 3:I:872:ARG:NH1   | 1.58                     | 1.16              |
| 2:C:1097:LEU:HD11 | 3:D:1451:ALA:HB2  | 1.23                     | 1.15              |
| 3:I:1254:GLN:HG2  | 3:I:1255:GLY:H    | 1.02                     | 1.15              |
| 2:M:660:ALA:HB1   | 2:M:667:ALA:O     | 1.46                     | 1.15              |
| 2:M:84:ARG:NE     | 2:M:133:ASP:OD1   | 1.79                     | 1.15              |
| 2:M:564:MET:HE1   | 2:M:846:LYS:HE2   | 1.24                     | 1.15              |
| 3:D:480:GLU:O     | 3:D:484:PRO:HD2   | 1.43                     | 1.15              |
| 3:N:809:PRO:HB2   | 3:N:812:ALA:HB2   | 1.27                     | 1.15              |
| 3:N:783:ARG:HD2   | 7:Z:41:ASP:OD2    | 1.40                     | 1.15              |
| 3:N:996:TRP:CD2   | 3:N:1056:PRO:HG2  | 1.80                     | 1.15              |
| 2:C:175:GLU:HG2   | 2:C:183:SER:HB3   | 1.22                     | 1.14              |
| 2:H:603:VAL:HA    | 2:H:613:VAL:HG12  | 1.25                     | 1.14              |
| 3:I:126:VAL:O     | 3:I:130:SER:HB3   | 1.45                     | 1.14              |
| 7:X:57:ARG:HB2    | 7:X:57:ARG:HH21   | 1.12                     | 1.14              |
| 2:H:267:TYR:HB2   | 2:H:272:ALA:HB1   | 1.29                     | 1.14              |
| 3:D:134:VAL:HG21  | 3:D:460:ALA:CB    | 1.77                     | 1.14              |
| 3:D:161:LEU:HD12  | 3:D:161:LEU:N     | 1.55                     | 1.14              |
| 2:M:1092:LEU:HD13 | 2:M:1099:VAL:HG21 | 1.20                     | 1.14              |
| 3:D:28:LYS:O      | 3:D:43:GLY:HA2    | 1.47                     | 1.14              |
| 2:M:197:LEU:HA    | 2:M:200:LEU:HD12  | 1.27                     | 1.14              |
| 7:Z:6:LYS:HD2     | 7:Z:85:LEU:HD12   | 1.30                     | 1.14              |
| 2:M:111:ASP:CB    | 2:M:369:PRO:HG2   | 1.77                     | 1.14              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:313:LEU:HG    | 2:H:320:HIS:CE1   | 1.83                     | 1.14              |
| 1:G:187:GLY:O     | 3:I:688:TRP:HD1   | 1.28                     | 1.14              |
| 2:C:660:ALA:HB1   | 2:C:667:ALA:O     | 1.46                     | 1.13              |
| 2:H:660:ALA:HB1   | 2:H:667:ALA:O     | 1.46                     | 1.13              |
| 3:I:116:LEU:HD22  | 3:I:118:LEU:HG    | 1.30                     | 1.13              |
| 2:M:676:ILE:CG2   | 2:M:988:VAL:HG13  | 1.78                     | 1.13              |
| 2:H:1092:LEU:HD13 | 2:H:1099:VAL:HG21 | 1.20                     | 1.13              |
| 3:D:28:LYS:HD2    | 3:D:29:PRO:HD2    | 1.29                     | 1.13              |
| 3:D:762:GLN:HE21  | 4:E:20:THR:CG2    | 1.60                     | 1.13              |
| 2:M:243:ARG:HB3   | 2:M:244:PRO:HD2   | 1.31                     | 1.13              |
| 1:G:112:ARG:HD3   | 1:G:125:PRO:HB3   | 1.31                     | 1.13              |
| 3:N:1481:VAL:HG11 | 4:O:18:ARG:HA     | 1.27                     | 1.12              |
| 3:D:172:PRO:HG2   | 3:D:175:VAL:HG21  | 1.23                     | 1.12              |
| 2:M:129:ILE:HG22  | 2:M:130:ASN:H     | 0.96                     | 1.12              |
| 2:C:185:LYS:CG    | 2:C:190:LYS:HG2   | 1.79                     | 1.12              |
| 2:M:70:GLU:HB2    | 2:M:97:ARG:HH21   | 1.12                     | 1.12              |
| 3:D:991:GLN:NE2   | 7:X:112:VAL:HB    | 1.62                     | 1.12              |
| 3:I:871:LYS:NZ    | 1:L:60:ASP:HA     | 1.64                     | 1.12              |
| 3:I:142:LEU:HB3   | 3:I:145:VAL:O     | 1.46                     | 1.12              |
| 3:I:50:PHE:O      | 3:I:89:ARG:HD3    | 1.37                     | 1.12              |
| 3:N:680:GLN:HG3   | 3:N:682:ASP:O     | 1.50                     | 1.12              |
| 2:M:834:GLN:HE22  | 3:N:724:GLN:HG3   | 1.06                     | 1.12              |
| 1:K:25:LEU:HD22   | 1:L:225:PHE:CE2   | 1.83                     | 1.12              |
| 2:M:987:ILE:HG23  | 3:N:948:THR:HG21  | 1.24                     | 1.12              |
| 2:C:193:LEU:CD2   | 2:C:307:LEU:CD2   | 2.27                     | 1.12              |
| 3:N:28:LYS:O      | 3:N:43:GLY:HA2    | 1.47                     | 1.12              |
| 2:H:1097:LEU:HD11 | 3:I:1451:ALA:HB2  | 1.23                     | 1.11              |
| 2:H:181:VAL:HG12  | 2:H:182:VAL:H     | 1.03                     | 1.11              |
| 3:I:611:GLN:HE22  | 6:S:9:U:H4'       | 1.09                     | 1.11              |
| 2:M:290:LEU:HB3   | 2:M:302:VAL:HG11  | 1.29                     | 1.11              |
| 3:I:408:GLU:HG3   | 3:I:409:VAL:H     | 1.08                     | 1.11              |
| 2:C:193:LEU:HD23  | 2:C:307:LEU:CD2   | 1.81                     | 1.11              |
| 3:N:116:LEU:HD22  | 3:N:118:LEU:HG    | 1.30                     | 1.11              |
| 3:N:1211:MET:HG2  | 3:N:1212:ALA:H    | 1.15                     | 1.11              |
| 2:H:111:ASP:CB    | 2:H:369:PRO:HG2   | 1.79                     | 1.11              |
| 3:N:86:ARG:CD     | 3:N:523:ASP:OD2   | 1.99                     | 1.11              |
| 2:C:1092:LEU:HD13 | 2:C:1099:VAL:HG21 | 1.20                     | 1.10              |
| 2:M:84:ARG:HE     | 2:M:133:ASP:CG    | 1.53                     | 1.10              |
| 3:N:970:LYS:HZ1   | 7:Z:113:LEU:CB    | 1.64                     | 1.10              |
| 2:C:304:LEU:HD23  | 2:C:305:PRO:HD3   | 1.32                     | 1.10              |
| 2:C:193:LEU:HD21  | 2:C:307:LEU:HD22  | 1.18                     | 1.10              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:28:LYS:HD2    | 3:N:29:PRO:HD2    | 1.33                     | 1.10              |
| 2:H:685:GLU:HG3   | 7:Y:41:ASP:OD1    | 1.50                     | 1.10              |
| 3:D:116:LEU:HD22  | 3:D:118:LEU:HG    | 1.22                     | 1.10              |
| 3:D:139:GLY:HA3   | 3:D:162:ARG:HH22  | 0.94                     | 1.10              |
| 2:H:987:ILE:HG23  | 3:I:948:THR:HG21  | 1.32                     | 1.10              |
| 2:H:565:GLN:HE21  | 2:H:842:ARG:HG2   | 1.17                     | 1.10              |
| 2:C:196:LEU:HD23  | 2:C:200:LEU:HD11  | 1.18                     | 1.10              |
| 2:H:1090:LYS:HE3  | 3:I:90:MET:CG     | 1.79                     | 1.10              |
| 2:H:878:SER:HA    | 3:I:1034:GLN:HE22 | 1.09                     | 1.09              |
| 1:L:41:ARG:HG3    | 1:L:177:VAL:HG21  | 1.34                     | 1.09              |
| 3:N:1362:LYS:HD2  | 7:Z:34:GLN:NE2    | 1.67                     | 1.09              |
| 2:C:987:ILE:HG23  | 3:D:948:THR:HG21  | 1.29                     | 1.09              |
| 1:L:74:ASP:HB2    | 3:N:872:ARG:HH22  | 1.05                     | 1.09              |
| 3:I:783:ARG:NH1   | 7:Y:41:ASP:HB2    | 1.52                     | 1.09              |
| 1:B:187:GLY:HA3   | 3:D:685:ASP:CA    | 1.80                     | 1.09              |
| 2:H:1052:MET:SD   | 3:I:623:VAL:HG11  | 1.92                     | 1.09              |
| 3:D:1359:GLN:HE22 | 7:X:52:LYS:HE2    | 1.01                     | 1.09              |
| 1:G:112:ARG:HH11  | 1:G:125:PRO:HB2   | 0.96                     | 1.09              |
| 2:H:193:LEU:H     | 2:H:193:LEU:CD1   | 1.64                     | 1.09              |
| 2:M:1074:GLU:HG2  | 2:M:1075:ASP:H    | 1.18                     | 1.09              |
| 1:B:187:GLY:HA3   | 3:D:685:ASP:HB3   | 1.32                     | 1.09              |
| 3:D:785:ILE:HD12  | 3:D:785:ILE:H     | 1.00                     | 1.09              |
| 2:H:182:VAL:HG12  | 2:H:193:LEU:HD11  | 1.35                     | 1.09              |
| 3:I:520:LEU:HD11  | 3:I:524:LEU:HD22  | 1.20                     | 1.09              |
| 2:M:217:LEU:HB2   | 2:M:311:PHE:CD1   | 1.88                     | 1.09              |
| 2:H:266:ARG:HA    | 2:H:288:ARG:HD3   | 1.30                     | 1.08              |
| 3:D:1211:MET:HG2  | 3:D:1212:ALA:H    | 1.15                     | 1.08              |
| 2:C:1074:GLU:HG2  | 2:C:1075:ASP:H    | 1.18                     | 1.08              |
| 3:D:160:GLU:HA    | 3:D:165:LYS:HB2   | 1.35                     | 1.08              |
| 2:H:188:LYS:HB2   | 2:H:188:LYS:NZ    | 1.60                     | 1.08              |
| 3:N:397:LYS:HE2   | 3:N:448:GLU:HB3   | 1.31                     | 1.08              |
| 1:A:67:THR:HG21   | 2:C:609:ASN:HD21  | 1.09                     | 1.08              |
| 3:D:126:VAL:HG13  | 3:D:132:TYR:CD2   | 1.88                     | 1.08              |
| 3:D:136:ASP:CG    | 3:D:137:PRO:CD    | 2.21                     | 1.08              |
| 2:C:1065:ALA:HB1  | 2:C:1077:PRO:HG2  | 1.27                     | 1.08              |
| 2:C:564:MET:HE1   | 2:C:846:LYS:HE2   | 1.35                     | 1.08              |
| 2:M:1097:LEU:HD11 | 3:N:1451:ALA:HB2  | 1.33                     | 1.08              |
| 3:I:119:SER:HB2   | 3:I:123:LEU:HB2   | 1.33                     | 1.08              |
| 2:M:1004:LYS:HD2  | 3:N:744:GLN:HE22  | 1.12                     | 1.08              |
| 2:C:911:GLU:OE1   | 3:D:951:ILE:HD13  | 1.51                     | 1.08              |
| 2:H:1019:GLN:CG   | 3:I:621:LYS:HD2   | 1.84                     | 1.08              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:224:GLU:HB3   | 2:C:228:ALA:HB2   | 1.36                     | 1.07              |
| 2:H:260:LEU:HB2   | 2:H:291:ALA:HB1   | 1.36                     | 1.07              |
| 3:I:1211:MET:HG2  | 3:I:1212:ALA:H    | 1.15                     | 1.07              |
| 3:N:1257:PRO:HA   | 3:N:1260:ILE:HD12 | 1.30                     | 1.07              |
| 2:C:1099:VAL:HG22 | 3:D:10:ILE:HG12   | 1.34                     | 1.07              |
| 3:D:762:GLN:NE2   | 4:E:20:THR:HG21   | 1.68                     | 1.07              |
| 3:I:131:LYS:HB2   | 3:I:568:ARG:HD2   | 1.14                     | 1.07              |
| 2:H:1084:SER:HB3  | 3:I:617:ASN:OD1   | 1.51                     | 1.07              |
| 2:M:6:PHE:HZ      | 2:M:901:TYR:CD2   | 1.70                     | 1.07              |
| 3:N:131:LYS:CG    | 3:N:568:ARG:HD3   | 1.60                     | 1.07              |
| 2:H:1081:VAL:HG21 | 2:H:1111:ILE:HG22 | 1.29                     | 1.07              |
| 2:H:165:LEU:O     | 2:H:265:ARG:HD2   | 1.54                     | 1.07              |
| 2:H:328:LEU:HD13  | 2:H:433:THR:HB    | 1.33                     | 1.07              |
| 2:M:170:PRO:HD3   | 2:M:263:ASP:HB3   | 1.17                     | 1.07              |
| 2:M:328:LEU:HD13  | 2:M:433:THR:HB    | 1.36                     | 1.07              |
| 3:D:161:LEU:HD12  | 3:D:161:LEU:H     | 1.09                     | 1.07              |
| 2:H:576:ALA:HB3   | 2:H:900:ARG:NH1   | 1.69                     | 1.07              |
| 3:D:136:ASP:CB    | 3:D:137:PRO:CD    | 2.32                     | 1.07              |
| 3:D:809:PRO:HB2   | 3:D:812:ALA:HB2   | 1.36                     | 1.07              |
| 3:N:1362:LYS:HD2  | 7:Z:34:GLN:HE22   | 1.19                     | 1.07              |
| 2:C:193:LEU:HD23  | 2:C:307:LEU:HD22  | 1.16                     | 1.07              |
| 2:H:309:TYR:O     | 2:H:313:LEU:CD1   | 2.03                     | 1.07              |
| 2:C:111:ASP:CB    | 2:C:369:PRO:HG2   | 1.85                     | 1.07              |
| 2:M:140:ILE:HD13  | 2:M:331:ARG:HH21  | 1.19                     | 1.07              |
| 2:M:334:ARG:HH12  | 2:M:415:PRO:HG2   | 1.19                     | 1.07              |
| 2:M:217:LEU:HD12  | 2:M:311:PHE:CD1   | 1.89                     | 1.07              |
| 3:D:1481:VAL:HG11 | 4:E:18:ARG:HA     | 1.31                     | 1.07              |
| 2:H:160:ALA:HB3   | 2:H:174:LEU:HB2   | 1.32                     | 1.07              |
| 2:H:245:GLY:O     | 2:H:246:ASP:CG    | 1.93                     | 1.07              |
| 2:C:267:TYR:HB2   | 2:C:272:ALA:HB1   | 1.36                     | 1.06              |
| 1:B:74:ASP:HB2    | 3:D:872:ARG:HH22  | 1.15                     | 1.06              |
| 2:H:182:VAL:HB    | 2:H:193:LEU:CD1   | 1.83                     | 1.06              |
| 3:N:432:TYR:HD2   | 3:N:450:TYR:CE2   | 1.73                     | 1.06              |
| 2:C:1093:GLN:HB3  | 3:D:21:TRP:CZ3    | 1.90                     | 1.06              |
| 2:M:675:ALA:HA    | 2:M:989:VAL:HG12  | 1.34                     | 1.06              |
| 3:N:15:PRO:HB3    | 3:N:515:GLU:OE1   | 1.53                     | 1.06              |
| 2:H:685:GLU:CG    | 7:Y:41:ASP:OD1    | 2.03                     | 1.06              |
| 2:H:267:TYR:HB2   | 2:H:272:ALA:CB    | 1.85                     | 1.06              |
| 3:D:119:SER:HB2   | 3:D:123:LEU:HB2   | 1.07                     | 1.06              |
| 7:X:24:GLU:HA     | 7:X:27:GLN:HE21   | 1.16                     | 1.06              |
| 2:C:185:LYS:HD2   | 2:C:190:LYS:HG2   | 1.11                     | 1.06              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1258:ARG:HH12 | 3:D:1262:LEU:HD13 | 1.16                     | 1.06              |
| 2:H:290:LEU:HB3   | 2:H:302:VAL:HG11  | 1.34                     | 1.06              |
| 3:I:134:VAL:HG21  | 3:I:460:ALA:HB1   | 1.30                     | 1.06              |
| 2:M:39:ARG:HG2    | 2:M:45:GLN:OE1    | 0.88                     | 1.06              |
| 3:N:119:SER:HB2   | 3:N:123:LEU:HB2   | 1.33                     | 1.06              |
| 1:B:185:ARG:CZ    | 3:D:692:GLU:HG2   | 1.85                     | 1.06              |
| 2:M:188:LYS:HB2   | 2:M:188:LYS:HZ3   | 0.90                     | 1.05              |
| 3:N:996:TRP:CG    | 3:N:1056:PRO:HG2  | 1.89                     | 1.05              |
| 2:C:565:GLN:HE21  | 2:C:842:ARG:HG2   | 1.21                     | 1.05              |
| 3:I:89:ARG:O      | 3:I:521:PRO:HG3   | 1.56                     | 1.05              |
| 3:I:28:LYS:HD2    | 3:I:29:PRO:HD2    | 1.33                     | 1.05              |
| 3:I:204:LEU:HB3   | 3:I:394:LEU:HG    | 1.39                     | 1.05              |
| 3:I:785:ILE:HD12  | 3:I:785:ILE:H     | 1.20                     | 1.05              |
| 3:D:1121:PRO:HB2  | 3:D:1135:ARG:HH12 | 1.13                     | 1.05              |
| 2:C:111:ASP:HB3   | 2:C:369:PRO:HG2   | 1.06                     | 1.05              |
| 3:D:176:ASP:HB3   | 3:D:389:GLU:HG2   | 1.39                     | 1.05              |
| 1:G:185:ARG:CZ    | 3:I:692:GLU:CG    | 2.34                     | 1.05              |
| 3:I:762:GLN:HE21  | 4:J:20:THR:HG21   | 0.89                     | 1.05              |
| 3:N:81:THR:CG2    | 3:N:82:LYS:H      | 1.68                     | 1.05              |
| 2:C:879:ARG:NH2   | 7:X:42:ASP:CG     | 2.10                     | 1.05              |
| 2:M:1099:VAL:HG22 | 3:N:10:ILE:HG12   | 1.38                     | 1.05              |
| 2:M:157:ARG:HD3   | 2:M:314:THR:OG1   | 1.56                     | 1.05              |
| 2:C:129:ILE:HG22  | 2:C:130:ASN:H     | 1.22                     | 1.05              |
| 2:M:109:LYS:HD3   | 2:M:368:THR:CG2   | 1.87                     | 1.05              |
| 2:M:432:ARG:HH22  | 3:N:1047:LYS:HD3  | 0.97                     | 1.05              |
| 1:K:90:LEU:HD13   | 1:K:119:ASP:O     | 1.57                     | 1.04              |
| 1:F:90:LEU:HD13   | 1:F:119:ASP:O     | 1.57                     | 1.04              |
| 2:M:129:ILE:HD13  | 2:M:134:ARG:HG3   | 1.08                     | 1.04              |
| 2:H:193:LEU:N     | 2:H:193:LEU:HD12  | 1.68                     | 1.04              |
| 2:H:265:ARG:HB3   | 2:H:267:TYR:CE2   | 1.91                     | 1.04              |
| 2:M:41:ASN:O      | 2:M:46:ALA:CB     | 2.05                     | 1.04              |
| 1:K:226:SER:O     | 1:K:228:PRO:HD3   | 1.56                     | 1.04              |
| 3:N:783:ARG:NH1   | 7:Z:41:ASP:HB3    | 1.69                     | 1.04              |
| 3:D:139:GLY:HA3   | 3:D:162:ARG:NH2   | 1.73                     | 1.04              |
| 2:M:200:LEU:HD13  | 2:M:300:ASP:OD2   | 1.58                     | 1.04              |
| 2:M:39:ARG:CG     | 2:M:45:GLN:CD     | 2.24                     | 1.04              |
| 3:D:1122:LEU:HD11 | 3:D:1186:VAL:HG23 | 1.39                     | 1.04              |
| 1:F:42:ARG:NH1    | 1:G:34:VAL:HB     | 1.73                     | 1.04              |
| 2:H:196:LEU:HD23  | 2:H:200:LEU:HD11  | 1.40                     | 1.04              |
| 2:H:1005:MET:SD   | 3:I:724:GLN:OE1   | 2.15                     | 1.04              |
| 3:N:187:LYS:HB2   | 3:N:200:ASP:HB2   | 1.34                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1099:VAL:HG22 | 3:D:10:ILE:CG1    | 1.88                     | 1.04              |
| 3:D:129:PHE:CZ    | 3:D:587:ARG:NE    | 2.25                     | 1.03              |
| 3:I:50:PHE:O      | 3:I:89:ARG:CG     | 2.06                     | 1.03              |
| 3:N:785:ILE:HD12  | 3:N:785:ILE:H     | 1.20                     | 1.03              |
| 3:N:81:THR:HG22   | 3:N:82:LYS:N      | 1.68                     | 1.03              |
| 3:I:136:ASP:HB3   | 3:I:137:PRO:HD3   | 1.34                     | 1.03              |
| 3:I:762:GLN:NE2   | 4:J:20:THR:HG21   | 1.72                     | 1.03              |
| 2:H:1104:GLU:OE2  | 3:I:3:LYS:NZ      | 1.91                     | 1.03              |
| 3:D:165:LYS:HD3   | 3:D:167:GLU:HB2   | 1.39                     | 1.03              |
| 2:H:1074:GLU:HG2  | 2:H:1075:ASP:H    | 1.18                     | 1.03              |
| 2:H:111:ASP:HB2   | 2:H:369:PRO:CG    | 1.89                     | 1.03              |
| 3:I:162:ARG:HD2   | 3:I:452:ILE:HG21  | 1.36                     | 1.03              |
| 2:M:217:LEU:HD12  | 2:M:311:PHE:CG    | 1.92                     | 1.03              |
| 2:M:263:ASP:HB2   | 2:M:264:PRO:HD3   | 1.37                     | 1.03              |
| 1:A:90:LEU:HD13   | 1:A:119:ASP:O     | 1.57                     | 1.03              |
| 2:M:565:GLN:HE21  | 2:M:842:ARG:HG2   | 1.22                     | 1.03              |
| 1:A:56:VAL:HG13   | 1:A:142:VAL:HG12  | 1.40                     | 1.03              |
| 2:C:383:ARG:HH11  | 2:C:383:ARG:HB2   | 1.21                     | 1.03              |
| 3:I:991:GLN:HE22  | 7:Y:112:VAL:CG2   | 1.71                     | 1.03              |
| 2:H:109:LYS:HD3   | 2:H:368:THR:HG23  | 1.40                     | 1.03              |
| 2:M:432:ARG:HH22  | 3:N:1047:LYS:CD   | 1.71                     | 1.03              |
| 2:H:21:ILE:H      | 2:H:21:ILE:HD12   | 1.16                     | 1.02              |
| 2:M:122:THR:HG21  | 2:M:124:ASP:OD1   | 1.55                     | 1.02              |
| 2:M:564:MET:HE1   | 2:M:846:LYS:CE    | 1.88                     | 1.02              |
| 3:N:131:LYS:CG    | 3:N:568:ARG:CD    | 2.26                     | 1.02              |
| 2:C:224:GLU:HB3   | 2:C:228:ALA:CB    | 1.88                     | 1.02              |
| 2:C:211:LEU:HD23  | 2:C:221:LEU:CD2   | 1.88                     | 1.02              |
| 3:D:124:GLU:HG3   | 3:D:128:TYR:CD1   | 1.94                     | 1.02              |
| 3:N:1305:LEU:HD12 | 3:N:1311:LEU:HD22 | 1.42                     | 1.02              |
| 7:Z:119:ILE:HG13  | 7:Z:125:MET:HE1   | 1.04                     | 1.02              |
| 1:G:112:ARG:HH11  | 1:G:125:PRO:CB    | 1.73                     | 1.02              |
| 1:A:24:VAL:HG13   | 1:A:196:THR:HG22  | 1.42                     | 1.02              |
| 3:D:159:ARG:NH2   | 2:H:218:VAL:HG11  | 1.75                     | 1.02              |
| 2:H:1090:LYS:CD   | 3:I:90:MET:SD     | 2.47                     | 1.02              |
| 2:M:129:ILE:HG22  | 2:M:130:ASN:N     | 1.74                     | 1.02              |
| 1:B:62:LEU:HD13   | 1:B:63:HIS:H      | 1.24                     | 1.02              |
| 3:D:762:GLN:HE21  | 4:E:20:THR:HG21   | 0.85                     | 1.02              |
| 3:N:1256:LEU:O    | 3:N:1260:ILE:HG13 | 1.59                     | 1.02              |
| 3:N:214:GLU:HG2   | 3:N:342:PRO:HB3   | 1.42                     | 1.01              |
| 3:N:432:TYR:HD2   | 3:N:450:TYR:CD2   | 1.73                     | 1.01              |
| 2:M:1090:LYS:HE3  | 3:N:90:MET:HG2    | 1.42                     | 1.01              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:407:VAL:HG22  | 3:N:408:GLU:H     | 1.21                     | 1.01              |
| 1:B:62:LEU:HD12   | 1:B:62:LEU:H      | 1.21                     | 1.01              |
| 3:D:166:GLN:HG2   | 3:D:396:VAL:HG12  | 1.42                     | 1.01              |
| 2:H:36:PRO:O      | 2:H:39:ARG:HG3    | 1.59                     | 1.01              |
| 2:H:332:ARG:HG3   | 2:H:465:GLY:HA3   | 1.41                     | 1.01              |
| 2:H:1093:GLN:HB3  | 3:I:21:TRP:CZ3    | 1.94                     | 1.01              |
| 3:N:1031:ASN:HD21 | 7:Z:32:ILE:HG23   | 1.23                     | 1.01              |
| 2:C:224:GLU:HB2   | 2:C:228:ALA:HB2   | 1.43                     | 1.01              |
| 3:D:1359:GLN:NE2  | 7:X:52:LYS:HE2    | 1.74                     | 1.01              |
| 2:M:1004:LYS:HD2  | 3:N:744:GLN:NE2   | 1.75                     | 1.01              |
| 1:B:41:ARG:HG3    | 1:B:177:VAL:HG21  | 1.40                     | 1.01              |
| 2:C:1037:VAL:HG13 | 2:C:1049:LEU:HD11 | 1.36                     | 1.01              |
| 1:F:56:VAL:HG13   | 1:F:142:VAL:HG12  | 1.40                     | 1.01              |
| 2:C:115:LEU:HA    | 2:C:375:SER:OG    | 1.59                     | 1.01              |
| 3:D:1106:VAL:HB   | 3:D:1108:ARG:HE   | 1.21                     | 1.01              |
| 2:C:325:ILE:HD12  | 2:C:325:ILE:H     | 1.20                     | 1.01              |
| 3:D:119:SER:CB    | 3:D:123:LEU:HB2   | 1.90                     | 1.01              |
| 2:H:564:MET:HE1   | 2:H:846:LYS:HE2   | 1.43                     | 1.01              |
| 2:M:265:ARG:HH12  | 2:M:332:ARG:HH12  | 1.02                     | 1.01              |
| 3:D:136:ASP:HB3   | 3:D:137:PRO:HD2   | 1.41                     | 1.01              |
| 3:D:677:LEU:HD23  | 3:D:683:ILE:HD11  | 1.42                     | 1.01              |
| 3:N:783:ARG:HD2   | 7:Z:41:ASP:CG     | 1.81                     | 1.01              |
| 3:N:81:THR:HG22   | 3:N:82:LYS:H      | 1.19                     | 1.01              |
| 3:D:50:PHE:CD2    | 3:D:522:PRO:CD    | 2.42                     | 1.00              |
| 2:M:129:ILE:HD13  | 2:M:134:ARG:CG    | 1.91                     | 1.00              |
| 2:M:172:ILE:HG23  | 2:M:186:VAL:HG12  | 1.40                     | 1.00              |
| 2:M:676:ILE:HG21  | 2:M:988:VAL:HG13  | 1.38                     | 1.00              |
| 3:N:783:ARG:HD3   | 7:Z:41:ASP:OD2    | 1.55                     | 1.00              |
| 1:B:185:ARG:NE    | 3:D:692:GLU:HG2   | 1.76                     | 1.00              |
| 2:C:576:ALA:HB3   | 2:C:900:ARG:NH1   | 1.76                     | 1.00              |
| 3:D:136:ASP:HB3   | 3:D:137:PRO:CD    | 1.92                     | 1.00              |
| 2:C:175:GLU:HG2   | 2:C:183:SER:CB    | 1.91                     | 1.00              |
| 3:D:1123:PHE:HE2  | 3:D:1184:GLN:HA   | 1.24                     | 1.00              |
| 3:I:36:THR:OG1    | 3:I:40:GLU:OE2    | 1.77                     | 1.00              |
| 2:H:1056:LYS:HD3  | 3:I:623:VAL:CG1   | 1.91                     | 1.00              |
| 1:G:185:ARG:NH1   | 3:I:692:GLU:HB3   | 1.77                     | 1.00              |
| 3:D:15:PRO:HB3    | 3:D:515:GLU:OE1   | 1.59                     | 1.00              |
| 3:D:28:LYS:CD     | 3:D:29:PRO:HD2    | 1.91                     | 1.00              |
| 2:H:182:VAL:CG1   | 2:H:193:LEU:CD2   | 1.91                     | 1.00              |
| 3:N:1256:LEU:HG   | 3:N:1260:ILE:HD11 | 1.42                     | 1.00              |
| 7:Z:14:ARG:HB3    | 7:Z:14:ARG:HH11   | 1.21                     | 1.00              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1254:GLN:HG2  | 3:I:1255:GLY:N    | 1.75                     | 1.00              |
| 2:M:267:TYR:HB2   | 2:M:272:ALA:CB    | 1.91                     | 1.00              |
| 3:N:1233:GLY:HA2  | 3:N:1236:LEU:HD12 | 1.43                     | 1.00              |
| 2:C:1081:VAL:HG21 | 2:C:1111:ILE:CG2  | 1.91                     | 1.00              |
| 2:M:84:ARG:HH11   | 2:M:84:ARG:HG3    | 1.27                     | 1.00              |
| 2:H:675:ALA:HA    | 2:H:989:VAL:HG12  | 1.43                     | 1.00              |
| 2:C:1011:GLY:HA3  | 2:C:1026:GLN:HG2  | 1.44                     | 0.99              |
| 2:H:122:THR:HG21  | 2:H:124:ASP:OD1   | 1.55                     | 0.99              |
| 2:H:451:LEU:C     | 2:H:452:ILE:HD12  | 1.81                     | 0.99              |
| 2:H:432:ARG:HH22  | 3:I:1047:LYS:HD3  | 1.25                     | 0.99              |
| 4:J:6:ILE:HA      | 4:J:9:LEU:HD12    | 1.42                     | 0.99              |
| 2:M:6:PHE:HE1     | 2:M:901:TYR:HB3   | 1.25                     | 0.99              |
| 2:M:80:GLN:CG     | 2:M:90:TYR:CE2    | 2.44                     | 0.99              |
| 2:M:6:PHE:CZ      | 2:M:901:TYR:HD2   | 1.79                     | 0.99              |
| 7:X:57:ARG:HB2    | 7:X:57:ARG:NH2    | 1.75                     | 0.99              |
| 1:G:112:ARG:NH1   | 1:G:125:PRO:HB2   | 1.77                     | 0.99              |
| 2:H:111:ASP:HB2   | 2:H:369:PRO:HG2   | 1.00                     | 0.99              |
| 2:M:211:LEU:HD23  | 2:M:221:LEU:HD21  | 1.42                     | 0.99              |
| 3:I:40:GLU:OE1    | 3:I:40:GLU:HA     | 1.61                     | 0.99              |
| 1:K:56:VAL:HG13   | 1:K:142:VAL:HG12  | 1.40                     | 0.99              |
| 2:C:1004:LYS:CD   | 3:D:744:GLN:NE2   | 2.25                     | 0.99              |
| 3:N:387:LEU:H     | 3:N:387:LEU:HD12  | 1.27                     | 0.99              |
| 2:C:197:LEU:HD13  | 2:C:207:LEU:HD11  | 1.41                     | 0.99              |
| 2:M:274:ARG:HD2   | 2:M:285:LEU:HD22  | 1.44                     | 0.99              |
| 1:K:42:ARG:NH1    | 1:L:34:VAL:HB     | 1.78                     | 0.99              |
| 3:D:31:THR:HG23   | 3:D:545:ARG:HD3   | 1.42                     | 0.99              |
| 2:C:1090:LYS:HE3  | 3:D:90:MET:CG     | 1.92                     | 0.99              |
| 2:M:1093:GLN:HB3  | 3:N:21:TRP:HZ3    | 1.16                     | 0.99              |
| 3:D:126:VAL:HG13  | 3:D:132:TYR:CG    | 1.96                     | 0.99              |
| 2:M:188:LYS:NZ    | 2:M:188:LYS:HB2   | 1.63                     | 0.99              |
| 2:M:52:PHE:CZ     | 2:M:98:LEU:HG     | 1.98                     | 0.99              |
| 3:N:141:ILE:HD13  | 3:N:142:LEU:N     | 1.78                     | 0.99              |
| 1:L:185:ARG:NE    | 3:N:692:GLU:HG2   | 1.76                     | 0.99              |
| 3:N:639:LEU:HD13  | 3:N:766:ALA:HB2   | 1.44                     | 0.99              |
| 2:C:111:ASP:HB3   | 2:C:369:PRO:CG    | 1.92                     | 0.98              |
| 3:N:133:ILE:O     | 3:N:152:LEU:HB2   | 1.63                     | 0.98              |
| 3:N:1468:LEU:HD22 | 3:N:1470:ARG:HB2  | 1.45                     | 0.98              |
| 5:T:18:DC:H2''    | 5:T:19:DC:H5'     | 1.43                     | 0.98              |
| 2:C:185:LYS:CG    | 2:C:190:LYS:CG    | 2.40                     | 0.98              |
| 3:D:119:SER:HB2   | 3:D:123:LEU:CB    | 1.93                     | 0.98              |
| 1:L:74:ASP:HB2    | 3:N:872:ARG:NH2   | 1.76                     | 0.98              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:1085:PHE:HE2  | 3:N:1468:LEU:HG   | 1.29                     | 0.98              |
| 2:C:267:TYR:HB2   | 2:C:272:ALA:CB    | 1.93                     | 0.98              |
| 3:D:116:LEU:CD2   | 3:D:118:LEU:HG    | 1.91                     | 0.98              |
| 7:Z:57:ARG:HB2    | 7:Z:57:ARG:HH21   | 1.27                     | 0.98              |
| 1:G:76:VAL:HB     | 3:I:872:ARG:HH12  | 1.15                     | 0.98              |
| 3:I:404:GLU:N     | 3:I:423:ASP:OD2   | 1.97                     | 0.98              |
| 2:M:115:LEU:HD23  | 2:M:115:LEU:H     | 1.26                     | 0.98              |
| 2:C:1086:ARG:HD3  | 3:D:88:TYR:CE1    | 1.97                     | 0.98              |
| 2:H:1086:ARG:NH1  | 3:I:88:TYR:CD2    | 2.31                     | 0.98              |
| 1:B:187:GLY:CA    | 3:D:685:ASP:CA    | 2.41                     | 0.98              |
| 3:D:145:VAL:HG22  | 3:D:146:PRO:HD2   | 1.42                     | 0.98              |
| 3:D:162:ARG:HG3   | 3:D:452:ILE:HG13  | 1.45                     | 0.98              |
| 2:M:1095:LEU:HD11 | 2:M:1097:LEU:HB2  | 1.45                     | 0.98              |
| 3:N:1484:THR:HG21 | 4:O:22:VAL:HG22   | 1.45                     | 0.98              |
| 3:D:991:GLN:HE22  | 7:X:112:VAL:CB    | 1.75                     | 0.98              |
| 3:I:809:PRO:HB2   | 3:I:812:ALA:HB2   | 1.42                     | 0.98              |
| 2:M:1065:ALA:HB1  | 2:M:1077:PRO:HG2  | 1.43                     | 0.98              |
| 2:M:293:PHE:HD1   | 2:M:293:PHE:H     | 1.05                     | 0.98              |
| 2:M:52:PHE:HZ     | 2:M:98:LEU:HG     | 1.26                     | 0.98              |
| 1:F:58:ILE:HD13   | 1:F:140:MET:HB3   | 1.45                     | 0.98              |
| 3:N:141:ILE:HG13  | 3:N:448:GLU:CD    | 1.84                     | 0.98              |
| 3:N:432:TYR:CD2   | 3:N:450:TYR:CE2   | 2.52                     | 0.98              |
| 3:I:1305:LEU:HD12 | 3:I:1311:LEU:HD22 | 1.42                     | 0.98              |
| 3:I:177:ALA:HB2   | 3:I:390:PRO:HG3   | 1.41                     | 0.98              |
| 1:K:58:ILE:HD13   | 1:K:140:MET:HB3   | 1.45                     | 0.98              |
| 2:C:185:LYS:HG2   | 2:C:190:LYS:CG    | 1.93                     | 0.97              |
| 2:H:313:LEU:HA    | 2:H:320:HIS:ND1   | 1.78                     | 0.97              |
| 2:H:136:ILE:HG21  | 2:H:336:VAL:HG13  | 1.46                     | 0.97              |
| 2:H:1085:PHE:HE2  | 3:I:1468:LEU:HG   | 1.25                     | 0.97              |
| 3:I:87:ARG:O      | 3:I:88:TYR:CD2    | 2.16                     | 0.97              |
| 3:D:677:LEU:HD23  | 3:D:683:ILE:CD1   | 1.95                     | 0.97              |
| 3:D:785:ILE:H     | 3:D:785:ILE:CD1   | 1.75                     | 0.97              |
| 3:I:1465:ASN:HD21 | 3:I:1470:ARG:NH2  | 1.63                     | 0.97              |
| 1:G:187:GLY:O     | 3:I:688:TRP:CD1   | 2.18                     | 0.97              |
| 3:D:170:PRO:HD2   | 2:H:318:PRO:HB3   | 1.46                     | 0.97              |
| 2:H:1095:LEU:HD11 | 2:H:1097:LEU:HB2  | 1.45                     | 0.97              |
| 2:H:676:ILE:CG2   | 2:H:988:VAL:HG13  | 1.94                     | 0.97              |
| 3:D:116:LEU:HD22  | 3:D:118:LEU:CG    | 1.93                     | 0.97              |
| 2:M:6:PHE:CE1     | 2:M:901:TYR:HB3   | 1.98                     | 0.97              |
| 3:D:134:VAL:HG21  | 3:D:460:ALA:HB1   | 1.44                     | 0.97              |
| 2:H:1029:GLY:O    | 3:I:622:ARG:HD3   | 1.64                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1103:ASP:OD1  | 3:D:3:LYS:HB2     | 1.62                     | 0.97              |
| 2:M:290:LEU:CB    | 2:M:302:VAL:HG11  | 1.94                     | 0.97              |
| 3:D:806:PHE:CE1   | 3:D:813:LEU:HB3   | 1.99                     | 0.97              |
| 1:G:112:ARG:CD    | 1:G:125:PRO:HB3   | 1.94                     | 0.97              |
| 3:I:41:ARG:HA     | 3:I:46:ASP:OD1    | 1.63                     | 0.97              |
| 3:I:50:PHE:O      | 3:I:89:ARG:HD2    | 1.65                     | 0.97              |
| 1:K:42:ARG:HH12   | 1:L:34:VAL:HB     | 1.29                     | 0.97              |
| 3:D:991:GLN:HE22  | 7:X:112:VAL:HB    | 0.82                     | 0.96              |
| 3:I:540:LEU:HA    | 3:I:543:LEU:HD12  | 1.44                     | 0.96              |
| 2:C:199:VAL:HG21  | 2:C:238:LEU:HD12  | 1.44                     | 0.96              |
| 3:D:411:THR:HG23  | 3:D:436:GLU:HA    | 1.44                     | 0.96              |
| 3:D:785:ILE:HD12  | 3:D:785:ILE:N     | 1.78                     | 0.96              |
| 2:C:1081:VAL:HG21 | 2:C:1111:ILE:HG22 | 1.42                     | 0.96              |
| 3:D:18:ILE:HG23   | 3:D:518:PRO:HG3   | 1.47                     | 0.96              |
| 3:I:991:GLN:NE2   | 7:Y:112:VAL:CG2   | 2.27                     | 0.96              |
| 2:M:129:ILE:CG2   | 2:M:130:ASN:H     | 1.78                     | 0.96              |
| 2:M:170:PRO:CD    | 2:M:263:ASP:HB3   | 1.94                     | 0.96              |
| 2:M:71:TYR:HA     | 2:M:96:ALA:HB2    | 1.47                     | 0.96              |
| 2:M:565:GLN:NE2   | 2:M:842:ARG:HG2   | 1.78                     | 0.96              |
| 1:A:42:ARG:HH12   | 1:B:34:VAL:CG1    | 1.79                     | 0.96              |
| 2:C:1095:LEU:HD11 | 2:C:1097:LEU:HB2  | 1.45                     | 0.96              |
| 2:H:182:VAL:CG1   | 2:H:193:LEU:HD11  | 1.95                     | 0.96              |
| 2:M:101:ILE:HA    | 2:M:108:ILE:HG12  | 1.47                     | 0.96              |
| 2:H:1097:LEU:HD11 | 3:I:1451:ALA:CB   | 1.94                     | 0.96              |
| 3:I:160:GLU:HG2   | 3:I:165:LYS:HG3   | 1.48                     | 0.96              |
| 3:N:432:TYR:CD2   | 3:N:450:TYR:HD2   | 1.74                     | 0.96              |
| 3:N:970:LYS:CE    | 7:Z:113:LEU:CD2   | 2.33                     | 0.96              |
| 3:D:139:GLY:O     | 3:D:147:VAL:HG11  | 1.65                     | 0.96              |
| 1:G:41:ARG:HH11   | 1:G:177:VAL:HG23  | 1.26                     | 0.96              |
| 3:I:639:LEU:HD13  | 3:I:766:ALA:HB2   | 1.44                     | 0.96              |
| 2:M:235:LEU:HD11  | 2:M:298:PHE:CZ    | 2.01                     | 0.96              |
| 2:M:317:VAL:HG13  | 2:M:320:HIS:NE2   | 1.79                     | 0.96              |
| 2:M:109:LYS:HD3   | 2:M:368:THR:HG23  | 1.45                     | 0.96              |
| 3:D:407:VAL:HG22  | 3:D:408:GLU:H     | 1.31                     | 0.96              |
| 3:N:50:PHE:CG     | 3:N:522:PRO:CD    | 2.46                     | 0.96              |
| 1:A:58:ILE:HD13   | 1:A:140:MET:HB3   | 1.45                     | 0.96              |
| 2:C:939:ARG:HA    | 2:C:939:ARG:HE    | 1.30                     | 0.96              |
| 2:H:560:MET:O     | 2:H:564:MET:HG2   | 1.66                     | 0.96              |
| 3:I:407:VAL:HG22  | 3:I:408:GLU:H     | 1.28                     | 0.96              |
| 2:H:1019:GLN:HG3  | 3:I:621:LYS:HD2   | 1.48                     | 0.96              |
| 3:I:762:GLN:HE21  | 4:J:20:THR:CG2    | 1.77                     | 0.96              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:G:76:VAL:CB     | 3:I:872:ARG:HH12 | 1.78                     | 0.96              |
| 1:B:122:ILE:HD12  | 1:B:122:ILE:H    | 1.29                     | 0.95              |
| 2:H:195:LEU:CD1   | 2:H:234:ALA:HB1  | 1.96                     | 0.95              |
| 2:H:451:LEU:O     | 2:H:452:ILE:HD12 | 1.65                     | 0.95              |
| 3:N:103:TRP:HE1   | 3:N:604:THR:HG1  | 1.03                     | 0.95              |
| 2:C:260:LEU:HB2   | 2:C:291:ALA:HB1  | 1.47                     | 0.95              |
| 3:I:947:ILE:O     | 3:I:947:ILE:HD12 | 1.66                     | 0.95              |
| 1:L:41:ARG:HH11   | 1:L:177:VAL:HG23 | 1.32                     | 0.95              |
| 2:M:1011:GLY:HA3  | 2:M:1026:GLN:HG2 | 1.47                     | 0.95              |
| 2:M:140:ILE:HD13  | 2:M:331:ARG:NH2  | 1.80                     | 0.95              |
| 2:C:305:PRO:HG3   | 2:C:308:ARG:HH21 | 1.31                     | 0.95              |
| 3:I:1161:GLU:OE2  | 3:I:1164:ARG:HD2 | 1.67                     | 0.95              |
| 3:N:347:VAL:HG13  | 3:N:351:MET:HB2  | 1.49                     | 0.95              |
| 3:D:639:LEU:HD13  | 3:D:766:ALA:HB2  | 1.44                     | 0.95              |
| 2:H:304:LEU:HG    | 2:H:305:PRO:HD3  | 1.45                     | 0.95              |
| 3:N:603:LEU:O     | 3:N:606:ILE:HG22 | 1.64                     | 0.95              |
| 2:M:242:LEU:CD1   | 2:M:254:VAL:HG11 | 1.96                     | 0.95              |
| 1:K:161:ARG:NH1   | 1:K:161:ARG:HB2  | 1.81                     | 0.95              |
| 2:M:267:TYR:HB2   | 2:M:272:ALA:HB1  | 1.45                     | 0.95              |
| 2:M:74:GLY:O      | 2:M:76:PRO:HD3   | 1.66                     | 0.95              |
| 3:D:1052:THR:HG22 | 7:X:57:ARG:HH11  | 1.31                     | 0.95              |
| 1:A:161:ARG:HB2   | 1:A:161:ARG:NH1  | 1.81                     | 0.95              |
| 3:D:1209:LEU:HD23 | 3:D:1211:MET:H   | 1.30                     | 0.95              |
| 2:H:170:PRO:HD3   | 2:H:263:ASP:HB3  | 1.48                     | 0.95              |
| 3:D:160:GLU:HG2   | 3:D:165:LYS:CB   | 1.97                     | 0.95              |
| 2:H:170:PRO:CD    | 2:H:263:ASP:HB3  | 1.95                     | 0.95              |
| 2:H:172:ILE:HG13  | 2:H:186:VAL:HG12 | 1.49                     | 0.95              |
| 3:I:871:LYS:HZ2   | 1:L:60:ASP:HA    | 1.23                     | 0.95              |
| 2:M:437:ARG:NH2   | 2:M:488:ALA:HA   | 1.82                     | 0.95              |
| 3:D:161:LEU:CD1   | 3:D:161:LEU:N    | 2.30                     | 0.95              |
| 1:K:86:VAL:HG12   | 1:K:124:ASN:HB2  | 1.49                     | 0.95              |
| 2:C:1097:LEU:CD1  | 3:D:1451:ALA:CB  | 2.44                     | 0.95              |
| 1:F:161:ARG:NH1   | 1:F:161:ARG:HB2  | 1.81                     | 0.95              |
| 3:N:970:LYS:NZ    | 7:Z:113:LEU:CG   | 2.20                     | 0.95              |
| 3:N:997:THR:HG21  | 7:Z:61:ARG:CZ    | 1.97                     | 0.95              |
| 2:H:1004:LYS:HD2  | 3:I:744:GLN:HE22 | 1.27                     | 0.94              |
| 2:M:129:ILE:CD1   | 2:M:134:ARG:HG3  | 1.96                     | 0.94              |
| 2:M:861:LEU:HG    | 2:M:862:PRO:HD2  | 1.49                     | 0.94              |
| 1:A:109:VAL:HG12  | 1:A:129:ILE:HD12 | 1.49                     | 0.94              |
| 2:C:363:SER:HB3   | 3:I:1130:ARG:O   | 1.67                     | 0.94              |
| 2:H:313:LEU:HG    | 2:H:320:HIS:ND1  | 1.83                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:615:ARG:HG3   | 3:I:619:LEU:CG    | 1.97                     | 0.94              |
| 1:F:86:VAL:HG12   | 1:F:124:ASN:HB2   | 1.49                     | 0.94              |
| 3:D:349:PRO:HB3   | 2:H:274:ARG:NH1   | 1.81                     | 0.94              |
| 2:H:182:VAL:CB    | 2:H:193:LEU:CD1   | 2.45                     | 0.94              |
| 3:N:214:GLU:HA    | 3:N:342:PRO:HA    | 1.49                     | 0.94              |
| 3:D:654:LYS:HB3   | 3:D:655:PRO:HD3   | 1.49                     | 0.94              |
| 2:H:408:ARG:HH21  | 2:H:455:LEU:CD1   | 1.79                     | 0.94              |
| 2:M:140:ILE:CD1   | 2:M:331:ARG:NH2   | 2.30                     | 0.94              |
| 5:R:20:DG:H1      | 6:S:11:C:N4       | 1.64                     | 0.94              |
| 2:C:182:VAL:HG11  | 2:C:193:LEU:CD2   | 1.97                     | 0.94              |
| 2:H:293:PHE:HD1   | 2:H:293:PHE:H     | 1.12                     | 0.94              |
| 2:M:560:MET:O     | 2:M:564:MET:HG2   | 1.66                     | 0.94              |
| 2:M:80:GLN:HG2    | 2:M:90:TYR:CE2    | 2.03                     | 0.94              |
| 2:M:939:ARG:HA    | 2:M:939:ARG:HE    | 1.30                     | 0.94              |
| 2:C:160:ALA:HB3   | 2:C:174:LEU:HB2   | 1.48                     | 0.94              |
| 3:D:161:LEU:CD1   | 3:D:161:LEU:H     | 1.79                     | 0.94              |
| 2:M:118:ILE:HG22  | 2:M:382:ILE:HD13  | 1.48                     | 0.94              |
| 3:N:654:LYS:HB3   | 3:N:655:PRO:HD3   | 1.49                     | 0.94              |
| 7:Y:13:GLU:HG2    | 7:Y:17:GLN:HE21   | 1.31                     | 0.94              |
| 1:A:35:THR:HG21   | 1:B:43:ILE:HD11   | 1.49                     | 0.94              |
| 2:C:478:VAL:HA    | 2:C:506:ASN:O     | 1.68                     | 0.94              |
| 2:H:794:PRO:HD2   | 2:H:1024:LYS:O    | 1.68                     | 0.94              |
| 1:K:109:VAL:HG12  | 1:K:129:ILE:HD12  | 1.49                     | 0.94              |
| 2:M:597:ALA:HB2   | 2:M:655:LEU:HD21  | 1.50                     | 0.94              |
| 3:D:1052:THR:CG2  | 7:X:57:ARG:HH11   | 1.81                     | 0.94              |
| 7:Z:119:ILE:HG13  | 7:Z:125:MET:CE    | 1.97                     | 0.94              |
| 2:H:182:VAL:HG11  | 2:H:193:LEU:HD22  | 1.50                     | 0.94              |
| 2:M:188:LYS:HZ3   | 2:M:188:LYS:CB    | 1.79                     | 0.94              |
| 3:N:1263:PHE:CE2  | 3:N:1371:VAL:HG11 | 2.03                     | 0.94              |
| 2:C:861:LEU:HG    | 2:C:862:PRO:HD2   | 1.49                     | 0.93              |
| 3:D:1263:PHE:CE2  | 3:D:1371:VAL:HG11 | 2.03                     | 0.93              |
| 2:H:1110:ASP:OD1  | 2:H:1112:PHE:CD1  | 2.20                     | 0.93              |
| 2:H:355:VAL:HG23  | 2:H:372:LEU:HG    | 1.50                     | 0.93              |
| 3:I:1481:VAL:HG11 | 4:J:18:ARG:HA     | 1.47                     | 0.93              |
| 1:L:187:GLY:O     | 3:N:688:TRP:HD1   | 1.51                     | 0.93              |
| 2:H:313:LEU:CG    | 2:H:320:HIS:CE1   | 2.51                     | 0.93              |
| 2:M:408:ARG:HH21  | 2:M:455:LEU:CD1   | 1.80                     | 0.93              |
| 2:M:572:ILE:HD12  | 2:M:573:ARG:H     | 1.32                     | 0.93              |
| 3:N:970:LYS:CD    | 7:Z:113:LEU:HD23  | 1.97                     | 0.93              |
| 2:C:560:MET:O     | 2:C:564:MET:HG2   | 1.67                     | 0.93              |
| 3:D:1112:CYS:HB2  | 3:D:1195:GLN:HG2  | 1.48                     | 0.93              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:603:LEU:O    | 3:I:606:ILE:HG22  | 1.68                     | 0.93              |
| 2:C:676:ILE:CG2  | 2:C:988:VAL:HG13  | 1.99                     | 0.93              |
| 2:M:564:MET:CE   | 2:M:846:LYS:HD2   | 1.98                     | 0.93              |
| 1:A:86:VAL:HG12  | 1:A:124:ASN:HB2   | 1.49                     | 0.93              |
| 2:H:939:ARG:HE   | 2:H:939:ARG:HA    | 1.30                     | 0.93              |
| 2:M:101:ILE:HD12 | 2:M:108:ILE:HD11  | 1.50                     | 0.93              |
| 3:D:1106:VAL:HB  | 3:D:1108:ARG:NE   | 1.82                     | 0.93              |
| 3:D:1254:GLN:HA  | 3:D:1258:ARG:HB2  | 1.50                     | 0.93              |
| 3:D:127:LEU:CD2  | 3:D:134:VAL:HG13  | 1.97                     | 0.93              |
| 3:D:480:GLU:O    | 3:D:484:PRO:CD    | 2.16                     | 0.93              |
| 3:D:563:PRO:HA   | 2:H:223:ASP:HB2   | 1.48                     | 0.93              |
| 3:D:631:ILE:HD12 | 3:D:743:ASP:O     | 1.69                     | 0.93              |
| 2:H:64:LEU:HB2   | 2:H:359:MET:HG3   | 1.50                     | 0.93              |
| 2:H:565:GLN:NE2  | 2:H:842:ARG:HG2   | 1.83                     | 0.93              |
| 2:M:200:LEU:HD22 | 2:M:300:ASP:CG    | 1.89                     | 0.93              |
| 2:M:111:ASP:CG   | 2:M:369:PRO:HG2   | 1.88                     | 0.93              |
| 3:N:631:ILE:HD12 | 3:N:743:ASP:O     | 1.68                     | 0.93              |
| 2:C:477:GLY:O    | 2:C:507:ARG:HA    | 1.69                     | 0.93              |
| 3:D:134:VAL:HG21 | 3:D:460:ALA:HB2   | 1.49                     | 0.93              |
| 1:F:42:ARG:HH12  | 1:G:34:VAL:HB     | 1.25                     | 0.93              |
| 1:G:170:VAL:HG11 | 3:I:848:GLU:OE2   | 1.69                     | 0.93              |
| 1:L:75:VAL:O     | 1:L:79:ILE:HG23   | 1.67                     | 0.93              |
| 3:N:166:GLN:HE22 | 3:N:394:LEU:HB2   | 1.31                     | 0.93              |
| 3:N:520:LEU:HD12 | 3:N:521:PRO:HD2   | 1.51                     | 0.93              |
| 2:H:10:ARG:HA    | 2:H:10:ARG:HH11   | 1.34                     | 0.93              |
| 3:I:631:ILE:HD12 | 3:I:743:ASP:O     | 1.69                     | 0.93              |
| 1:K:67:THR:HG21  | 2:M:609:ASN:HD21  | 1.31                     | 0.93              |
| 2:M:80:GLN:HG3   | 2:M:90:TYR:CE2    | 2.02                     | 0.93              |
| 3:I:142:LEU:HD23 | 3:I:146:PRO:HA    | 1.51                     | 0.93              |
| 2:C:572:ILE:HD12 | 2:C:573:ARG:H     | 1.32                     | 0.92              |
| 1:F:221:HIS:HE2  | 1:G:32:PHE:HE2    | 0.95                     | 0.92              |
| 1:G:41:ARG:NH1   | 1:G:177:VAL:HG23  | 1.83                     | 0.92              |
| 2:H:1011:GLY:HA3 | 2:H:1026:GLN:HG2  | 1.51                     | 0.92              |
| 2:M:836:GLY:HA3  | 2:M:1001:VAL:HG21 | 1.49                     | 0.92              |
| 2:M:325:ILE:HD12 | 2:M:325:ILE:H     | 1.32                     | 0.92              |
| 3:N:131:LYS:O    | 3:N:132:TYR:C     | 2.08                     | 0.92              |
| 3:N:809:PRO:HB2  | 3:N:812:ALA:CB    | 1.97                     | 0.92              |
| 3:I:783:ARG:HH12 | 7:Y:41:ASP:HB3    | 1.31                     | 0.92              |
| 3:I:486:ARG:HA   | 3:I:489:ARG:HG2   | 1.51                     | 0.92              |
| 1:F:109:VAL:HG12 | 1:F:129:ILE:HD12  | 1.49                     | 0.92              |
| 3:I:107:ASP:OD1  | 3:I:1444:THR:HG22 | 1.68                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1046:ALA:HB1  | 3:I:1471:LEU:HD11 | 1.52                     | 0.92              |
| 2:C:36:PRO:O      | 2:C:39:ARG:HG3    | 1.68                     | 0.92              |
| 2:H:188:LYS:HB2   | 2:H:188:LYS:HZ2   | 1.14                     | 0.92              |
| 2:H:432:ARG:NH2   | 3:I:1047:LYS:HD3  | 1.84                     | 0.92              |
| 3:D:1412:LYS:O    | 3:D:1414:PRO:HD3  | 1.70                     | 0.92              |
| 2:H:1106:ASP:OD1  | 3:I:7:LYS:CD      | 2.17                     | 0.92              |
| 2:H:572:ILE:HD12  | 2:H:573:ARG:H     | 1.32                     | 0.92              |
| 2:M:36:PRO:HA     | 2:M:39:ARG:HB2    | 1.52                     | 0.92              |
| 3:N:87:ARG:O      | 3:N:521:PRO:HB3   | 1.69                     | 0.92              |
| 7:Y:7:LEU:HD21    | 7:Y:72:ALA:HB1    | 1.51                     | 0.92              |
| 2:C:565:GLN:NE2   | 2:C:842:ARG:HG2   | 1.85                     | 0.92              |
| 3:D:127:LEU:HD23  | 3:D:134:VAL:HG13  | 1.52                     | 0.92              |
| 1:F:112:ARG:HH21  | 1:F:125:PRO:HB2   | 1.35                     | 0.92              |
| 1:G:80:LEU:HG     | 3:I:844:ALA:HA    | 1.52                     | 0.92              |
| 3:I:1112:CYS:HB2  | 3:I:1195:GLN:HG2  | 1.51                     | 0.92              |
| 3:I:1263:PHE:CE2  | 3:I:1371:VAL:HG11 | 2.03                     | 0.92              |
| 3:I:28:LYS:O      | 3:I:43:GLY:HA2    | 1.69                     | 0.92              |
| 3:I:41:ARG:CB     | 3:I:46:ASP:OD1    | 2.17                     | 0.92              |
| 2:H:1019:GLN:OE1  | 3:I:621:LYS:CG    | 2.17                     | 0.92              |
| 2:M:21:ILE:HD12   | 2:M:21:ILE:H      | 1.34                     | 0.92              |
| 3:I:406:ASP:O     | 3:I:422:ALA:HB1   | 1.68                     | 0.92              |
| 3:I:615:ARG:O     | 3:I:619:LEU:HG    | 1.69                     | 0.92              |
| 2:M:129:ILE:HG12  | 2:M:134:ARG:HD3   | 1.52                     | 0.92              |
| 1:A:218:LEU:HD23  | 1:B:222:LEU:HD21  | 1.52                     | 0.92              |
| 2:C:879:ARG:NH2   | 7:X:42:ASP:CB     | 2.31                     | 0.92              |
| 2:H:288:ARG:HH11  | 2:H:288:ARG:HB2   | 1.33                     | 0.92              |
| 3:I:398:ALA:HB2   | 3:I:447:VAL:HA    | 1.51                     | 0.92              |
| 2:M:48:PHE:CD1    | 2:M:348:LEU:HD21  | 2.05                     | 0.92              |
| 3:N:1209:LEU:HD21 | 4:O:16:LYS:NZ     | 1.85                     | 0.92              |
| 2:C:182:VAL:HG21  | 2:C:193:LEU:HB3   | 1.50                     | 0.92              |
| 1:L:212:ASN:O     | 1:L:215:VAL:HG22  | 1.70                     | 0.92              |
| 2:M:834:GLN:NE2   | 3:N:724:GLN:HG3   | 1.85                     | 0.92              |
| 5:R:20:DG:H1      | 6:S:11:C:H42      | 0.94                     | 0.92              |
| 2:C:685:GLU:OE2   | 7:X:41:ASP:HB2    | 1.69                     | 0.92              |
| 2:C:834:GLN:HE22  | 3:D:724:GLN:HG3   | 1.34                     | 0.91              |
| 2:H:181:VAL:HG12  | 2:H:182:VAL:N     | 1.84                     | 0.91              |
| 3:I:554:LEU:O     | 3:I:558:LEU:HG    | 1.70                     | 0.91              |
| 2:H:1106:ASP:OD1  | 3:I:7:LYS:HD2     | 1.69                     | 0.91              |
| 3:I:908:LYS:HB2   | 3:I:1027:GLY:HA3  | 1.52                     | 0.91              |
| 3:D:50:PHE:CG     | 3:D:522:PRO:HG2   | 2.04                     | 0.91              |
| 2:H:40:GLU:HG3    | 2:H:41:ASN:H      | 1.35                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:861:LEU:HG   | 2:H:862:PRO:HD2  | 1.49                     | 0.91              |
| 3:N:162:ARG:HB3  | 3:N:452:ILE:HG21 | 1.51                     | 0.91              |
| 2:C:675:ALA:HA   | 2:C:989:VAL:HG12 | 1.51                     | 0.91              |
| 3:I:41:ARG:HB3   | 3:I:46:ASP:OD1   | 1.69                     | 0.91              |
| 3:N:373:PRO:HA   | 3:N:376:GLU:OE2  | 1.70                     | 0.91              |
| 3:D:158:TYR:O    | 3:D:162:ARG:HB2  | 1.71                     | 0.91              |
| 2:H:1065:ALA:HB1 | 2:H:1077:PRO:HG2 | 1.51                     | 0.91              |
| 2:H:1093:GLN:HB3 | 3:I:21:TRP:HZ3   | 1.33                     | 0.91              |
| 2:M:260:LEU:HB2  | 2:M:291:ALA:HB1  | 1.49                     | 0.91              |
| 3:N:997:THR:HG21 | 7:Z:61:ARG:NH2   | 1.85                     | 0.91              |
| 1:B:212:ASN:O    | 1:B:215:VAL:HG22 | 1.70                     | 0.91              |
| 2:C:374:ASN:H    | 2:C:374:ASN:HD22 | 1.18                     | 0.91              |
| 2:C:943:VAL:HG23 | 2:C:985:GLY:H    | 1.36                     | 0.91              |
| 2:H:99:GLN:HE21  | 2:H:101:ILE:HD11 | 1.33                     | 0.91              |
| 2:M:689:VAL:HB   | 2:M:870:ILE:HG12 | 1.49                     | 0.91              |
| 2:H:943:VAL:HG23 | 2:H:985:GLY:H    | 1.36                     | 0.91              |
| 3:I:141:ILE:HD13 | 3:I:142:LEU:N    | 1.85                     | 0.91              |
| 3:I:654:LYS:HB3  | 3:I:655:PRO:HD3  | 1.49                     | 0.91              |
| 2:M:6:PHE:CZ     | 2:M:901:TYR:CD2  | 2.55                     | 0.91              |
| 3:N:50:PHE:CD1   | 3:N:522:PRO:HG2  | 2.04                     | 0.91              |
| 1:G:212:ASN:O    | 1:G:215:VAL:HG22 | 1.70                     | 0.91              |
| 2:H:1086:ARG:CZ  | 3:I:88:TYR:HE2   | 1.70                     | 0.91              |
| 3:I:12:LEU:CD2   | 3:I:104:PHE:HE1  | 1.84                     | 0.91              |
| 3:I:1412:LYS:O   | 3:I:1414:PRO:HD3 | 1.69                     | 0.91              |
| 1:K:112:ARG:HH21 | 1:K:125:PRO:HB2  | 1.35                     | 0.91              |
| 1:B:187:GLY:O    | 3:D:688:TRP:HD1  | 1.54                     | 0.91              |
| 2:C:564:MET:HE1  | 2:C:846:LYS:CE   | 2.01                     | 0.91              |
| 3:D:139:GLY:O    | 3:D:147:VAL:CG1  | 2.18                     | 0.91              |
| 3:D:28:LYS:O     | 3:D:43:GLY:CA    | 2.19                     | 0.91              |
| 2:M:39:ARG:CD    | 2:M:45:GLN:CD    | 2.39                     | 0.91              |
| 3:D:134:VAL:O    | 3:D:454:ALA:HB1  | 1.70                     | 0.91              |
| 1:F:218:LEU:HD23 | 1:G:222:LEU:HD21 | 1.52                     | 0.91              |
| 3:I:1111:ASP:OD1 | 3:I:1203:LYS:HD2 | 1.70                     | 0.91              |
| 3:I:615:ARG:HG3  | 3:I:619:LEU:HG   | 1.53                     | 0.91              |
| 2:H:834:GLN:HE22 | 3:I:724:GLN:HG3  | 1.34                     | 0.91              |
| 1:L:165:ILE:HD13 | 1:L:165:ILE:H    | 1.36                     | 0.91              |
| 3:I:12:LEU:HD21  | 3:I:104:PHE:HE1  | 1.02                     | 0.91              |
| 2:H:1075:ASP:OD1 | 4:J:31:LEU:HD11  | 1.71                     | 0.91              |
| 3:N:783:ARG:HH11 | 7:Z:41:ASP:HB2   | 0.75                     | 0.91              |
| 2:C:958:THR:HG23 | 2:C:961:GLU:HG3  | 1.52                     | 0.90              |
| 1:F:36:LEU:O     | 1:F:39:PRO:HD2   | 1.71                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:21:ILE:H      | 2:H:21:ILE:CD1    | 1.82                     | 0.90              |
| 2:H:958:THR:HG23  | 2:H:961:GLU:HG3   | 1.51                     | 0.90              |
| 3:N:676:MET:HE1   | 3:N:684:LYS:HE3   | 1.52                     | 0.90              |
| 1:A:36:LEU:O      | 1:A:39:PRO:HD2    | 1.71                     | 0.90              |
| 3:I:764:LEU:HD12  | 3:I:765:SER:H     | 1.36                     | 0.90              |
| 2:M:242:LEU:HD11  | 2:M:254:VAL:HG11  | 1.52                     | 0.90              |
| 3:D:1258:ARG:NH1  | 3:D:1262:LEU:HD13 | 1.85                     | 0.90              |
| 3:I:1257:PRO:HA   | 3:I:1260:ILE:HD12 | 1.54                     | 0.90              |
| 2:H:1030:GLN:NE2  | 3:I:628:ARG:CD    | 2.34                     | 0.90              |
| 3:N:168:THR:HG22  | 3:N:170:PRO:HD3   | 1.53                     | 0.90              |
| 2:H:1083:GLU:OE2  | 2:H:1086:ARG:HD2  | 1.71                     | 0.90              |
| 3:N:373:PRO:HA    | 3:N:376:GLU:CD    | 1.91                     | 0.90              |
| 3:N:486:ARG:HA    | 3:N:489:ARG:HG2   | 1.51                     | 0.90              |
| 3:N:86:ARG:CZ     | 3:N:523:ASP:OD1   | 2.19                     | 0.90              |
| 7:X:81:GLU:O      | 7:X:154:ILE:HD12  | 1.69                     | 0.90              |
| 3:D:683:ILE:HD13  | 3:D:687:VAL:HG21  | 1.52                     | 0.90              |
| 2:H:129:ILE:HG12  | 2:H:386:PHE:HB3   | 1.53                     | 0.90              |
| 2:H:140:ILE:HD11  | 2:H:412:ALA:HA    | 1.54                     | 0.90              |
| 2:C:1083:GLU:OE2  | 2:C:1086:ARG:HD2  | 1.71                     | 0.90              |
| 2:C:221:LEU:HD12  | 2:C:222:MET:N     | 1.86                     | 0.90              |
| 2:C:854:PRO:HB2   | 2:C:856:GLU:HG3   | 1.54                     | 0.90              |
| 3:D:1286:THR:HG22 | 3:D:1287:GLU:H    | 1.36                     | 0.90              |
| 1:K:36:LEU:O      | 1:K:39:PRO:HD2    | 1.71                     | 0.90              |
| 3:N:137:PRO:HD3   | 3:N:453:ASP:HB2   | 1.53                     | 0.90              |
| 3:N:1412:LYS:O    | 3:N:1414:PRO:HD3  | 1.70                     | 0.90              |
| 3:D:1114:THR:CG2  | 3:D:1195:GLN:HB3  | 2.02                     | 0.90              |
| 3:N:806:PHE:CE1   | 3:N:813:LEU:HB3   | 2.06                     | 0.90              |
| 3:D:50:PHE:CG     | 3:D:522:PRO:CG    | 2.54                     | 0.90              |
| 1:G:41:ARG:HG3    | 1:G:177:VAL:HG21  | 1.53                     | 0.90              |
| 1:G:67:THR:OG1    | 1:L:159:LYS:HG3   | 1.72                     | 0.90              |
| 2:M:1083:GLU:OE2  | 2:M:1086:ARG:HD2  | 1.71                     | 0.90              |
| 3:D:127:LEU:O     | 3:D:457:GLY:CA    | 2.16                     | 0.90              |
| 2:H:292:ARG:HG2   | 2:H:299:LYS:HB3   | 1.51                     | 0.90              |
| 2:H:676:ILE:HG21  | 2:H:988:VAL:HG13  | 1.53                     | 0.90              |
| 2:M:943:VAL:HG23  | 2:M:985:GLY:H     | 1.36                     | 0.90              |
| 1:A:67:THR:HG21   | 2:C:609:ASN:ND2   | 1.87                     | 0.90              |
| 3:I:482:LYS:HE2   | 3:I:1388:ARG:NH2  | 1.87                     | 0.90              |
| 2:M:188:LYS:NZ    | 2:M:188:LYS:CB    | 2.35                     | 0.90              |
| 1:B:74:ASP:CB     | 3:D:872:ARG:HH22  | 1.85                     | 0.89              |
| 2:H:54:ILE:HG22   | 2:H:66:LEU:H      | 1.37                     | 0.89              |
| 3:I:181:ASP:HA    | 3:I:205:TYR:CD2   | 2.06                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:87:ARG:CG     | 3:I:523:ASP:HB2   | 2.01                     | 0.89              |
| 2:M:1030:GLN:NE2  | 3:N:628:ARG:CD    | 2.34                     | 0.89              |
| 2:M:111:ASP:OD2   | 2:M:369:PRO:CB    | 2.19                     | 0.89              |
| 2:C:208:ALA:CB    | 2:C:222:MET:SD    | 2.60                     | 0.89              |
| 3:D:1123:PHE:CE2  | 3:D:1184:GLN:HA   | 2.08                     | 0.89              |
| 2:C:1097:LEU:CD1  | 3:D:1451:ALA:HB2  | 2.03                     | 0.89              |
| 3:D:392:SER:C     | 3:D:393:ILE:HD12  | 1.91                     | 0.89              |
| 3:D:102:ILE:HB    | 3:D:579:ASP:OD1   | 1.72                     | 0.89              |
| 3:I:204:LEU:O     | 3:I:393:ILE:HA    | 1.72                     | 0.89              |
| 1:L:228:PRO:O     | 1:L:229:GLN:HG3   | 1.72                     | 0.89              |
| 3:N:764:LEU:HD12  | 3:N:765:SER:H     | 1.36                     | 0.89              |
| 3:D:153:LEU:CD1   | 3:D:158:TYR:HB2   | 2.02                     | 0.89              |
| 2:H:182:VAL:CG1   | 2:H:193:LEU:CD1   | 2.49                     | 0.89              |
| 2:H:878:SER:CA    | 3:I:1034:GLN:HE22 | 1.84                     | 0.89              |
| 2:M:1099:VAL:HG22 | 3:N:10:ILE:CG1    | 2.02                     | 0.89              |
| 2:M:854:PRO:HB2   | 2:M:856:GLU:HG3   | 1.54                     | 0.89              |
| 3:D:982:PHE:CE1   | 7:X:100:LEU:HD21  | 2.07                     | 0.89              |
| 2:H:878:SER:HA    | 3:I:1034:GLN:NE2  | 1.87                     | 0.89              |
| 3:I:774:SER:HB3   | 3:I:1362:LYS:O    | 1.72                     | 0.89              |
| 2:M:564:MET:SD    | 2:M:846:LYS:HD2   | 2.13                     | 0.89              |
| 2:M:958:THR:HG23  | 2:M:961:GLU:HG3   | 1.52                     | 0.89              |
| 3:N:28:LYS:O      | 3:N:43:GLY:CA     | 2.19                     | 0.89              |
| 3:D:1263:PHE:HE2  | 3:D:1371:VAL:HG11 | 1.38                     | 0.89              |
| 1:B:187:GLY:CA    | 3:D:685:ASP:CB    | 2.46                     | 0.89              |
| 2:H:601:GLY:HA2   | 2:H:616:GLU:HG2   | 1.55                     | 0.89              |
| 2:H:576:ALA:HB3   | 2:H:900:ARG:HH11  | 1.33                     | 0.89              |
| 2:H:1019:GLN:OE1  | 3:I:621:LYS:CD    | 2.19                     | 0.89              |
| 2:C:193:LEU:HD21  | 2:C:307:LEU:CD2   | 1.99                     | 0.89              |
| 2:C:455:LEU:HD13  | 2:C:459:ALA:HB3   | 1.54                     | 0.89              |
| 3:I:131:LYS:HG3   | 3:I:568:ARG:NE    | 1.85                     | 0.89              |
| 3:I:154:THR:HG23  | 3:I:157:GLU:HB2   | 1.54                     | 0.89              |
| 3:I:615:ARG:CD    | 3:I:619:LEU:HD21  | 2.02                     | 0.89              |
| 2:M:1085:PHE:CE2  | 3:N:1468:LEU:HG   | 2.07                     | 0.89              |
| 2:M:140:ILE:HD11  | 2:M:331:ARG:HH21  | 1.34                     | 0.89              |
| 1:B:56:VAL:HG22   | 1:B:142:VAL:HG12  | 1.55                     | 0.89              |
| 2:C:185:LYS:HD2   | 2:C:190:LYS:CG    | 2.02                     | 0.89              |
| 3:D:124:GLU:CG    | 3:D:128:TYR:CE1   | 2.56                     | 0.89              |
| 3:D:139:GLY:O     | 3:D:147:VAL:CB    | 2.21                     | 0.89              |
| 2:C:1093:GLN:HB3  | 3:D:21:TRP:HZ3    | 1.36                     | 0.89              |
| 3:D:520:LEU:HD12  | 3:D:521:PRO:HD2   | 1.50                     | 0.89              |
| 2:H:195:LEU:O     | 2:H:199:VAL:HG23  | 1.72                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1256:LEU:HB3  | 3:I:1257:PRO:HD3  | 1.55                     | 0.89              |
| 2:M:502:PRO:HB2   | 2:M:509:ALA:HB3   | 1.55                     | 0.89              |
| 2:M:654:LEU:HD23  | 2:M:654:LEU:H     | 1.38                     | 0.89              |
| 4:O:18:ARG:HB2    | 4:O:18:ARG:HH21   | 1.37                     | 0.89              |
| 1:B:41:ARG:NH1    | 1:B:177:VAL:HG23  | 1.88                     | 0.89              |
| 3:D:387:LEU:H     | 3:D:387:LEU:HD12  | 1.38                     | 0.89              |
| 2:M:697:ARG:HD2   | 2:M:699:PHE:CD1   | 2.08                     | 0.89              |
| 3:N:1468:LEU:HD13 | 3:N:1470:ARG:HE   | 1.35                     | 0.89              |
| 3:N:81:THR:CG2    | 3:N:82:LYS:N      | 2.30                     | 0.89              |
| 2:C:215:GLY:O     | 2:C:216:GLU:HB3   | 1.72                     | 0.89              |
| 2:C:911:GLU:OE1   | 3:D:951:ILE:CD1   | 2.19                     | 0.89              |
| 3:I:408:GLU:CG    | 3:I:409:VAL:H     | 1.85                     | 0.89              |
| 1:G:76:VAL:CB     | 3:I:872:ARG:NH1   | 2.35                     | 0.89              |
| 2:M:794:PRO:HD2   | 2:M:1024:LYS:O    | 1.72                     | 0.89              |
| 1:A:112:ARG:HH21  | 1:A:125:PRO:HB2   | 1.35                     | 0.88              |
| 1:B:54:THR:O      | 1:B:167:VAL:HG23  | 1.73                     | 0.88              |
| 3:N:356:PRO:HG2   | 3:N:359:ALA:HB2   | 1.55                     | 0.88              |
| 1:A:42:ARG:HH12   | 1:B:34:VAL:CB     | 1.86                     | 0.88              |
| 1:A:42:ARG:NH1    | 1:B:34:VAL:CG1    | 2.35                     | 0.88              |
| 2:M:368:THR:O     | 2:M:372:LEU:HD12  | 1.72                     | 0.88              |
| 3:D:1066:THR:HG22 | 3:D:1069:GLU:HB2  | 1.55                     | 0.88              |
| 3:D:764:LEU:HD12  | 3:D:765:SER:H     | 1.35                     | 0.88              |
| 3:I:1292:VAL:HG11 | 3:I:1325:LEU:HG   | 1.54                     | 0.88              |
| 2:C:642:ARG:HD3   | 2:C:642:ARG:O     | 1.74                     | 0.88              |
| 2:H:455:LEU:HD13  | 2:H:459:ALA:HB3   | 1.54                     | 0.88              |
| 2:M:457:ALA:HB3   | 2:M:538:GLN:HA    | 1.56                     | 0.88              |
| 3:N:1031:ASN:ND2  | 7:Z:32:ILE:HG23   | 1.88                     | 0.88              |
| 3:N:44:LEU:O      | 3:N:50:PHE:CE1    | 2.27                     | 0.88              |
| 3:N:868:TYR:CD1   | 3:N:869:MET:HG3   | 2.09                     | 0.88              |
| 1:L:74:ASP:CB     | 3:N:872:ARG:HH22  | 1.86                     | 0.88              |
| 1:B:87:VAL:HG21   | 1:B:144:VAL:HG11  | 1.55                     | 0.88              |
| 4:J:54:LEU:HG     | 4:J:58:PRO:HG2    | 1.55                     | 0.88              |
| 2:M:455:LEU:HD13  | 2:M:459:ALA:HB3   | 1.54                     | 0.88              |
| 2:M:69:LEU:HD11   | 2:M:99:GLN:HG2    | 1.56                     | 0.88              |
| 3:N:15:PRO:CB     | 3:N:515:GLU:OE1   | 2.21                     | 0.88              |
| 2:C:265:ARG:H     | 2:C:289:THR:HG21  | 1.36                     | 0.88              |
| 3:D:145:VAL:HG22  | 3:D:146:PRO:CD    | 2.03                     | 0.88              |
| 3:D:164:GLY:HA3   | 3:D:449:SER:HB3   | 1.54                     | 0.88              |
| 2:H:642:ARG:HD3   | 2:H:642:ARG:O     | 1.74                     | 0.88              |
| 3:N:1266:ARG:O    | 3:N:1268:PRO:HD3  | 1.73                     | 0.88              |
| 2:C:1081:VAL:CG2  | 2:C:1111:ILE:HG22 | 2.04                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:98:LEU:HD12   | 2:H:98:LEU:N      | 1.89                     | 0.88              |
| 2:C:198:ARG:HD3   | 2:C:228:ALA:HA    | 1.56                     | 0.88              |
| 3:D:142:LEU:HB3   | 3:D:145:VAL:O     | 1.73                     | 0.88              |
| 3:D:868:TYR:CD1   | 3:D:869:MET:HG3   | 2.09                     | 0.88              |
| 2:H:457:ALA:HB3   | 2:H:538:GLN:HA    | 1.56                     | 0.88              |
| 2:H:73:LEU:HD22   | 2:H:118:ILE:HD11  | 1.56                     | 0.88              |
| 2:M:113:VAL:HG21  | 2:M:373:VAL:HG11  | 1.56                     | 0.88              |
| 1:B:228:PRO:O     | 1:B:229:GLN:HG3   | 1.72                     | 0.88              |
| 2:M:100:LEU:O     | 2:M:108:ILE:HG23  | 1.73                     | 0.88              |
| 1:B:75:VAL:O      | 1:B:79:ILE:HG23   | 1.74                     | 0.88              |
| 2:C:129:ILE:HG22  | 2:C:130:ASN:N     | 1.89                     | 0.88              |
| 3:D:809:PRO:HB2   | 3:D:812:ALA:CB    | 2.04                     | 0.88              |
| 1:K:9:PRO:HB2     | 1:L:224:TYR:HB3   | 1.56                     | 0.88              |
| 1:G:165:ILE:H     | 1:G:165:ILE:HD13  | 1.37                     | 0.87              |
| 3:I:982:PHE:CD1   | 7:Y:125:MET:SD    | 2.66                     | 0.87              |
| 2:H:21:ILE:N      | 2:H:21:ILE:HD12   | 1.88                     | 0.87              |
| 2:H:654:LEU:HD23  | 2:H:654:LEU:H     | 1.39                     | 0.87              |
| 3:I:661:MET:O     | 3:I:664:LYS:O     | 1.92                     | 0.87              |
| 2:C:290:LEU:HB3   | 2:C:302:VAL:HG11  | 1.55                     | 0.87              |
| 2:H:469:THR:HG23  | 2:H:470:PRO:HD2   | 1.56                     | 0.87              |
| 3:I:13:ALA:HB1    | 3:I:18:ILE:HD11   | 1.56                     | 0.87              |
| 2:M:174:LEU:HD22  | 2:M:193:LEU:HD21  | 1.56                     | 0.87              |
| 2:M:282:GLY:O     | 2:M:283:ILE:HG12  | 1.73                     | 0.87              |
| 2:C:21:ILE:HD12   | 2:C:21:ILE:H      | 1.40                     | 0.87              |
| 3:D:1266:ARG:O    | 3:D:1268:PRO:HD3  | 1.73                     | 0.87              |
| 3:D:152:LEU:HD23  | 3:D:152:LEU:H     | 1.40                     | 0.87              |
| 2:H:854:PRO:HB2   | 2:H:856:GLU:HG3   | 1.54                     | 0.87              |
| 2:M:165:LEU:HG    | 2:M:166:PRO:HA    | 1.56                     | 0.87              |
| 2:C:185:LYS:HG3   | 2:C:190:LYS:HB3   | 1.56                     | 0.87              |
| 3:D:661:MET:O     | 3:D:664:LYS:O     | 1.92                     | 0.87              |
| 3:I:41:ARG:CA     | 3:I:46:ASP:OD1    | 2.22                     | 0.87              |
| 2:M:129:ILE:HG12  | 2:M:134:ARG:CD    | 2.04                     | 0.87              |
| 3:N:1095:THR:O    | 3:N:1099:VAL:HG23 | 1.75                     | 0.87              |
| 3:N:166:GLN:HG2   | 3:N:396:VAL:HG12  | 1.53                     | 0.87              |
| 3:N:675:ARG:O     | 3:N:679:ARG:CB    | 2.21                     | 0.87              |
| 3:D:206:ARG:HD3   | 3:D:394:LEU:HD21  | 1.56                     | 0.87              |
| 3:D:166:GLN:HE22  | 3:D:394:LEU:HB2   | 1.37                     | 0.87              |
| 3:D:706:PRO:HD3   | 6:Q:16:G:H21      | 1.39                     | 0.87              |
| 3:D:89:ARG:O      | 3:D:521:PRO:HG3   | 1.75                     | 0.87              |
| 2:H:182:VAL:HG12  | 2:H:193:LEU:CD1   | 2.05                     | 0.87              |
| 3:I:1066:THR:HG22 | 3:I:1069:GLU:HB2  | 1.56                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:119:SER:CB    | 3:I:123:LEU:HB2   | 2.05                     | 0.87              |
| 3:N:661:MET:O     | 3:N:664:LYS:O     | 1.92                     | 0.87              |
| 2:C:208:ALA:HB2   | 2:C:222:MET:SD    | 2.15                     | 0.87              |
| 3:D:157:GLU:O     | 3:D:161:LEU:HD13  | 1.74                     | 0.87              |
| 3:D:353:VAL:HA    | 3:D:368:VAL:HG22  | 1.54                     | 0.87              |
| 2:H:15:LEU:HD12   | 2:H:15:LEU:H      | 1.39                     | 0.87              |
| 2:H:1085:PHE:CE2  | 3:I:1468:LEU:HG   | 2.09                     | 0.87              |
| 2:M:642:ARG:HD3   | 2:M:642:ARG:O     | 1.74                     | 0.87              |
| 4:O:54:LEU:HD23   | 4:O:58:PRO:HD2    | 1.56                     | 0.87              |
| 7:X:24:GLU:HA     | 7:X:27:GLN:NE2    | 1.89                     | 0.87              |
| 2:C:170:PRO:HG2   | 2:C:258:TYR:CD1   | 2.10                     | 0.87              |
| 1:F:156:HIS:HD2   | 1:F:157:GLY:H     | 1.23                     | 0.87              |
| 1:F:91:ASN:OD1    | 1:F:92:PRO:HD2    | 1.75                     | 0.87              |
| 3:I:1266:ARG:O    | 3:I:1268:PRO:HD3  | 1.73                     | 0.87              |
| 3:I:115:LEU:HD12  | 3:I:502:PHE:HE1   | 1.40                     | 0.87              |
| 3:I:606:ILE:O     | 3:I:613:ARG:HG2   | 1.73                     | 0.87              |
| 3:I:868:TYR:CD1   | 3:I:869:MET:HG3   | 2.09                     | 0.87              |
| 1:K:91:ASN:OD1    | 1:K:92:PRO:HD2    | 1.75                     | 0.87              |
| 2:M:235:LEU:HD11  | 2:M:298:PHE:HZ    | 1.39                     | 0.87              |
| 2:M:399:ASN:HD22  | 2:M:568:ALA:HB3   | 1.39                     | 0.87              |
| 7:X:59:GLU:O      | 7:X:62:ILE:HG22   | 1.74                     | 0.87              |
| 3:N:970:LYS:NZ    | 7:Z:113:LEU:CB    | 2.34                     | 0.87              |
| 1:B:74:ASP:HB2    | 3:D:872:ARG:NH2   | 1.89                     | 0.87              |
| 2:C:113:VAL:O     | 2:C:115:LEU:HD23  | 1.73                     | 0.87              |
| 2:C:276:LYS:HA    | 2:C:280:LYS:HD2   | 1.56                     | 0.87              |
| 2:H:1014:SER:HB2  | 2:H:1021:LEU:HD13 | 1.56                     | 0.87              |
| 2:H:69:LEU:HD12   | 2:H:97:ARG:HB3    | 1.56                     | 0.87              |
| 1:F:54:THR:HG22   | 1:F:158:ILE:CD1   | 2.05                     | 0.86              |
| 2:H:1081:VAL:HG21 | 2:H:1111:ILE:CG2  | 2.05                     | 0.86              |
| 2:H:185:LYS:HD2   | 2:H:190:LYS:CG    | 2.03                     | 0.86              |
| 1:L:76:VAL:HB     | 3:N:872:ARG:HH12  | 1.38                     | 0.86              |
| 3:N:1066:THR:HG22 | 3:N:1069:GLU:HB2  | 1.56                     | 0.86              |
| 3:N:1095:THR:HG23 | 3:N:1230:GLY:HA3  | 1.56                     | 0.86              |
| 2:C:879:ARG:CZ    | 7:X:42:ASP:CG     | 2.44                     | 0.86              |
| 2:M:79:PRO:HG2    | 2:M:82:GLU:HB2    | 1.56                     | 0.86              |
| 1:B:41:ARG:HG3    | 1:B:177:VAL:CG2   | 2.04                     | 0.86              |
| 2:C:182:VAL:HG11  | 2:C:193:LEU:HD22  | 1.54                     | 0.86              |
| 2:C:878:SER:OG    | 3:D:1029:ARG:NE   | 2.07                     | 0.86              |
| 3:I:131:LYS:HB2   | 3:I:568:ARG:NE    | 1.90                     | 0.86              |
| 3:I:141:ILE:HD13  | 3:I:142:LEU:H     | 1.39                     | 0.86              |
| 2:M:831:ARG:HD2   | 2:M:1000:MET:SD   | 2.15                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:564:MET:CE    | 2:M:846:LYS:CE    | 2.53                     | 0.86              |
| 3:D:186:VAL:HA    | 3:D:200:ASP:OD1   | 1.74                     | 0.86              |
| 3:I:991:GLN:NE2   | 7:Y:112:VAL:HG23  | 1.88                     | 0.86              |
| 2:M:172:ILE:N     | 2:M:172:ILE:HD12  | 1.90                     | 0.86              |
| 2:M:88:LEU:HD22   | 2:M:814:GLU:HG2   | 1.57                     | 0.86              |
| 3:N:50:PHE:CE2    | 3:N:522:PRO:HD3   | 2.08                     | 0.86              |
| 1:A:54:THR:HG22   | 1:A:158:ILE:CD1   | 2.05                     | 0.86              |
| 2:C:654:LEU:HD23  | 2:C:654:LEU:H     | 1.38                     | 0.86              |
| 3:N:1384:PRO:HG3  | 3:N:1389:LEU:HB3  | 1.57                     | 0.86              |
| 3:N:676:MET:O     | 3:N:680:GLN:CB    | 2.24                     | 0.86              |
| 2:C:408:ARG:HH21  | 2:C:455:LEU:CD1   | 1.88                     | 0.86              |
| 3:D:136:ASP:CB    | 3:D:137:PRO:HD3   | 2.01                     | 0.86              |
| 2:H:18:LEU:HD13   | 2:H:590:ASP:OD2   | 1.75                     | 0.86              |
| 2:M:1105:LYS:NZ   | 2:M:1107:ASN:HB2  | 1.90                     | 0.86              |
| 3:N:135:LEU:HD13  | 3:N:148:GLU:O     | 1.75                     | 0.86              |
| 3:N:203:ALA:HB1   | 3:N:393:ILE:HG21  | 1.57                     | 0.86              |
| 2:C:950:LEU:HB3   | 2:C:952:LEU:HD23  | 1.58                     | 0.86              |
| 2:H:200:LEU:HD13  | 2:H:300:ASP:CG    | 1.95                     | 0.86              |
| 3:I:23:TYR:O      | 3:I:49:ILE:HG23   | 1.75                     | 0.86              |
| 2:H:245:GLY:O     | 2:H:246:ASP:OD1   | 1.93                     | 0.86              |
| 3:I:1263:PHE:HE2  | 3:I:1371:VAL:HG11 | 1.38                     | 0.86              |
| 3:I:202:VAL:O     | 3:I:395:VAL:HA    | 1.75                     | 0.86              |
| 3:I:421:LEU:HD22  | 3:I:444:VAL:HG11  | 1.58                     | 0.86              |
| 3:N:1263:PHE:HE2  | 3:N:1371:VAL:HG11 | 1.38                     | 0.86              |
| 3:N:625:TYR:HB3   | 3:N:749:VAL:HG23  | 1.56                     | 0.86              |
| 3:I:813:LEU:O     | 3:I:817:GLU:HB2   | 1.76                     | 0.86              |
| 1:K:54:THR:HG22   | 1:K:158:ILE:CD1   | 2.05                     | 0.86              |
| 2:M:1088:LEU:HD23 | 2:M:1092:LEU:HD12 | 1.56                     | 0.86              |
| 2:C:831:ARG:HD2   | 2:C:1000:MET:SD   | 2.15                     | 0.86              |
| 2:C:316:GLY:C     | 2:C:318:PRO:HD3   | 1.96                     | 0.86              |
| 3:I:127:LEU:HD12  | 3:I:127:LEU:O     | 1.76                     | 0.86              |
| 3:I:181:ASP:HA    | 3:I:205:TYR:HD2   | 1.39                     | 0.86              |
| 2:M:569:VAL:HG12  | 2:M:996:LYS:O     | 1.76                     | 0.86              |
| 2:C:879:ARG:NH2   | 7:X:42:ASP:HB2    | 1.90                     | 0.86              |
| 2:H:879:ARG:NH2   | 7:Y:42:ASP:HB2    | 1.90                     | 0.86              |
| 1:A:156:HIS:HD2   | 1:A:157:GLY:H     | 1.23                     | 0.85              |
| 1:A:42:ARG:HH12   | 1:B:34:VAL:HB     | 1.38                     | 0.85              |
| 2:C:473:ARG:HB2   | 2:C:531:PHE:CE1   | 2.11                     | 0.85              |
| 2:C:979:THR:HG23  | 2:C:981:GLU:H     | 1.41                     | 0.85              |
| 3:D:1102:THR:HA   | 3:D:1105:ILE:HD13 | 1.58                     | 0.85              |
| 3:I:1211:MET:HG2  | 3:I:1212:ALA:N    | 1.91                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1288:GLU:O    | 3:N:1289:LYS:HG3  | 1.76                     | 0.85              |
| 3:N:1359:GLN:HE22 | 7:Z:52:LYS:HD3    | 1.41                     | 0.85              |
| 2:C:457:ALA:HB3   | 2:C:538:GLN:HA    | 1.56                     | 0.85              |
| 1:G:112:ARG:CG    | 1:G:125:PRO:HB3   | 2.06                     | 0.85              |
| 2:H:1097:LEU:CD1  | 3:I:1451:ALA:HB2  | 2.06                     | 0.85              |
| 3:N:119:SER:CB    | 3:N:123:LEU:HB2   | 2.05                     | 0.85              |
| 3:N:18:ILE:HG23   | 3:N:518:PRO:HG3   | 1.56                     | 0.85              |
| 1:A:91:ASN:OD1    | 1:A:92:PRO:HD2    | 1.75                     | 0.85              |
| 2:C:1088:LEU:HD23 | 2:C:1092:LEU:HD12 | 1.56                     | 0.85              |
| 2:H:1105:LYS:NZ   | 2:H:1107:ASN:HB2  | 1.90                     | 0.85              |
| 2:M:184:MET:SD    | 2:M:303:PHE:HE2   | 2.00                     | 0.85              |
| 2:M:157:ARG:HH12  | 2:M:217:LEU:HD22  | 1.41                     | 0.85              |
| 2:M:64:LEU:HD22   | 2:M:359:MET:HB2   | 1.54                     | 0.85              |
| 2:M:1046:ALA:HA   | 3:N:1472:ILE:HD11 | 1.58                     | 0.85              |
| 3:N:764:LEU:HD12  | 3:N:765:SER:N     | 1.91                     | 0.85              |
| 3:D:1211:MET:HG2  | 3:D:1212:ALA:N    | 1.91                     | 0.85              |
| 2:H:181:VAL:CG1   | 2:H:182:VAL:H     | 1.86                     | 0.85              |
| 4:J:54:LEU:HD23   | 4:J:58:PRO:HD2    | 1.58                     | 0.85              |
| 2:M:31:GLN:HG3    | 2:M:34:VAL:HG22   | 1.57                     | 0.85              |
| 2:M:987:ILE:HG23  | 3:N:948:THR:CG2   | 2.07                     | 0.85              |
| 3:N:108:VAL:HB    | 3:N:109:PRO:HD3   | 1.59                     | 0.85              |
| 2:C:1105:LYS:NZ   | 2:C:1107:ASN:HB2  | 1.90                     | 0.85              |
| 1:G:62:LEU:HD12   | 1:G:63:HIS:H      | 1.42                     | 0.85              |
| 3:I:182:GLY:HA3   | 3:I:441:ARG:HH11  | 1.41                     | 0.85              |
| 2:M:188:LYS:HG3   | 2:M:188:LYS:O     | 1.73                     | 0.85              |
| 1:A:73:GLU:HB2    | 1:A:78:ILE:HD11   | 1.57                     | 0.85              |
| 3:D:643:GLY:HA3   | 3:D:727:GLN:HB2   | 1.57                     | 0.85              |
| 2:H:1088:LEU:HD23 | 2:H:1092:LEU:HD12 | 1.56                     | 0.85              |
| 2:H:265:ARG:HG2   | 2:H:267:TYR:CG    | 2.10                     | 0.85              |
| 3:I:611:GLN:NE2   | 6:S:9:U:H4'       | 1.92                     | 0.85              |
| 3:D:1133:ARG:HH12 | 7:X:23:ARG:HH12   | 1.24                     | 0.85              |
| 3:D:355:VAL:HG11  | 3:D:385:VAL:HG21  | 1.57                     | 0.85              |
| 3:D:50:PHE:HD2    | 3:D:522:PRO:HD3   | 1.40                     | 0.85              |
| 2:H:408:ARG:HH21  | 2:H:455:LEU:HD11  | 1.39                     | 0.85              |
| 2:M:408:ARG:HH21  | 2:M:455:LEU:HD11  | 1.39                     | 0.85              |
| 2:M:979:THR:HG23  | 2:M:981:GLU:H     | 1.41                     | 0.85              |
| 3:N:1211:MET:HG2  | 3:N:1212:ALA:N    | 1.91                     | 0.85              |
| 2:C:502:PRO:HB2   | 2:C:509:ALA:HB3   | 1.55                     | 0.85              |
| 4:E:25:LYS:HA     | 4:E:28:GLN:NE2    | 1.92                     | 0.85              |
| 3:I:1122:LEU:HD11 | 3:I:1186:VAL:HG23 | 1.58                     | 0.85              |
| 3:I:131:LYS:CG    | 3:I:568:ARG:NE    | 2.39                     | 0.85              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:I:764:LEU:HD12  | 3:I:765:SER:N    | 1.91                     | 0.85              |
| 3:I:771:SER:HB2   | 3:I:778:LEU:HD13 | 1.59                     | 0.85              |
| 2:M:958:THR:HG23  | 2:M:961:GLU:CG   | 2.07                     | 0.85              |
| 3:N:481:MET:HE3   | 3:N:493:ARG:HA   | 1.59                     | 0.85              |
| 3:D:996:TRP:CD2   | 3:D:1056:PRO:HG2 | 2.11                     | 0.85              |
| 3:D:172:PRO:CG    | 3:D:175:VAL:HG21 | 2.07                     | 0.85              |
| 2:H:342:ASP:O     | 2:H:345:ARG:HG2  | 1.77                     | 0.85              |
| 3:I:1468:LEU:HD22 | 3:I:1470:ARG:HB2 | 1.57                     | 0.85              |
| 3:I:813:LEU:HD12  | 3:I:814:ALA:N    | 1.92                     | 0.85              |
| 1:K:156:HIS:HD2   | 1:K:157:GLY:H    | 1.23                     | 0.85              |
| 2:M:317:VAL:CG1   | 2:M:320:HIS:NE2  | 2.39                     | 0.85              |
| 3:N:1031:ASN:HD21 | 7:Z:32:ILE:CG2   | 1.90                     | 0.85              |
| 3:N:813:LEU:O     | 3:N:817:GLU:HB2  | 1.77                     | 0.85              |
| 2:C:1056:LYS:HD3  | 3:D:623:VAL:CG1  | 2.07                     | 0.85              |
| 2:C:170:PRO:CD    | 2:C:263:ASP:HB3  | 2.07                     | 0.85              |
| 3:D:139:GLY:CA    | 3:D:162:ARG:HH22 | 1.85                     | 0.85              |
| 3:I:483:HIS:HB2   | 3:I:484:PRO:HD3  | 1.59                     | 0.85              |
| 3:N:87:ARG:O      | 3:N:521:PRO:CB   | 2.24                     | 0.85              |
| 2:C:676:ILE:HG21  | 2:C:988:VAL:HG13 | 1.58                     | 0.84              |
| 3:D:108:VAL:HB    | 3:D:109:PRO:HD3  | 1.58                     | 0.84              |
| 3:N:1037:GLN:HG2  | 3:N:1042:ARG:HB3 | 1.59                     | 0.84              |
| 2:C:170:PRO:HD2   | 2:C:263:ASP:HB3  | 1.59                     | 0.84              |
| 2:C:958:THR:HG23  | 2:C:961:GLU:CG   | 2.07                     | 0.84              |
| 3:D:157:GLU:O     | 3:D:161:LEU:HD11 | 1.76                     | 0.84              |
| 2:H:242:LEU:O     | 2:H:243:ARG:HG3  | 1.77                     | 0.84              |
| 2:H:678:PRO:HG2   | 3:I:947:ILE:HD11 | 1.58                     | 0.84              |
| 3:I:810:GLU:O     | 3:I:813:LEU:HG   | 1.77                     | 0.84              |
| 2:M:305:PRO:HA    | 2:M:308:ARG:HB3  | 1.58                     | 0.84              |
| 2:M:399:ASN:ND2   | 2:M:568:ALA:HB3  | 1.93                     | 0.84              |
| 2:M:564:MET:CE    | 2:M:846:LYS:CD   | 2.55                     | 0.84              |
| 2:M:78:PHE:HB3    | 2:M:79:PRO:HD2   | 1.58                     | 0.84              |
| 7:Z:119:ILE:CG1   | 7:Z:125:MET:HE1  | 2.00                     | 0.84              |
| 1:A:39:PRO:HG3    | 1:B:39:PRO:CG    | 2.08                     | 0.84              |
| 2:H:197:LEU:HD13  | 2:H:207:LEU:HD11 | 1.58                     | 0.84              |
| 2:H:383:ARG:HH11  | 2:H:383:ARG:HB2  | 1.41                     | 0.84              |
| 2:H:572:ILE:HD12  | 2:H:573:ARG:N    | 1.92                     | 0.84              |
| 3:I:1288:GLU:O    | 3:I:1289:LYS:HG3 | 1.76                     | 0.84              |
| 3:I:465:LEU:HD13  | 3:I:510:GLU:HA   | 1.59                     | 0.84              |
| 1:L:27:PRO:O      | 1:L:28:LEU:HD23  | 1.76                     | 0.84              |
| 2:M:383:ARG:HH11  | 2:M:383:ARG:HB2  | 1.42                     | 0.84              |
| 3:N:169:TYR:OH    | 3:N:198:ARG:HG3  | 1.76                     | 0.84              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:643:GLY:HA3   | 3:N:727:GLN:HB2  | 1.58                     | 0.84              |
| 1:B:187:GLY:HA3   | 3:D:685:ASP:HB2  | 1.58                     | 0.84              |
| 2:C:305:PRO:HG3   | 2:C:308:ARG:NH2  | 1.91                     | 0.84              |
| 3:D:764:LEU:HD12  | 3:D:765:SER:N    | 1.91                     | 0.84              |
| 2:H:571:LEU:HD11  | 2:H:701:THR:N    | 1.92                     | 0.84              |
| 2:H:979:THR:HG23  | 2:H:981:GLU:H    | 1.41                     | 0.84              |
| 3:I:1037:GLN:HG2  | 3:I:1042:ARG:HB3 | 1.59                     | 0.84              |
| 3:I:1209:LEU:HD21 | 4:J:16:LYS:NZ    | 1.90                     | 0.84              |
| 2:M:139:GLN:OE1   | 2:M:418:LEU:HD22 | 1.77                     | 0.84              |
| 2:C:304:LEU:CD2   | 2:C:305:PRO:HD3  | 2.06                     | 0.84              |
| 3:D:160:GLU:OE2   | 3:D:397:LYS:HD2  | 1.78                     | 0.84              |
| 3:D:174:GLY:H     | 3:D:209:ARG:NH1  | 1.76                     | 0.84              |
| 1:G:27:PRO:O      | 1:G:28:LEU:HD23  | 1.76                     | 0.84              |
| 3:I:643:GLY:HA3   | 3:I:727:GLN:HB2  | 1.57                     | 0.84              |
| 1:K:42:ARG:HH12   | 1:L:34:VAL:CB    | 1.89                     | 0.84              |
| 2:M:503:LEU:HD23  | 2:M:507:ARG:O    | 1.76                     | 0.84              |
| 2:M:576:ALA:HB3   | 2:M:900:ARG:NH1  | 1.92                     | 0.84              |
| 4:O:6:ILE:HD11    | 4:O:10:PHE:CZ    | 2.12                     | 0.84              |
| 2:C:198:ARG:NH1   | 2:C:228:ALA:O    | 2.10                     | 0.84              |
| 3:I:554:LEU:HD11  | 3:I:558:LEU:HD21 | 1.58                     | 0.84              |
| 3:D:31:THR:CG2    | 3:D:545:ARG:HD3  | 2.08                     | 0.84              |
| 3:D:771:SER:HB2   | 3:D:778:LEU:HD13 | 1.59                     | 0.84              |
| 3:D:813:LEU:HD12  | 3:D:814:ALA:N    | 1.92                     | 0.84              |
| 3:I:108:VAL:HB    | 3:I:109:PRO:HD3  | 1.58                     | 0.84              |
| 3:I:1114:THR:CG2  | 3:I:1195:GLN:HB3 | 2.08                     | 0.84              |
| 3:N:1103:HIS:HD2  | 3:N:1463:LYS:HB2 | 1.41                     | 0.84              |
| 1:A:153:ALA:HA    | 1:A:156:HIS:NE2  | 1.93                     | 0.84              |
| 2:C:1098:ASP:HB3  | 3:D:11:ALA:O     | 1.76                     | 0.84              |
| 3:D:96:ALA:HB3    | 3:D:554:LEU:HD23 | 1.59                     | 0.84              |
| 2:H:395:LYS:O     | 2:H:397:GLU:HG3  | 1.78                     | 0.84              |
| 2:H:958:THR:HG23  | 2:H:961:GLU:CG   | 2.07                     | 0.84              |
| 3:I:809:PRO:HB2   | 3:I:812:ALA:CB   | 2.08                     | 0.84              |
| 3:D:813:LEU:O     | 3:D:817:GLU:HB2  | 1.77                     | 0.84              |
| 3:D:987:GLU:OE1   | 7:X:120:SER:HB2  | 1.78                     | 0.84              |
| 2:H:182:VAL:CG1   | 2:H:193:LEU:CG   | 2.56                     | 0.84              |
| 2:H:261:ILE:CD1   | 2:H:262:ALA:H    | 1.90                     | 0.84              |
| 3:I:14:SER:O      | 3:I:18:ILE:HG12  | 1.76                     | 0.84              |
| 2:M:1089:VAL:O    | 2:M:1093:GLN:HG2 | 1.78                     | 0.84              |
| 3:N:465:LEU:HD13  | 3:N:510:GLU:HA   | 1.59                     | 0.84              |
| 7:X:111:ASN:OD1   | 7:X:113:LEU:HD12 | 1.76                     | 0.84              |
| 1:F:221:HIS:NE2   | 1:G:32:PHE:CE2   | 2.46                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:218:VAL:HG13  | 2:H:221:LEU:HD11  | 1.57                     | 0.84              |
| 2:H:950:LEU:HB3   | 2:H:952:LEU:HD23  | 1.57                     | 0.84              |
| 3:I:142:LEU:CB    | 3:I:145:VAL:O     | 2.24                     | 0.84              |
| 1:K:25:LEU:CD2    | 1:L:225:PHE:CE2   | 2.61                     | 0.84              |
| 2:M:334:ARG:HH21  | 2:M:339:LEU:HD23  | 1.42                     | 0.84              |
| 2:M:675:ALA:CA    | 2:M:989:VAL:HG12  | 2.07                     | 0.84              |
| 2:M:950:LEU:HB3   | 2:M:952:LEU:HD23  | 1.58                     | 0.84              |
| 3:N:813:LEU:HD12  | 3:N:814:ALA:N     | 1.92                     | 0.84              |
| 3:D:181:ASP:HA    | 3:D:205:TYR:CD2   | 2.13                     | 0.83              |
| 3:D:465:LEU:HD13  | 3:D:510:GLU:HA    | 1.59                     | 0.83              |
| 2:M:1005:MET:SD   | 3:N:724:GLN:OE1   | 2.36                     | 0.83              |
| 3:N:1029:ARG:CB   | 3:N:1029:ARG:HH11 | 1.90                     | 0.83              |
| 3:N:956:ILE:HD11  | 3:N:1062:ARG:CB   | 2.08                     | 0.83              |
| 2:C:501:THR:HG22  | 2:C:513:VAL:HG13  | 1.61                     | 0.83              |
| 1:F:153:ALA:HA    | 1:F:156:HIS:NE2   | 1.93                     | 0.83              |
| 3:I:28:LYS:CD     | 3:I:29:PRO:HD2    | 2.08                     | 0.83              |
| 1:B:27:PRO:O      | 1:B:28:LEU:HD23   | 1.76                     | 0.83              |
| 2:C:579:VAL:HG11  | 2:C:887:GLU:HG3   | 1.59                     | 0.83              |
| 3:I:1209:LEU:HD21 | 4:J:16:LYS:CE     | 2.07                     | 0.83              |
| 2:H:1052:MET:SD   | 3:I:623:VAL:CG1   | 2.66                     | 0.83              |
| 1:L:41:ARG:HG3    | 1:L:177:VAL:CG2   | 2.07                     | 0.83              |
| 3:I:1359:GLN:HE22 | 7:Y:52:LYS:HD3    | 1.43                     | 0.83              |
| 3:D:810:GLU:O     | 3:D:813:LEU:HG    | 1.77                     | 0.83              |
| 2:H:572:ILE:HG23  | 2:H:703:ILE:HD11  | 1.60                     | 0.83              |
| 2:H:831:ARG:HD2   | 2:H:1000:MET:SD   | 2.19                     | 0.83              |
| 3:I:101:HIS:HD1   | 3:I:103:TRP:HB2   | 1.42                     | 0.83              |
| 3:I:1235:GLN:NE2  | 7:Y:37:MET:HG3    | 1.93                     | 0.83              |
| 2:M:111:ASP:HB3   | 2:M:369:PRO:CG    | 2.07                     | 0.83              |
| 3:N:1359:GLN:O    | 7:Z:37:MET:SD     | 2.36                     | 0.83              |
| 3:N:771:SER:HB2   | 3:N:778:LEU:HD13  | 1.59                     | 0.83              |
| 3:N:984:THR:HG22  | 3:N:987:GLU:CG    | 2.08                     | 0.83              |
| 7:Z:111:ASN:OD1   | 7:Z:113:LEU:HD12  | 1.76                     | 0.83              |
| 2:C:122:THR:HB    | 2:C:124:ASP:OD1   | 1.78                     | 0.83              |
| 2:C:557:ARG:NH1   | 2:C:560:MET:HG3   | 1.93                     | 0.83              |
| 3:D:1387:SER:HB3  | 3:D:1391:GLU:OE2  | 1.77                     | 0.83              |
| 2:C:1085:PHE:HE2  | 3:D:1468:LEU:HG   | 1.44                     | 0.83              |
| 3:D:153:LEU:HD13  | 3:D:158:TYR:HB2   | 1.60                     | 0.83              |
| 2:H:557:ARG:NH1   | 2:H:560:MET:HG3   | 1.93                     | 0.83              |
| 3:I:160:GLU:HG2   | 3:I:165:LYS:CG    | 2.08                     | 0.83              |
| 3:I:997:THR:HG21  | 7:Y:61:ARG:CZ     | 2.09                     | 0.83              |
| 2:M:368:THR:HB    | 2:M:369:PRO:HD2   | 1.60                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:166:GLN:HB3   | 2:H:210:GLU:HG3   | 1.60                     | 0.83              |
| 1:F:42:ARG:HH12   | 1:G:34:VAL:CB     | 1.90                     | 0.83              |
| 3:I:1025:GLN:HE21 | 3:I:1025:GLN:HA   | 1.43                     | 0.83              |
| 3:I:1256:LEU:O    | 3:I:1260:ILE:HG13 | 1.79                     | 0.83              |
| 1:L:86:VAL:CG1    | 1:L:124:ASN:HB2   | 2.08                     | 0.83              |
| 3:N:421:LEU:HD22  | 3:N:444:VAL:HG11  | 1.58                     | 0.83              |
| 3:N:581:LEU:H     | 3:N:581:LEU:HD23  | 1.43                     | 0.83              |
| 1:B:44:LEU:HA     | 1:B:48:ILE:HD13   | 1.61                     | 0.83              |
| 2:C:195:LEU:O     | 2:C:199:VAL:HG23  | 1.79                     | 0.83              |
| 2:C:572:ILE:HD12  | 2:C:573:ARG:N     | 1.92                     | 0.83              |
| 3:D:637:LEU:HD21  | 3:D:642:CYS:HA    | 1.61                     | 0.83              |
| 2:C:1004:LYS:HD2  | 3:D:744:GLN:HE22  | 1.04                     | 0.83              |
| 3:N:1007:VAL:HG11 | 3:N:1039:CYS:HB2  | 1.59                     | 0.83              |
| 3:D:207:PHE:O     | 3:D:390:PRO:HA    | 1.79                     | 0.83              |
| 2:H:193:LEU:N     | 2:H:193:LEU:CD1   | 2.30                     | 0.83              |
| 2:H:196:LEU:O     | 2:H:200:LEU:HG    | 1.78                     | 0.83              |
| 1:L:133:GLU:HG3   | 1:L:134:GLU:H     | 1.40                     | 0.83              |
| 3:I:991:GLN:HE22  | 7:Y:112:VAL:CB    | 1.91                     | 0.83              |
| 2:H:170:PRO:HD3   | 2:H:263:ASP:CB    | 2.08                     | 0.83              |
| 2:H:182:VAL:CB    | 2:H:193:LEU:HD11  | 2.08                     | 0.83              |
| 2:H:258:TYR:CE2   | 2:H:290:LEU:HD11  | 2.14                     | 0.83              |
| 2:M:172:ILE:H     | 2:M:172:ILE:HD12  | 1.43                     | 0.83              |
| 2:M:557:ARG:NH1   | 2:M:560:MET:HG3   | 1.94                     | 0.83              |
| 2:M:572:ILE:HD12  | 2:M:573:ARG:N     | 1.92                     | 0.83              |
| 2:M:579:VAL:HG11  | 2:M:887:GLU:HG3   | 1.60                     | 0.83              |
| 3:N:810:GLU:O     | 3:N:813:LEU:HG    | 1.77                     | 0.83              |
| 1:B:42:ARG:HH11   | 1:B:42:ARG:HG2    | 1.44                     | 0.83              |
| 2:C:1099:VAL:CG2  | 3:D:10:ILE:HG12   | 2.09                     | 0.83              |
| 3:D:483:HIS:HB2   | 3:D:484:PRO:HD3   | 1.59                     | 0.83              |
| 2:H:502:PRO:HB2   | 2:H:509:ALA:HB3   | 1.59                     | 0.83              |
| 1:G:185:ARG:HD3   | 3:I:692:GLU:OE2   | 1.79                     | 0.83              |
| 2:M:69:LEU:HD11   | 2:M:99:GLN:CG     | 2.09                     | 0.83              |
| 3:N:1123:PHE:HE2  | 3:N:1184:GLN:HA   | 1.44                     | 0.83              |
| 3:N:637:LEU:HD21  | 3:N:642:CYS:HA    | 1.61                     | 0.83              |
| 7:Y:57:ARG:NH2    | 7:Y:57:ARG:HB2    | 1.94                     | 0.83              |
| 7:Z:115:THR:HB    | 7:Z:116:PRO:HD3   | 1.60                     | 0.83              |
| 3:D:1099:VAL:O    | 3:D:1103:HIS:HB3  | 1.78                     | 0.82              |
| 3:D:481:MET:SD    | 3:D:1388:ARG:HD3  | 2.19                     | 0.82              |
| 3:I:432:TYR:HB3   | 3:I:450:TYR:HB2   | 1.59                     | 0.82              |
| 3:N:28:LYS:CD     | 3:N:29:PRO:HD2    | 2.08                     | 0.82              |
| 2:H:92:ALA:HB2    | 2:H:120:LEU:HD11  | 1.60                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:675:ALA:HA    | 2:M:989:VAL:CG1   | 2.09                     | 0.82              |
| 3:N:1106:VAL:HG12 | 3:N:1107:VAL:H    | 1.43                     | 0.82              |
| 2:M:1097:LEU:HD11 | 3:N:1451:ALA:CB   | 2.07                     | 0.82              |
| 3:N:189:GLN:NE2   | 3:N:190:GLU:H     | 1.77                     | 0.82              |
| 7:X:115:THR:HB    | 7:X:116:PRO:HD3   | 1.60                     | 0.82              |
| 3:I:997:THR:HG21  | 7:Y:61:ARG:NH2    | 1.94                     | 0.82              |
| 2:C:1081:VAL:CG1  | 2:C:1085:PHE:HB3  | 2.09                     | 0.82              |
| 2:C:987:ILE:HG23  | 3:D:948:THR:CG2   | 2.09                     | 0.82              |
| 3:D:620:GLY:O     | 3:D:621:LYS:HG2   | 1.78                     | 0.82              |
| 3:D:984:THR:HG22  | 3:D:987:GLU:CG    | 2.08                     | 0.82              |
| 1:G:133:GLU:HG3   | 1:G:134:GLU:H     | 1.45                     | 0.82              |
| 2:H:1081:VAL:CG1  | 2:H:1085:PHE:HB3  | 2.10                     | 0.82              |
| 2:H:500:ASN:HD22  | 2:H:500:ASN:N     | 1.76                     | 0.82              |
| 3:I:513:ILE:HD12  | 3:I:513:ILE:O     | 1.80                     | 0.82              |
| 3:I:1476:THR:HG23 | 4:J:21:VAL:HG22   | 1.59                     | 0.82              |
| 3:D:1037:GLN:HG2  | 3:D:1042:ARG:HB3  | 1.59                     | 0.82              |
| 3:I:581:LEU:H     | 3:I:581:LEU:HD23  | 1.43                     | 0.82              |
| 2:M:162:ILE:HD11  | 2:M:306:THR:HG21  | 1.61                     | 0.82              |
| 2:M:333:ILE:N     | 2:M:333:ILE:HD12  | 1.95                     | 0.82              |
| 3:N:107:ASP:OD1   | 3:N:1444:THR:HG22 | 1.79                     | 0.82              |
| 3:N:483:HIS:HB2   | 3:N:484:PRO:HD3   | 1.59                     | 0.82              |
| 2:M:1030:GLN:HE21 | 3:N:628:ARG:HD3   | 1.44                     | 0.82              |
| 2:M:1090:LYS:HE3  | 3:N:90:MET:HG3    | 1.57                     | 0.82              |
| 3:N:970:LYS:HD3   | 7:Z:113:LEU:CD2   | 2.09                     | 0.82              |
| 2:C:140:ILE:HD11  | 2:C:412:ALA:HA    | 1.62                     | 0.82              |
| 3:D:164:GLY:CA    | 3:D:449:SER:HB3   | 2.09                     | 0.82              |
| 2:M:111:ASP:CB    | 2:M:369:PRO:CG    | 2.56                     | 0.82              |
| 1:A:39:PRO:HG3    | 1:B:39:PRO:HG2    | 1.60                     | 0.82              |
| 1:B:62:LEU:CD1    | 1:B:63:HIS:H      | 1.91                     | 0.82              |
| 1:F:73:GLU:HB2    | 1:F:78:ILE:HD11   | 1.61                     | 0.82              |
| 2:H:1072:LYS:O    | 3:I:659:LYS:HE2   | 1.80                     | 0.82              |
| 3:I:584:ASN:ND2   | 3:I:590:PRO:HD2   | 1.94                     | 0.82              |
| 3:I:984:THR:HG22  | 3:I:987:GLU:CG    | 2.08                     | 0.82              |
| 2:M:52:PHE:HZ     | 2:M:98:LEU:CG     | 1.93                     | 0.82              |
| 3:N:1292:VAL:HG23 | 3:N:1305:LEU:HG   | 1.60                     | 0.82              |
| 3:N:977:ALA:HB1   | 3:N:983:LEU:HD21  | 1.62                     | 0.82              |
| 3:D:1137:ARG:HH11 | 3:D:1137:ARG:HB2  | 1.45                     | 0.82              |
| 2:H:1089:VAL:O    | 2:H:1093:GLN:HG2  | 1.79                     | 0.82              |
| 2:H:1103:ASP:OD2  | 3:I:2:LYS:CA      | 2.22                     | 0.82              |
| 2:H:274:ARG:HD2   | 2:H:285:LEU:HD22  | 1.59                     | 0.82              |
| 2:H:351:LEU:HD12  | 2:H:374:ASN:ND2   | 1.95                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:637:LEU:HD21  | 3:I:642:CYS:HA    | 1.61                     | 0.82              |
| 2:C:1089:VAL:O    | 2:C:1093:GLN:HG2  | 1.78                     | 0.82              |
| 2:C:88:LEU:HD13   | 2:C:89:THR:N      | 1.95                     | 0.82              |
| 2:H:1095:LEU:HD12 | 2:H:1097:LEU:H    | 1.45                     | 0.82              |
| 2:H:265:ARG:HB3   | 2:H:267:TYR:CZ    | 2.15                     | 0.82              |
| 2:H:579:VAL:HG11  | 2:H:887:GLU:HG3   | 1.62                     | 0.82              |
| 2:M:274:ARG:CD    | 2:M:285:LEU:HD22  | 2.10                     | 0.82              |
| 2:M:317:VAL:HG13  | 2:M:320:HIS:CE1   | 2.15                     | 0.82              |
| 2:M:578:VAL:HG23  | 2:M:579:VAL:HG12  | 1.62                     | 0.82              |
| 2:M:850:ALA:HA    | 3:N:632:VAL:CG1   | 2.10                     | 0.82              |
| 3:N:133:ILE:HG22  | 3:N:134:VAL:H     | 1.45                     | 0.82              |
| 7:X:134:VAL:HG23  | 7:X:154:ILE:HG13  | 1.61                     | 0.82              |
| 1:B:133:GLU:HG3   | 1:B:134:GLU:H     | 1.44                     | 0.81              |
| 2:H:578:VAL:HG23  | 2:H:579:VAL:HG12  | 1.62                     | 0.81              |
| 2:M:111:ASP:HB3   | 2:M:369:PRO:HG2   | 1.62                     | 0.81              |
| 2:M:557:ARG:HG2   | 2:M:881:ASN:ND2   | 1.94                     | 0.81              |
| 3:N:111:LYS:HG2   | 3:N:1452:ILE:HD11 | 1.61                     | 0.81              |
| 3:N:142:LEU:HB3   | 3:N:144:GLY:H     | 1.45                     | 0.81              |
| 3:N:814:ALA:HB1   | 3:N:818:ARG:HH21  | 1.45                     | 0.81              |
| 2:H:188:LYS:NZ    | 2:H:188:LYS:CB    | 2.43                     | 0.81              |
| 2:M:71:TYR:HA     | 2:M:96:ALA:CB     | 2.10                     | 0.81              |
| 2:M:1004:LYS:O    | 3:N:629:SER:HA    | 1.80                     | 0.81              |
| 2:C:139:GLN:HE22  | 2:C:415:PRO:HD3   | 1.43                     | 0.81              |
| 2:C:282:GLY:O     | 2:C:283:ILE:HD13  | 1.80                     | 0.81              |
| 3:D:126:VAL:HG12  | 3:D:132:TYR:HB2   | 1.59                     | 0.81              |
| 3:D:513:ILE:O     | 3:D:513:ILE:HD12  | 1.80                     | 0.81              |
| 1:K:153:ALA:HA    | 1:K:156:HIS:NE2   | 1.93                     | 0.81              |
| 2:M:516:ARG:NE    | 3:N:1068:LEU:HD22 | 1.95                     | 0.81              |
| 3:N:520:LEU:HD23  | 3:N:525:ARG:HD2   | 1.62                     | 0.81              |
| 1:B:187:GLY:HA2   | 3:D:685:ASP:HA    | 1.62                     | 0.81              |
| 2:H:148:PHE:CE1   | 2:H:309:TYR:HD1   | 1.98                     | 0.81              |
| 2:H:182:VAL:C     | 2:H:193:LEU:HD11  | 1.99                     | 0.81              |
| 3:I:1106:VAL:HG12 | 3:I:1107:VAL:H    | 1.43                     | 0.81              |
| 3:I:166:GLN:HE22  | 3:I:394:LEU:HD12  | 1.46                     | 0.81              |
| 3:I:977:ALA:HB1   | 3:I:983:LEU:HD21  | 1.62                     | 0.81              |
| 1:L:76:VAL:HB     | 3:N:872:ARG:NH1   | 1.94                     | 0.81              |
| 2:M:1081:VAL:CG1  | 2:M:1085:PHE:HB3  | 2.09                     | 0.81              |
| 3:D:989:TYR:CE2   | 3:D:993:LEU:HD11  | 2.16                     | 0.81              |
| 4:E:54:LEU:HD23   | 4:E:58:PRO:HD2    | 1.63                     | 0.81              |
| 3:I:205:TYR:HB2   | 3:I:393:ILE:HG13  | 1.62                     | 0.81              |
| 2:M:12:VAL:HG11   | 2:M:472:ARG:HD3   | 1.61                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:98:LEU:HD11   | 2:C:113:VAL:HG22  | 1.63                     | 0.81              |
| 3:D:982:PHE:HE1   | 7:X:100:LEU:HD21  | 1.43                     | 0.81              |
| 1:G:190:THR:CB    | 3:I:722:GLU:OE1   | 2.29                     | 0.81              |
| 3:I:1264:GLU:OE2  | 3:I:1424:VAL:HG13 | 1.81                     | 0.81              |
| 1:K:156:HIS:CD2   | 1:K:157:GLY:H     | 1.99                     | 0.81              |
| 1:L:59:GLU:HG3    | 1:L:60:ASP:H      | 1.45                     | 0.81              |
| 3:N:1283:ILE:HD12 | 3:N:1315:ASP:OD2  | 1.80                     | 0.81              |
| 3:N:1288:GLU:O    | 3:N:1307:LYS:HE2  | 1.79                     | 0.81              |
| 3:N:1297:GLU:HG2  | 3:N:1298:GLY:N    | 1.94                     | 0.81              |
| 2:C:1074:GLU:HG2  | 2:C:1075:ASP:N    | 1.96                     | 0.81              |
| 1:F:156:HIS:CD2   | 1:F:157:GLY:H     | 1.98                     | 0.81              |
| 2:H:3:ILE:HA      | 2:H:900:ARG:O     | 1.81                     | 0.81              |
| 2:M:70:GLU:HB2    | 2:M:97:ARG:NH2    | 1.94                     | 0.81              |
| 2:C:24:GLU:OE2    | 2:C:27:ARG:HD3    | 1.81                     | 0.81              |
| 2:C:473:ARG:HH11  | 2:C:473:ARG:HG2   | 1.45                     | 0.81              |
| 2:C:576:ALA:HB3   | 2:C:900:ARG:HH11  | 1.43                     | 0.81              |
| 4:J:54:LEU:CG     | 4:J:58:PRO:HG2    | 2.11                     | 0.81              |
| 2:M:193:LEU:O     | 2:M:197:LEU:HG    | 1.80                     | 0.81              |
| 3:D:18:ILE:CG2    | 3:D:518:PRO:HG3   | 2.11                     | 0.81              |
| 1:G:42:ARG:HH11   | 1:G:42:ARG:HG2    | 1.43                     | 0.81              |
| 3:I:99:ALA:O      | 3:I:514:LEU:N     | 2.14                     | 0.81              |
| 1:K:206:THR:HG22  | 1:K:209:GLU:H     | 1.46                     | 0.81              |
| 3:N:1264:GLU:OE2  | 3:N:1424:VAL:HG13 | 1.80                     | 0.81              |
| 2:C:408:ARG:HH21  | 2:C:455:LEU:HD11  | 1.45                     | 0.81              |
| 3:D:482:LYS:HE2   | 3:D:1388:ARG:NH2  | 1.96                     | 0.81              |
| 3:D:160:GLU:HG2   | 3:D:165:LYS:HB3   | 1.61                     | 0.81              |
| 2:H:109:LYS:HD3   | 2:H:368:THR:CG2   | 2.10                     | 0.81              |
| 3:I:176:ASP:HA    | 3:I:390:PRO:HD2   | 1.61                     | 0.81              |
| 3:I:408:GLU:HG3   | 3:I:409:VAL:N     | 1.92                     | 0.81              |
| 2:H:1004:LYS:CD   | 3:I:744:GLN:NE2   | 2.37                     | 0.81              |
| 2:M:1032:PHE:O    | 2:M:1036:GLU:HB2  | 1.80                     | 0.81              |
| 3:N:1443:THR:O    | 3:N:1447:LEU:HD13 | 1.80                     | 0.81              |
| 3:N:86:ARG:NE     | 3:N:523:ASP:OD2   | 2.12                     | 0.81              |
| 1:A:39:PRO:O      | 1:A:43:ILE:HG13   | 1.81                     | 0.81              |
| 1:B:24:VAL:HG22   | 1:B:196:THR:HG22  | 1.62                     | 0.81              |
| 2:C:588:VAL:HG21  | 2:C:664:GLY:O     | 1.81                     | 0.81              |
| 3:D:170:PRO:HB2   | 2:H:318:PRO:O     | 1.80                     | 0.81              |
| 2:H:364:GLU:O     | 2:H:367:LEU:HG    | 1.81                     | 0.81              |
| 3:I:1137:ARG:O    | 3:I:1141:GLU:HG3  | 1.81                     | 0.81              |
| 2:M:1012:PRO:HD2  | 2:M:1026:GLN:HG2  | 1.63                     | 0.81              |
| 3:N:996:TRP:O     | 3:N:1000:THR:HG22 | 1.81                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:206:THR:HG22  | 1:A:209:GLU:H     | 1.46                     | 0.80              |
| 2:C:325:ILE:HD12  | 2:C:325:ILE:N     | 1.95                     | 0.80              |
| 3:D:28:LYS:CG     | 3:D:29:PRO:HD2    | 2.10                     | 0.80              |
| 3:I:680:GLN:O     | 3:I:683:ILE:HD12  | 1.80                     | 0.80              |
| 3:N:1000:THR:O    | 3:N:1003:VAL:HG12 | 1.81                     | 0.80              |
| 3:N:513:ILE:HD12  | 3:N:513:ILE:O     | 1.80                     | 0.80              |
| 7:X:139:SER:HB3   | 7:X:148:GLU:HG3   | 1.62                     | 0.80              |
| 7:Z:83:ILE:HD11   | 7:Z:151:VAL:HG11  | 1.61                     | 0.80              |
| 3:D:15:PRO:CB     | 3:D:515:GLU:OE1   | 2.29                     | 0.80              |
| 2:H:404:LEU:HA    | 2:H:407:LYS:HD3   | 1.63                     | 0.80              |
| 2:H:689:VAL:HB    | 2:H:870:ILE:HG12  | 1.63                     | 0.80              |
| 3:D:1264:GLU:OE2  | 3:D:1424:VAL:HG13 | 1.80                     | 0.80              |
| 1:G:112:ARG:HD3   | 1:G:125:PRO:CB    | 2.12                     | 0.80              |
| 2:H:309:TYR:CD1   | 2:H:313:LEU:HD11  | 2.16                     | 0.80              |
| 2:H:668:LEU:N     | 2:H:668:LEU:HD12  | 1.96                     | 0.80              |
| 2:M:1095:LEU:HD12 | 2:M:1097:LEU:H    | 1.45                     | 0.80              |
| 2:H:135:VAL:HG11  | 2:H:407:LYS:HA    | 1.61                     | 0.80              |
| 2:H:726:ILE:HG13  | 2:H:734:LEU:HD11  | 1.62                     | 0.80              |
| 1:G:80:LEU:HD21   | 3:I:867:ARG:HB2   | 1.62                     | 0.80              |
| 1:K:39:PRO:O      | 1:K:43:ILE:HG13   | 1.81                     | 0.80              |
| 1:L:44:LEU:HA     | 1:L:48:ILE:HD13   | 1.63                     | 0.80              |
| 1:A:156:HIS:CD2   | 1:A:157:GLY:H     | 1.98                     | 0.80              |
| 2:C:1082:PRO:HG2  | 3:D:1469:GLY:HA3  | 1.61                     | 0.80              |
| 2:H:2:GLU:O       | 2:H:899:GLN:HB2   | 1.80                     | 0.80              |
| 1:K:25:LEU:HD22   | 1:L:225:PHE:CD2   | 2.17                     | 0.80              |
| 2:M:274:ARG:HD2   | 2:M:285:LEU:CD2   | 2.11                     | 0.80              |
| 2:M:545:ASN:HB3   | 2:M:583:LEU:HD22  | 1.64                     | 0.80              |
| 2:M:70:GLU:CB     | 2:M:97:ARG:HH21   | 1.92                     | 0.80              |
| 3:N:434:ARG:O     | 3:N:447:VAL:HG22  | 1.79                     | 0.80              |
| 3:N:650:LEU:HD13  | 3:N:688:TRP:HZ3   | 1.47                     | 0.80              |
| 2:C:571:LEU:HD11  | 2:C:701:THR:N     | 1.96                     | 0.80              |
| 2:C:758:ARG:HB3   | 2:C:788:THR:O     | 1.82                     | 0.80              |
| 2:H:657:ASP:OD1   | 2:H:662:GLU:HA    | 1.82                     | 0.80              |
| 3:I:1256:LEU:HG   | 3:I:1260:ILE:HD11 | 1.63                     | 0.80              |
| 3:I:989:TYR:CE2   | 3:I:993:LEU:HD11  | 2.16                     | 0.80              |
| 2:M:1031:ARG:HH21 | 3:N:621:LYS:HZ2   | 1.27                     | 0.80              |
| 2:M:292:ARG:HG2   | 2:M:299:LYS:HB2   | 1.64                     | 0.80              |
| 2:M:676:ILE:HG22  | 2:M:988:VAL:O     | 1.80                     | 0.80              |
| 3:N:989:TYR:CE2   | 3:N:993:LEU:HD11  | 2.16                     | 0.80              |
| 2:C:657:ASP:OD1   | 2:C:662:GLU:HA    | 1.81                     | 0.80              |
| 2:C:668:LEU:HD12  | 2:C:668:LEU:N     | 1.96                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:188:LYS:HG3   | 2:H:188:LYS:O     | 1.79                     | 0.80              |
| 2:M:243:ARG:CB    | 2:M:244:PRO:HD2   | 1.98                     | 0.80              |
| 2:M:399:ASN:OD1   | 2:M:402:SER:HB2   | 1.81                     | 0.80              |
| 2:M:657:ASP:OD1   | 2:M:662:GLU:HA    | 1.82                     | 0.80              |
| 3:D:209:ARG:HB3   | 3:D:389:GLU:HB3   | 1.63                     | 0.80              |
| 3:D:9:ARG:HD2     | 3:D:1456:LYS:HE2  | 1.64                     | 0.80              |
| 2:H:758:ARG:HB3   | 2:H:788:THR:O     | 1.82                     | 0.80              |
| 3:I:1468:LEU:HD13 | 3:I:1470:ARG:HE   | 1.46                     | 0.80              |
| 3:I:204:LEU:HD11  | 3:I:441:ARG:HH22  | 1.46                     | 0.80              |
| 3:I:400:VAL:HG13  | 3:I:443:VAL:HG21  | 1.64                     | 0.80              |
| 3:I:877:PRO:O     | 3:I:880:ILE:HG22  | 1.81                     | 0.80              |
| 3:I:89:ARG:O      | 3:I:521:PRO:CG    | 2.30                     | 0.80              |
| 3:N:1112:CYS:HB2  | 3:N:1195:GLN:HG2  | 1.64                     | 0.80              |
| 2:C:73:LEU:HB2    | 2:C:93:PRO:O      | 1.81                     | 0.80              |
| 3:D:1133:ARG:HH12 | 7:X:23:ARG:NH1    | 1.80                     | 0.80              |
| 3:D:877:PRO:O     | 3:D:880:ILE:HG22  | 1.81                     | 0.80              |
| 3:I:996:TRP:O     | 3:I:1000:THR:HG22 | 1.81                     | 0.80              |
| 3:I:134:VAL:HG21  | 3:I:460:ALA:CB    | 2.12                     | 0.80              |
| 3:I:1472:ILE:HD12 | 3:I:1472:ILE:H    | 1.47                     | 0.80              |
| 1:L:24:VAL:HG22   | 1:L:196:THR:HG22  | 1.61                     | 0.80              |
| 2:M:115:LEU:CD2   | 2:M:115:LEU:H     | 1.94                     | 0.80              |
| 2:M:334:ARG:NH2   | 2:M:339:LEU:HD23  | 1.97                     | 0.80              |
| 2:M:668:LEU:HD12  | 2:M:668:LEU:N     | 1.96                     | 0.80              |
| 3:N:877:PRO:O     | 3:N:880:ILE:HG22  | 1.81                     | 0.80              |
| 3:D:158:TYR:HD1   | 3:D:162:ARG:HG2   | 1.46                     | 0.80              |
| 3:D:172:PRO:HG2   | 3:D:175:VAL:CG2   | 2.07                     | 0.80              |
| 3:D:814:ALA:HB1   | 3:D:818:ARG:HH21  | 1.45                     | 0.80              |
| 2:H:193:LEU:H     | 2:H:193:LEU:HD12  | 1.25                     | 0.80              |
| 3:I:996:TRP:CD2   | 3:I:1056:PRO:HG2  | 2.17                     | 0.80              |
| 3:I:814:ALA:HB1   | 3:I:818:ARG:HH21  | 1.45                     | 0.80              |
| 2:M:84:ARG:NE     | 2:M:133:ASP:CG    | 2.31                     | 0.80              |
| 2:C:471:TYR:O     | 2:C:483:VAL:HG13  | 1.83                     | 0.79              |
| 2:C:578:VAL:HG23  | 2:C:579:VAL:HG12  | 1.62                     | 0.79              |
| 1:F:206:THR:HG22  | 1:F:209:GLU:H     | 1.46                     | 0.79              |
| 2:H:1037:VAL:HG13 | 2:H:1049:LEU:HD11 | 1.65                     | 0.79              |
| 1:B:41:ARG:HH11   | 1:B:177:VAL:HG23  | 1.45                     | 0.79              |
| 3:D:1494:ALA:HA   | 3:D:1497:GLU:HG3  | 1.64                     | 0.79              |
| 3:D:970:LYS:NZ    | 7:X:113:LEU:HD23  | 1.96                     | 0.79              |
| 2:M:316:GLY:C     | 2:M:318:PRO:HD3   | 2.02                     | 0.79              |
| 2:M:404:LEU:HA    | 2:M:407:LYS:HD3   | 1.63                     | 0.79              |
| 2:M:564:MET:HE2   | 2:M:846:LYS:HD2   | 1.62                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1494:ALA:HA   | 3:N:1497:GLU:HG3  | 1.65                     | 0.79              |
| 3:N:554:LEU:O     | 3:N:558:LEU:HG    | 1.82                     | 0.79              |
| 3:N:676:MET:O     | 3:N:680:GLN:HB3   | 1.81                     | 0.79              |
| 3:D:358:GLY:HA2   | 3:D:385:VAL:O     | 1.82                     | 0.79              |
| 1:G:24:VAL:HG22   | 1:G:196:THR:HG22  | 1.62                     | 0.79              |
| 2:H:203:ASP:HB2   | 2:H:205:GLU:OE2   | 1.82                     | 0.79              |
| 3:I:1000:THR:O    | 3:I:1003:VAL:HG12 | 1.81                     | 0.79              |
| 2:M:374:ASN:HD22  | 2:M:374:ASN:H     | 1.30                     | 0.79              |
| 3:N:365:ASP:O     | 3:N:379:ALA:HB2   | 1.81                     | 0.79              |
| 2:C:545:ASN:HB3   | 2:C:583:LEU:HD22  | 1.64                     | 0.79              |
| 3:D:139:GLY:O     | 3:D:147:VAL:HB    | 1.80                     | 0.79              |
| 2:H:545:ASN:HB3   | 2:H:583:LEU:HD22  | 1.64                     | 0.79              |
| 2:M:31:GLN:CG     | 2:M:34:VAL:HG22   | 2.13                     | 0.79              |
| 3:N:1301:LYS:HG3  | 3:N:1303:TYR:CE1  | 2.18                     | 0.79              |
| 7:X:24:GLU:CA     | 7:X:27:GLN:HE21   | 1.96                     | 0.79              |
| 3:D:1147:ARG:HB3  | 3:D:1188:VAL:HG21 | 1.64                     | 0.79              |
| 1:F:39:PRO:O      | 1:F:43:ILE:HG13   | 1.81                     | 0.79              |
| 2:H:1095:LEU:HB2  | 3:I:101:HIS:CE1   | 2.18                     | 0.79              |
| 2:H:98:LEU:HD12   | 2:H:98:LEU:H      | 1.46                     | 0.79              |
| 3:N:136:ASP:HB3   | 3:N:137:PRO:HD3   | 1.64                     | 0.79              |
| 3:N:166:GLN:NE2   | 3:N:394:LEU:HD12  | 1.97                     | 0.79              |
| 2:C:437:ARG:NH2   | 2:C:488:ALA:HA    | 1.98                     | 0.79              |
| 3:D:977:ALA:HB1   | 3:D:983:LEU:HD21  | 1.62                     | 0.79              |
| 4:E:54:LEU:HG     | 4:E:58:PRO:HG2    | 1.64                     | 0.79              |
| 2:H:317:VAL:N     | 2:H:318:PRO:HD3   | 1.96                     | 0.79              |
| 3:I:1235:GLN:HE21 | 7:Y:37:MET:HG3    | 1.46                     | 0.79              |
| 3:I:1288:GLU:HG2  | 3:I:1307:LYS:HE2  | 1.64                     | 0.79              |
| 4:J:18:ARG:HB2    | 4:J:18:ARG:HH21   | 1.48                     | 0.79              |
| 2:M:305:PRO:HG3   | 2:M:308:ARG:HH21  | 1.46                     | 0.79              |
| 3:N:387:LEU:N     | 3:N:387:LEU:HD12  | 1.97                     | 0.79              |
| 2:C:1095:LEU:HD12 | 2:C:1097:LEU:H    | 1.45                     | 0.79              |
| 3:D:1330:ILE:HD13 | 3:D:1347:TYR:OH   | 1.83                     | 0.79              |
| 3:D:520:LEU:HD23  | 3:D:525:ARG:HD2   | 1.62                     | 0.79              |
| 1:F:211:LEU:O     | 1:F:215:VAL:HG23  | 1.82                     | 0.79              |
| 3:D:207:PHE:CE1   | 2:H:283:ILE:HB    | 2.18                     | 0.79              |
| 3:I:1209:LEU:HD21 | 4:J:16:LYS:HE3    | 1.64                     | 0.79              |
| 2:M:66:LEU:HD22   | 2:M:372:LEU:HD22  | 1.65                     | 0.79              |
| 3:N:1330:ILE:HD13 | 3:N:1347:TYR:OH   | 1.83                     | 0.79              |
| 1:A:211:LEU:O     | 1:A:215:VAL:HG23  | 1.82                     | 0.79              |
| 2:C:1095:LEU:CD1  | 2:C:1097:LEU:HB2  | 2.13                     | 0.79              |
| 3:D:1326:THR:HG22 | 3:D:1327:ARG:H    | 1.47                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:33:ASN:HD21   | 3:D:35:ARG:NH2    | 1.80                     | 0.79              |
| 3:I:1301:LYS:HG3  | 3:I:1303:TYR:CE1  | 2.18                     | 0.79              |
| 1:K:211:LEU:O     | 1:K:215:VAL:HG23  | 1.82                     | 0.79              |
| 1:L:57:TYR:CE2    | 1:L:161:ARG:HG2   | 2.18                     | 0.79              |
| 3:N:1233:GLY:HA2  | 3:N:1236:LEU:CD1  | 2.11                     | 0.79              |
| 3:N:213:VAL:HG13  | 3:N:384:VAL:O     | 1.82                     | 0.79              |
| 2:C:537:LYS:HG3   | 2:C:545:ASN:OD1   | 1.83                     | 0.79              |
| 3:D:996:TRP:O     | 3:D:1000:THR:HG22 | 1.81                     | 0.79              |
| 2:H:1032:PHE:O    | 2:H:1036:GLU:HB2  | 1.82                     | 0.79              |
| 3:I:9:ARG:HD3     | 3:I:1456:LYS:HE2  | 1.64                     | 0.79              |
| 2:M:996:LYS:NZ    | 2:M:1000:MET:SD   | 2.55                     | 0.79              |
| 2:M:70:GLU:O      | 2:M:96:ALA:HB1    | 1.81                     | 0.79              |
| 3:N:1209:LEU:HD23 | 3:N:1211:MET:H    | 1.48                     | 0.79              |
| 3:N:1496:GLU:HA   | 3:N:1499:ARG:NE   | 1.97                     | 0.79              |
| 2:C:30:LEU:HD12   | 2:C:30:LEU:O      | 1.83                     | 0.79              |
| 2:C:395:LYS:HG2   | 2:C:397:GLU:HG3   | 1.65                     | 0.79              |
| 2:C:603:VAL:HA    | 2:C:613:VAL:HG12  | 1.64                     | 0.79              |
| 3:D:1000:THR:O    | 3:D:1003:VAL:HG12 | 1.81                     | 0.79              |
| 3:D:204:LEU:O     | 3:D:393:ILE:HG23  | 1.81                     | 0.79              |
| 3:D:413:ASP:O     | 3:D:435:VAL:HG23  | 1.82                     | 0.78              |
| 2:H:632:ASN:HB3   | 2:H:633:GLN:HE21  | 1.48                     | 0.78              |
| 3:N:137:PRO:CD    | 3:N:453:ASP:HB2   | 2.13                     | 0.78              |
| 3:N:128:TYR:HE2   | 3:N:458:ALA:HA    | 1.47                     | 0.78              |
| 3:N:857:ILE:HG22  | 3:N:858:VAL:HG13  | 1.65                     | 0.78              |
| 1:A:87:VAL:HG21   | 1:A:144:VAL:HG11  | 1.65                     | 0.78              |
| 2:C:1012:PRO:HD2  | 2:C:1026:GLN:HG2  | 1.65                     | 0.78              |
| 2:C:861:LEU:HD23  | 2:C:863:ASP:H     | 1.49                     | 0.78              |
| 3:I:177:ALA:H     | 3:I:390:PRO:HD3   | 1.46                     | 0.78              |
| 2:H:1029:GLY:O    | 3:I:622:ARG:CD    | 2.31                     | 0.78              |
| 3:I:1485:GLN:HE21 | 4:J:79:LEU:H      | 1.31                     | 0.78              |
| 3:N:1035:ILE:HA   | 3:N:1038:LEU:HD12 | 1.65                     | 0.78              |
| 3:N:1156:LEU:CD1  | 3:N:1176:LYS:HE3  | 2.12                     | 0.78              |
| 3:N:11:ALA:HB1    | 3:N:507:ASN:ND2   | 1.98                     | 0.78              |
| 3:N:792:ILE:HD11  | 3:N:881:LEU:HD23  | 1.65                     | 0.78              |
| 3:D:481:MET:CE    | 3:D:493:ARG:HA    | 2.13                     | 0.78              |
| 2:H:267:TYR:CB    | 2:H:272:ALA:HB1   | 2.12                     | 0.78              |
| 2:H:305:PRO:HA    | 2:H:308:ARG:HB3   | 1.65                     | 0.78              |
| 2:H:437:ARG:NH2   | 2:H:488:ALA:HA    | 1.98                     | 0.78              |
| 2:H:537:LYS:HG3   | 2:H:545:ASN:OD1   | 1.83                     | 0.78              |
| 3:I:142:LEU:HB3   | 3:I:145:VAL:C     | 2.02                     | 0.78              |
| 3:I:481:MET:CE    | 3:I:493:ARG:HA    | 2.13                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:792:ILE:HD11  | 3:I:881:LEU:HD23  | 1.65                     | 0.78              |
| 3:I:50:PHE:HA     | 3:I:89:ARG:HB3    | 1.64                     | 0.78              |
| 2:C:185:LYS:CG    | 2:C:190:LYS:CB    | 2.62                     | 0.78              |
| 3:D:1209:LEU:HD22 | 3:D:1211:MET:HB3  | 1.65                     | 0.78              |
| 3:D:857:ILE:HG22  | 3:D:858:VAL:HG13  | 1.65                     | 0.78              |
| 2:M:260:LEU:O     | 2:M:260:LEU:HD23  | 1.84                     | 0.78              |
| 3:N:211:VAL:HG12  | 3:N:213:VAL:CG2   | 2.12                     | 0.78              |
| 3:D:704:ARG:NH2   | 6:Q:16:G:O2'      | 2.16                     | 0.78              |
| 2:C:211:LEU:HD23  | 2:C:221:LEU:HD21  | 1.65                     | 0.78              |
| 2:C:374:ASN:HD22  | 2:C:374:ASN:N     | 1.79                     | 0.78              |
| 1:G:79:ILE:HA     | 1:G:82:LEU:HD12   | 1.65                     | 0.78              |
| 2:H:218:VAL:O     | 2:H:221:LEU:HG    | 1.83                     | 0.78              |
| 2:H:344:PHE:HE2   | 2:H:378:LEU:HD21  | 1.49                     | 0.78              |
| 2:H:508:ILE:HD12  | 2:H:526:PRO:HB3   | 1.65                     | 0.78              |
| 2:M:1074:GLU:HG2  | 2:M:1075:ASP:N    | 1.96                     | 0.78              |
| 3:N:1209:LEU:HD21 | 4:O:16:LYS:CE     | 2.12                     | 0.78              |
| 3:N:1326:THR:HG22 | 3:N:1327:ARG:H    | 1.46                     | 0.78              |
| 2:C:266:ARG:O     | 2:C:266:ARG:HD3   | 1.84                     | 0.78              |
| 3:D:171:LEU:HD23  | 3:D:172:PRO:HD2   | 1.63                     | 0.78              |
| 3:D:365:ASP:O     | 3:D:379:ALA:CB    | 2.32                     | 0.78              |
| 3:I:1209:LEU:HD23 | 3:I:1211:MET:H    | 1.48                     | 0.78              |
| 3:I:1330:ILE:HD13 | 3:I:1347:TYR:OH   | 1.83                     | 0.78              |
| 2:M:364:GLU:O     | 2:M:367:LEU:HG    | 1.82                     | 0.78              |
| 3:N:481:MET:CE    | 3:N:493:ARG:HA    | 2.13                     | 0.78              |
| 7:X:6:LYS:HD3     | 7:X:75:LEU:HD21   | 1.63                     | 0.78              |
| 3:D:1281:VAL:HG21 | 3:D:1313:VAL:HG21 | 1.65                     | 0.78              |
| 2:H:334:ARG:HA    | 2:H:338:GLU:OE2   | 1.83                     | 0.78              |
| 3:I:160:GLU:HA    | 3:I:165:LYS:HB2   | 1.66                     | 0.78              |
| 3:I:857:ILE:HG22  | 3:I:858:VAL:HG13  | 1.65                     | 0.78              |
| 2:M:129:ILE:HD12  | 2:M:129:ILE:N     | 1.98                     | 0.78              |
| 3:N:838:ARG:HB3   | 3:N:865:THR:HG23  | 1.66                     | 0.78              |
| 2:C:144:PRO:HB3   | 2:C:164:PRO:HA    | 1.66                     | 0.78              |
| 3:D:160:GLU:CA    | 3:D:165:LYS:HB2   | 2.14                     | 0.78              |
| 3:D:95:LEU:HA     | 3:D:551:ASN:OD1   | 1.84                     | 0.78              |
| 1:F:128:HIS:CE1   | 1:F:131:THR:HG23  | 2.19                     | 0.78              |
| 2:M:1095:LEU:CD1  | 2:M:1097:LEU:HB2  | 2.13                     | 0.78              |
| 2:M:537:LYS:HG3   | 2:M:545:ASN:OD1   | 1.83                     | 0.78              |
| 2:M:601:GLY:HA2   | 2:M:616:GLU:HG2   | 1.66                     | 0.78              |
| 2:M:861:LEU:HD23  | 2:M:863:ASP:H     | 1.49                     | 0.78              |
| 3:N:82:LYS:O      | 3:N:85:VAL:HG22   | 1.84                     | 0.78              |
| 3:N:956:ILE:CD1   | 3:N:1062:ARG:HG3  | 2.14                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:99:ALA:HB1    | 3:D:575:GLN:OE1   | 1.82                     | 0.78              |
| 2:H:288:ARG:HB2   | 2:H:288:ARG:NH1   | 1.98                     | 0.78              |
| 2:H:474:VAL:CG2   | 2:H:479:VAL:HG12  | 2.14                     | 0.78              |
| 3:I:39:PRO:HB3    | 3:I:45:PHE:HB2    | 1.66                     | 0.78              |
| 2:H:1090:LYS:HE3  | 3:I:90:MET:HG3    | 1.63                     | 0.78              |
| 2:M:127:PHE:CE1   | 2:M:136:ILE:HD13  | 2.18                     | 0.78              |
| 3:N:50:PHE:CD1    | 3:N:522:PRO:CG    | 2.63                     | 0.78              |
| 7:Z:57:ARG:HH21   | 7:Z:57:ARG:CB     | 1.97                     | 0.78              |
| 1:A:35:THR:HG21   | 1:B:43:ILE:CD1    | 2.13                     | 0.78              |
| 2:C:1105:LYS:HD2  | 2:C:1107:ASN:HD22 | 1.49                     | 0.78              |
| 2:C:325:ILE:H     | 2:C:325:ILE:CD1   | 1.93                     | 0.78              |
| 2:C:632:ASN:HB3   | 2:C:633:GLN:HE21  | 1.48                     | 0.78              |
| 2:H:182:VAL:HG12  | 2:H:193:LEU:HD21  | 1.56                     | 0.78              |
| 2:H:679:PHE:HB2   | 2:H:683:ASN:HD21  | 1.48                     | 0.78              |
| 2:H:1052:MET:SD   | 3:I:623:VAL:HG21  | 2.24                     | 0.78              |
| 3:N:1084:THR:HA   | 3:N:1087:ARG:HD2  | 1.64                     | 0.78              |
| 3:N:347:VAL:HG13  | 3:N:351:MET:CB    | 2.14                     | 0.78              |
| 3:N:510:GLU:O     | 3:N:513:ILE:HG13  | 1.84                     | 0.78              |
| 2:C:679:PHE:HB2   | 2:C:683:ASN:HD21  | 1.49                     | 0.77              |
| 2:H:304:LEU:CG    | 2:H:305:PRO:HD3   | 2.14                     | 0.77              |
| 3:I:510:GLU:O     | 3:I:513:ILE:HG13  | 1.84                     | 0.77              |
| 1:G:74:ASP:HB3    | 3:I:872:ARG:HH22  | 1.48                     | 0.77              |
| 3:N:1361:VAL:HG23 | 7:Z:37:MET:SD     | 2.24                     | 0.77              |
| 1:A:128:HIS:CE1   | 1:A:131:THR:HG23  | 2.19                     | 0.77              |
| 2:C:1097:LEU:HD11 | 3:D:1451:ALA:CA   | 2.14                     | 0.77              |
| 2:C:148:PHE:HE1   | 2:C:309:TYR:HD2   | 1.31                     | 0.77              |
| 2:H:95:TYR:HB3    | 2:H:114:PHE:HA    | 1.65                     | 0.77              |
| 2:H:118:ILE:HG22  | 2:H:382:ILE:HD13  | 1.65                     | 0.77              |
| 2:M:329:GLY:HA3   | 2:M:489:THR:HG23  | 1.64                     | 0.77              |
| 7:Z:14:ARG:HB3    | 7:Z:14:ARG:NH1    | 1.99                     | 0.77              |
| 1:B:44:LEU:HA     | 1:B:48:ILE:CD1    | 2.14                     | 0.77              |
| 3:D:838:ARG:HB3   | 3:D:865:THR:HG23  | 1.66                     | 0.77              |
| 2:H:794:PRO:CG    | 2:H:1025:ALA:HA   | 2.14                     | 0.77              |
| 2:H:1095:LEU:CD1  | 2:H:1097:LEU:HB2  | 2.13                     | 0.77              |
| 2:H:290:LEU:CB    | 2:H:302:VAL:HG11  | 2.14                     | 0.77              |
| 2:H:391:LEU:O     | 2:H:391:LEU:HD23  | 1.83                     | 0.77              |
| 2:H:564:MET:HE1   | 2:H:846:LYS:CE    | 2.13                     | 0.77              |
| 3:I:25:GLU:HG3    | 3:I:92:HIS:O      | 1.85                     | 0.77              |
| 2:H:1103:ASP:CG   | 3:I:2:LYS:HA      | 2.04                     | 0.77              |
| 1:K:79:ILE:HG13   | 1:K:80:LEU:N      | 1.97                     | 0.77              |
| 1:L:86:VAL:HG12   | 1:L:124:ASN:HB2   | 1.64                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:157:ARG:CZ    | 2:M:314:THR:HG21  | 2.14                     | 0.77              |
| 3:N:543:LEU:HD22  | 3:N:580:ALA:HB1   | 1.66                     | 0.77              |
| 3:D:367:ILE:HB    | 3:D:377:VAL:HG12  | 1.65                     | 0.77              |
| 3:D:650:LEU:HD13  | 3:D:688:TRP:HZ3   | 1.47                     | 0.77              |
| 2:C:1009:SER:HB3  | 3:D:651:GLU:O     | 1.85                     | 0.77              |
| 3:D:804:LEU:HD23  | 3:D:804:LEU:N     | 1.99                     | 0.77              |
| 4:E:36:LYS:NZ     | 4:E:36:LYS:HA     | 1.99                     | 0.77              |
| 4:E:36:LYS:HA     | 4:E:36:LYS:HZ3    | 1.46                     | 0.77              |
| 1:G:94:LEU:HD11   | 1:G:119:ASP:HB2   | 1.67                     | 0.77              |
| 2:H:1012:PRO:HD2  | 2:H:1026:GLN:HG2  | 1.65                     | 0.77              |
| 2:H:52:PHE:CD2    | 2:H:68:PHE:HB2    | 2.19                     | 0.77              |
| 2:H:754:ILE:HG13  | 2:H:791:ARG:NH1   | 2.00                     | 0.77              |
| 3:I:1061:PHE:HE1  | 3:I:1065:LEU:HD22 | 1.50                     | 0.77              |
| 3:I:555:LYS:HA    | 3:I:558:LEU:HD12  | 1.67                     | 0.77              |
| 3:I:584:ASN:HB2   | 3:I:602:SER:OG    | 1.84                     | 0.77              |
| 3:I:838:ARG:HB3   | 3:I:865:THR:HG23  | 1.66                     | 0.77              |
| 2:M:141:HIS:NE2   | 2:M:332:ARG:HB3   | 1.99                     | 0.77              |
| 2:M:334:ARG:HH11  | 2:M:418:LEU:HD21  | 1.48                     | 0.77              |
| 2:M:794:PRO:HG2   | 2:M:1025:ALA:HA   | 1.66                     | 0.77              |
| 3:N:501:ALA:CB    | 3:N:1452:ILE:HG22 | 2.13                     | 0.77              |
| 3:I:991:GLN:HE22  | 7:Y:112:VAL:HB    | 1.48                     | 0.77              |
| 3:D:398:ALA:HB2   | 3:D:447:VAL:HA    | 1.67                     | 0.77              |
| 3:I:1326:THR:HG22 | 3:I:1327:ARG:H    | 1.47                     | 0.77              |
| 3:I:398:ALA:CB    | 3:I:447:VAL:HA    | 2.13                     | 0.77              |
| 1:K:128:HIS:CE1   | 1:K:131:THR:HG23  | 2.19                     | 0.77              |
| 3:N:1442:ASN:ND2  | 3:N:1445:HIS:H    | 1.82                     | 0.77              |
| 3:I:204:LEU:O     | 3:I:393:ILE:CA    | 2.33                     | 0.77              |
| 3:I:650:LEU:HD13  | 3:I:688:TRP:HZ3   | 1.47                     | 0.77              |
| 3:N:676:MET:CE    | 3:N:684:LYS:HE3   | 2.15                     | 0.77              |
| 3:D:25:GLU:HG3    | 3:D:92:HIS:O      | 1.85                     | 0.77              |
| 3:D:792:ILE:HD11  | 3:D:881:LEU:HD23  | 1.65                     | 0.77              |
| 3:D:984:THR:HG22  | 3:D:987:GLU:CD    | 2.05                     | 0.77              |
| 2:H:202:TYR:CE2   | 2:H:304:LEU:HD22  | 2.20                     | 0.77              |
| 2:H:5:ARG:HB2     | 2:H:902:ILE:HB    | 1.67                     | 0.77              |
| 3:I:1254:GLN:CG   | 3:I:1255:GLY:H    | 1.92                     | 0.77              |
| 2:H:1004:LYS:O    | 3:I:629:SER:HA    | 1.85                     | 0.77              |
| 1:K:87:VAL:HG21   | 1:K:144:VAL:HG11  | 1.65                     | 0.77              |
| 2:M:834:GLN:HE22  | 3:N:724:GLN:CG    | 1.93                     | 0.77              |
| 3:N:1061:PHE:HE1  | 3:N:1065:LEU:HD22 | 1.50                     | 0.77              |
| 3:N:1166:LEU:HD23 | 3:N:1166:LEU:H    | 1.48                     | 0.77              |
| 2:C:267:TYR:CB    | 2:C:272:ALA:HB1   | 2.15                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:473:ARG:HA    | 2:C:531:PHE:CD1   | 2.19                     | 0.77              |
| 3:D:1042:ARG:O    | 3:D:1057:VAL:HB   | 1.85                     | 0.77              |
| 3:D:365:ASP:O     | 3:D:379:ALA:HB2   | 1.85                     | 0.77              |
| 1:G:165:ILE:HD13  | 1:G:165:ILE:N     | 1.99                     | 0.77              |
| 2:H:1074:GLU:HG2  | 2:H:1075:ASP:N    | 1.96                     | 0.77              |
| 2:H:218:VAL:HG22  | 2:H:221:LEU:HD21  | 1.66                     | 0.77              |
| 3:I:482:LYS:HE2   | 3:I:1388:ARG:HH22 | 1.46                     | 0.77              |
| 2:H:1019:GLN:OE1  | 3:I:621:LYS:HG3   | 1.81                     | 0.77              |
| 1:G:83:LYS:HD3    | 3:I:844:ALA:HB2   | 1.65                     | 0.77              |
| 4:J:25:LYS:HA     | 4:J:28:GLN:HG3    | 1.67                     | 0.77              |
| 2:M:109:LYS:HD3   | 2:M:368:THR:HG22  | 1.65                     | 0.77              |
| 2:M:30:LEU:CD1    | 2:M:30:LEU:O      | 2.30                     | 0.77              |
| 3:N:956:ILE:HD11  | 3:N:1062:ARG:HB3  | 1.66                     | 0.77              |
| 1:B:86:VAL:HG12   | 1:B:124:ASN:HB2   | 1.65                     | 0.77              |
| 2:C:874:LEU:O     | 3:D:1029:ARG:HD2  | 1.85                     | 0.77              |
| 3:D:112:ILE:C     | 3:D:112:ILE:HD13  | 2.05                     | 0.77              |
| 3:D:207:PHE:CZ    | 2:H:284:ARG:HB2   | 2.20                     | 0.77              |
| 3:N:1152:GLU:HG2  | 3:N:1161:GLU:HA   | 1.67                     | 0.77              |
| 4:O:28:GLN:O      | 4:O:31:LEU:HD12   | 1.85                     | 0.77              |
| 3:D:510:GLU:O     | 3:D:513:ILE:HG13  | 1.84                     | 0.77              |
| 3:I:1288:GLU:HG2  | 3:I:1307:LYS:CE   | 2.15                     | 0.77              |
| 3:I:138:LYS:H     | 3:I:138:LYS:HD3   | 1.50                     | 0.77              |
| 1:L:190:THR:CB    | 3:N:722:GLU:OE1   | 2.33                     | 0.77              |
| 2:M:18:LEU:H      | 2:M:18:LEU:HD12   | 1.48                     | 0.77              |
| 2:M:157:ARG:CZ    | 2:M:314:THR:CG2   | 2.63                     | 0.77              |
| 1:A:42:ARG:NH1    | 1:B:34:VAL:HB     | 1.98                     | 0.76              |
| 2:C:196:LEU:CD2   | 2:C:200:LEU:HD11  | 2.09                     | 0.76              |
| 3:D:1061:PHE:HE1  | 3:D:1065:LEU:HD22 | 1.50                     | 0.76              |
| 2:C:1085:PHE:CE2  | 3:D:1468:LEU:HG   | 2.19                     | 0.76              |
| 3:D:1468:LEU:HD22 | 3:D:1470:ARG:HB2  | 1.65                     | 0.76              |
| 3:D:208:PRO:O     | 3:D:347:VAL:HB    | 1.85                     | 0.76              |
| 1:F:74:ASP:O      | 1:F:78:ILE:HG12   | 1.85                     | 0.76              |
| 2:H:136:ILE:CG2   | 2:H:336:VAL:HG13  | 2.15                     | 0.76              |
| 2:H:754:ILE:HD12  | 2:H:754:ILE:N     | 2.00                     | 0.76              |
| 3:I:1035:ILE:HA   | 3:I:1038:LEU:HD12 | 1.65                     | 0.76              |
| 3:I:112:ILE:C     | 3:I:112:ILE:HD13  | 2.05                     | 0.76              |
| 2:M:436:GLY:HA2   | 2:M:538:GLN:O     | 1.85                     | 0.76              |
| 3:N:1101:VAL:HG11 | 3:N:1424:VAL:HG23 | 1.67                     | 0.76              |
| 3:N:970:LYS:CD    | 7:Z:113:LEU:CD2   | 2.60                     | 0.76              |
| 2:H:274:ARG:HH11  | 2:H:274:ARG:HG2   | 1.48                     | 0.76              |
| 2:H:474:VAL:HG23  | 2:H:478:VAL:O     | 1.84                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1042:ARG:O    | 3:I:1057:VAL:HB   | 1.85                     | 0.76              |
| 3:I:470:LEU:HB2   | 3:I:503:LEU:HD21  | 1.67                     | 0.76              |
| 3:I:984:THR:HG22  | 3:I:987:GLU:CD    | 2.05                     | 0.76              |
| 2:M:189:ARG:NE    | 2:M:189:ARG:HA    | 2.00                     | 0.76              |
| 2:M:261:ILE:H     | 2:M:261:ILE:HD12  | 1.48                     | 0.76              |
| 2:M:679:PHE:HB2   | 2:M:683:ASN:HD21  | 1.48                     | 0.76              |
| 3:N:1101:VAL:HG23 | 3:N:1102:THR:HG23 | 1.67                     | 0.76              |
| 3:N:25:GLU:HG3    | 3:N:92:HIS:O      | 1.85                     | 0.76              |
| 4:O:41:GLU:O      | 4:O:45:ARG:HD2    | 1.86                     | 0.76              |
| 2:H:857:ASP:HB2   | 2:H:978:ARG:HG2   | 1.68                     | 0.76              |
| 3:I:1384:PRO:HG3  | 3:I:1389:LEU:HB3  | 1.67                     | 0.76              |
| 3:I:203:ALA:HB1   | 3:I:393:ILE:HG21  | 1.67                     | 0.76              |
| 1:L:156:HIS:ND1   | 1:L:158:ILE:HG12  | 2.00                     | 0.76              |
| 2:M:200:LEU:CD1   | 2:M:300:ASP:OD2   | 2.32                     | 0.76              |
| 2:M:54:ILE:HG13   | 2:M:356:ARG:NH2   | 1.99                     | 0.76              |
| 2:M:79:PRO:HG2    | 2:M:82:GLU:CB     | 2.14                     | 0.76              |
| 2:M:1086:ARG:NH1  | 3:N:88:TYR:CD1    | 2.53                     | 0.76              |
| 7:Y:13:GLU:HG2    | 7:Y:17:GLN:NE2    | 2.01                     | 0.76              |
| 2:C:274:ARG:HH11  | 2:C:274:ARG:HG2   | 1.51                     | 0.76              |
| 2:C:754:ILE:N     | 2:C:754:ILE:HD12  | 2.00                     | 0.76              |
| 2:C:857:ASP:HB2   | 2:C:978:ARG:HG2   | 1.67                     | 0.76              |
| 3:D:581:LEU:HD23  | 3:D:582:LEU:N     | 2.01                     | 0.76              |
| 3:D:603:LEU:O     | 3:D:606:ILE:HG22  | 1.85                     | 0.76              |
| 1:G:80:LEU:HG     | 3:I:844:ALA:CA    | 2.14                     | 0.76              |
| 3:I:1395:LEU:HD23 | 3:I:1396:GLU:N    | 2.00                     | 0.76              |
| 3:I:1481:VAL:HG13 | 4:J:18:ARG:HD3    | 1.67                     | 0.76              |
| 2:M:39:ARG:HE     | 2:M:45:GLN:HE21   | 1.25                     | 0.76              |
| 2:M:754:ILE:HD12  | 2:M:754:ILE:N     | 2.00                     | 0.76              |
| 2:C:175:GLU:CG    | 2:C:183:SER:HB3   | 2.12                     | 0.76              |
| 2:C:12:VAL:HG11   | 2:C:472:ARG:HD3   | 1.68                     | 0.76              |
| 3:D:728:LEU:HD12  | 3:D:729:HIS:H     | 1.51                     | 0.76              |
| 3:D:800:LYS:HD3   | 3:D:830:ALA:HB3   | 1.67                     | 0.76              |
| 2:H:18:LEU:H      | 2:H:18:LEU:HD12   | 1.51                     | 0.76              |
| 2:H:144:PRO:HG2   | 2:H:265:ARG:NH1   | 2.01                     | 0.76              |
| 3:I:398:ALA:HB2   | 3:I:447:VAL:CG1   | 2.16                     | 0.76              |
| 2:M:79:PRO:HG2    | 2:M:82:GLU:HG3    | 1.67                     | 0.76              |
| 3:N:134:VAL:HG22  | 3:N:455:ARG:O     | 1.85                     | 0.76              |
| 3:N:984:THR:HG22  | 3:N:987:GLU:CD    | 2.05                     | 0.76              |
| 4:O:33:HIS:CD2    | 4:O:89:MET:HG2    | 2.20                     | 0.76              |
| 1:B:71:VAL:HG13   | 1:B:132:LEU:HD12  | 1.68                     | 0.76              |
| 3:D:614:PHE:CD2   | 3:D:1438:ALA:HB1  | 2.20                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1105:LYS:HD2  | 2:H:1107:ASN:HD22 | 1.50                     | 0.76              |
| 2:H:304:LEU:H     | 2:H:304:LEU:HD23  | 1.50                     | 0.76              |
| 3:I:1161:GLU:HG2  | 3:I:1164:ARG:HB2  | 1.67                     | 0.76              |
| 3:I:87:ARG:HG2    | 3:I:523:ASP:HB2   | 1.68                     | 0.76              |
| 2:M:1105:LYS:HD2  | 2:M:1107:ASN:HD22 | 1.50                     | 0.76              |
| 2:M:39:ARG:NE     | 2:M:45:GLN:CD     | 2.39                     | 0.76              |
| 2:M:707:ARG:HG3   | 2:M:826:TYR:CE1   | 2.21                     | 0.76              |
| 3:N:1288:GLU:HG2  | 3:N:1307:LYS:HE2  | 1.68                     | 0.76              |
| 7:Y:7:LEU:HD21    | 7:Y:72:ALA:CB     | 2.14                     | 0.76              |
| 2:C:101:ILE:HD12  | 2:C:108:ILE:HD13  | 1.68                     | 0.76              |
| 3:D:192:ALA:HB1   | 3:D:193:PRO:HD2   | 1.68                     | 0.76              |
| 1:F:87:VAL:HG21   | 1:F:144:VAL:HG11  | 1.65                     | 0.76              |
| 2:H:436:GLY:HA2   | 2:H:538:GLN:O     | 1.86                     | 0.76              |
| 3:I:105:VAL:HG21  | 3:I:128:TYR:HE1   | 1.50                     | 0.76              |
| 3:I:728:LEU:HD12  | 3:I:729:HIS:H     | 1.51                     | 0.76              |
| 2:M:1056:LYS:HD3  | 3:N:623:VAL:HG13  | 1.66                     | 0.76              |
| 2:M:48:PHE:HD1    | 2:M:348:LEU:HD21  | 1.47                     | 0.76              |
| 3:N:116:LEU:HD22  | 3:N:118:LEU:CG    | 2.15                     | 0.76              |
| 1:A:226:SER:O     | 1:A:228:PRO:HD3   | 1.86                     | 0.76              |
| 2:C:165:LEU:HB2   | 2:C:265:ARG:NH1   | 2.01                     | 0.76              |
| 3:D:800:LYS:HG3   | 3:D:829:VAL:CG1   | 2.16                     | 0.76              |
| 4:J:59:ASN:OD1    | 4:J:61:VAL:HG22   | 1.86                     | 0.76              |
| 2:M:176:VAL:HG12  | 2:M:182:VAL:HG13  | 1.67                     | 0.76              |
| 2:M:632:ASN:HB3   | 2:M:633:GLN:HE21  | 1.48                     | 0.76              |
| 3:N:178:LEU:HD13  | 3:N:179:VAL:HG23  | 1.68                     | 0.76              |
| 3:N:470:LEU:HB2   | 3:N:503:LEU:HD21  | 1.67                     | 0.76              |
| 1:A:66:SER:O      | 1:A:75:VAL:HG23   | 1.86                     | 0.76              |
| 2:C:754:ILE:HG13  | 2:C:791:ARG:NH1   | 2.00                     | 0.76              |
| 3:D:1166:LEU:HD23 | 3:D:1166:LEU:H    | 1.51                     | 0.76              |
| 3:D:1359:GLN:O    | 7:X:37:MET:HE1    | 1.85                     | 0.76              |
| 2:H:165:LEU:O     | 2:H:265:ARG:CD    | 2.33                     | 0.76              |
| 2:H:294:GLU:HG2   | 2:H:295:ASP:CG    | 2.06                     | 0.76              |
| 2:H:794:PRO:HG2   | 2:H:1025:ALA:HA   | 1.67                     | 0.76              |
| 3:N:1078:ARG:HG2  | 3:N:1078:ARG:NH1  | 2.00                     | 0.76              |
| 3:N:112:ILE:HD13  | 3:N:112:ILE:C     | 2.05                     | 0.76              |
| 3:N:357:GLU:HG2   | 3:N:441:ARG:HG2   | 1.68                     | 0.76              |
| 3:N:984:THR:HG23  | 3:N:987:GLU:H     | 1.51                     | 0.76              |
| 3:N:1362:LYS:CD   | 7:Z:34:GLN:NE2    | 2.47                     | 0.76              |
| 2:C:412:ALA:O     | 2:C:419:THR:HG23  | 1.86                     | 0.76              |
| 2:C:564:MET:CE    | 2:C:846:LYS:CE    | 2.63                     | 0.76              |
| 3:D:984:THR:HG23  | 3:D:987:GLU:H     | 1.51                     | 0.76              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:H:15:LEU:HD12   | 2:H:15:LEU:N     | 2.00                     | 0.76              |
| 2:H:342:ASP:HA    | 2:H:345:ARG:HD3  | 1.67                     | 0.76              |
| 2:M:274:ARG:HB2   | 2:M:285:LEU:HD13 | 1.66                     | 0.76              |
| 2:M:557:ARG:HH11  | 2:M:560:MET:HG3  | 1.51                     | 0.76              |
| 3:N:100:ALA:HB2   | 3:N:128:TYR:OH   | 1.86                     | 0.76              |
| 3:D:1123:PHE:HD2  | 3:D:1184:GLN:HG3 | 1.52                     | 0.75              |
| 3:D:127:LEU:CD2   | 3:D:134:VAL:CG1  | 2.64                     | 0.75              |
| 3:D:618:LEU:CD2   | 3:D:1463:LYS:HE2 | 2.16                     | 0.75              |
| 3:N:1264:GLU:OE2  | 3:N:1424:VAL:CG1 | 2.34                     | 0.75              |
| 7:X:33:LEU:HD11   | 7:X:52:LYS:HG3   | 1.67                     | 0.75              |
| 7:Z:7:LEU:HA      | 7:Z:109:GLU:OE2  | 1.86                     | 0.75              |
| 1:B:62:LEU:HD12   | 1:B:62:LEU:N     | 2.01                     | 0.75              |
| 3:D:347:VAL:HG13  | 3:D:351:MET:CB   | 2.16                     | 0.75              |
| 3:I:571:LYS:O     | 3:I:574:LEU:HB3  | 1.86                     | 0.75              |
| 2:M:139:GLN:HE22  | 2:M:414:GLY:HA3  | 1.50                     | 0.75              |
| 3:N:1468:LEU:HD13 | 3:N:1470:ARG:NE  | 2.01                     | 0.75              |
| 2:C:436:GLY:HA2   | 2:C:538:GLN:O    | 1.86                     | 0.75              |
| 2:H:1095:LEU:HD11 | 2:H:1097:LEU:CD2 | 2.17                     | 0.75              |
| 3:I:131:LYS:CB    | 3:I:568:ARG:NE   | 2.46                     | 0.75              |
| 3:I:543:LEU:HD21  | 3:I:600:LEU:HB2  | 1.69                     | 0.75              |
| 1:L:106:PRO:HG3   | 1:L:134:GLU:HA   | 1.68                     | 0.75              |
| 5:R:17:DG:H2''    | 5:R:18:DC:H5'    | 1.69                     | 0.75              |
| 2:C:196:LEU:HD22  | 2:C:303:PHE:CE2  | 2.21                     | 0.75              |
| 2:C:265:ARG:HB3   | 2:C:267:TYR:CE1  | 2.22                     | 0.75              |
| 3:D:1146:GLY:CA   | 3:D:1207:TYR:HB2 | 2.16                     | 0.75              |
| 3:D:347:VAL:HG13  | 3:D:351:MET:HB3  | 1.66                     | 0.75              |
| 3:D:176:ASP:CB    | 3:D:389:GLU:HG2  | 2.16                     | 0.75              |
| 3:D:470:LEU:HB2   | 3:D:503:LEU:HD21 | 1.67                     | 0.75              |
| 2:H:69:LEU:HD21   | 2:H:99:GLN:HG2   | 1.67                     | 0.75              |
| 3:I:87:ARG:HG2    | 3:I:523:ASP:CB   | 2.15                     | 0.75              |
| 2:M:63:GLY:HA3    | 2:M:103:LYS:CE   | 2.17                     | 0.75              |
| 2:M:678:PRO:HG2   | 3:N:947:ILE:HD11 | 1.67                     | 0.75              |
| 3:N:1042:ARG:O    | 3:N:1057:VAL:HB  | 1.85                     | 0.75              |
| 3:N:1379:VAL:HG12 | 3:N:1419:PRO:HA  | 1.68                     | 0.75              |
| 3:N:890:VAL:HG11  | 3:N:922:LEU:HD12 | 1.69                     | 0.75              |
| 1:B:123:MET:C     | 1:B:125:PRO:HD3  | 2.06                     | 0.75              |
| 3:D:969:ARG:HG3   | 3:D:970:LYS:N    | 2.02                     | 0.75              |
| 1:G:38:ASN:HB3    | 1:G:39:PRO:HD3   | 1.68                     | 0.75              |
| 3:I:1078:ARG:HG2  | 3:I:1078:ARG:NH1 | 2.00                     | 0.75              |
| 2:M:1090:LYS:HE3  | 3:N:90:MET:SD    | 2.27                     | 0.75              |
| 2:M:304:LEU:HG    | 2:M:305:PRO:HD3  | 1.67                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:65:VAL:HB     | 2:M:101:ILE:O     | 1.87                     | 0.75              |
| 1:A:18:ARG:O      | 1:A:207:PRO:HD3   | 1.86                     | 0.75              |
| 2:C:181:VAL:HG11  | 2:C:223:ASP:OD2   | 1.87                     | 0.75              |
| 3:D:169:TYR:CE2   | 3:D:197:SER:HA    | 2.21                     | 0.75              |
| 3:D:677:LEU:CD2   | 3:D:683:ILE:CD1   | 2.65                     | 0.75              |
| 2:H:165:LEU:HD12  | 2:H:166:PRO:C     | 2.06                     | 0.75              |
| 2:H:242:LEU:O     | 2:H:243:ARG:CG    | 2.34                     | 0.75              |
| 2:H:265:ARG:HB3   | 2:H:267:TYR:CD2   | 2.21                     | 0.75              |
| 3:I:1379:VAL:HG12 | 3:I:1419:PRO:HA   | 1.69                     | 0.75              |
| 3:I:166:GLN:HE21  | 3:I:396:VAL:CG1   | 1.99                     | 0.75              |
| 3:I:871:LYS:HZ1   | 1:L:60:ASP:HA     | 1.47                     | 0.75              |
| 2:M:1095:LEU:HD11 | 2:M:1097:LEU:CD2  | 2.17                     | 0.75              |
| 2:M:265:ARG:HH12  | 2:M:332:ARG:NH1   | 1.80                     | 0.75              |
| 7:Y:19:LEU:HD21   | 7:Y:23:ARG:NH2    | 2.02                     | 0.75              |
| 7:Z:11:GLY:O      | 7:Z:15:LEU:HG     | 1.87                     | 0.75              |
| 1:A:102:LYS:HD3   | 1:A:139:ASN:ND2   | 2.01                     | 0.75              |
| 1:A:75:VAL:O      | 1:A:79:ILE:HG23   | 1.86                     | 0.75              |
| 3:D:1109:GLU:OE1  | 3:D:1201:CYS:HB2  | 1.86                     | 0.75              |
| 1:G:44:LEU:HA     | 1:G:48:ILE:HD13   | 1.67                     | 0.75              |
| 2:H:442:GLU:HG2   | 2:H:454:SER:CB    | 2.17                     | 0.75              |
| 2:H:730:SER:O     | 2:H:734:LEU:HD13  | 1.86                     | 0.75              |
| 2:H:965:GLU:HA    | 2:H:968:LEU:HD12  | 1.69                     | 0.75              |
| 3:I:143:ASN:HA    | 3:I:161:LEU:HD11  | 1.69                     | 0.75              |
| 3:I:690:ALA:O     | 3:I:694:VAL:HG23  | 1.86                     | 0.75              |
| 2:M:850:ALA:HA    | 3:N:632:VAL:HG11  | 1.68                     | 0.75              |
| 2:M:9:ILE:HG12    | 2:M:907:ASP:CG    | 2.07                     | 0.75              |
| 3:N:1384:PRO:CG   | 3:N:1389:LEU:HB3  | 2.17                     | 0.75              |
| 1:B:152:PRO:HG2   | 3:D:857:ILE:HD11  | 1.69                     | 0.75              |
| 2:C:73:LEU:HD22   | 2:C:118:ILE:HD11  | 1.68                     | 0.75              |
| 3:D:1281:VAL:HG21 | 3:D:1313:VAL:CG2  | 2.17                     | 0.75              |
| 3:D:190:GLU:HG2   | 3:D:196:VAL:HG22  | 1.69                     | 0.75              |
| 1:F:102:LYS:HD3   | 1:F:139:ASN:ND2   | 2.01                     | 0.75              |
| 2:H:89:THR:O      | 2:H:91:GLN:HG3    | 1.87                     | 0.75              |
| 3:I:1095:THR:O    | 3:I:1099:VAL:HG23 | 1.86                     | 0.75              |
| 3:I:123:LEU:HD21  | 3:I:151:GLN:NE2   | 2.00                     | 0.75              |
| 1:K:102:LYS:HD3   | 1:K:139:ASN:ND2   | 2.01                     | 0.75              |
| 2:M:129:ILE:HD11  | 2:M:134:ARG:HB2   | 1.69                     | 0.75              |
| 3:D:481:MET:O     | 3:D:489:ARG:HB2   | 1.87                     | 0.75              |
| 3:D:519:VAL:HG13  | 3:D:544:TYR:CE1   | 2.22                     | 0.75              |
| 3:D:890:VAL:HG11  | 3:D:922:LEU:HD12  | 1.68                     | 0.75              |
| 1:G:178:ALA:HB3   | 1:G:198:ARG:HG3   | 1.69                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:185:ARG:NE    | 3:I:692:GLU:CG    | 2.39                     | 0.75              |
| 2:H:1097:LEU:CD1  | 3:I:1451:ALA:CB   | 2.64                     | 0.75              |
| 2:H:363:SER:HB2   | 2:H:366:SER:HB2   | 1.68                     | 0.75              |
| 2:M:1105:LYS:HD2  | 2:M:1107:ASN:ND2  | 2.02                     | 0.75              |
| 2:M:1086:ARG:HD3  | 3:N:88:TYR:CE2    | 2.21                     | 0.75              |
| 7:X:3:ARG:O       | 7:X:4:GLU:HG3     | 1.86                     | 0.75              |
| 1:B:150:TYR:HE1   | 1:B:170:VAL:HG12  | 1.51                     | 0.74              |
| 2:C:965:GLU:HA    | 2:C:968:LEU:HD12  | 1.69                     | 0.74              |
| 3:D:1264:GLU:OE2  | 3:D:1424:VAL:CG1  | 2.35                     | 0.74              |
| 1:K:220:GLU:O     | 1:K:223:THR:HG22  | 1.87                     | 0.74              |
| 2:M:114:PHE:O     | 2:M:114:PHE:CD2   | 2.40                     | 0.74              |
| 2:M:129:ILE:CD1   | 2:M:134:ARG:CG    | 2.61                     | 0.74              |
| 3:N:571:LYS:O     | 3:N:574:LEU:HB3   | 1.86                     | 0.74              |
| 3:N:899:LEU:HD12  | 3:N:900:ILE:HG22  | 1.69                     | 0.74              |
| 3:N:950:GLY:O     | 3:N:953:ASP:HB2   | 1.87                     | 0.74              |
| 2:C:1095:LEU:HD11 | 2:C:1097:LEU:CD2  | 2.17                     | 0.74              |
| 2:C:207:LEU:CD2   | 2:C:221:LEU:HD22  | 2.17                     | 0.74              |
| 3:D:124:GLU:HG3   | 3:D:128:TYR:HE1   | 1.51                     | 0.74              |
| 3:D:134:VAL:HG23  | 3:D:455:ARG:O     | 1.87                     | 0.74              |
| 2:C:1046:ALA:HA   | 3:D:1472:ILE:HD11 | 1.69                     | 0.74              |
| 3:D:706:PRO:HG3   | 5:P:15:DC:O2      | 1.86                     | 0.74              |
| 3:I:1109:GLU:HG2  | 3:I:1201:CYS:HA   | 1.69                     | 0.74              |
| 3:I:135:LEU:HD13  | 3:I:148:GLU:O     | 1.85                     | 0.74              |
| 3:I:202:VAL:HG11  | 3:I:445:ARG:HE    | 1.52                     | 0.74              |
| 2:C:185:LYS:HG2   | 2:C:190:LYS:CB    | 2.17                     | 0.74              |
| 2:C:395:LYS:HG2   | 2:C:397:GLU:CG    | 2.17                     | 0.74              |
| 3:D:1078:ARG:HG2  | 3:D:1078:ARG:NH1  | 2.00                     | 0.74              |
| 2:H:836:GLY:HA3   | 2:H:1001:VAL:HG21 | 1.68                     | 0.74              |
| 2:H:151:ASP:CG    | 2:H:152:PRO:HD2   | 2.08                     | 0.74              |
| 2:H:26:TYR:CD2    | 2:H:30:LEU:HD11   | 2.22                     | 0.74              |
| 2:H:861:LEU:HD23  | 2:H:863:ASP:H     | 1.49                     | 0.74              |
| 3:I:1264:GLU:OE2  | 3:I:1424:VAL:CG1  | 2.35                     | 0.74              |
| 3:I:480:GLU:O     | 3:I:484:PRO:HD2   | 1.88                     | 0.74              |
| 1:G:190:THR:HB    | 3:I:722:GLU:OE1   | 1.87                     | 0.74              |
| 3:I:970:LYS:NZ    | 7:Y:113:LEU:HD23  | 2.01                     | 0.74              |
| 1:L:87:VAL:HG21   | 1:L:144:VAL:HG11  | 1.69                     | 0.74              |
| 3:N:1257:PRO:HA   | 3:N:1260:ILE:CD1  | 2.13                     | 0.74              |
| 3:N:432:TYR:HB3   | 3:N:450:TYR:HB2   | 1.69                     | 0.74              |
| 2:M:1009:SER:HB3  | 3:N:651:GLU:O     | 1.88                     | 0.74              |
| 2:C:1032:PHE:O    | 2:C:1036:GLU:HB2  | 1.88                     | 0.74              |
| 2:C:1105:LYS:HD2  | 2:C:1107:ASN:ND2  | 2.01                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:31:GLN:OE1    | 2:C:39:ARG:HA     | 1.87                     | 0.74              |
| 2:C:557:ARG:HH11  | 2:C:560:MET:HG3   | 1.51                     | 0.74              |
| 3:D:1312:LEU:HD11 | 3:D:1327:ARG:NH2  | 2.03                     | 0.74              |
| 1:B:187:GLY:C     | 3:D:685:ASP:HA    | 2.08                     | 0.74              |
| 1:F:124:ASN:HD21  | 1:F:127:LEU:HD22  | 1.53                     | 0.74              |
| 2:H:603:VAL:CA    | 2:H:613:VAL:HG12  | 2.13                     | 0.74              |
| 2:H:946:ARG:HH11  | 2:H:946:ARG:HB3   | 1.52                     | 0.74              |
| 3:I:1286:THR:HG22 | 3:I:1287:GLU:H    | 1.51                     | 0.74              |
| 3:I:131:LYS:HB2   | 3:I:568:ARG:CZ    | 2.16                     | 0.74              |
| 2:C:211:LEU:HD23  | 2:C:221:LEU:HD23  | 1.69                     | 0.74              |
| 3:D:1442:ASN:HD21 | 3:D:1444:THR:HB   | 1.50                     | 0.74              |
| 3:D:690:ALA:O     | 3:D:694:VAL:HG23  | 1.86                     | 0.74              |
| 1:F:220:GLU:O     | 1:F:223:THR:HG22  | 1.87                     | 0.74              |
| 1:F:226:SER:O     | 1:F:228:PRO:HD3   | 1.86                     | 0.74              |
| 2:H:412:ALA:O     | 2:H:419:THR:HG23  | 1.87                     | 0.74              |
| 2:H:557:ARG:HH11  | 2:H:560:MET:HG3   | 1.51                     | 0.74              |
| 3:I:872:ARG:NE    | 1:L:162:ILE:HG21  | 2.02                     | 0.74              |
| 1:L:165:ILE:HD13  | 1:L:165:ILE:N     | 2.03                     | 0.74              |
| 3:N:1459:LEU:HB3  | 3:N:1465:ASN:OD1  | 1.87                     | 0.74              |
| 2:C:442:GLU:HG2   | 2:C:454:SER:CB    | 2.17                     | 0.74              |
| 3:D:86:ARG:HB3    | 3:D:86:ARG:CZ     | 2.15                     | 0.74              |
| 2:H:1105:LYS:HZ3  | 2:H:1107:ASN:HB2  | 1.52                     | 0.74              |
| 3:I:890:VAL:HG11  | 3:I:922:LEU:HD12  | 1.68                     | 0.74              |
| 4:J:33:HIS:CD2    | 4:J:89:MET:HG2    | 2.23                     | 0.74              |
| 1:K:86:VAL:CG1    | 1:K:124:ASN:HB2   | 2.16                     | 0.74              |
| 2:M:965:GLU:HA    | 2:M:968:LEU:HD12  | 1.69                     | 0.74              |
| 3:N:728:LEU:HD12  | 3:N:729:HIS:H     | 1.50                     | 0.74              |
| 7:X:24:GLU:O      | 7:X:27:GLN:HG2    | 1.87                     | 0.74              |
| 7:Y:89:VAL:CG1    | 7:Y:91:LEU:HD21   | 2.16                     | 0.74              |
| 7:Z:114:ASP:OD2   | 7:Z:118:LYS:HE3   | 1.88                     | 0.74              |
| 1:A:86:VAL:CG1    | 1:A:124:ASN:HB2   | 2.16                     | 0.74              |
| 2:C:140:ILE:HD12  | 2:C:140:ILE:O     | 1.88                     | 0.74              |
| 2:C:144:PRO:HA    | 2:C:163:ILE:O     | 1.88                     | 0.74              |
| 3:I:1205:TYR:CD2  | 3:I:1215:VAL:HG21 | 2.23                     | 0.74              |
| 3:I:1288:GLU:O    | 3:I:1307:LYS:HG2  | 1.86                     | 0.74              |
| 3:I:606:ILE:O     | 3:I:613:ARG:CG    | 2.36                     | 0.74              |
| 4:J:37:ASN:HD22   | 4:J:37:ASN:N      | 1.85                     | 0.74              |
| 2:M:368:THR:HB    | 2:M:369:PRO:CD    | 2.17                     | 0.74              |
| 2:M:442:GLU:HG2   | 2:M:454:SER:CB    | 2.17                     | 0.74              |
| 3:N:1326:THR:HG22 | 3:N:1327:ARG:N    | 2.02                     | 0.74              |
| 3:N:690:ALA:O     | 3:N:694:VAL:HG23  | 1.87                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:134:GLU:HG3   | 3:N:821:VAL:CG1   | 2.18                     | 0.74              |
| 3:D:899:LEU:HD12  | 3:D:900:ILE:HG22  | 1.69                     | 0.74              |
| 2:H:1105:LYS:HD2  | 2:H:1107:ASN:ND2  | 2.02                     | 0.74              |
| 2:H:313:LEU:CB    | 2:H:320:HIS:CE1   | 2.69                     | 0.74              |
| 3:I:521:PRO:O     | 3:I:524:LEU:HB2   | 1.87                     | 0.74              |
| 3:I:520:LEU:HD23  | 3:I:525:ARG:HD2   | 1.69                     | 0.74              |
| 3:I:899:LEU:HD12  | 3:I:900:ILE:HG22  | 1.70                     | 0.74              |
| 3:I:984:THR:HG23  | 3:I:987:GLU:H     | 1.51                     | 0.74              |
| 2:M:857:ASP:HB2   | 2:M:978:ARG:HG2   | 1.68                     | 0.74              |
| 2:M:984:GLU:HG2   | 3:N:944:THR:O     | 1.88                     | 0.74              |
| 3:N:115:LEU:HD12  | 3:N:502:PHE:HE1   | 1.51                     | 0.74              |
| 2:H:144:PRO:HA    | 2:H:163:ILE:O     | 1.88                     | 0.74              |
| 2:H:707:ARG:HG3   | 2:H:826:TYR:CE1   | 2.23                     | 0.74              |
| 3:I:1254:GLN:CG   | 3:I:1255:GLY:N    | 2.50                     | 0.74              |
| 3:I:139:GLY:HA3   | 3:I:162:ARG:CZ    | 2.17                     | 0.74              |
| 3:I:95:LEU:HB2    | 3:I:515:GLU:O     | 1.88                     | 0.74              |
| 2:M:48:PHE:O      | 2:M:52:PHE:HB2    | 1.88                     | 0.74              |
| 3:N:1078:ARG:HG2  | 3:N:1078:ARG:HH11 | 1.53                     | 0.74              |
| 2:C:1067:TYR:CZ   | 2:C:1071:ILE:HD11 | 2.23                     | 0.74              |
| 3:D:1326:THR:HG22 | 3:D:1327:ARG:N    | 2.02                     | 0.74              |
| 3:D:159:ARG:NH2   | 2:H:218:VAL:CG1   | 2.50                     | 0.74              |
| 2:H:676:ILE:HG22  | 2:H:988:VAL:O     | 1.86                     | 0.74              |
| 3:I:187:LYS:HG3   | 3:I:198:ARG:O     | 1.88                     | 0.74              |
| 3:I:554:LEU:CD1   | 3:I:558:LEU:HD21  | 2.17                     | 0.74              |
| 3:N:178:LEU:H     | 3:N:178:LEU:HD12  | 1.53                     | 0.74              |
| 3:N:50:PHE:CB     | 3:N:522:PRO:HG2   | 2.17                     | 0.74              |
| 4:O:6:ILE:HA      | 4:O:9:LEU:HD12    | 1.69                     | 0.74              |
| 7:X:103:GLN:HE21  | 7:X:105:VAL:HG13  | 1.50                     | 0.74              |
| 2:C:185:LYS:CD    | 2:C:190:LYS:CG    | 2.58                     | 0.73              |
| 2:C:54:ILE:HG22   | 2:C:66:LEU:HB3    | 1.68                     | 0.73              |
| 3:D:804:LEU:HD23  | 3:D:804:LEU:H     | 1.53                     | 0.73              |
| 3:D:52:PRO:O      | 3:D:86:ARG:HD3    | 1.88                     | 0.73              |
| 1:F:86:VAL:CG1    | 1:F:124:ASN:HB2   | 2.16                     | 0.73              |
| 2:H:144:PRO:HG2   | 2:H:265:ARG:HH11  | 1.53                     | 0.73              |
| 3:I:405:ASP:H     | 3:I:423:ASP:CG    | 1.92                     | 0.73              |
| 1:K:124:ASN:HD21  | 1:K:127:LEU:HD22  | 1.53                     | 0.73              |
| 1:L:56:VAL:HG22   | 1:L:142:VAL:HG12  | 1.70                     | 0.73              |
| 1:L:58:ILE:N      | 1:L:58:ILE:HD12   | 2.03                     | 0.73              |
| 2:M:334:ARG:NH1   | 2:M:415:PRO:HG2   | 2.00                     | 0.73              |
| 2:M:86:LYS:O      | 2:M:87:ASP:HB2    | 1.86                     | 0.73              |
| 3:N:1209:LEU:HD21 | 4:O:16:LYS:HE3    | 1.68                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:44:LEU:O      | 3:N:50:PHE:HE1    | 1.70                     | 0.73              |
| 2:M:988:VAL:HG12  | 3:N:948:THR:OG1   | 1.88                     | 0.73              |
| 1:B:178:ALA:HB3   | 1:B:198:ARG:HG3   | 1.69                     | 0.73              |
| 2:C:207:LEU:HD22  | 2:C:221:LEU:HD22  | 1.70                     | 0.73              |
| 2:C:516:ARG:HG3   | 3:D:1068:LEU:CD1  | 2.18                     | 0.73              |
| 2:C:516:ARG:HG3   | 3:D:1068:LEU:HD11 | 1.70                     | 0.73              |
| 2:H:1019:GLN:NE2  | 3:I:621:LYS:HG2   | 1.99                     | 0.73              |
| 2:H:1067:TYR:CZ   | 2:H:1071:ILE:HD11 | 2.23                     | 0.73              |
| 3:I:525:ARG:HB2   | 3:I:538:SER:HB3   | 1.68                     | 0.73              |
| 2:M:109:LYS:NZ    | 2:M:367:LEU:O     | 2.21                     | 0.73              |
| 3:N:1235:GLN:HG2  | 7:Z:48:LEU:CD1    | 2.18                     | 0.73              |
| 2:C:199:VAL:HG21  | 2:C:238:LEU:CD1   | 2.17                     | 0.73              |
| 3:D:1205:TYR:CD2  | 3:D:1215:VAL:HG21 | 2.23                     | 0.73              |
| 3:D:126:VAL:CG1   | 3:D:132:TYR:CG    | 2.72                     | 0.73              |
| 3:D:682:ASP:O     | 3:D:683:ILE:HB    | 1.88                     | 0.73              |
| 4:E:47:LYS:HA     | 4:E:54:LEU:HB3    | 1.70                     | 0.73              |
| 2:H:9:ILE:HG12    | 2:H:907:ASP:HB2   | 1.70                     | 0.73              |
| 3:I:1114:THR:HG21 | 3:I:1195:GLN:HB3  | 1.68                     | 0.73              |
| 3:I:1326:THR:HG22 | 3:I:1327:ARG:N    | 2.02                     | 0.73              |
| 3:I:1312:LEU:HD11 | 3:I:1327:ARG:NH2  | 2.02                     | 0.73              |
| 3:I:87:ARG:HG3    | 3:I:523:ASP:HB2   | 1.69                     | 0.73              |
| 3:N:356:PRO:HB3   | 3:N:441:ARG:HA    | 1.70                     | 0.73              |
| 3:N:480:GLU:O     | 3:N:484:PRO:HD2   | 1.87                     | 0.73              |
| 3:I:997:THR:HG21  | 7:Y:61:ARG:NH1    | 2.03                     | 0.73              |
| 1:B:94:LEU:HD11   | 1:B:119:ASP:HB2   | 1.68                     | 0.73              |
| 2:C:1092:LEU:HD13 | 2:C:1099:VAL:CG2  | 2.10                     | 0.73              |
| 2:C:21:ILE:H      | 2:C:21:ILE:CD1    | 2.01                     | 0.73              |
| 2:C:872:ASN:HD21  | 2:C:874:LEU:HB2   | 1.54                     | 0.73              |
| 2:C:91:GLN:HE22   | 2:C:383:ARG:HH12  | 1.36                     | 0.73              |
| 3:D:957:PRO:HG2   | 3:D:1007:VAL:HG22 | 1.70                     | 0.73              |
| 3:D:1122:LEU:HD13 | 3:D:1185:GLU:HA   | 1.69                     | 0.73              |
| 3:D:142:LEU:HD23  | 3:D:146:PRO:HA    | 1.70                     | 0.73              |
| 1:F:186:LEU:HD23  | 1:F:187:GLY:N     | 2.03                     | 0.73              |
| 2:H:172:ILE:N     | 2:H:172:ILE:HD12  | 2.03                     | 0.73              |
| 3:I:957:PRO:HG2   | 3:I:1007:VAL:HG22 | 1.70                     | 0.73              |
| 3:I:143:ASN:HB3   | 3:I:161:LEU:CD1   | 2.19                     | 0.73              |
| 3:I:969:ARG:HG3   | 3:I:970:LYS:N     | 2.02                     | 0.73              |
| 1:L:190:THR:HB    | 3:N:722:GLU:OE1   | 1.88                     | 0.73              |
| 2:M:187:ASN:O     | 2:M:188:LYS:HB3   | 1.87                     | 0.73              |
| 2:M:449:ILE:HG21  | 3:N:1082:ALA:HA   | 1.70                     | 0.73              |
| 3:N:141:ILE:HG21  | 3:N:448:GLU:OE1   | 1.89                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:392:SER:C     | 3:N:393:ILE:HD12  | 2.08                     | 0.73              |
| 1:A:220:GLU:O     | 1:A:223:THR:HG22  | 1.87                     | 0.73              |
| 2:C:1004:LYS:CD   | 3:D:744:GLN:HE22  | 1.92                     | 0.73              |
| 2:H:1110:ASP:OD1  | 2:H:1112:PHE:CE1  | 2.41                     | 0.73              |
| 3:I:1369:GLU:O    | 3:I:1372:VAL:HG12 | 1.89                     | 0.73              |
| 3:I:407:VAL:HA    | 3:I:422:ALA:HA    | 1.71                     | 0.73              |
| 2:M:681:GLY:C     | 3:N:635:PRO:HG3   | 2.08                     | 0.73              |
| 2:M:957:LYS:HD3   | 2:M:961:GLU:HB3   | 1.70                     | 0.73              |
| 3:N:957:PRO:HG2   | 3:N:1007:VAL:HG22 | 1.70                     | 0.73              |
| 3:N:1312:LEU:HD11 | 3:N:1327:ARG:NH2  | 2.03                     | 0.73              |
| 1:B:66:SER:OG     | 1:B:75:VAL:HG21   | 1.89                     | 0.73              |
| 2:C:260:LEU:CB    | 2:C:291:ALA:HB1   | 2.16                     | 0.73              |
| 2:C:302:VAL:O     | 2:C:305:PRO:HD2   | 1.87                     | 0.73              |
| 3:D:127:LEU:HD11  | 3:D:461:ILE:HD11  | 1.70                     | 0.73              |
| 3:D:17:LYS:HG2    | 3:D:21:TRP:HE1    | 1.53                     | 0.73              |
| 2:H:1008:ARG:NH1  | 2:H:1010:THR:HA   | 2.04                     | 0.73              |
| 2:H:182:VAL:CB    | 2:H:193:LEU:CD2   | 2.65                     | 0.73              |
| 2:H:879:ARG:NH2   | 7:Y:42:ASP:CB     | 2.51                     | 0.73              |
| 1:K:18:ARG:O      | 1:K:207:PRO:HD3   | 1.88                     | 0.73              |
| 2:M:1094:ALA:HB1  | 3:N:603:LEU:HD11  | 1.68                     | 0.73              |
| 7:Y:82:VAL:CG2    | 7:Y:133:ARG:HH21  | 2.02                     | 0.73              |
| 2:C:36:PRO:HA     | 2:C:39:ARG:HG3    | 1.71                     | 0.73              |
| 2:C:676:ILE:HG23  | 3:D:948:THR:HB    | 1.71                     | 0.73              |
| 3:D:165:LYS:NZ    | 3:D:199:LEU:HD22  | 2.04                     | 0.73              |
| 1:G:86:VAL:HG12   | 1:G:124:ASN:ND2   | 2.03                     | 0.73              |
| 3:I:1098:LEU:O    | 3:I:1102:THR:HG23 | 1.87                     | 0.73              |
| 1:L:178:ALA:HB3   | 1:L:198:ARG:HG3   | 1.69                     | 0.73              |
| 2:M:1067:TYR:CZ   | 2:M:1071:ILE:HD11 | 2.24                     | 0.73              |
| 2:M:84:ARG:CZ     | 2:M:133:ASP:OD2   | 2.37                     | 0.73              |
| 2:M:897:LEU:HB3   | 2:M:899:GLN:HE21  | 1.54                     | 0.73              |
| 3:N:996:TRP:CG    | 3:N:1056:PRO:CG   | 2.72                     | 0.73              |
| 2:M:1056:LYS:HD3  | 3:N:623:VAL:CG1   | 2.18                     | 0.73              |
| 7:X:114:ASP:OD2   | 7:X:118:LYS:HE3   | 1.88                     | 0.73              |
| 7:X:134:VAL:CG2   | 7:X:154:ILE:HG13  | 2.19                     | 0.73              |
| 1:A:186:LEU:HD23  | 1:A:187:GLY:N     | 2.03                     | 0.73              |
| 2:C:1044:GLY:HA3  | 4:E:17:TYR:CE1    | 2.23                     | 0.73              |
| 3:D:908:LYS:HB2   | 3:D:1027:GLY:HA3  | 1.69                     | 0.73              |
| 3:D:1146:GLY:HA2  | 3:D:1207:TYR:HB2  | 1.70                     | 0.73              |
| 3:D:187:LYS:HE2   | 3:D:199:LEU:HD12  | 1.69                     | 0.73              |
| 3:D:827:ILE:H     | 3:D:827:ILE:HD12  | 1.54                     | 0.73              |
| 2:H:794:PRO:HG2   | 2:H:1025:ALA:O    | 1.88                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:675:ALA:CA    | 2:H:989:VAL:HG12  | 2.18                     | 0.73              |
| 3:I:477:LEU:HD22  | 3:I:492:ALA:HB1   | 1.71                     | 0.73              |
| 2:M:1031:ARG:HH21 | 3:N:621:LYS:NZ    | 1.86                     | 0.73              |
| 2:M:31:GLN:CG     | 2:M:34:VAL:CG2    | 2.67                     | 0.73              |
| 2:C:47:ALA:O      | 2:C:50:GLU:HB3    | 1.88                     | 0.73              |
| 3:D:205:TYR:OH    | 3:D:208:PRO:HB3   | 1.88                     | 0.73              |
| 3:D:207:PHE:HE1   | 2:H:283:ILE:HG13  | 1.54                     | 0.73              |
| 3:D:982:PHE:N     | 3:D:982:PHE:HD2   | 1.87                     | 0.73              |
| 2:H:144:PRO:HB3   | 2:H:164:PRO:HA    | 1.71                     | 0.73              |
| 2:H:195:LEU:HD12  | 2:H:234:ALA:HB1   | 1.68                     | 0.73              |
| 2:H:47:ALA:O      | 2:H:50:GLU:HB3    | 1.88                     | 0.73              |
| 3:I:908:LYS:CB    | 3:I:1027:GLY:HA3  | 2.17                     | 0.73              |
| 3:I:12:LEU:CD2    | 3:I:104:PHE:CE1   | 2.61                     | 0.73              |
| 1:L:85:LEU:HD12   | 1:L:86:VAL:N      | 2.03                     | 0.73              |
| 3:N:1205:TYR:CD2  | 3:N:1215:VAL:HG21 | 2.23                     | 0.73              |
| 3:N:187:LYS:HG3   | 3:N:199:LEU:HA    | 1.71                     | 0.73              |
| 3:N:50:PHE:CD2    | 3:N:522:PRO:HG3   | 2.24                     | 0.73              |
| 3:N:704:ARG:HD3   | 3:N:738:ALA:HB2   | 1.71                     | 0.73              |
| 3:D:1263:PHE:O    | 3:D:1424:VAL:HG12 | 1.89                     | 0.73              |
| 2:H:1092:LEU:HD13 | 2:H:1099:VAL:CG2  | 2.10                     | 0.73              |
| 2:H:1056:LYS:HD3  | 3:I:623:VAL:HG12  | 1.68                     | 0.73              |
| 2:M:412:ALA:O     | 2:M:419:THR:HG23  | 1.89                     | 0.73              |
| 3:N:1369:GLU:O    | 3:N:1372:VAL:HG12 | 1.89                     | 0.73              |
| 3:N:165:LYS:HD3   | 3:N:165:LYS:O     | 1.88                     | 0.73              |
| 3:N:477:LEU:HD22  | 3:N:492:ALA:HB1   | 1.71                     | 0.73              |
| 7:Y:115:THR:CB    | 7:Y:116:PRO:HD3   | 2.19                     | 0.73              |
| 2:C:897:LEU:HB3   | 2:C:899:GLN:HE21  | 1.53                     | 0.72              |
| 1:F:54:THR:O      | 1:F:158:ILE:HD13  | 1.89                     | 0.72              |
| 2:H:632:ASN:HB3   | 2:H:633:GLN:NE2   | 2.03                     | 0.72              |
| 2:H:74:GLY:O      | 2:H:76:PRO:HD3    | 1.89                     | 0.72              |
| 3:I:982:PHE:N     | 3:I:982:PHE:HD2   | 1.87                     | 0.72              |
| 1:K:73:GLU:OE1    | 1:K:130:ALA:HA    | 1.88                     | 0.72              |
| 2:M:9:ILE:HG13    | 2:M:9:ILE:O       | 1.88                     | 0.72              |
| 3:N:190:GLU:HG2   | 3:N:196:VAL:HG22  | 1.70                     | 0.72              |
| 3:N:17:LYS:HG2    | 3:N:21:TRP:HE1    | 1.53                     | 0.72              |
| 3:N:456:MET:CE    | 3:N:568:ARG:NH2   | 2.52                     | 0.72              |
| 3:D:1078:ARG:HG2  | 3:D:1078:ARG:HH11 | 1.53                     | 0.72              |
| 3:D:1369:GLU:O    | 3:D:1372:VAL:HG12 | 1.89                     | 0.72              |
| 3:D:1101:VAL:HG11 | 3:D:1424:VAL:HG23 | 1.69                     | 0.72              |
| 2:C:1100:GLN:N    | 3:D:9:ARG:O       | 2.21                     | 0.72              |
| 2:H:1037:VAL:HG13 | 2:H:1049:LEU:CD1  | 2.19                     | 0.72              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:H:957:LYS:HD3   | 2:H:961:GLU:HB3  | 1.71                     | 0.72              |
| 3:I:143:ASN:HB3   | 3:I:161:LEU:HD11 | 1.71                     | 0.72              |
| 3:I:203:ALA:HB1   | 3:I:393:ILE:CG2  | 2.18                     | 0.72              |
| 3:I:41:ARG:O      | 3:I:42:ASP:HB2   | 1.87                     | 0.72              |
| 2:M:217:LEU:CB    | 2:M:311:PHE:CD1  | 2.71                     | 0.72              |
| 3:N:827:ILE:H     | 3:N:827:ILE:HD12 | 1.54                     | 0.72              |
| 1:A:58:ILE:HD13   | 1:A:140:MET:CB   | 2.19                     | 0.72              |
| 2:C:432:ARG:HH22  | 3:D:1047:LYS:HD3 | 1.53                     | 0.72              |
| 3:D:800:LYS:NZ    | 3:D:804:LEU:HD22 | 2.04                     | 0.72              |
| 1:G:106:PRO:HG3   | 1:G:134:GLU:HA   | 1.70                     | 0.72              |
| 1:G:137:ARG:NH1   | 1:G:137:ARG:HB3  | 2.03                     | 0.72              |
| 1:G:39:PRO:O      | 1:G:43:ILE:HG12  | 1.89                     | 0.72              |
| 2:H:498:GLN:NE2   | 2:H:498:GLN:HA   | 2.04                     | 0.72              |
| 2:H:872:ASN:HD21  | 2:H:874:LEU:HB2  | 1.54                     | 0.72              |
| 1:K:54:THR:O      | 1:K:158:ILE:HD13 | 1.89                     | 0.72              |
| 2:M:872:ASN:HD21  | 2:M:874:LEU:HB2  | 1.54                     | 0.72              |
| 1:B:73:GLU:OE1    | 1:B:130:ALA:HA   | 1.88                     | 0.72              |
| 2:C:957:LYS:HD3   | 2:C:961:GLU:HB3  | 1.71                     | 0.72              |
| 3:D:1114:THR:HG21 | 3:D:1195:GLN:HB3 | 1.70                     | 0.72              |
| 3:D:1256:LEU:HB3  | 3:D:1257:PRO:HD3 | 1.72                     | 0.72              |
| 3:D:1280:VAL:HA   | 3:D:1318:TYR:HA  | 1.71                     | 0.72              |
| 3:D:1379:VAL:HG12 | 3:D:1419:PRO:HA  | 1.69                     | 0.72              |
| 1:F:24:VAL:HG22   | 1:F:196:THR:CG2  | 2.18                     | 0.72              |
| 1:F:18:ARG:HH22   | 1:F:88:ARG:HH21  | 1.37                     | 0.72              |
| 2:H:432:ARG:HH22  | 3:I:1047:LYS:CD  | 2.01                     | 0.72              |
| 3:I:982:PHE:HA    | 7:Y:125:MET:HB2  | 1.72                     | 0.72              |
| 2:M:576:ALA:HB3   | 2:M:900:ARG:HH11 | 1.53                     | 0.72              |
| 1:A:124:ASN:HD21  | 1:A:127:LEU:HD22 | 1.53                     | 0.72              |
| 3:D:432:TYR:HB3   | 3:D:450:TYR:HB2  | 1.71                     | 0.72              |
| 3:D:687:VAL:HG13  | 3:D:688:TRP:CE3  | 2.25                     | 0.72              |
| 1:G:20:TYR:HD2    | 1:G:21:GLY:H     | 1.36                     | 0.72              |
| 2:H:1008:ARG:HH12 | 2:H:1010:THR:HA  | 1.52                     | 0.72              |
| 3:I:17:LYS:HG2    | 3:I:21:TRP:HE1   | 1.53                     | 0.72              |
| 2:M:758:ARG:HB3   | 2:M:788:THR:O    | 1.89                     | 0.72              |
| 2:M:859:PRO:O     | 2:M:867:VAL:HG22 | 1.89                     | 0.72              |
| 2:M:557:ARG:HH21  | 2:M:879:ARG:HE   | 1.37                     | 0.72              |
| 2:M:946:ARG:HB3   | 2:M:946:ARG:HH11 | 1.52                     | 0.72              |
| 1:B:58:ILE:HD12   | 1:B:58:ILE:N     | 2.04                     | 0.72              |
| 2:C:165:LEU:CB    | 2:C:265:ARG:NH1  | 2.52                     | 0.72              |
| 2:C:332:ARG:HG3   | 2:C:465:GLY:HA3  | 1.71                     | 0.72              |
| 2:C:632:ASN:HB3   | 2:C:633:GLN:NE2  | 2.04                     | 0.72              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1047:LYS:HB3 | 3:D:1048:PRO:CD   | 2.20                     | 0.72              |
| 3:D:205:TYR:HD1  | 3:D:390:PRO:HG3   | 1.54                     | 0.72              |
| 3:D:52:PRO:N     | 3:D:86:ARG:HD3    | 2.05                     | 0.72              |
| 3:D:683:ILE:O    | 3:D:687:VAL:HG12  | 1.88                     | 0.72              |
| 1:G:185:ARG:NH1  | 3:I:692:GLU:CB    | 2.53                     | 0.72              |
| 2:H:266:ARG:CA   | 2:H:288:ARG:HD3   | 2.14                     | 0.72              |
| 2:H:56:GLU:HG2   | 2:H:356:ARG:HG2   | 1.72                     | 0.72              |
| 2:H:681:GLY:C    | 3:I:635:PRO:HG3   | 2.09                     | 0.72              |
| 1:K:161:ARG:HB2  | 1:K:161:ARG:CZ    | 2.20                     | 0.72              |
| 2:M:221:LEU:C    | 2:M:223:ASP:H     | 1.91                     | 0.72              |
| 2:M:265:ARG:HD3  | 2:M:267:TYR:CD1   | 2.25                     | 0.72              |
| 2:M:260:LEU:CB   | 2:M:291:ALA:HB1   | 2.18                     | 0.72              |
| 2:M:52:PHE:CD2   | 2:M:68:PHE:HB2    | 2.23                     | 0.72              |
| 3:N:1236:LEU:O   | 3:N:1237:THR:HG23 | 1.89                     | 0.72              |
| 2:M:984:GLU:CG   | 3:N:944:THR:O     | 2.38                     | 0.72              |
| 3:N:982:PHE:HD2  | 3:N:982:PHE:N     | 1.86                     | 0.72              |
| 7:Z:12:TYR:CZ    | 7:Z:16:MET:HE3    | 2.24                     | 0.72              |
| 3:D:1137:ARG:NH2 | 3:D:1172:HIS:CD2  | 2.58                     | 0.72              |
| 1:F:13:VAL:HG22  | 1:F:23:PHE:CD1    | 2.24                     | 0.72              |
| 1:G:112:ARG:NH1  | 1:G:126:ASP:OD1   | 2.22                     | 0.72              |
| 2:H:170:PRO:HD2  | 2:H:263:ASP:HB3   | 1.72                     | 0.72              |
| 3:I:1109:GLU:HG3 | 3:I:1217:ILE:HD12 | 1.71                     | 0.72              |
| 3:I:162:ARG:CD   | 3:I:452:ILE:HG21  | 2.17                     | 0.72              |
| 3:I:827:ILE:HD12 | 3:I:827:ILE:H     | 1.54                     | 0.72              |
| 2:M:69:LEU:HD21  | 2:M:99:GLN:NE2    | 2.05                     | 0.72              |
| 3:N:1047:LYS:HB3 | 3:N:1048:PRO:CD   | 2.20                     | 0.72              |
| 3:N:176:ASP:HA   | 3:N:389:GLU:HA    | 1.72                     | 0.72              |
| 2:C:879:ARG:CZ   | 7:X:42:ASP:OD1    | 2.37                     | 0.72              |
| 7:Z:8:THR:HG23   | 7:Z:109:GLU:OE1   | 1.88                     | 0.72              |
| 2:C:657:ASP:OD1  | 2:C:662:GLU:CA    | 2.38                     | 0.72              |
| 2:C:988:VAL:HG12 | 3:D:948:THR:OG1   | 1.88                     | 0.72              |
| 1:F:221:HIS:NE2  | 1:G:32:PHE:HE2    | 1.78                     | 0.72              |
| 2:H:196:LEU:CD2  | 2:H:200:LEU:HD11  | 2.17                     | 0.72              |
| 2:H:564:MET:CE   | 2:H:846:LYS:HE2   | 2.19                     | 0.72              |
| 2:M:200:LEU:HD22 | 2:M:300:ASP:OD1   | 1.89                     | 0.72              |
| 2:M:632:ASN:HB3  | 2:M:633:GLN:NE2   | 2.03                     | 0.72              |
| 3:N:187:LYS:CB   | 3:N:200:ASP:HB2   | 2.17                     | 0.72              |
| 3:D:520:LEU:CD1  | 3:D:521:PRO:HD2   | 2.20                     | 0.72              |
| 2:H:524:VAL:HG12 | 2:H:525:SER:N     | 2.05                     | 0.72              |
| 2:H:657:ASP:OD1  | 2:H:662:GLU:CA    | 2.38                     | 0.72              |
| 3:I:1047:LYS:HB3 | 3:I:1048:PRO:CD   | 2.19                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:54:THR:HG22   | 1:L:156:HIS:CE1   | 2.24                     | 0.72              |
| 2:M:217:LEU:CD1   | 2:M:311:PHE:CD1   | 2.70                     | 0.72              |
| 2:M:697:ARG:HD2   | 2:M:699:PHE:HD1   | 1.53                     | 0.72              |
| 3:N:181:ASP:HA    | 3:N:205:TYR:CD2   | 2.25                     | 0.72              |
| 3:N:671:LYS:O     | 3:N:675:ARG:HG3   | 1.89                     | 0.72              |
| 2:C:292:ARG:HB2   | 2:C:299:LYS:HE2   | 1.70                     | 0.72              |
| 3:D:179:VAL:HG22  | 3:D:183:GLU:OE2   | 1.89                     | 0.72              |
| 1:F:218:LEU:HD23  | 1:G:222:LEU:CD2   | 2.20                     | 0.72              |
| 2:H:193:LEU:H     | 2:H:193:LEU:HD13  | 1.53                     | 0.72              |
| 3:D:159:ARG:HH22  | 2:H:218:VAL:HG11  | 1.51                     | 0.72              |
| 2:H:408:ARG:HH21  | 2:H:455:LEU:HD12  | 1.54                     | 0.72              |
| 2:H:474:VAL:HG21  | 2:H:479:VAL:HG12  | 1.72                     | 0.72              |
| 3:I:1106:VAL:HG12 | 3:I:1107:VAL:N    | 2.04                     | 0.72              |
| 3:I:495:ARG:O     | 3:I:499:VAL:HG23  | 1.90                     | 0.72              |
| 3:I:704:ARG:HD3   | 3:I:738:ALA:HB2   | 1.71                     | 0.72              |
| 1:K:62:LEU:N      | 1:K:62:LEU:HD12   | 2.04                     | 0.72              |
| 2:M:367:LEU:HB3   | 2:M:371:LYS:HG2   | 1.72                     | 0.72              |
| 2:M:79:PRO:HG2    | 2:M:82:GLU:CG     | 2.19                     | 0.72              |
| 3:N:1281:VAL:HG21 | 3:N:1313:VAL:HG21 | 1.72                     | 0.72              |
| 3:N:131:LYS:HG3   | 3:N:568:ARG:CD    | 2.09                     | 0.72              |
| 3:N:365:ASP:H     | 3:N:379:ALA:HB3   | 1.54                     | 0.72              |
| 1:A:54:THR:O      | 1:A:158:ILE:HD13  | 1.89                     | 0.71              |
| 2:C:524:VAL:HG12  | 2:C:525:SER:N     | 2.04                     | 0.71              |
| 2:C:946:ARG:HB3   | 2:C:946:ARG:HH11  | 1.53                     | 0.71              |
| 1:F:62:LEU:N      | 1:F:62:LEU:HD12   | 2.04                     | 0.71              |
| 2:H:859:PRO:O     | 2:H:867:VAL:HG22  | 1.89                     | 0.71              |
| 3:I:160:GLU:HG2   | 3:I:165:LYS:HB2   | 1.71                     | 0.71              |
| 1:K:67:THR:HG21   | 2:M:609:ASN:ND2   | 2.05                     | 0.71              |
| 2:M:22:GLN:NE2    | 2:M:336:VAL:HG22  | 2.05                     | 0.71              |
| 2:M:99:GLN:OE1    | 2:M:110:GLU:HG3   | 1.90                     | 0.71              |
| 3:N:452:ILE:CD1   | 3:N:452:ILE:O     | 2.30                     | 0.71              |
| 3:N:970:LYS:HZ1   | 7:Z:113:LEU:HG    | 1.54                     | 0.71              |
| 1:B:20:TYR:HD2    | 1:B:21:GLY:H      | 1.36                     | 0.71              |
| 3:D:158:TYR:CD1   | 3:D:162:ARG:CB    | 2.74                     | 0.71              |
| 2:H:1090:LYS:HD2  | 3:I:90:MET:SD     | 2.29                     | 0.71              |
| 3:I:1263:PHE:O    | 3:I:1424:VAL:HG12 | 1.90                     | 0.71              |
| 3:I:204:LEU:CD1   | 3:I:441:ARG:HH22  | 2.01                     | 0.71              |
| 3:I:843:PHE:HE1   | 3:I:864:VAL:HG11  | 1.55                     | 0.71              |
| 2:H:988:VAL:HG11  | 3:I:949:ILE:O     | 1.89                     | 0.71              |
| 2:M:1099:VAL:CG2  | 3:N:10:ILE:HG12   | 2.19                     | 0.71              |
| 3:N:1103:HIS:CD2  | 3:N:1463:LYS:HB2  | 2.25                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:495:ARG:O     | 3:N:499:VAL:HG23  | 1.90                     | 0.71              |
| 7:Y:14:ARG:HB3    | 7:Y:14:ARG:NH1    | 2.04                     | 0.71              |
| 1:A:23:PHE:CD2    | 1:A:211:LEU:HD22  | 2.25                     | 0.71              |
| 2:C:148:PHE:HE1   | 2:C:309:TYR:CD2   | 2.07                     | 0.71              |
| 2:C:689:VAL:HB    | 2:C:870:ILE:HG12  | 1.72                     | 0.71              |
| 3:D:1041:LEU:HD23 | 3:D:1041:LEU:O    | 1.90                     | 0.71              |
| 3:D:645:PRO:HD3   | 3:D:726:ILE:HG12  | 1.72                     | 0.71              |
| 3:D:704:ARG:HD3   | 3:D:738:ALA:HB2   | 1.71                     | 0.71              |
| 1:F:98:THR:CG2    | 1:F:141:GLU:HG3   | 2.20                     | 0.71              |
| 3:I:1078:ARG:HG2  | 3:I:1078:ARG:HH11 | 1.52                     | 0.71              |
| 3:I:1101:VAL:HG21 | 3:I:1424:VAL:HG23 | 1.72                     | 0.71              |
| 2:M:1090:LYS:HA   | 2:M:1093:GLN:HG3  | 1.72                     | 0.71              |
| 2:M:722:ILE:HD13  | 2:M:722:ILE:O     | 1.89                     | 0.71              |
| 3:N:1263:PHE:O    | 3:N:1424:VAL:HG12 | 1.89                     | 0.71              |
| 3:N:432:TYR:HB3   | 3:N:450:TYR:CD2   | 2.24                     | 0.71              |
| 2:C:859:PRO:O     | 2:C:867:VAL:HG22  | 1.89                     | 0.71              |
| 2:C:987:ILE:HD12  | 3:D:948:THR:CG2   | 2.19                     | 0.71              |
| 3:D:159:ARG:CZ    | 2:H:222:MET:HE2   | 2.21                     | 0.71              |
| 3:D:477:LEU:HD22  | 3:D:492:ALA:HB1   | 1.71                     | 0.71              |
| 3:D:783:ARG:HG2   | 3:D:784:ASP:H     | 1.55                     | 0.71              |
| 1:F:18:ARG:O      | 1:F:207:PRO:HD3   | 1.91                     | 0.71              |
| 1:G:59:GLU:HG3    | 1:G:60:ASP:H      | 1.54                     | 0.71              |
| 2:H:42:VAL:HG23   | 2:H:43:GLY:N      | 2.04                     | 0.71              |
| 2:H:597:ALA:HB2   | 2:H:655:LEU:HD21  | 1.72                     | 0.71              |
| 3:I:1286:THR:O    | 3:I:1287:GLU:HB2  | 1.90                     | 0.71              |
| 1:G:185:ARG:CD    | 3:I:692:GLU:HG2   | 2.20                     | 0.71              |
| 3:N:817:GLU:O     | 3:N:821:VAL:HG23  | 1.90                     | 0.71              |
| 7:Z:6:LYS:CD      | 7:Z:85:LEU:HD12   | 2.17                     | 0.71              |
| 2:C:1090:LYS:HA   | 2:C:1093:GLN:HG3  | 1.72                     | 0.71              |
| 2:C:492:ASP:OD2   | 2:C:518:LYS:HG3   | 1.90                     | 0.71              |
| 2:C:501:THR:CG2   | 2:C:513:VAL:HG13  | 2.20                     | 0.71              |
| 3:D:1384:PRO:HG3  | 3:D:1389:LEU:HB3  | 1.72                     | 0.71              |
| 3:D:87:ARG:HB2    | 3:D:524:LEU:HD12  | 1.72                     | 0.71              |
| 2:H:675:ALA:HA    | 2:H:989:VAL:CG1   | 2.21                     | 0.71              |
| 3:I:1147:ARG:HB3  | 3:I:1188:VAL:HG21 | 1.73                     | 0.71              |
| 1:L:42:ARG:HG2    | 1:L:42:ARG:HH11   | 1.55                     | 0.71              |
| 3:N:1111:ASP:OD1  | 3:N:1203:LYS:HD2  | 1.90                     | 0.71              |
| 3:N:151:GLN:HG3   | 3:N:152:LEU:H     | 1.53                     | 0.71              |
| 3:N:452:ILE:HD13  | 3:N:452:ILE:C     | 2.11                     | 0.71              |
| 1:B:122:ILE:HD12  | 1:B:122:ILE:N     | 2.02                     | 0.71              |
| 2:C:273:GLY:HA2   | 2:C:276:LYS:NZ    | 2.05                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:124:GLU:CG    | 3:D:128:TYR:HE1   | 2.02                     | 0.71              |
| 1:G:75:VAL:O      | 1:G:79:ILE:HG23   | 1.90                     | 0.71              |
| 2:H:1090:LYS:HA   | 2:H:1093:GLN:HG3  | 1.72                     | 0.71              |
| 3:N:1041:LEU:O    | 3:N:1041:LEU:HD23 | 1.90                     | 0.71              |
| 3:N:1147:ARG:HB3  | 3:N:1188:VAL:HG21 | 1.70                     | 0.71              |
| 1:B:132:LEU:HD21  | 1:B:138:LEU:HB3   | 1.72                     | 0.71              |
| 2:C:118:ILE:HG22  | 2:C:382:ILE:HD13  | 1.72                     | 0.71              |
| 2:C:95:TYR:HD2    | 2:C:114:PHE:HB3   | 1.56                     | 0.71              |
| 3:D:116:LEU:HD22  | 3:D:118:LEU:CD1   | 2.20                     | 0.71              |
| 1:G:71:VAL:HG21   | 1:G:138:LEU:HD12  | 1.73                     | 0.71              |
| 2:H:193:LEU:HD23  | 2:H:307:LEU:HD22  | 1.72                     | 0.71              |
| 2:H:897:LEU:HB3   | 2:H:899:GLN:HE21  | 1.53                     | 0.71              |
| 3:I:1025:GLN:HA   | 3:I:1025:GLN:NE2  | 2.03                     | 0.71              |
| 3:I:398:ALA:HB2   | 3:I:447:VAL:HG12  | 1.71                     | 0.71              |
| 1:K:98:THR:CG2    | 1:K:141:GLU:HG3   | 2.21                     | 0.71              |
| 3:I:872:ARG:HE    | 1:L:162:ILE:HG21  | 1.56                     | 0.71              |
| 2:M:265:ARG:HB3   | 2:M:267:TYR:CE2   | 2.25                     | 0.71              |
| 3:N:211:VAL:O     | 3:N:213:VAL:HG23  | 1.91                     | 0.71              |
| 3:N:623:VAL:HG12  | 3:N:624:ASP:O     | 1.90                     | 0.71              |
| 2:C:64:LEU:HB2    | 2:C:359:MET:CG    | 2.20                     | 0.71              |
| 3:D:168:THR:HG22  | 3:D:169:TYR:N     | 2.05                     | 0.71              |
| 2:C:987:ILE:CG2   | 3:D:948:THR:HG21  | 2.17                     | 0.71              |
| 2:H:221:LEU:C     | 2:H:223:ASP:H     | 1.93                     | 0.71              |
| 3:I:139:GLY:O     | 3:I:147:VAL:HB    | 1.90                     | 0.71              |
| 3:I:26:VAL:CG2    | 3:I:93:ILE:HG12   | 2.21                     | 0.71              |
| 3:I:615:ARG:NE    | 3:I:619:LEU:HD21  | 2.05                     | 0.71              |
| 3:I:817:GLU:O     | 3:I:821:VAL:HG23  | 1.91                     | 0.71              |
| 1:L:41:ARG:NH1    | 1:L:177:VAL:HG23  | 2.03                     | 0.71              |
| 3:N:1156:LEU:HD12 | 3:N:1176:LYS:HE3  | 1.71                     | 0.71              |
| 3:N:1211:MET:CG   | 3:N:1212:ALA:H    | 2.00                     | 0.71              |
| 3:N:676:MET:SD    | 3:N:684:LYS:CE    | 2.78                     | 0.71              |
| 1:A:170:VAL:O     | 1:A:170:VAL:HG23  | 1.91                     | 0.71              |
| 1:A:26:GLU:OE2    | 1:A:194:LYS:HE3   | 1.90                     | 0.71              |
| 1:A:62:LEU:HD12   | 1:A:62:LEU:N      | 2.04                     | 0.71              |
| 2:C:182:VAL:CG2   | 2:C:193:LEU:HB3   | 2.20                     | 0.71              |
| 2:C:195:LEU:HG    | 2:C:238:LEU:HG    | 1.73                     | 0.71              |
| 2:C:328:LEU:HD11  | 2:C:434:HIS:CD2   | 2.25                     | 0.71              |
| 2:C:564:MET:CE    | 2:C:846:LYS:HD2   | 2.20                     | 0.71              |
| 3:D:174:GLY:H     | 3:D:209:ARG:HH11  | 1.36                     | 0.71              |
| 3:D:817:GLU:O     | 3:D:821:VAL:HG23  | 1.91                     | 0.71              |
| 1:F:58:ILE:HD13   | 1:F:140:MET:CB    | 2.19                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:159:ARG:HH22  | 2:H:218:VAL:CB    | 2.04                     | 0.71              |
| 2:H:313:LEU:CA    | 2:H:320:HIS:ND1   | 2.54                     | 0.71              |
| 3:I:1453:ALA:O    | 3:I:1455:LYS:N    | 2.23                     | 0.71              |
| 3:I:408:GLU:OE2   | 3:I:409:VAL:HG23  | 1.91                     | 0.71              |
| 3:I:645:PRO:HD3   | 3:I:726:ILE:HG12  | 1.72                     | 0.71              |
| 2:M:141:HIS:HB3   | 2:M:418:LEU:HB3   | 1.71                     | 0.71              |
| 3:N:26:VAL:CG2    | 3:N:93:ILE:HG12   | 2.21                     | 0.71              |
| 3:N:843:PHE:HE1   | 3:N:864:VAL:HG11  | 1.55                     | 0.71              |
| 3:I:734:GLU:OE1   | 7:Y:38:GLU:O      | 2.09                     | 0.71              |
| 2:C:224:GLU:CB    | 2:C:228:ALA:CB    | 2.53                     | 0.71              |
| 2:C:512:ARG:HA    | 2:C:523:ILE:HD11  | 1.72                     | 0.71              |
| 3:D:181:ASP:O     | 3:D:204:LEU:HA    | 1.91                     | 0.71              |
| 3:D:54:LYS:HD2    | 3:D:55:ASP:H      | 1.54                     | 0.71              |
| 1:F:170:VAL:HG23  | 1:F:170:VAL:O     | 1.91                     | 0.71              |
| 1:F:80:LEU:HD23   | 1:F:81:ASN:N      | 2.05                     | 0.71              |
| 1:G:74:ASP:HB2    | 3:I:872:ARG:NH2   | 2.04                     | 0.71              |
| 2:H:1081:VAL:CG2  | 2:H:1111:ILE:HG22 | 2.15                     | 0.71              |
| 3:I:561:GLY:O     | 3:I:563:PRO:HD3   | 1.90                     | 0.71              |
| 3:I:606:ILE:HD11  | 3:I:613:ARG:HE    | 1.54                     | 0.71              |
| 1:L:20:TYR:HD2    | 1:L:21:GLY:H      | 1.36                     | 0.71              |
| 2:M:1045:ALA:HB1  | 2:M:1048:THR:HB   | 1.72                     | 0.71              |
| 2:M:1105:LYS:HZ3  | 2:M:1107:ASN:HB2  | 1.54                     | 0.71              |
| 2:M:66:LEU:HD22   | 2:M:372:LEU:CD2   | 2.20                     | 0.71              |
| 3:N:1029:ARG:HB3  | 3:N:1029:ARG:HH11 | 1.56                     | 0.71              |
| 3:N:165:LYS:HZ2   | 3:N:199:LEU:HD22  | 1.55                     | 0.71              |
| 1:L:187:GLY:O     | 3:N:688:TRP:CD1   | 2.41                     | 0.71              |
| 2:C:292:ARG:HG2   | 2:C:299:LYS:HB3   | 1.73                     | 0.70              |
| 2:C:347:GLY:HA3   | 2:C:378:LEU:HD12  | 1.73                     | 0.70              |
| 2:C:720:GLU:HA    | 2:C:759:THR:O     | 1.91                     | 0.70              |
| 3:D:26:VAL:CG2    | 3:D:93:ILE:HG12   | 2.21                     | 0.70              |
| 2:H:358:ARG:HH22  | 2:H:374:ASN:CG    | 1.94                     | 0.70              |
| 2:H:167:LYS:HD2   | 2:H:415:PRO:O     | 1.90                     | 0.70              |
| 3:I:127:LEU:HD12  | 3:I:457:GLY:HA2   | 1.72                     | 0.70              |
| 2:M:1008:ARG:HH12 | 2:M:1010:THR:HA   | 1.56                     | 0.70              |
| 2:M:270:GLY:O     | 2:M:274:ARG:HD3   | 1.91                     | 0.70              |
| 3:D:414:ARG:HB3   | 3:D:450:TYR:CE1   | 2.26                     | 0.70              |
| 3:D:23:TYR:O      | 3:D:49:ILE:HG23   | 1.90                     | 0.70              |
| 3:I:939:PHE:O     | 3:I:942:SER:HB3   | 1.91                     | 0.70              |
| 1:K:183:ASP:O     | 1:K:192:LEU:O     | 2.09                     | 0.70              |
| 2:M:172:ILE:HG23  | 2:M:186:VAL:CG1   | 2.20                     | 0.70              |
| 2:M:242:LEU:HD12  | 2:M:254:VAL:HG11  | 1.73                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:253:ALA:O     | 2:M:256:TYR:HB3   | 1.91                     | 0.70              |
| 2:M:401:LEU:HD13  | 2:M:587:VAL:HG11  | 1.71                     | 0.70              |
| 2:M:498:GLN:OE1   | 3:N:1068:LEU:HD12 | 1.90                     | 0.70              |
| 3:N:1273:VAL:HG22 | 3:N:1326:THR:OG1  | 1.92                     | 0.70              |
| 3:N:1487:VAL:HG12 | 3:N:1488:ASP:N    | 2.04                     | 0.70              |
| 3:N:166:GLN:NE2   | 3:N:394:LEU:HB2   | 2.06                     | 0.70              |
| 3:N:617:ASN:ND2   | 3:N:1467:ILE:HA   | 2.05                     | 0.70              |
| 7:Y:89:VAL:HG11   | 7:Y:91:LEU:HD21   | 1.73                     | 0.70              |
| 3:D:127:LEU:CD1   | 3:D:461:ILE:HD11  | 2.21                     | 0.70              |
| 3:D:181:ASP:HA    | 3:D:205:TYR:HD2   | 1.56                     | 0.70              |
| 2:H:1106:ASP:OD1  | 3:I:7:LYS:HD3     | 1.90                     | 0.70              |
| 2:H:260:LEU:CB    | 2:H:291:ALA:HB1   | 2.19                     | 0.70              |
| 2:M:39:ARG:HE     | 2:M:45:GLN:HE22   | 1.31                     | 0.70              |
| 2:M:496:ILE:HD12  | 2:M:496:ILE:N     | 2.06                     | 0.70              |
| 2:M:524:VAL:HG12  | 2:M:525:SER:N     | 2.04                     | 0.70              |
| 2:M:52:PHE:O      | 2:M:54:ILE:N      | 2.24                     | 0.70              |
| 2:M:657:ASP:OD1   | 2:M:662:GLU:CA    | 2.38                     | 0.70              |
| 3:N:762:GLN:NE2   | 4:O:20:THR:OG1    | 2.24                     | 0.70              |
| 1:B:165:ILE:N     | 1:B:165:ILE:HD13  | 2.06                     | 0.70              |
| 2:C:139:GLN:HE22  | 2:C:415:PRO:CD    | 2.03                     | 0.70              |
| 2:C:12:VAL:HG22   | 2:C:13:ILE:HG23   | 1.74                     | 0.70              |
| 2:C:148:PHE:CE1   | 2:C:309:TYR:HD2   | 2.09                     | 0.70              |
| 2:C:36:PRO:C      | 2:C:39:ARG:HG3    | 2.12                     | 0.70              |
| 2:C:141:HIS:HB3   | 2:C:418:LEU:HD23  | 1.73                     | 0.70              |
| 2:C:516:ARG:NE    | 3:D:1068:LEU:HD13 | 2.07                     | 0.70              |
| 3:D:141:ILE:HG13  | 3:D:448:GLU:CD    | 2.12                     | 0.70              |
| 2:H:1082:PRO:HG2  | 3:I:1469:GLY:HA3  | 1.73                     | 0.70              |
| 2:H:73:LEU:HB2    | 2:H:93:PRO:O      | 1.92                     | 0.70              |
| 3:I:115:LEU:HD12  | 3:I:502:PHE:CE1   | 2.24                     | 0.70              |
| 3:I:116:LEU:HD22  | 3:I:118:LEU:CG    | 2.15                     | 0.70              |
| 3:I:1438:ALA:O    | 3:I:1443:THR:HG22 | 1.90                     | 0.70              |
| 3:I:166:GLN:HG2   | 3:I:396:VAL:HG12  | 1.72                     | 0.70              |
| 1:G:74:ASP:HB2    | 1:L:162:ILE:HB    | 1.72                     | 0.70              |
| 3:N:205:TYR:HD1   | 3:N:390:PRO:HB3   | 1.55                     | 0.70              |
| 3:N:949:ILE:N     | 3:N:949:ILE:HD12  | 2.05                     | 0.70              |
| 7:Z:13:GLU:HG2    | 7:Z:17:GLN:HE21   | 1.56                     | 0.70              |
| 2:C:1105:LYS:HZ3  | 2:C:1107:ASN:HB2  | 1.56                     | 0.70              |
| 2:C:447:ALA:O     | 2:C:448:ASN:HB2   | 1.91                     | 0.70              |
| 2:C:1004:LYS:O    | 3:D:629:SER:HA    | 1.90                     | 0.70              |
| 3:D:781:PRO:HB2   | 3:D:786:ILE:HD11  | 1.73                     | 0.70              |
| 4:E:73:LEU:H      | 4:E:73:LEU:HD12   | 1.55                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:13:VAL:HG22   | 1:F:23:PHE:HD1    | 1.57                     | 0.70              |
| 2:H:1015:LEU:N    | 2:H:1015:LEU:HD12 | 2.06                     | 0.70              |
| 2:H:261:ILE:HD13  | 2:H:262:ALA:H     | 1.56                     | 0.70              |
| 2:H:64:LEU:HB2    | 2:H:359:MET:CG    | 2.20                     | 0.70              |
| 2:H:496:ILE:H     | 2:H:496:ILE:HD12  | 1.57                     | 0.70              |
| 2:H:996:LYS:NZ    | 2:H:1000:MET:SD   | 2.62                     | 0.70              |
| 3:I:1156:LEU:HD12 | 3:I:1176:LYS:HE3  | 1.73                     | 0.70              |
| 2:M:1012:PRO:HD2  | 2:M:1026:GLN:CG   | 2.21                     | 0.70              |
| 2:M:154:ARG:NH1   | 2:M:178:PRO:HD3   | 2.05                     | 0.70              |
| 2:M:516:ARG:HG3   | 3:N:1068:LEU:HD11 | 1.74                     | 0.70              |
| 2:M:571:LEU:HD11  | 2:M:701:THR:N     | 2.06                     | 0.70              |
| 3:N:1114:THR:CG2  | 3:N:1195:GLN:HB3  | 2.20                     | 0.70              |
| 3:N:809:PRO:O     | 3:N:812:ALA:HB3   | 1.90                     | 0.70              |
| 3:D:631:ILE:HD13  | 3:D:631:ILE:O     | 1.92                     | 0.70              |
| 2:H:15:LEU:CD1    | 2:H:15:LEU:H      | 2.05                     | 0.70              |
| 2:H:512:ARG:HA    | 2:H:523:ILE:HD11  | 1.72                     | 0.70              |
| 3:I:1041:LEU:O    | 3:I:1041:LEU:HD23 | 1.90                     | 0.70              |
| 2:M:100:LEU:HD12  | 2:M:100:LEU:O     | 1.92                     | 0.70              |
| 3:N:1468:LEU:CD1  | 3:N:1470:ARG:HE   | 2.05                     | 0.70              |
| 3:N:362:GLU:O     | 3:N:379:ALA:HB1   | 1.91                     | 0.70              |
| 1:A:150:TYR:HB2   | 2:C:696:LYS:HE2   | 1.73                     | 0.70              |
| 1:B:106:PRO:HG3   | 1:B:134:GLU:HA    | 1.74                     | 0.70              |
| 1:B:55:SER:OG     | 1:B:158:ILE:HB    | 1.90                     | 0.70              |
| 2:C:191:PHE:HZ    | 2:C:196:LEU:HB2   | 1.57                     | 0.70              |
| 2:C:593:ALA:HB1   | 2:C:659:PRO:HD2   | 1.74                     | 0.70              |
| 2:C:676:ILE:HG22  | 2:C:988:VAL:O     | 1.92                     | 0.70              |
| 2:C:949:LYS:HD3   | 3:D:796:ARG:NH2   | 2.07                     | 0.70              |
| 2:C:1090:LYS:HE3  | 3:D:90:MET:HG2    | 1.74                     | 0.70              |
| 2:H:344:PHE:CE2   | 2:H:378:LEU:HD21  | 2.26                     | 0.70              |
| 2:H:472:ARG:HD2   | 2:H:480:THR:O     | 1.91                     | 0.70              |
| 3:I:1472:ILE:HG22 | 3:I:1473:PRO:HD2  | 1.74                     | 0.70              |
| 2:H:1084:SER:CB   | 3:I:617:ASN:OD1   | 2.37                     | 0.70              |
| 1:K:54:THR:HG22   | 1:K:158:ILE:HD11  | 1.73                     | 0.70              |
| 1:L:38:ASN:HB3    | 1:L:39:PRO:HD3    | 1.72                     | 0.70              |
| 3:N:992:ILE:HD12  | 3:N:1054:GLU:OE2  | 1.91                     | 0.70              |
| 3:N:1122:LEU:N    | 3:N:1122:LEU:HD12 | 2.06                     | 0.70              |
| 3:N:631:ILE:HD13  | 3:N:631:ILE:O     | 1.92                     | 0.70              |
| 3:N:680:GLN:CG    | 3:N:682:ASP:O     | 2.36                     | 0.70              |
| 3:N:982:PHE:N     | 3:N:982:PHE:CD2   | 2.60                     | 0.70              |
| 3:D:126:VAL:CG1   | 3:D:132:TYR:HB2   | 2.21                     | 0.70              |
| 3:D:141:ILE:HD13  | 3:D:142:LEU:N     | 2.06                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:158:TYR:HD1   | 3:D:162:ARG:CG    | 2.04                     | 0.70              |
| 3:D:685:ASP:O     | 3:D:689:ASP:CG    | 2.30                     | 0.70              |
| 1:G:173:PRO:O     | 1:G:201:THR:HG22  | 1.92                     | 0.70              |
| 3:I:906:GLN:HB3   | 3:I:911:LEU:HD11  | 1.74                     | 0.70              |
| 1:K:170:VAL:O     | 1:K:170:VAL:HG23  | 1.91                     | 0.70              |
| 2:M:564:MET:CE    | 2:M:846:LYS:HE2   | 2.10                     | 0.70              |
| 3:N:347:VAL:HG22  | 3:N:368:VAL:HG11  | 1.72                     | 0.70              |
| 3:N:643:GLY:O     | 3:N:726:ILE:HG23  | 1.92                     | 0.70              |
| 2:M:911:GLU:OE1   | 3:N:951:ILE:CG1   | 2.39                     | 0.70              |
| 1:A:98:THR:CG2    | 1:A:141:GLU:HG3   | 2.21                     | 0.70              |
| 2:C:89:THR:HG21   | 2:C:383:ARG:NH2   | 2.05                     | 0.70              |
| 3:D:1312:LEU:CD1  | 3:D:1327:ARG:NH2  | 2.55                     | 0.70              |
| 3:D:484:PRO:HB3   | 3:D:488:ARG:HE    | 1.56                     | 0.70              |
| 3:I:126:VAL:O     | 3:I:130:SER:CB    | 2.32                     | 0.70              |
| 2:M:101:ILE:CA    | 2:M:108:ILE:HG12  | 2.22                     | 0.70              |
| 2:M:1092:LEU:HD13 | 2:M:1099:VAL:CG2  | 2.10                     | 0.70              |
| 3:N:1312:LEU:CD1  | 3:N:1327:ARG:NH2  | 2.55                     | 0.70              |
| 3:N:18:ILE:CG2    | 3:N:518:PRO:HG3   | 2.21                     | 0.70              |
| 3:N:561:GLY:O     | 3:N:563:PRO:HD2   | 1.91                     | 0.70              |
| 3:N:645:PRO:HD3   | 3:N:726:ILE:HG12  | 1.72                     | 0.70              |
| 7:Y:102:VAL:HG21  | 7:Y:125:MET:CE    | 2.22                     | 0.70              |
| 7:Z:14:ARG:HH11   | 7:Z:14:ARG:CB     | 2.00                     | 0.70              |
| 2:C:11:GLU:HG2    | 2:C:537:LYS:HZ1   | 1.56                     | 0.70              |
| 2:C:136:ILE:N     | 2:C:136:ILE:HD12  | 2.06                     | 0.70              |
| 2:C:516:ARG:HE    | 3:D:1068:LEU:HD13 | 1.57                     | 0.70              |
| 2:C:611:ILE:CD1   | 2:C:625:LEU:HD21  | 2.22                     | 0.70              |
| 2:C:729:LEU:HG    | 2:C:729:LEU:O     | 1.92                     | 0.70              |
| 3:D:484:PRO:HB3   | 3:D:488:ARG:HG3   | 1.74                     | 0.70              |
| 3:D:50:PHE:CD2    | 3:D:522:PRO:CG    | 2.75                     | 0.70              |
| 3:D:643:GLY:O     | 3:D:726:ILE:HG23  | 1.92                     | 0.70              |
| 3:D:843:PHE:HE1   | 3:D:864:VAL:HG11  | 1.56                     | 0.70              |
| 2:H:185:LYS:CD    | 2:H:190:LYS:HG2   | 2.15                     | 0.70              |
| 2:H:258:TYR:CD2   | 2:H:290:LEU:HD11  | 2.26                     | 0.70              |
| 2:H:322:VAL:O     | 2:H:322:VAL:HG23  | 1.92                     | 0.70              |
| 2:H:906:PHE:CE1   | 3:I:1067:VAL:HA   | 2.27                     | 0.70              |
| 3:I:696:HIS:CD2   | 4:J:58:PRO:HB3    | 2.26                     | 0.70              |
| 1:L:33:GLY:O      | 1:L:195:LEU:HD22  | 1.92                     | 0.70              |
| 2:M:1014:SER:HB2  | 2:M:1021:LEU:HD13 | 1.73                     | 0.70              |
| 2:M:1111:ILE:HG12 | 2:M:1112:PHE:N    | 2.05                     | 0.70              |
| 3:N:774:SER:HB3   | 3:N:1362:LYS:O    | 1.91                     | 0.70              |
| 3:N:584:ASN:HB2   | 3:N:602:SER:HB3   | 1.74                     | 0.70              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:676:MET:SD    | 3:N:684:LYS:HE3  | 2.32                     | 0.70              |
| 1:B:173:PRO:O     | 1:B:201:THR:HG22 | 1.92                     | 0.69              |
| 2:C:64:LEU:HB2    | 2:C:359:MET:HG3  | 1.74                     | 0.69              |
| 3:D:154:THR:HG23  | 3:D:157:GLU:OE2  | 1.92                     | 0.69              |
| 3:D:87:ARG:HB3    | 3:D:523:ASP:HB2  | 0.78                     | 0.69              |
| 3:I:166:GLN:NE2   | 3:I:394:LEU:HD12 | 2.07                     | 0.69              |
| 3:I:804:LEU:HB2   | 3:I:831:GLY:HA2  | 1.73                     | 0.69              |
| 1:L:185:ARG:CZ    | 3:N:692:GLU:CG   | 2.62                     | 0.69              |
| 3:N:108:VAL:CB    | 3:N:109:PRO:HD3  | 2.22                     | 0.69              |
| 3:N:126:VAL:O     | 3:N:130:SER:HB3  | 1.91                     | 0.69              |
| 3:N:1292:VAL:HG11 | 3:N:1325:LEU:HG  | 1.74                     | 0.69              |
| 3:N:939:PHE:O     | 3:N:942:SER:HB3  | 1.92                     | 0.69              |
| 3:D:44:LEU:O      | 3:D:50:PHE:CE1   | 2.45                     | 0.69              |
| 2:C:1030:GLN:NE2  | 3:D:628:ARG:HG2  | 2.07                     | 0.69              |
| 3:D:734:GLU:OE1   | 7:X:38:GLU:O     | 2.09                     | 0.69              |
| 3:D:980:MET:HB3   | 3:D:982:PHE:CE2  | 2.27                     | 0.69              |
| 4:E:36:LYS:NZ     | 4:E:36:LYS:CA    | 2.55                     | 0.69              |
| 1:G:122:ILE:HD12  | 1:G:122:ILE:N    | 2.07                     | 0.69              |
| 2:H:442:GLU:HG2   | 2:H:454:SER:HB2  | 1.74                     | 0.69              |
| 2:H:18:LEU:HD13   | 2:H:590:ASP:CG   | 2.13                     | 0.69              |
| 3:I:1277:ILE:HD13 | 3:I:1301:LYS:HB2 | 1.74                     | 0.69              |
| 3:I:44:LEU:O      | 3:I:522:PRO:HG2  | 1.90                     | 0.69              |
| 2:H:1091:GLU:HB3  | 3:I:607:LEU:HD21 | 1.72                     | 0.69              |
| 1:G:185:ARG:HH11  | 3:I:692:GLU:HB3  | 1.54                     | 0.69              |
| 1:K:58:ILE:HD13   | 1:K:140:MET:CB   | 2.19                     | 0.69              |
| 2:M:191:PHE:HD2   | 2:M:195:LEU:HD23 | 1.57                     | 0.69              |
| 2:M:408:ARG:HH21  | 2:M:455:LEU:HD12 | 1.55                     | 0.69              |
| 2:M:447:ALA:O     | 2:M:448:ASN:HB2  | 1.91                     | 0.69              |
| 3:N:1109:GLU:HG2  | 3:N:1202:GLN:H   | 1.57                     | 0.69              |
| 3:D:1273:VAL:HG22 | 3:D:1326:THR:OG1 | 1.92                     | 0.69              |
| 3:D:1442:ASN:ND2  | 3:D:1444:THR:HB  | 2.07                     | 0.69              |
| 3:D:1453:ALA:O    | 3:D:1455:LYS:N   | 2.25                     | 0.69              |
| 3:D:484:PRO:CB    | 3:D:488:ARG:HG3  | 2.23                     | 0.69              |
| 1:F:54:THR:HG22   | 1:F:158:ILE:HD11 | 1.74                     | 0.69              |
| 2:H:101:ILE:HD13  | 2:H:108:ILE:HG23 | 1.73                     | 0.69              |
| 2:H:9:ILE:HG12    | 2:H:907:ASP:CB   | 2.21                     | 0.69              |
| 1:G:80:LEU:CD2    | 3:I:867:ARG:HB2  | 2.21                     | 0.69              |
| 2:M:588:VAL:HG21  | 2:M:664:GLY:O    | 1.92                     | 0.69              |
| 1:B:152:PRO:HG2   | 3:D:857:ILE:CD1  | 2.22                     | 0.69              |
| 2:C:151:ASP:CG    | 2:C:152:PRO:HD2  | 2.13                     | 0.69              |
| 2:C:15:LEU:HD12   | 2:C:15:LEU:H     | 1.57                     | 0.69              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:885:ILE:HG13  | 3:D:949:ILE:CG2  | 2.23                     | 0.69              |
| 3:D:1102:THR:OG1  | 3:D:1226:ALA:HB2 | 1.92                     | 0.69              |
| 3:D:111:LYS:HG2   | 3:D:1452:ILE:CD1 | 2.23                     | 0.69              |
| 3:D:495:ARG:O     | 3:D:499:VAL:HG23 | 1.90                     | 0.69              |
| 2:C:1036:GLU:HG3  | 3:D:707:THR:OG1  | 1.92                     | 0.69              |
| 3:D:906:GLN:HB3   | 3:D:911:LEU:HD11 | 1.74                     | 0.69              |
| 3:D:159:ARG:HH22  | 2:H:218:VAL:CG1  | 2.06                     | 0.69              |
| 2:H:242:LEU:CD1   | 2:H:254:VAL:HG11 | 2.22                     | 0.69              |
| 3:I:1273:VAL:HG22 | 3:I:1326:THR:OG1 | 1.92                     | 0.69              |
| 3:I:465:LEU:HD21  | 3:I:509:PRO:HB2  | 1.75                     | 0.69              |
| 4:J:41:GLU:O      | 4:J:45:ARG:HD2   | 1.93                     | 0.69              |
| 2:M:80:GLN:HG2    | 2:M:90:TYR:CD2   | 2.27                     | 0.69              |
| 3:N:394:LEU:HD23  | 3:N:394:LEU:H    | 1.56                     | 0.69              |
| 3:N:134:VAL:O     | 3:N:454:ALA:HB1  | 1.92                     | 0.69              |
| 1:L:185:ARG:NH1   | 3:N:692:GLU:HB3  | 2.07                     | 0.69              |
| 3:N:639:LEU:CD1   | 3:N:766:ALA:HB2  | 2.22                     | 0.69              |
| 2:C:182:VAL:HG11  | 2:C:193:LEU:CB   | 2.23                     | 0.69              |
| 3:D:133:ILE:HG22  | 3:D:134:VAL:N    | 2.06                     | 0.69              |
| 4:E:41:GLU:O      | 4:E:45:ARG:HD2   | 1.93                     | 0.69              |
| 1:F:24:VAL:HG22   | 1:F:196:THR:HG22 | 1.73                     | 0.69              |
| 2:H:1036:GLU:OE1  | 2:H:1036:GLU:N   | 2.25                     | 0.69              |
| 2:H:1102:LEU:N    | 3:I:7:LYS:O      | 2.25                     | 0.69              |
| 2:H:564:MET:CE    | 2:H:846:LYS:CE   | 2.70                     | 0.69              |
| 3:I:160:GLU:HG2   | 3:I:165:LYS:CB   | 2.21                     | 0.69              |
| 3:I:982:PHE:N     | 3:I:982:PHE:CD2  | 2.60                     | 0.69              |
| 1:L:173:PRO:O     | 1:L:201:THR:HG22 | 1.92                     | 0.69              |
| 2:M:211:LEU:HD23  | 2:M:221:LEU:CD2  | 2.22                     | 0.69              |
| 2:M:243:ARG:HB3   | 2:M:244:PRO:CD   | 2.16                     | 0.69              |
| 2:M:69:LEU:HD21   | 2:M:99:GLN:HE21  | 1.57                     | 0.69              |
| 2:M:1095:LEU:HB2  | 3:N:101:HIS:CE1  | 2.27                     | 0.69              |
| 3:N:1109:GLU:HG2  | 3:N:1201:CYS:HA  | 1.75                     | 0.69              |
| 3:N:1256:LEU:HG   | 3:N:1260:ILE:CD1 | 2.21                     | 0.69              |
| 3:N:465:LEU:HD21  | 3:N:509:PRO:HB2  | 1.75                     | 0.69              |
| 3:N:50:PHE:CE2    | 3:N:522:PRO:HG3  | 2.27                     | 0.69              |
| 3:N:681:ARG:HG3   | 3:N:682:ASP:N    | 2.07                     | 0.69              |
| 2:C:1012:PRO:HD2  | 2:C:1026:GLN:CG  | 2.22                     | 0.69              |
| 2:C:364:GLU:O     | 2:C:367:LEU:HG   | 1.91                     | 0.69              |
| 2:C:877:PRO:HG3   | 3:D:1023:MET:SD  | 2.32                     | 0.69              |
| 3:D:108:VAL:CB    | 3:D:109:PRO:HD3  | 2.22                     | 0.69              |
| 3:D:352:ASN:OD1   | 2:H:284:ARG:NH2  | 2.25                     | 0.69              |
| 2:H:906:PHE:CZ    | 3:I:1067:VAL:HA  | 2.28                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:119:SER:HB2   | 3:I:123:LEU:CB    | 2.19                     | 0.69              |
| 3:I:415:VAL:HG13  | 3:I:419:ASP:HB2   | 1.75                     | 0.69              |
| 1:G:74:ASP:CB     | 3:I:872:ARG:HH22  | 2.04                     | 0.69              |
| 3:I:980:MET:HB3   | 3:I:982:PHE:CE2   | 2.27                     | 0.69              |
| 4:J:54:LEU:HA     | 4:J:58:PRO:HG2    | 1.74                     | 0.69              |
| 2:M:512:ARG:HA    | 2:M:523:ILE:HD11  | 1.72                     | 0.69              |
| 2:M:723:THR:HG23  | 2:M:725:ASP:H     | 1.58                     | 0.69              |
| 3:N:1025:GLN:HE21 | 3:N:1025:GLN:HA   | 1.55                     | 0.69              |
| 3:N:407:VAL:HG22  | 3:N:408:GLU:N     | 2.02                     | 0.69              |
| 2:C:603:VAL:HG13  | 2:C:613:VAL:HG12  | 1.74                     | 0.69              |
| 2:C:9:ILE:HG12    | 2:C:907:ASP:CG    | 2.13                     | 0.69              |
| 3:D:1146:GLY:CA   | 3:D:1207:TYR:CB   | 2.69                     | 0.69              |
| 3:D:939:PHE:O     | 3:D:942:SER:HB3   | 1.92                     | 0.69              |
| 4:J:54:LEU:HD23   | 4:J:58:PRO:CD     | 2.23                     | 0.69              |
| 2:M:31:GLN:HG3    | 2:M:34:VAL:CG2    | 2.22                     | 0.69              |
| 3:N:171:LEU:HD21  | 3:N:175:VAL:HB    | 1.72                     | 0.69              |
| 3:N:980:MET:HB3   | 3:N:982:PHE:CE2   | 2.27                     | 0.69              |
| 7:Y:57:ARG:HB2    | 7:Y:57:ARG:HH21   | 1.56                     | 0.69              |
| 3:D:1095:THR:O    | 3:D:1099:VAL:HG23 | 1.92                     | 0.69              |
| 3:D:1438:ALA:O    | 3:D:1443:THR:HG22 | 1.93                     | 0.69              |
| 4:E:54:LEU:HA     | 4:E:58:PRO:HG2    | 1.75                     | 0.69              |
| 2:H:129:ILE:HG22  | 2:H:130:ASN:N     | 2.07                     | 0.69              |
| 2:H:187:ASN:O     | 2:H:188:LYS:HB3   | 1.90                     | 0.69              |
| 3:I:1442:ASN:ND2  | 3:I:1445:HIS:H    | 1.91                     | 0.69              |
| 3:I:1462:LEU:HD22 | 3:I:1472:ILE:CG2  | 2.23                     | 0.69              |
| 2:H:987:ILE:HD11  | 3:I:946:GLY:CA    | 2.22                     | 0.69              |
| 1:K:11:PHE:HB2    | 1:K:25:LEU:HD13   | 1.75                     | 0.69              |
| 2:M:571:LEU:HD21  | 2:M:699:PHE:O     | 1.92                     | 0.69              |
| 3:N:1124:GLN:OE1  | 3:N:1135:ARG:HA   | 1.92                     | 0.69              |
| 3:N:116:LEU:CD2   | 3:N:118:LEU:HG    | 2.18                     | 0.69              |
| 3:N:415:VAL:HG13  | 3:N:419:ASP:HB2   | 1.75                     | 0.69              |
| 3:I:982:PHE:CG    | 7:Y:125:MET:SD    | 2.86                     | 0.69              |
| 3:D:1211:MET:CG   | 3:D:1212:ALA:H    | 2.00                     | 0.69              |
| 2:H:276:LYS:HA    | 2:H:280:LYS:HD2   | 1.75                     | 0.69              |
| 2:H:374:ASN:H     | 2:H:374:ASN:HD22  | 1.40                     | 0.69              |
| 1:K:75:VAL:O      | 1:K:79:ILE:HG23   | 1.92                     | 0.69              |
| 2:M:135:VAL:HG11  | 2:M:407:LYS:HA    | 1.75                     | 0.69              |
| 2:M:754:ILE:HD12  | 2:M:754:ILE:H     | 1.57                     | 0.69              |
| 3:N:1359:GLN:HE22 | 7:Z:52:LYS:CD     | 2.06                     | 0.69              |
| 3:N:1489:GLN:O    | 3:N:1493:LYS:HG2  | 1.93                     | 0.69              |
| 3:N:432:TYR:CG    | 3:N:450:TYR:HD2   | 2.11                     | 0.69              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:99:ALA:HA     | 3:N:575:GLN:HE22 | 1.57                     | 0.69              |
| 1:A:42:ARG:NH1    | 1:B:34:VAL:HG12  | 2.07                     | 0.69              |
| 1:B:153:ALA:HA    | 1:B:156:HIS:HE2  | 1.58                     | 0.69              |
| 2:C:885:ILE:HG13  | 3:D:949:ILE:HG22 | 1.75                     | 0.69              |
| 2:H:89:THR:HA     | 2:H:129:ILE:O    | 1.92                     | 0.69              |
| 2:H:580:MET:SD    | 2:H:584:GLU:HG3  | 2.33                     | 0.69              |
| 3:I:1123:PHE:HE2  | 3:I:1184:GLN:HA  | 1.58                     | 0.69              |
| 3:I:452:ILE:HD13  | 3:I:452:ILE:O    | 1.93                     | 0.69              |
| 2:M:52:PHE:CZ     | 2:M:98:LEU:CG    | 2.73                     | 0.69              |
| 3:N:1256:LEU:HB3  | 3:N:1257:PRO:HD3 | 1.74                     | 0.69              |
| 3:N:379:ALA:O     | 3:N:380:GLU:HG3  | 1.92                     | 0.69              |
| 2:M:987:ILE:CG2   | 3:N:948:THR:HG21 | 2.13                     | 0.69              |
| 7:Y:83:ILE:HD13   | 7:Y:89:VAL:HG21  | 1.75                     | 0.69              |
| 1:A:161:ARG:HB2   | 1:A:161:ARG:CZ   | 2.20                     | 0.69              |
| 1:A:31:GLY:N      | 1:A:193:ASP:OD1  | 2.23                     | 0.69              |
| 2:C:1019:GLN:NE2  | 3:D:621:LYS:HG3  | 2.08                     | 0.69              |
| 2:C:124:ASP:HB2   | 2:C:407:LYS:HZ1  | 1.58                     | 0.69              |
| 3:D:116:LEU:O     | 3:D:117:ASP:HB3  | 1.93                     | 0.69              |
| 3:D:403:PHE:HB2   | 3:D:423:ASP:OD1  | 1.93                     | 0.69              |
| 3:D:481:MET:HE3   | 3:D:493:ARG:HA   | 1.74                     | 0.69              |
| 3:D:715:ALA:HB3   | 3:D:764:LEU:HA   | 1.75                     | 0.69              |
| 1:F:62:LEU:H      | 1:F:62:LEU:HD12  | 1.58                     | 0.69              |
| 1:F:7:LYS:O       | 1:F:7:LYS:HE2    | 1.92                     | 0.69              |
| 1:F:218:LEU:CD2   | 1:G:222:LEU:HD21 | 2.23                     | 0.69              |
| 1:G:41:ARG:HG3    | 1:G:177:VAL:CG2  | 2.22                     | 0.69              |
| 2:H:565:GLN:HE21  | 2:H:842:ARG:CG   | 2.02                     | 0.69              |
| 2:H:863:ASP:OD1   | 2:H:865:THR:HG22 | 1.93                     | 0.69              |
| 2:H:987:ILE:HD11  | 3:I:946:GLY:HA2  | 1.73                     | 0.69              |
| 3:I:127:LEU:O     | 3:I:457:GLY:HA2  | 1.92                     | 0.69              |
| 3:I:1280:VAL:HA   | 3:I:1318:TYR:HA  | 1.74                     | 0.69              |
| 3:I:643:GLY:O     | 3:I:726:ILE:HG23 | 1.92                     | 0.69              |
| 1:L:62:LEU:H      | 1:L:62:LEU:HD12  | 1.57                     | 0.69              |
| 3:N:1258:ARG:HH21 | 3:N:1351:GLU:HG2 | 1.57                     | 0.69              |
| 3:N:1261:GLU:OE1  | 3:N:1268:PRO:HA  | 1.93                     | 0.69              |
| 3:N:906:GLN:HB3   | 3:N:911:LEU:HD11 | 1.74                     | 0.69              |
| 2:C:101:ILE:HG23  | 2:C:108:ILE:HG12 | 1.75                     | 0.68              |
| 3:D:1288:GLU:O    | 3:D:1289:LYS:HG3 | 1.93                     | 0.68              |
| 3:D:996:TRP:CG    | 3:D:1056:PRO:HG2 | 2.28                     | 0.68              |
| 1:G:87:VAL:HG21   | 1:G:144:VAL:HG11 | 1.76                     | 0.68              |
| 2:H:309:TYR:C     | 2:H:313:LEU:HD13 | 2.11                     | 0.68              |
| 2:H:316:GLY:C     | 2:H:318:PRO:HD3  | 2.14                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:395:LYS:HD3   | 2:H:397:GLU:OE2   | 1.93                     | 0.68              |
| 2:H:497:ALA:HA    | 2:H:515:ALA:HA    | 1.75                     | 0.68              |
| 3:I:1026:SER:C    | 3:I:1028:ALA:H    | 1.96                     | 0.68              |
| 1:K:11:PHE:HE1    | 1:K:23:PHE:HB3    | 1.58                     | 0.68              |
| 2:M:129:ILE:O     | 2:M:131:GLY:N     | 2.26                     | 0.68              |
| 2:M:261:ILE:CD1   | 2:M:261:ILE:H     | 2.04                     | 0.68              |
| 2:M:309:TYR:O     | 2:M:313:LEU:HB2   | 1.92                     | 0.68              |
| 3:N:1481:VAL:CG1  | 4:O:18:ARG:HA     | 2.17                     | 0.68              |
| 4:O:33:HIS:CG     | 4:O:89:MET:HG2    | 2.28                     | 0.68              |
| 2:C:996:LYS:NZ    | 2:C:1000:MET:SD   | 2.64                     | 0.68              |
| 2:C:984:GLU:HG2   | 3:D:944:THR:O     | 1.94                     | 0.68              |
| 3:D:1276:GLU:C    | 3:D:1277:ILE:HD12 | 2.13                     | 0.68              |
| 3:D:783:ARG:NH1   | 7:X:41:ASP:HB2    | 2.09                     | 0.68              |
| 1:F:161:ARG:HB2   | 1:F:161:ARG:CZ    | 2.20                     | 0.68              |
| 2:H:1045:ALA:HB1  | 2:H:1048:THR:HB   | 1.75                     | 0.68              |
| 2:H:113:VAL:O     | 2:H:115:LEU:HD23  | 1.93                     | 0.68              |
| 3:I:1312:LEU:CD1  | 3:I:1327:ARG:NH2  | 2.55                     | 0.68              |
| 3:I:153:LEU:HD13  | 3:I:158:TYR:HB2   | 1.75                     | 0.68              |
| 3:I:631:ILE:O     | 3:I:631:ILE:HD13  | 1.92                     | 0.68              |
| 3:I:799:LYS:HD3   | 3:I:826:PRO:HG2   | 1.74                     | 0.68              |
| 2:H:1060:ILE:HD11 | 3:I:85:VAL:H      | 1.56                     | 0.68              |
| 2:M:184:MET:HB2   | 2:M:193:LEU:HG    | 1.73                     | 0.68              |
| 2:M:224:GLU:O     | 2:M:228:ALA:HB3   | 1.93                     | 0.68              |
| 2:M:357:GLU:O     | 2:M:360:LEU:HD23  | 1.93                     | 0.68              |
| 2:M:516:ARG:HE    | 3:N:1068:LEU:HD13 | 1.57                     | 0.68              |
| 3:N:780:LYS:NZ    | 7:Z:38:GLU:HB3    | 2.08                     | 0.68              |
| 3:N:881:LEU:HD21  | 3:N:941:PHE:CZ    | 2.28                     | 0.68              |
| 1:B:33:GLY:O      | 1:B:195:LEU:HD22  | 1.93                     | 0.68              |
| 1:B:38:ASN:HB3    | 1:B:39:PRO:HD3    | 1.74                     | 0.68              |
| 2:C:408:ARG:NH2   | 2:C:455:LEU:HD11  | 2.08                     | 0.68              |
| 2:C:328:LEU:HD11  | 2:C:434:HIS:HD2   | 1.56                     | 0.68              |
| 2:C:580:MET:SD    | 2:C:584:GLU:HG3   | 2.33                     | 0.68              |
| 2:C:950:LEU:HD12  | 2:C:952:LEU:HD21  | 1.75                     | 0.68              |
| 3:D:1111:ASP:OD1  | 3:D:1203:LYS:HD2  | 1.93                     | 0.68              |
| 1:F:24:VAL:HG13   | 1:F:196:THR:HG22  | 1.76                     | 0.68              |
| 3:N:406:ASP:O     | 3:N:422:ALA:HB1   | 1.93                     | 0.68              |
| 3:N:81:THR:HG21   | 3:N:85:VAL:HG11   | 1.76                     | 0.68              |
| 7:Y:102:VAL:HG21  | 7:Y:125:MET:HE1   | 1.75                     | 0.68              |
| 2:C:258:TYR:CE2   | 2:C:290:LEU:HD11  | 2.29                     | 0.68              |
| 2:C:673:LEU:HD22  | 2:C:867:VAL:HG12  | 1.75                     | 0.68              |
| 3:D:1101:VAL:CG1  | 3:D:1424:VAL:O    | 2.41                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1105:ILE:HD12 | 3:D:1105:ILE:N    | 2.09                     | 0.68              |
| 3:D:881:LEU:HD21  | 3:D:941:PHE:CZ    | 2.28                     | 0.68              |
| 3:I:1166:LEU:HD23 | 3:I:1166:LEU:H    | 1.59                     | 0.68              |
| 3:I:143:ASN:CA    | 3:I:161:LEU:HD11  | 2.24                     | 0.68              |
| 3:I:615:ARG:HG3   | 3:I:619:LEU:CD2   | 2.23                     | 0.68              |
| 3:I:799:LYS:HD3   | 3:I:799:LYS:O     | 1.93                     | 0.68              |
| 2:M:580:MET:SD    | 2:M:584:GLU:HG3   | 2.34                     | 0.68              |
| 2:M:854:PRO:HB2   | 2:M:856:GLU:CG    | 2.24                     | 0.68              |
| 3:N:128:TYR:CE2   | 3:N:458:ALA:HA    | 2.28                     | 0.68              |
| 3:N:520:LEU:CD1   | 3:N:521:PRO:HD2   | 2.20                     | 0.68              |
| 2:C:1056:LYS:HD3  | 3:D:623:VAL:HG13  | 1.74                     | 0.68              |
| 2:C:432:ARG:NH2   | 3:D:1047:LYS:HD3  | 2.08                     | 0.68              |
| 2:C:473:ARG:HB2   | 2:C:531:PHE:HE1   | 1.56                     | 0.68              |
| 2:H:274:ARG:NH1   | 2:H:274:ARG:HG2   | 2.09                     | 0.68              |
| 2:M:139:GLN:NE2   | 2:M:414:GLY:HA3   | 2.07                     | 0.68              |
| 2:M:22:GLN:HE21   | 2:M:336:VAL:HG22  | 1.59                     | 0.68              |
| 2:M:666:LEU:HG    | 2:M:668:LEU:HD11  | 1.75                     | 0.68              |
| 3:N:501:ALA:HB3   | 3:N:1452:ILE:HG22 | 1.73                     | 0.68              |
| 3:N:187:LYS:HE2   | 3:N:199:LEU:HG    | 1.75                     | 0.68              |
| 3:N:843:PHE:CE1   | 3:N:864:VAL:HG11  | 2.28                     | 0.68              |
| 1:A:186:LEU:HD23  | 1:A:186:LEU:C     | 2.14                     | 0.68              |
| 1:A:218:LEU:HD23  | 1:B:222:LEU:CD2   | 2.22                     | 0.68              |
| 2:C:294:GLU:O     | 2:C:295:ASP:HB2   | 1.94                     | 0.68              |
| 2:C:878:SER:HB3   | 3:D:1029:ARG:NH1  | 2.07                     | 0.68              |
| 3:D:166:GLN:HE21  | 3:D:396:VAL:HG12  | 1.58                     | 0.68              |
| 3:D:458:ALA:HB2   | 3:D:575:GLN:NE2   | 2.09                     | 0.68              |
| 2:H:39:ARG:HB2    | 2:H:45:GLN:NE2    | 2.07                     | 0.68              |
| 2:H:570:PRO:HD2   | 2:H:635:THR:HG21  | 1.76                     | 0.68              |
| 2:H:705:ILE:HG12  | 2:H:828:ALA:HB2   | 1.74                     | 0.68              |
| 3:I:1261:GLU:OE1  | 3:I:1268:PRO:HA   | 1.93                     | 0.68              |
| 1:L:152:PRO:HG2   | 3:N:857:ILE:CD1   | 2.23                     | 0.68              |
| 1:L:206:THR:HG22  | 1:L:209:GLU:H     | 1.58                     | 0.68              |
| 2:M:111:ASP:OD2   | 2:M:369:PRO:HB3   | 1.91                     | 0.68              |
| 2:M:334:ARG:HG2   | 2:M:338:GLU:CD    | 2.14                     | 0.68              |
| 2:M:611:ILE:HG13  | 2:M:625:LEU:HD21  | 1.74                     | 0.68              |
| 2:M:84:ARG:NH1    | 2:M:84:ARG:HG3    | 2.01                     | 0.68              |
| 3:N:115:LEU:HD12  | 3:N:502:PHE:CE1   | 2.28                     | 0.68              |
| 3:N:715:ALA:HB3   | 3:N:764:LEU:HA    | 1.75                     | 0.68              |
| 3:N:781:PRO:HB2   | 3:N:786:ILE:HD11  | 1.74                     | 0.68              |
| 3:N:88:TYR:N      | 3:N:88:TYR:CD2    | 2.58                     | 0.68              |
| 2:C:1055:LEU:HD22 | 2:C:1066:ALA:HB2  | 1.75                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1081:VAL:HG13 | 2:C:1085:PHE:HB3  | 1.76                     | 0.68              |
| 1:G:74:ASP:CB     | 3:I:872:ARG:NH2   | 2.57                     | 0.68              |
| 2:H:1081:VAL:HG13 | 2:H:1085:PHE:HB3  | 1.76                     | 0.68              |
| 3:I:1101:VAL:HG13 | 3:I:1428:ALA:HB2  | 1.76                     | 0.68              |
| 3:I:781:PRO:HB2   | 3:I:786:ILE:HD11  | 1.74                     | 0.68              |
| 3:I:881:LEU:HD21  | 3:I:941:PHE:CZ    | 2.28                     | 0.68              |
| 1:K:62:LEU:H      | 1:K:62:LEU:HD12   | 1.59                     | 0.68              |
| 2:M:1081:VAL:HG13 | 2:M:1085:PHE:HB3  | 1.75                     | 0.68              |
| 2:M:236:ILE:N     | 2:M:236:ILE:HD12  | 2.08                     | 0.68              |
| 2:M:570:PRO:HD2   | 2:M:635:THR:HG21  | 1.76                     | 0.68              |
| 3:N:1277:ILE:HD13 | 3:N:1301:LYS:HB2  | 1.74                     | 0.68              |
| 3:N:180:LYS:HZ1   | 3:N:386:HIS:CA    | 2.06                     | 0.68              |
| 2:M:1036:GLU:HG3  | 3:N:707:THR:OG1   | 1.92                     | 0.68              |
| 2:M:987:ILE:HD12  | 3:N:948:THR:CG2   | 2.24                     | 0.68              |
| 1:A:128:HIS:HE1   | 1:A:131:THR:HG23  | 1.58                     | 0.68              |
| 1:A:54:THR:HG22   | 1:A:158:ILE:HD11  | 1.73                     | 0.68              |
| 1:A:62:LEU:HD12   | 1:A:62:LEU:H      | 1.58                     | 0.68              |
| 1:B:19:GLU:HG3    | 1:B:201:THR:O     | 1.94                     | 0.68              |
| 2:C:754:ILE:H     | 2:C:754:ILE:HD12  | 1.57                     | 0.68              |
| 3:D:1128:VAL:HG13 | 3:D:1129:THR:HG22 | 1.76                     | 0.68              |
| 3:D:126:VAL:CG1   | 3:D:132:TYR:CB    | 2.71                     | 0.68              |
| 3:D:205:TYR:CD1   | 3:D:390:PRO:HG3   | 2.29                     | 0.68              |
| 3:I:108:VAL:CB    | 3:I:109:PRO:HD3   | 2.22                     | 0.68              |
| 3:I:843:PHE:CE1   | 3:I:864:VAL:HG11  | 2.29                     | 0.68              |
| 1:K:176:ARG:HG3   | 1:K:200:TRP:CE3   | 2.29                     | 0.68              |
| 1:L:123:MET:C     | 1:L:125:PRO:HD3   | 2.14                     | 0.68              |
| 2:M:1012:PRO:HD2  | 2:M:1026:GLN:CB   | 2.24                     | 0.68              |
| 2:M:442:GLU:HG2   | 2:M:454:SER:HB2   | 1.74                     | 0.68              |
| 2:M:661:SER:HA    | 2:M:665:PHE:O     | 1.94                     | 0.68              |
| 3:N:1003:VAL:HG11 | 3:N:1041:LEU:HD22 | 1.76                     | 0.68              |
| 3:N:361:VAL:HG11  | 3:N:367:ILE:HD11  | 1.75                     | 0.68              |
| 7:Z:102:VAL:HG11  | 7:Z:125:MET:CE    | 2.24                     | 0.68              |
| 2:C:1105:LYS:HZ1  | 2:C:1107:ASN:HB2  | 1.59                     | 0.68              |
| 2:C:257:VAL:HG12  | 2:C:263:ASP:OD1   | 1.94                     | 0.68              |
| 2:C:148:PHE:CE1   | 2:C:309:TYR:HB3   | 2.29                     | 0.68              |
| 3:D:465:LEU:HD21  | 3:D:509:PRO:HB2   | 1.74                     | 0.68              |
| 3:D:987:GLU:OE1   | 7:X:120:SER:CB    | 2.42                     | 0.68              |
| 1:G:88:ARG:HD2    | 1:G:123:MET:SD    | 2.33                     | 0.68              |
| 2:H:224:GLU:O     | 2:H:228:ALA:HB3   | 1.94                     | 0.68              |
| 2:H:195:LEU:HD11  | 2:H:234:ALA:O     | 1.94                     | 0.68              |
| 2:H:503:LEU:HD23  | 2:H:507:ARG:O     | 1.93                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:666:LEU:HG    | 2:H:668:LEU:HD11  | 1.76                     | 0.68              |
| 3:I:590:PRO:HB2   | 3:I:600:LEU:CD1   | 2.24                     | 0.68              |
| 4:J:64:ALA:O      | 4:J:68:LEU:HD13   | 1.94                     | 0.68              |
| 1:K:58:ILE:CD1    | 1:K:140:MET:HB3   | 2.23                     | 0.68              |
| 3:N:1485:GLN:O    | 4:O:75:PHE:HA     | 1.93                     | 0.68              |
| 3:N:881:LEU:HD21  | 3:N:941:PHE:HZ    | 1.58                     | 0.68              |
| 2:H:879:ARG:NH2   | 7:Y:42:ASP:OD1    | 2.27                     | 0.68              |
| 2:C:666:LEU:HG    | 2:C:668:LEU:HD11  | 1.76                     | 0.68              |
| 3:D:158:TYR:CD1   | 3:D:162:ARG:CG    | 2.77                     | 0.68              |
| 3:D:806:PHE:CZ    | 3:D:813:LEU:HB3   | 2.28                     | 0.68              |
| 2:H:754:ILE:H     | 2:H:754:ILE:HD12  | 1.57                     | 0.68              |
| 2:H:950:LEU:HD12  | 2:H:952:LEU:HD21  | 1.75                     | 0.68              |
| 3:I:115:LEU:CD1   | 3:I:502:PHE:CE1   | 2.77                     | 0.68              |
| 3:I:481:MET:HE3   | 3:I:493:ARG:HA    | 1.76                     | 0.68              |
| 2:M:418:LEU:HD12  | 2:M:418:LEU:N     | 2.08                     | 0.68              |
| 2:M:97:ARG:N      | 2:M:97:ARG:HD3    | 2.07                     | 0.68              |
| 4:O:47:LYS:HA     | 4:O:54:LEU:HB3    | 1.75                     | 0.68              |
| 2:C:863:ASP:OD1   | 2:C:865:THR:HG22  | 1.93                     | 0.67              |
| 3:D:1101:VAL:HG11 | 3:D:1424:VAL:O    | 1.93                     | 0.67              |
| 1:F:161:ARG:HH11  | 1:F:161:ARG:HB2   | 1.57                     | 0.67              |
| 1:G:19:GLU:HG3    | 1:G:201:THR:O     | 1.94                     | 0.67              |
| 2:H:1098:ASP:N    | 3:I:11:ALA:O      | 2.27                     | 0.67              |
| 2:H:171:TRP:CH2   | 2:H:417:GLY:O     | 2.47                     | 0.67              |
| 2:H:471:TYR:O     | 2:H:483:VAL:HG13  | 1.93                     | 0.67              |
| 3:I:398:ALA:HB2   | 3:I:447:VAL:CA    | 2.24                     | 0.67              |
| 1:K:161:ARG:HH11  | 1:K:161:ARG:HB2   | 1.57                     | 0.67              |
| 2:M:863:ASP:OD1   | 2:M:865:THR:HG22  | 1.93                     | 0.67              |
| 2:M:1034:GLU:OE1  | 3:N:1096:ARG:NH2  | 2.26                     | 0.67              |
| 3:N:190:GLU:HA    | 3:N:196:VAL:HA    | 1.76                     | 0.67              |
| 4:O:18:ARG:NH2    | 4:O:18:ARG:HB2    | 2.09                     | 0.67              |
| 3:N:991:GLN:HE22  | 7:Z:112:VAL:HB    | 1.59                     | 0.67              |
| 1:A:161:ARG:HB2   | 1:A:161:ARG:HH11  | 1.57                     | 0.67              |
| 1:B:187:GLY:O     | 3:D:688:TRP:CD1   | 2.42                     | 0.67              |
| 2:C:154:ARG:NH1   | 2:C:178:PRO:HD3   | 2.09                     | 0.67              |
| 2:C:312:ALA:HB1   | 2:C:318:PRO:HG2   | 1.76                     | 0.67              |
| 3:D:393:ILE:N     | 3:D:393:ILE:HD12  | 2.08                     | 0.67              |
| 2:H:512:ARG:CB    | 2:H:523:ILE:HD11  | 2.24                     | 0.67              |
| 3:I:715:ALA:HB3   | 3:I:764:LEU:HA    | 1.75                     | 0.67              |
| 2:M:211:LEU:CD2   | 2:M:221:LEU:HD21  | 2.20                     | 0.67              |
| 2:M:571:LEU:HD11  | 2:M:700:TYR:HA    | 1.74                     | 0.67              |
| 2:M:516:ARG:CZ    | 3:N:1068:LEU:HD22 | 2.25                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:119:SER:HB2   | 3:N:123:LEU:H     | 1.58                     | 0.67              |
| 3:N:169:TYR:CE1   | 3:N:198:ARG:HG3   | 2.30                     | 0.67              |
| 1:A:42:ARG:NH1    | 1:B:34:VAL:CB     | 2.56                     | 0.67              |
| 1:B:206:THR:HG22  | 1:B:209:GLU:H     | 1.58                     | 0.67              |
| 2:C:211:LEU:HD11  | 2:C:311:PHE:CD1   | 2.30                     | 0.67              |
| 2:C:611:ILE:HG13  | 2:C:625:LEU:HD21  | 1.76                     | 0.67              |
| 3:D:179:VAL:HG13  | 3:D:183:GLU:HB3   | 1.76                     | 0.67              |
| 3:D:521:PRO:HB2   | 3:D:524:LEU:HD13  | 1.76                     | 0.67              |
| 2:C:988:VAL:HG11  | 3:D:949:ILE:O     | 1.94                     | 0.67              |
| 2:H:1056:LYS:CD   | 3:I:623:VAL:CG1   | 2.70                     | 0.67              |
| 3:I:785:ILE:HD12  | 3:I:785:ILE:N     | 2.02                     | 0.67              |
| 2:M:63:GLY:HA3    | 2:M:103:LYS:HE2   | 1.74                     | 0.67              |
| 2:M:676:ILE:HG21  | 2:M:988:VAL:CG1   | 2.21                     | 0.67              |
| 3:N:1106:VAL:HG12 | 3:N:1107:VAL:N    | 2.09                     | 0.67              |
| 2:M:1043:TYR:CE2  | 3:N:710:ARG:HD2   | 2.29                     | 0.67              |
| 7:X:155:HIS:O     | 7:X:156:GLY:C     | 2.32                     | 0.67              |
| 7:Y:139:SER:HB3   | 7:Y:148:GLU:HG3   | 1.76                     | 0.67              |
| 2:C:272:ALA:HA    | 2:C:464:LEU:HD22  | 1.76                     | 0.67              |
| 2:C:442:GLU:HG2   | 2:C:454:SER:HB2   | 1.74                     | 0.67              |
| 2:C:54:ILE:CG2    | 2:C:66:LEU:HB3    | 2.24                     | 0.67              |
| 2:C:678:PRO:HG3   | 2:C:873:PRO:HD2   | 1.75                     | 0.67              |
| 3:D:1321:ALA:O    | 3:D:1339:LYS:HD2  | 1.95                     | 0.67              |
| 3:D:982:PHE:N     | 3:D:982:PHE:CD2   | 2.60                     | 0.67              |
| 3:I:205:TYR:CB    | 3:I:393:ILE:HG13  | 2.24                     | 0.67              |
| 2:M:98:LEU:N      | 2:M:98:LEU:HD12   | 2.09                     | 0.67              |
| 3:N:1257:PRO:CA   | 3:N:1260:ILE:HD12 | 2.15                     | 0.67              |
| 3:N:1367:HIS:HA   | 3:N:1370:ILE:HD12 | 1.77                     | 0.67              |
| 3:N:970:LYS:HD3   | 7:Z:113:LEU:HD21  | 1.76                     | 0.67              |
| 7:Y:22:GLU:HB3    | 7:Y:62:ILE:HD11   | 1.77                     | 0.67              |
| 2:C:305:PRO:HA    | 2:C:308:ARG:HB3   | 1.76                     | 0.67              |
| 2:C:661:SER:HA    | 2:C:665:PHE:O     | 1.94                     | 0.67              |
| 3:D:843:PHE:CE1   | 3:D:864:VAL:HG11  | 2.29                     | 0.67              |
| 3:D:890:VAL:HG11  | 3:D:922:LEU:CD1   | 2.25                     | 0.67              |
| 1:F:128:HIS:HE1   | 1:F:131:THR:HG23  | 1.59                     | 0.67              |
| 2:H:838:LYS:O     | 2:H:838:LYS:HG3   | 1.94                     | 0.67              |
| 1:L:19:GLU:HG3    | 1:L:201:THR:O     | 1.93                     | 0.67              |
| 2:M:99:GLN:HA     | 2:M:109:LYS:O     | 1.95                     | 0.67              |
| 2:M:140:ILE:HG22  | 2:M:333:ILE:HG13  | 1.76                     | 0.67              |
| 2:M:47:ALA:O      | 2:M:50:GLU:HB3    | 1.94                     | 0.67              |
| 2:C:3:ILE:N       | 2:C:3:ILE:HD12    | 2.10                     | 0.67              |
| 2:C:80:GLN:HB2    | 2:C:84:ARG:HH12   | 1.60                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1197:ARG:HB3  | 3:D:1396:GLU:CD   | 2.15                     | 0.67              |
| 3:D:139:GLY:N     | 3:D:147:VAL:HG21  | 2.10                     | 0.67              |
| 1:F:176:ARG:HG3   | 1:F:200:TRP:CE3   | 2.29                     | 0.67              |
| 1:G:33:GLY:O      | 1:G:195:LEU:HD22  | 1.94                     | 0.67              |
| 2:H:289:THR:O     | 2:H:291:ALA:N     | 2.26                     | 0.67              |
| 2:H:428:ARG:HA    | 2:H:450:GLY:O     | 1.95                     | 0.67              |
| 2:H:678:PRO:HG3   | 2:H:873:PRO:HD2   | 1.76                     | 0.67              |
| 2:H:878:SER:O     | 3:I:1034:GLN:NE2  | 2.27                     | 0.67              |
| 3:I:1459:LEU:HB3  | 3:I:1465:ASN:OD1  | 1.95                     | 0.67              |
| 3:I:639:LEU:CD1   | 3:I:766:ALA:HB2   | 2.21                     | 0.67              |
| 3:N:1094:LEU:HG   | 3:N:1098:LEU:CD2  | 2.25                     | 0.67              |
| 3:N:1102:THR:HA   | 3:N:1105:ILE:HD13 | 1.76                     | 0.67              |
| 3:N:1321:ALA:O    | 3:N:1339:LYS:HD2  | 1.95                     | 0.67              |
| 3:N:600:LEU:HD12  | 3:N:600:LEU:H     | 1.59                     | 0.67              |
| 7:X:57:ARG:CB     | 7:X:57:ARG:HH21   | 2.00                     | 0.67              |
| 3:N:783:ARG:CZ    | 7:Z:41:ASP:HB3    | 2.23                     | 0.67              |
| 1:A:176:ARG:HG3   | 1:A:200:TRP:CE3   | 2.29                     | 0.67              |
| 1:B:86:VAL:CG1    | 1:B:124:ASN:HB2   | 2.24                     | 0.67              |
| 2:C:273:GLY:HA2   | 2:C:276:LYS:HZ2   | 1.59                     | 0.67              |
| 2:C:512:ARG:CB    | 2:C:523:ILE:HD11  | 2.24                     | 0.67              |
| 2:C:878:SER:HA    | 3:D:1034:GLN:NE2  | 2.09                     | 0.67              |
| 3:D:367:ILE:HG22  | 3:D:368:VAL:HG23  | 1.77                     | 0.67              |
| 3:D:368:VAL:HB    | 3:D:377:VAL:CG2   | 2.24                     | 0.67              |
| 2:H:676:ILE:O     | 3:I:948:THR:HG22  | 1.95                     | 0.67              |
| 3:I:134:VAL:CG2   | 3:I:460:ALA:HB1   | 2.18                     | 0.67              |
| 3:I:800:LYS:HD2   | 3:I:804:LEU:HB3   | 1.77                     | 0.67              |
| 3:I:881:LEU:HD21  | 3:I:941:PHE:HZ    | 1.58                     | 0.67              |
| 2:M:1086:ARG:CZ   | 3:N:88:TYR:CZ     | 2.77                     | 0.67              |
| 2:M:101:ILE:CD1   | 2:M:108:ILE:HD11  | 2.22                     | 0.67              |
| 2:M:391:LEU:O     | 2:M:393:GLN:NE2   | 2.28                     | 0.67              |
| 2:M:512:ARG:CB    | 2:M:523:ILE:HD11  | 2.24                     | 0.67              |
| 3:N:860:LEU:O     | 3:N:877:PRO:HD2   | 1.95                     | 0.67              |
| 1:A:74:ASP:O      | 1:A:78:ILE:HG12   | 1.95                     | 0.67              |
| 2:C:185:LYS:CG    | 2:C:190:LYS:HB3   | 2.24                     | 0.67              |
| 2:C:368:THR:HB    | 2:C:369:PRO:HD2   | 1.75                     | 0.67              |
| 3:D:1283:ILE:HG22 | 3:D:1284:GLU:H    | 1.58                     | 0.67              |
| 3:D:1311:LEU:HD23 | 3:D:1311:LEU:N    | 2.10                     | 0.67              |
| 3:D:618:LEU:HD21  | 3:D:1463:LYS:HE2  | 1.75                     | 0.67              |
| 3:D:408:GLU:CG    | 3:D:409:VAL:H     | 2.07                     | 0.67              |
| 3:D:881:LEU:HD21  | 3:D:941:PHE:HZ    | 1.58                     | 0.67              |
| 3:D:991:GLN:NE2   | 7:X:112:VAL:CB    | 2.46                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:162:ILE:HG13  | 1:G:163:ASN:N     | 2.10                     | 0.67              |
| 3:I:131:LYS:HG3   | 3:I:568:ARG:HD3   | 0.68                     | 0.67              |
| 3:I:1462:LEU:HD22 | 3:I:1472:ILE:HG22 | 1.77                     | 0.67              |
| 3:I:1485:GLN:HE21 | 4:J:79:LEU:N      | 1.92                     | 0.67              |
| 3:I:115:LEU:CD1   | 3:I:502:PHE:HE1   | 2.08                     | 0.67              |
| 3:I:860:LEU:O     | 3:I:877:PRO:HD2   | 1.95                     | 0.67              |
| 3:I:890:VAL:HG11  | 3:I:922:LEU:CD1   | 2.25                     | 0.67              |
| 2:M:163:ILE:HD12  | 2:M:171:TRP:CH2   | 2.29                     | 0.67              |
| 2:M:480:THR:HB    | 2:M:482:GLU:H     | 1.60                     | 0.67              |
| 2:M:77:PRO:HD2    | 2:M:91:GLN:O      | 1.94                     | 0.67              |
| 6:Q:12:G:H2'      | 6:Q:13:G:C8       | 2.30                     | 0.67              |
| 7:X:19:LEU:O      | 7:X:23:ARG:HG3    | 1.93                     | 0.67              |
| 2:C:570:PRO:HD2   | 2:C:635:THR:HG21  | 1.75                     | 0.67              |
| 2:C:878:SER:OG    | 3:D:1029:ARG:CD   | 2.42                     | 0.67              |
| 3:D:860:LEU:O     | 3:D:877:PRO:HD2   | 1.95                     | 0.67              |
| 2:H:260:LEU:HD23  | 2:H:260:LEU:C     | 2.15                     | 0.67              |
| 2:H:697:ARG:HD2   | 2:H:699:PHE:CE1   | 2.30                     | 0.67              |
| 3:I:1403:LEU:O    | 3:I:1407:LEU:HB2  | 1.94                     | 0.67              |
| 3:I:996:TRP:CE3   | 3:I:999:THR:HG21  | 2.30                     | 0.67              |
| 2:M:1086:ARG:NH1  | 3:N:88:TYR:CE1    | 2.63                     | 0.67              |
| 3:N:1122:LEU:HD11 | 3:N:1186:VAL:HG23 | 1.76                     | 0.67              |
| 3:N:1403:LEU:O    | 3:N:1407:LEU:HB2  | 1.94                     | 0.67              |
| 3:N:26:VAL:HG23   | 3:N:26:VAL:O      | 1.95                     | 0.67              |
| 2:M:1070:ILE:HG23 | 3:N:656:PHE:CD1   | 2.29                     | 0.67              |
| 7:Z:16:MET:HE2    | 7:Z:69:LEU:HD13   | 1.77                     | 0.67              |
| 1:A:22:GLU:OE2    | 1:A:198:ARG:HB3   | 1.95                     | 0.67              |
| 1:A:56:VAL:HG13   | 1:A:142:VAL:CG1   | 2.23                     | 0.67              |
| 2:C:95:TYR:HD2    | 2:C:114:PHE:CB    | 2.07                     | 0.67              |
| 3:D:1299:PHE:HD2  | 3:D:1299:PHE:H    | 1.41                     | 0.67              |
| 2:C:1086:ARG:HD3  | 3:D:88:TYR:CD1    | 2.30                     | 0.67              |
| 2:H:854:PRO:HB2   | 2:H:856:GLU:CG    | 2.24                     | 0.67              |
| 2:H:997:LEU:C     | 2:H:999:HIS:H     | 1.99                     | 0.67              |
| 3:I:1437:ALA:HB1  | 3:I:1446:VAL:HG22 | 1.77                     | 0.67              |
| 3:I:26:VAL:O      | 3:I:26:VAL:HG23   | 1.95                     | 0.67              |
| 3:I:625:TYR:HB3   | 3:I:749:VAL:HG23  | 1.76                     | 0.67              |
| 3:N:1197:ARG:HB3  | 3:N:1396:GLU:CD   | 2.15                     | 0.67              |
| 3:N:407:VAL:HA    | 3:N:422:ALA:HB2   | 1.77                     | 0.67              |
| 2:C:685:GLU:OE2   | 7:X:41:ASP:CB     | 2.43                     | 0.67              |
| 2:C:473:ARG:HG2   | 2:C:473:ARG:NH1   | 2.09                     | 0.66              |
| 2:C:850:ALA:HA    | 3:D:632:VAL:CG1   | 2.26                     | 0.66              |
| 2:H:139:GLN:HE22  | 2:H:415:PRO:HD3   | 1.60                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:137:VAL:O     | 2:H:391:LEU:HD21  | 1.95                     | 0.66              |
| 2:H:713:ARG:HB3   | 2:H:720:GLU:OE2   | 1.95                     | 0.66              |
| 3:I:141:ILE:HG13  | 3:I:448:GLU:CG    | 2.25                     | 0.66              |
| 2:M:236:ILE:CD1   | 2:M:236:ILE:N     | 2.58                     | 0.66              |
| 2:M:137:VAL:O     | 2:M:391:LEU:HD21  | 1.95                     | 0.66              |
| 2:M:838:LYS:O     | 2:M:838:LYS:HG3   | 1.94                     | 0.66              |
| 3:N:139:GLY:O     | 3:N:147:VAL:HB    | 1.95                     | 0.66              |
| 3:N:521:PRO:HB2   | 3:N:524:LEU:HD13  | 1.76                     | 0.66              |
| 3:N:743:ASP:OD1   | 6:U:16:G:O3'      | 2.09                     | 0.66              |
| 1:A:156:HIS:HD2   | 1:A:157:GLY:N     | 1.92                     | 0.66              |
| 2:C:657:ASP:OD1   | 2:C:663:ASN:N     | 2.28                     | 0.66              |
| 3:D:119:SER:HB2   | 3:D:123:LEU:H     | 1.58                     | 0.66              |
| 3:D:1272:ALA:HA   | 3:D:1326:THR:HB   | 1.77                     | 0.66              |
| 3:D:1403:LEU:O    | 3:D:1407:LEU:HB2  | 1.94                     | 0.66              |
| 3:D:28:LYS:HD2    | 3:D:29:PRO:CD     | 2.17                     | 0.66              |
| 3:D:470:LEU:H     | 3:D:470:LEU:HD23  | 1.60                     | 0.66              |
| 3:D:774:SER:HB3   | 3:D:1362:LYS:O    | 1.95                     | 0.66              |
| 4:E:32:ARG:HB2    | 4:E:32:ARG:HH11   | 1.61                     | 0.66              |
| 4:E:31:LEU:HB3    | 4:E:35:PHE:HE1    | 1.60                     | 0.66              |
| 2:H:661:SER:HA    | 2:H:665:PHE:O     | 1.94                     | 0.66              |
| 3:I:1466:VAL:HG12 | 3:I:1467:ILE:HD13 | 1.76                     | 0.66              |
| 3:I:145:VAL:HG22  | 3:I:146:PRO:HD2   | 1.77                     | 0.66              |
| 2:H:987:ILE:HD12  | 3:I:948:THR:HG23  | 1.76                     | 0.66              |
| 2:M:1098:ASP:HB3  | 3:N:11:ALA:O      | 1.95                     | 0.66              |
| 2:M:144:PRO:HA    | 2:M:163:ILE:O     | 1.94                     | 0.66              |
| 2:M:142:ARG:NE    | 2:M:325:ILE:HG23  | 2.11                     | 0.66              |
| 2:M:879:ARG:NH2   | 7:Z:42:ASP:OD1    | 2.28                     | 0.66              |
| 3:N:705:ALA:CB    | 3:N:706:PRO:HD3   | 2.26                     | 0.66              |
| 3:N:996:TRP:CE3   | 3:N:999:THR:HG21  | 2.30                     | 0.66              |
| 1:B:24:VAL:HG22   | 1:B:196:THR:CG2   | 2.26                     | 0.66              |
| 2:C:316:GLY:O     | 2:C:318:PRO:HD3   | 1.95                     | 0.66              |
| 2:C:950:LEU:HD12  | 2:C:952:LEU:CD2   | 2.25                     | 0.66              |
| 3:D:1101:VAL:HG21 | 3:D:1424:VAL:HG23 | 1.78                     | 0.66              |
| 3:D:705:ALA:CB    | 3:D:706:PRO:HD3   | 2.25                     | 0.66              |
| 4:E:54:LEU:HD23   | 4:E:58:PRO:CD     | 2.24                     | 0.66              |
| 1:G:206:THR:HG22  | 1:G:209:GLU:H     | 1.58                     | 0.66              |
| 3:I:1321:ALA:O    | 3:I:1339:LYS:HD2  | 1.95                     | 0.66              |
| 3:I:1367:HIS:HA   | 3:I:1370:ILE:HD12 | 1.76                     | 0.66              |
| 3:I:179:VAL:HG21  | 3:I:189:GLN:HE22  | 1.58                     | 0.66              |
| 3:I:705:ALA:CB    | 3:I:706:PRO:HD3   | 2.25                     | 0.66              |
| 3:I:970:LYS:CE    | 7:Y:113:LEU:HD23  | 2.25                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:265:ARG:HB3   | 2:M:267:TYR:CD2   | 2.29                     | 0.66              |
| 2:M:64:LEU:CD2    | 2:M:359:MET:HB2   | 2.24                     | 0.66              |
| 2:M:473:ARG:HD3   | 2:M:531:PHE:CE1   | 2.29                     | 0.66              |
| 2:M:83:CYS:SG     | 2:M:90:TYR:HD2    | 2.18                     | 0.66              |
| 2:M:997:LEU:C     | 2:M:999:HIS:H     | 1.99                     | 0.66              |
| 3:N:1311:LEU:N    | 3:N:1311:LEU:HD23 | 2.10                     | 0.66              |
| 3:N:1481:VAL:HG13 | 4:O:18:ARG:HD3    | 1.76                     | 0.66              |
| 3:N:520:LEU:O     | 3:N:525:ARG:NH1   | 2.29                     | 0.66              |
| 3:N:669:ASN:HD21  | 3:N:671:LYS:HB2   | 1.59                     | 0.66              |
| 7:Z:115:THR:CB    | 7:Z:116:PRO:HD3   | 2.26                     | 0.66              |
| 2:C:597:ALA:HB2   | 2:C:655:LEU:HD21  | 1.76                     | 0.66              |
| 2:C:726:ILE:HG13  | 2:C:734:LEU:HD11  | 1.78                     | 0.66              |
| 2:C:997:LEU:C     | 2:C:999:HIS:H     | 1.98                     | 0.66              |
| 3:D:1109:GLU:HG2  | 3:D:1201:CYS:HA   | 1.78                     | 0.66              |
| 3:D:179:VAL:HG13  | 3:D:183:GLU:CD    | 2.15                     | 0.66              |
| 1:F:156:HIS:HD2   | 1:F:157:GLY:N     | 1.92                     | 0.66              |
| 2:H:188:LYS:O     | 2:H:188:LYS:CG    | 2.43                     | 0.66              |
| 2:H:657:ASP:OD1   | 2:H:663:ASN:N     | 2.28                     | 0.66              |
| 2:H:673:LEU:HD22  | 2:H:867:VAL:HG12  | 1.78                     | 0.66              |
| 2:H:950:LEU:HD12  | 2:H:952:LEU:CD2   | 2.25                     | 0.66              |
| 3:I:119:SER:HB2   | 3:I:123:LEU:H     | 1.58                     | 0.66              |
| 3:I:160:GLU:OE2   | 3:I:165:LYS:HD2   | 1.95                     | 0.66              |
| 3:I:204:LEU:N     | 3:I:394:LEU:O     | 2.23                     | 0.66              |
| 1:K:128:HIS:HE1   | 1:K:131:THR:HG23  | 1.59                     | 0.66              |
| 1:K:206:THR:HG22  | 1:K:209:GLU:CG    | 2.25                     | 0.66              |
| 2:M:374:ASN:N     | 2:M:374:ASN:HD22  | 1.93                     | 0.66              |
| 2:M:950:LEU:HD12  | 2:M:952:LEU:HD21  | 1.76                     | 0.66              |
| 3:N:1425:THR:O    | 3:N:1429:LEU:HD13 | 1.96                     | 0.66              |
| 3:N:412:GLY:HA2   | 3:N:434:ARG:HD3   | 1.77                     | 0.66              |
| 3:N:546:ARG:HG2   | 3:N:546:ARG:HH11  | 1.60                     | 0.66              |
| 2:M:987:ILE:HD12  | 3:N:948:THR:HG23  | 1.78                     | 0.66              |
| 1:A:91:ASN:ND2    | 1:A:93:SER:HB2    | 2.10                     | 0.66              |
| 2:C:258:TYR:CD2   | 2:C:290:LEU:HD11  | 2.31                     | 0.66              |
| 2:C:878:SER:HA    | 3:D:1034:GLN:HE22 | 1.60                     | 0.66              |
| 3:D:520:LEU:O     | 3:D:525:ARG:NH1   | 2.29                     | 0.66              |
| 4:E:36:LYS:HZ3    | 4:E:36:LYS:CA     | 2.08                     | 0.66              |
| 3:I:1311:LEU:N    | 3:I:1311:LEU:HD23 | 2.11                     | 0.66              |
| 1:K:156:HIS:HD2   | 1:K:157:GLY:N     | 1.92                     | 0.66              |
| 3:N:890:VAL:HG11  | 3:N:922:LEU:CD1   | 2.25                     | 0.66              |
| 7:X:133:ARG:HA    | 7:X:154:ILE:HD11  | 1.75                     | 0.66              |
| 2:C:191:PHE:HD2   | 2:C:195:LEU:HD23  | 1.61                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:196:LEU:O     | 2:C:199:VAL:HB    | 1.96                     | 0.66              |
| 2:C:36:PRO:CA     | 2:C:39:ARG:HG3    | 2.26                     | 0.66              |
| 2:C:569:VAL:HG12  | 2:C:996:LYS:O     | 1.95                     | 0.66              |
| 2:C:838:LYS:O     | 2:C:838:LYS:HG3   | 1.94                     | 0.66              |
| 2:C:854:PRO:HB2   | 2:C:856:GLU:CG    | 2.24                     | 0.66              |
| 3:D:1146:GLY:HA2  | 3:D:1207:TYR:CB   | 2.25                     | 0.66              |
| 3:D:47:GLU:O      | 3:D:51:GLY:N      | 2.29                     | 0.66              |
| 3:D:809:PRO:O     | 3:D:812:ALA:HB3   | 1.96                     | 0.66              |
| 1:F:206:THR:HG22  | 1:F:209:GLU:CG    | 2.26                     | 0.66              |
| 2:H:137:VAL:HG23  | 2:H:391:LEU:CD2   | 2.25                     | 0.66              |
| 2:H:63:GLY:HA3    | 2:H:103:LYS:HE2   | 1.76                     | 0.66              |
| 3:I:1472:ILE:O    | 3:I:1477:GLY:HA3  | 1.96                     | 0.66              |
| 3:I:470:LEU:HD23  | 3:I:470:LEU:H     | 1.61                     | 0.66              |
| 2:H:850:ALA:HA    | 3:I:632:VAL:CG1   | 2.25                     | 0.66              |
| 2:M:1094:ALA:HB1  | 3:N:603:LEU:CD1   | 2.25                     | 0.66              |
| 2:M:36:PRO:O      | 2:M:39:ARG:HB3    | 1.96                     | 0.66              |
| 7:Z:127:LYS:HD3   | 7:Z:127:LYS:C     | 2.16                     | 0.66              |
| 2:C:282:GLY:C     | 2:C:283:ILE:HD13  | 2.15                     | 0.66              |
| 2:C:26:TYR:HE1    | 2:C:340:MET:HE2   | 1.60                     | 0.66              |
| 2:C:512:ARG:CA    | 2:C:523:ILE:HD11  | 2.26                     | 0.66              |
| 3:D:452:ILE:N     | 3:D:452:ILE:HD13  | 2.10                     | 0.66              |
| 2:H:218:VAL:HG13  | 2:H:221:LEU:CD1   | 2.25                     | 0.66              |
| 3:I:1425:THR:O    | 3:I:1429:LEU:HD13 | 1.96                     | 0.66              |
| 1:K:150:TYR:CE2   | 1:K:152:PRO:HG3   | 2.31                     | 0.66              |
| 2:M:564:MET:HE2   | 2:M:846:LYS:CD    | 2.21                     | 0.66              |
| 3:N:1491:THR:O    | 3:N:1494:ALA:HB3  | 1.95                     | 0.66              |
| 3:N:658:LEU:O     | 3:N:661:MET:HB2   | 1.96                     | 0.66              |
| 7:Y:90:GLU:C      | 7:Y:91:LEU:HD23   | 2.16                     | 0.66              |
| 7:Z:54:GLU:O      | 7:Z:58:ILE:HG12   | 1.96                     | 0.66              |
| 1:A:206:THR:HG22  | 1:A:209:GLU:CG    | 2.25                     | 0.66              |
| 1:A:150:TYR:OH    | 2:C:695:LEU:HD22  | 1.96                     | 0.66              |
| 2:C:710:ILE:HD11  | 2:C:758:ARG:HE    | 1.60                     | 0.66              |
| 3:D:1223:ILE:HD11 | 3:D:1462:LEU:HD12 | 1.77                     | 0.66              |
| 3:D:154:THR:CG2   | 3:D:157:GLU:OE2   | 2.44                     | 0.66              |
| 3:D:50:PHE:CG     | 3:D:522:PRO:CD    | 2.78                     | 0.66              |
| 3:D:639:LEU:CD1   | 3:D:766:ALA:HB2   | 2.21                     | 0.66              |
| 3:D:947:ILE:H     | 3:D:947:ILE:HD12  | 1.61                     | 0.66              |
| 2:H:428:ARG:NH1   | 2:H:449:ILE:O     | 2.29                     | 0.66              |
| 3:I:1272:ALA:HA   | 3:I:1326:THR:HB   | 1.77                     | 0.66              |
| 3:I:159:ARG:O     | 3:I:164:GLY:O     | 2.13                     | 0.66              |
| 3:I:86:ARG:NH2    | 3:I:88:TYR:CE1    | 2.64                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:151:ASP:HB2   | 2:M:157:ARG:O     | 1.96                     | 0.66              |
| 2:M:554:ASP:OD2   | 2:M:556:ASN:HB3   | 1.96                     | 0.66              |
| 2:M:861:LEU:CG    | 2:M:862:PRO:HD2   | 2.25                     | 0.66              |
| 3:N:1434:TRP:NE1  | 3:N:1435:LEU:HD12 | 2.10                     | 0.66              |
| 3:N:172:PRO:HD3   | 3:N:195:VAL:CG2   | 2.26                     | 0.66              |
| 2:C:524:VAL:CG1   | 2:C:528:GLU:HB2   | 2.26                     | 0.66              |
| 3:D:1105:ILE:HB   | 3:D:1222:GLY:HA3  | 1.77                     | 0.66              |
| 3:D:1367:HIS:HA   | 3:D:1370:ILE:HD12 | 1.76                     | 0.66              |
| 4:E:25:LYS:HA     | 4:E:28:GLN:CD     | 2.16                     | 0.66              |
| 2:H:142:ARG:HE    | 2:H:325:ILE:HG13  | 1.59                     | 0.66              |
| 2:H:554:ASP:OD2   | 2:H:556:ASN:HB3   | 1.95                     | 0.66              |
| 2:H:65:VAL:O      | 2:H:100:LEU:HD12  | 1.96                     | 0.66              |
| 3:I:658:LEU:O     | 3:I:661:MET:HB2   | 1.95                     | 0.66              |
| 2:M:174:LEU:CD2   | 2:M:193:LEU:HD21  | 2.25                     | 0.66              |
| 2:M:950:LEU:HD12  | 2:M:952:LEU:CD2   | 2.26                     | 0.66              |
| 3:N:593:ASN:HB3   | 3:N:594:PRO:HD2   | 1.77                     | 0.66              |
| 1:A:73:GLU:HB2    | 1:A:78:ILE:CD1    | 2.23                     | 0.66              |
| 2:C:564:MET:HE2   | 2:C:846:LYS:HD2   | 1.78                     | 0.66              |
| 3:D:1123:PHE:CD2  | 3:D:1184:GLN:HG3  | 2.30                     | 0.66              |
| 3:D:139:GLY:CA    | 3:D:147:VAL:HG21  | 2.26                     | 0.66              |
| 3:D:686:GLU:HA    | 3:D:689:ASP:OD2   | 1.96                     | 0.66              |
| 2:H:524:VAL:CG1   | 2:H:528:GLU:HB2   | 2.26                     | 0.66              |
| 2:H:906:PHE:CE1   | 3:I:1067:VAL:HG13 | 2.31                     | 0.66              |
| 3:I:1211:MET:CG   | 3:I:1212:ALA:H    | 2.00                     | 0.66              |
| 4:J:31:LEU:HD12   | 4:J:32:ARG:N      | 2.10                     | 0.66              |
| 4:J:9:LEU:HB3     | 4:J:19:LEU:HD21   | 1.78                     | 0.66              |
| 1:L:27:PRO:C      | 1:L:28:LEU:HD23   | 2.17                     | 0.66              |
| 2:M:1105:LYS:HZ1  | 2:M:1107:ASN:HB2  | 1.61                     | 0.66              |
| 2:M:289:THR:O     | 2:M:291:ALA:N     | 2.28                     | 0.66              |
| 2:M:497:ALA:HA    | 2:M:515:ALA:HA    | 1.77                     | 0.66              |
| 3:N:347:VAL:CG2   | 3:N:368:VAL:HG11  | 2.24                     | 0.66              |
| 3:N:767:HIS:CE1   | 4:O:6:ILE:HG21    | 2.29                     | 0.66              |
| 3:N:95:LEU:HD21   | 3:N:574:LEU:HD11  | 1.76                     | 0.66              |
| 3:I:783:ARG:HH12  | 7:Y:41:ASP:CB     | 1.90                     | 0.66              |
| 7:Z:57:ARG:NH2    | 7:Z:57:ARG:HB2    | 2.05                     | 0.66              |
| 7:Z:64:SER:O      | 7:Z:68:ILE:HG12   | 1.96                     | 0.66              |
| 1:A:150:TYR:CE2   | 1:A:152:PRO:HG3   | 2.31                     | 0.65              |
| 2:C:138:SER:HB2   | 2:C:410:ILE:HG12  | 1.78                     | 0.65              |
| 2:C:681:GLY:C     | 3:D:635:PRO:HG3   | 2.17                     | 0.65              |
| 3:D:1459:LEU:HD21 | 3:D:1468:LEU:HD12 | 1.78                     | 0.65              |
| 3:D:157:GLU:O     | 3:D:161:LEU:HD12  | 1.94                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:996:TRP:CE3  | 3:D:999:THR:HG21  | 2.30                     | 0.65              |
| 1:F:186:LEU:C    | 1:F:186:LEU:HD23  | 2.14                     | 0.65              |
| 1:F:91:ASN:ND2   | 1:F:93:SER:HB2    | 2.10                     | 0.65              |
| 1:G:134:GLU:HG3  | 3:N:821:VAL:HG11  | 1.78                     | 0.65              |
| 2:H:1020:PRO:HD2 | 3:I:622:ARG:HB2   | 1.77                     | 0.65              |
| 2:H:338:GLU:O    | 2:H:341:THR:HG22  | 1.95                     | 0.65              |
| 2:H:129:ILE:CG1  | 2:H:386:PHE:HB3   | 2.27                     | 0.65              |
| 3:I:162:ARG:HD2  | 3:I:452:ILE:CG2   | 2.20                     | 0.65              |
| 2:M:142:ARG:HH11 | 2:M:142:ARG:HB3   | 1.61                     | 0.65              |
| 2:M:136:ILE:HG21 | 2:M:336:VAL:HG13  | 1.79                     | 0.65              |
| 2:M:630:ARG:HD3  | 2:M:705:ILE:HB    | 1.78                     | 0.65              |
| 3:N:470:LEU:H    | 3:N:470:LEU:HD23  | 1.61                     | 0.65              |
| 2:C:374:ASN:O    | 2:C:377:PRO:HD2   | 1.96                     | 0.65              |
| 2:C:508:ILE:HD12 | 2:C:526:PRO:HB3   | 1.77                     | 0.65              |
| 3:D:1261:GLU:OE1 | 3:D:1268:PRO:HA   | 1.96                     | 0.65              |
| 2:H:224:GLU:CB   | 2:H:228:ALA:HB2   | 2.26                     | 0.65              |
| 2:H:512:ARG:CA   | 2:H:523:ILE:HD11  | 2.26                     | 0.65              |
| 2:H:564:MET:SD   | 2:H:846:LYS:HD2   | 2.36                     | 0.65              |
| 2:H:976:ASP:CB   | 2:H:979:THR:HG22  | 2.26                     | 0.65              |
| 3:I:1397:LYS:NZ  | 3:I:1432:LYS:NZ   | 2.45                     | 0.65              |
| 1:K:91:ASN:ND2   | 1:K:93:SER:HB2    | 2.11                     | 0.65              |
| 2:M:1036:GLU:O   | 2:M:1039:ALA:HB3  | 1.95                     | 0.65              |
| 2:M:63:GLY:N     | 2:M:103:LYS:HG2   | 2.12                     | 0.65              |
| 2:M:657:ASP:OD1  | 2:M:663:ASN:N     | 2.29                     | 0.65              |
| 3:N:402:PRO:HA   | 3:N:443:VAL:HG23  | 1.78                     | 0.65              |
| 1:B:27:PRO:C     | 1:B:28:LEU:HD23   | 2.17                     | 0.65              |
| 2:C:383:ARG:HH11 | 2:C:383:ARG:CB    | 2.03                     | 0.65              |
| 3:D:1209:LEU:CD2 | 3:D:1211:MET:H    | 2.05                     | 0.65              |
| 3:D:153:LEU:HD11 | 3:D:158:TYR:HB2   | 1.76                     | 0.65              |
| 3:D:170:PRO:HD2  | 2:H:318:PRO:CB    | 2.24                     | 0.65              |
| 3:D:969:ARG:HG3  | 3:D:970:LYS:H     | 1.62                     | 0.65              |
| 2:H:141:HIS:HB3  | 2:H:418:LEU:HD23  | 1.76                     | 0.65              |
| 3:I:1197:ARG:HB3 | 3:I:1396:GLU:CD   | 2.15                     | 0.65              |
| 3:I:1258:ARG:NH2 | 3:I:1262:LEU:HD11 | 2.10                     | 0.65              |
| 3:I:50:PHE:HA    | 3:I:89:ARG:CB     | 2.26                     | 0.65              |
| 3:I:50:PHE:CD2   | 3:I:522:PRO:HD2   | 2.30                     | 0.65              |
| 2:M:205:GLU:HA   | 2:M:209:ARG:CZ    | 2.26                     | 0.65              |
| 2:M:22:GLN:HB3   | 2:M:121:MET:HE1   | 1.78                     | 0.65              |
| 2:M:36:PRO:CA    | 2:M:39:ARG:HB2    | 2.24                     | 0.65              |
| 3:N:180:LYS:HG2  | 3:N:183:GLU:OE1   | 1.96                     | 0.65              |
| 1:A:9:PRO:HB3    | 1:A:25:LEU:HD11   | 1.78                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:124:ASN:N    | 1:B:125:PRO:HD3  | 2.12                     | 0.65              |
| 2:C:150:PRO:HA   | 2:C:158:TYR:HB3  | 1.77                     | 0.65              |
| 2:C:554:ASP:OD2  | 2:C:556:ASN:HB3  | 1.96                     | 0.65              |
| 3:D:658:LEU:O    | 3:D:661:MET:HB2  | 1.95                     | 0.65              |
| 2:H:723:THR:HG23 | 2:H:725:ASP:H    | 1.61                     | 0.65              |
| 1:K:56:VAL:HG13  | 1:K:142:VAL:CG1  | 2.23                     | 0.65              |
| 3:N:17:LYS:HG2   | 3:N:21:TRP:NE1   | 2.11                     | 0.65              |
| 3:N:23:TYR:CD1   | 3:N:89:ARG:HG2   | 2.31                     | 0.65              |
| 2:M:1090:LYS:CE  | 3:N:90:MET:SD    | 2.85                     | 0.65              |
| 2:C:31:GLN:NE2   | 2:C:71:TYR:OH    | 2.28                     | 0.65              |
| 2:C:52:PHE:HB3   | 2:C:53:PRO:HD3   | 1.78                     | 0.65              |
| 3:D:26:VAL:HG23  | 3:D:26:VAL:O     | 1.95                     | 0.65              |
| 3:D:800:LYS:HG3  | 3:D:829:VAL:HG13 | 1.78                     | 0.65              |
| 1:G:24:VAL:HG22  | 1:G:196:THR:CG2  | 2.26                     | 0.65              |
| 3:I:6:ARG:HH21   | 3:I:1482:ARG:NH2 | 1.95                     | 0.65              |
| 2:M:218:VAL:HG22 | 2:M:222:MET:HG3  | 1.78                     | 0.65              |
| 2:M:263:ASP:HB2  | 2:M:264:PRO:CD   | 2.19                     | 0.65              |
| 2:M:343:GLN:HE21 | 2:M:343:GLN:HA   | 1.61                     | 0.65              |
| 3:N:122:GLU:O    | 3:N:126:VAL:HG23 | 1.96                     | 0.65              |
| 3:N:148:GLU:HG2  | 3:N:151:GLN:HB3  | 1.77                     | 0.65              |
| 2:C:196:LEU:O    | 2:C:200:LEU:HG   | 1.97                     | 0.65              |
| 2:C:199:VAL:CG2  | 2:C:238:LEU:HD12 | 2.24                     | 0.65              |
| 2:C:140:ILE:HG22 | 2:C:333:ILE:CD1  | 2.27                     | 0.65              |
| 3:D:1208:ASP:HB2 | 3:D:1366:LYS:HE3 | 1.78                     | 0.65              |
| 3:D:191:LEU:HD11 | 3:D:197:SER:OG   | 1.97                     | 0.65              |
| 2:H:267:TYR:HE2  | 2:H:289:THR:HG23 | 1.60                     | 0.65              |
| 3:I:177:ALA:CB   | 3:I:390:PRO:HG3  | 2.20                     | 0.65              |
| 3:I:484:PRO:HB3  | 3:I:488:ARG:HE   | 1.62                     | 0.65              |
| 3:I:676:MET:SD   | 3:I:684:LYS:HE3  | 2.36                     | 0.65              |
| 2:H:676:ILE:O    | 3:I:948:THR:CG2  | 2.44                     | 0.65              |
| 1:L:24:VAL:HG22  | 1:L:196:THR:CG2  | 2.26                     | 0.65              |
| 2:M:620:LEU:O    | 2:M:620:LEU:HD12 | 1.95                     | 0.65              |
| 3:N:1029:ARG:NH1 | 3:N:1030:GLY:H   | 1.94                     | 0.65              |
| 3:N:96:ALA:HB3   | 3:N:554:LEU:HD23 | 1.77                     | 0.65              |
| 3:N:577:ALA:O    | 3:N:580:ALA:HB3  | 1.97                     | 0.65              |
| 7:Y:93:ASP:OD1   | 7:Y:94:PRO:HD2   | 1.96                     | 0.65              |
| 2:C:154:ARG:CZ   | 2:C:178:PRO:HD3  | 2.26                     | 0.65              |
| 3:D:1168:MET:HE3 | 3:D:1171:VAL:HB  | 1.78                     | 0.65              |
| 3:D:600:LEU:HD12 | 3:D:600:LEU:H    | 1.61                     | 0.65              |
| 3:D:860:LEU:HD22 | 3:D:878:GLY:HA2  | 1.79                     | 0.65              |
| 2:H:1012:PRO:HD2 | 2:H:1026:GLN:CG  | 2.26                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:571:LEU:HD11  | 2:H:701:THR:H     | 1.59                     | 0.65              |
| 3:I:1066:THR:CG2  | 3:I:1069:GLU:HB2  | 2.26                     | 0.65              |
| 3:I:136:ASP:CB    | 3:I:137:PRO:HD3   | 2.20                     | 0.65              |
| 3:I:817:GLU:HG3   | 3:I:839:LEU:HD23  | 1.78                     | 0.65              |
| 3:I:894:LYS:O     | 3:I:898:GLU:HG3   | 1.97                     | 0.65              |
| 2:M:226:VAL:HG13  | 2:M:227:PHE:CD1   | 2.32                     | 0.65              |
| 2:M:342:ASP:O     | 2:M:346:VAL:HG23  | 1.97                     | 0.65              |
| 2:M:368:THR:CB    | 2:M:369:PRO:CD    | 2.75                     | 0.65              |
| 2:M:1046:ALA:CB   | 3:N:1476:THR:HB   | 2.27                     | 0.65              |
| 3:N:804:LEU:HB2   | 3:N:831:GLY:HA2   | 1.79                     | 0.65              |
| 7:X:115:THR:CB    | 7:X:116:PRO:HD3   | 2.26                     | 0.65              |
| 1:A:171:PHE:O     | 1:A:173:PRO:HD3   | 1.97                     | 0.65              |
| 1:B:206:THR:HG23  | 1:B:208:LEU:H     | 1.62                     | 0.65              |
| 1:A:218:LEU:CD2   | 1:B:222:LEU:HD21  | 2.24                     | 0.65              |
| 2:C:52:PHE:O      | 2:C:54:ILE:N      | 2.30                     | 0.65              |
| 3:D:1066:THR:CG2  | 3:D:1069:GLU:HB2  | 2.26                     | 0.65              |
| 2:C:1097:LEU:CD1  | 3:D:1451:ALA:HB1  | 2.26                     | 0.65              |
| 3:D:159:ARG:HH21  | 2:H:208:ALA:HB1   | 1.61                     | 0.65              |
| 3:I:1095:THR:OG1  | 3:I:1230:GLY:HA3  | 1.97                     | 0.65              |
| 3:I:808:THR:OG1   | 3:I:809:PRO:HD3   | 1.97                     | 0.65              |
| 2:M:113:VAL:CG2   | 2:M:373:VAL:HG11  | 2.27                     | 0.65              |
| 2:M:50:GLU:HG2    | 2:M:51:THR:HG23   | 1.78                     | 0.65              |
| 2:M:957:LYS:CD    | 2:M:961:GLU:HB3   | 2.26                     | 0.65              |
| 2:C:289:THR:O     | 2:C:291:ALA:N     | 2.27                     | 0.65              |
| 2:C:564:MET:SD    | 2:C:846:LYS:HD2   | 2.37                     | 0.65              |
| 2:C:878:SER:CB    | 3:D:1029:ARG:CZ   | 2.75                     | 0.65              |
| 3:D:1459:LEU:CD2  | 3:D:1468:LEU:HD12 | 2.27                     | 0.65              |
| 3:D:176:ASP:HB2   | 3:D:388:HIS:O     | 1.97                     | 0.65              |
| 3:D:480:GLU:O     | 3:D:484:PRO:CG    | 2.44                     | 0.65              |
| 1:B:185:ARG:CD    | 3:D:692:GLU:HG2   | 2.27                     | 0.65              |
| 4:E:59:ASN:HB3    | 4:E:62:THR:OG1    | 1.96                     | 0.65              |
| 1:G:44:LEU:HA     | 1:G:48:ILE:CD1    | 2.26                     | 0.65              |
| 3:I:1097:LYS:O    | 3:I:1100:ASP:HB2  | 1.97                     | 0.65              |
| 3:I:1223:ILE:HD11 | 3:I:1462:LEU:HD12 | 1.78                     | 0.65              |
| 3:I:1435:LEU:HB2  | 3:I:1457:ASP:OD2  | 1.97                     | 0.65              |
| 3:I:581:LEU:N     | 3:I:581:LEU:HD23  | 2.12                     | 0.65              |
| 3:I:680:GLN:O     | 3:I:683:ILE:CD1   | 2.44                     | 0.65              |
| 2:M:1072:LYS:O    | 3:N:659:LYS:HE2   | 1.97                     | 0.65              |
| 2:M:22:GLN:HB3    | 2:M:121:MET:CE    | 2.27                     | 0.65              |
| 2:M:987:ILE:HD11  | 3:N:946:GLY:HA2   | 1.79                     | 0.65              |
| 3:N:956:ILE:HD11  | 3:N:1062:ARG:CG   | 2.26                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:119:SER:HB2  | 3:N:123:LEU:CB    | 2.19                     | 0.65              |
| 3:N:408:GLU:HB2  | 3:N:421:LEU:O     | 1.97                     | 0.65              |
| 3:N:484:PRO:HB3  | 3:N:488:ARG:HE    | 1.62                     | 0.65              |
| 3:N:581:LEU:N    | 3:N:581:LEU:HD23  | 2.11                     | 0.65              |
| 7:Y:127:LYS:HD3  | 7:Y:127:LYS:C     | 2.18                     | 0.65              |
| 2:C:26:TYR:HD2   | 2:C:121:MET:HB2   | 1.61                     | 0.65              |
| 3:D:166:GLN:NE2  | 3:D:394:LEU:HB2   | 2.10                     | 0.65              |
| 3:D:354:VAL:HB   | 3:D:367:ILE:O     | 1.96                     | 0.65              |
| 4:E:54:LEU:CG    | 4:E:58:PRO:HG2    | 2.26                     | 0.65              |
| 2:H:18:LEU:H     | 2:H:18:LEU:CD1    | 2.10                     | 0.65              |
| 2:H:211:LEU:HG   | 2:H:218:VAL:CG2   | 2.26                     | 0.65              |
| 2:H:40:GLU:HG3   | 2:H:41:ASN:N      | 2.09                     | 0.65              |
| 2:H:564:MET:CE   | 2:H:846:LYS:HD2   | 2.27                     | 0.65              |
| 2:H:957:LYS:CD   | 2:H:961:GLU:HB3   | 2.26                     | 0.65              |
| 3:I:102:ILE:O    | 3:I:102:ILE:HD13  | 1.97                     | 0.65              |
| 3:I:206:ARG:HB3  | 3:I:207:PHE:CE1   | 2.31                     | 0.65              |
| 3:I:577:ALA:O    | 3:I:580:ALA:HB3   | 1.97                     | 0.65              |
| 2:M:293:PHE:N    | 2:M:293:PHE:CD1   | 2.59                     | 0.65              |
| 2:M:265:ARG:NH1  | 2:M:332:ARG:HH12  | 1.84                     | 0.65              |
| 2:M:714:ASP:OD1  | 2:M:719:PRO:HG3   | 1.97                     | 0.65              |
| 3:N:1272:ALA:HA  | 3:N:1326:THR:HB   | 1.77                     | 0.65              |
| 3:N:441:ARG:NH1  | 3:N:445:ARG:NH2   | 2.45                     | 0.65              |
| 3:N:826:PRO:O    | 3:N:829:VAL:HG23  | 1.97                     | 0.65              |
| 4:O:24:ALA:O     | 4:O:27:ALA:N      | 2.30                     | 0.65              |
| 2:C:265:ARG:HB3  | 2:C:267:TYR:CZ    | 2.31                     | 0.64              |
| 2:C:290:LEU:HB3  | 2:C:302:VAL:CG1   | 2.27                     | 0.64              |
| 3:D:102:ILE:O    | 3:D:102:ILE:HD13  | 1.98                     | 0.64              |
| 3:D:655:PRO:HA   | 3:D:658:LEU:HD12  | 1.79                     | 0.64              |
| 3:D:894:LYS:O    | 3:D:898:GLU:HG3   | 1.97                     | 0.64              |
| 3:D:23:TYR:CD1   | 3:D:89:ARG:HG2    | 2.32                     | 0.64              |
| 2:C:1090:LYS:HE3 | 3:D:90:MET:HG3    | 1.76                     | 0.64              |
| 1:F:150:TYR:CE2  | 1:F:152:PRO:HG3   | 2.31                     | 0.64              |
| 1:F:56:VAL:HG13  | 1:F:142:VAL:CG1   | 2.23                     | 0.64              |
| 1:G:59:GLU:OE2   | 1:G:139:ASN:HB3   | 1.97                     | 0.64              |
| 1:G:25:LEU:O     | 1:G:28:LEU:HD21   | 1.97                     | 0.64              |
| 2:H:50:GLU:HG2   | 2:H:51:THR:HG23   | 1.79                     | 0.64              |
| 2:H:557:ARG:HG2  | 2:H:881:ASN:ND2   | 2.12                     | 0.64              |
| 2:H:836:GLY:HA3  | 2:H:1001:VAL:CG2  | 2.27                     | 0.64              |
| 3:I:1025:GLN:CA  | 3:I:1025:GLN:HE21 | 2.06                     | 0.64              |
| 3:I:148:GLU:HB3  | 3:I:151:GLN:HB2   | 1.78                     | 0.64              |
| 3:I:655:PRO:HA   | 3:I:658:LEU:HD12  | 1.79                     | 0.64              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:I:704:ARG:NH2   | 6:S:16:G:O2'     | 2.29                     | 0.64              |
| 1:L:124:ASN:OD1   | 1:L:127:LEU:HB2  | 1.97                     | 0.64              |
| 1:L:185:ARG:HD3   | 3:N:692:GLU:OE2  | 1.97                     | 0.64              |
| 1:L:206:THR:HG23  | 1:L:208:LEU:H    | 1.62                     | 0.64              |
| 1:L:20:TYR:HD2    | 1:L:21:GLY:N     | 1.95                     | 0.64              |
| 2:M:109:LYS:CD    | 2:M:368:THR:HG23 | 2.24                     | 0.64              |
| 3:N:139:GLY:O     | 3:N:162:ARG:NH2  | 2.31                     | 0.64              |
| 3:N:50:PHE:HD2    | 3:N:522:PRO:HD3  | 0.84                     | 0.64              |
| 3:N:860:LEU:HD22  | 3:N:878:GLY:HA2  | 1.79                     | 0.64              |
| 2:C:861:LEU:HG    | 2:C:862:PRO:CD   | 2.26                     | 0.64              |
| 2:C:879:ARG:NE    | 7:X:42:ASP:CG    | 2.51                     | 0.64              |
| 3:D:1317:ASP:OD1  | 3:D:1318:TYR:N   | 2.30                     | 0.64              |
| 3:D:158:TYR:CD1   | 3:D:162:ARG:HG2  | 2.31                     | 0.64              |
| 3:D:17:LYS:HG2    | 3:D:21:TRP:NE1   | 2.12                     | 0.64              |
| 3:D:817:GLU:HG3   | 3:D:839:LEU:HD23 | 1.78                     | 0.64              |
| 3:D:826:PRO:O     | 3:D:829:VAL:HG23 | 1.97                     | 0.64              |
| 2:H:204:GLN:NE2   | 2:H:228:ALA:HB1  | 2.13                     | 0.64              |
| 2:H:170:PRO:HD3   | 2:H:263:ASP:CG   | 2.17                     | 0.64              |
| 2:H:317:VAL:HG12  | 2:H:317:VAL:O    | 1.95                     | 0.64              |
| 3:I:618:LEU:HD23  | 3:I:619:LEU:HD23 | 1.80                     | 0.64              |
| 2:M:217:LEU:HB2   | 2:M:311:PHE:HE1  | 1.56                     | 0.64              |
| 2:M:50:GLU:HG2    | 2:M:51:THR:N     | 2.12                     | 0.64              |
| 2:M:676:ILE:HG23  | 3:N:948:THR:HB   | 1.78                     | 0.64              |
| 2:M:976:ASP:CB    | 2:M:979:THR:HG22 | 2.26                     | 0.64              |
| 3:N:376:GLU:O     | 3:N:378:ILE:HG13 | 1.97                     | 0.64              |
| 1:A:64:GLU:O      | 1:A:75:VAL:HB    | 1.97                     | 0.64              |
| 3:D:187:LYS:HG3   | 3:D:198:ARG:O    | 1.97                     | 0.64              |
| 3:D:368:VAL:HB    | 3:D:377:VAL:HG21 | 1.77                     | 0.64              |
| 1:G:42:ARG:CG     | 1:G:42:ARG:HH11  | 2.08                     | 0.64              |
| 3:I:116:LEU:CD2   | 3:I:118:LEU:HG   | 2.18                     | 0.64              |
| 3:I:1109:GLU:HG2  | 3:I:1201:CYS:CA  | 2.26                     | 0.64              |
| 3:I:433:GLY:HA2   | 3:I:449:SER:H    | 1.61                     | 0.64              |
| 1:G:76:VAL:CG2    | 3:I:872:ARG:HH12 | 2.10                     | 0.64              |
| 2:M:1017:THR:O    | 2:M:1018:GLN:HB2 | 1.97                     | 0.64              |
| 2:M:512:ARG:CA    | 2:M:523:ILE:HD11 | 2.26                     | 0.64              |
| 3:N:1283:ILE:HD12 | 3:N:1315:ASP:CG  | 2.17                     | 0.64              |
| 3:N:398:ALA:HB2   | 3:N:447:VAL:HA   | 1.80                     | 0.64              |
| 3:N:53:ILE:O      | 3:N:53:ILE:HG13  | 1.96                     | 0.64              |
| 3:N:655:PRO:HA    | 3:N:658:LEU:HD12 | 1.79                     | 0.64              |
| 3:N:984:THR:HG22  | 3:N:987:GLU:HG3  | 1.79                     | 0.64              |
| 2:C:101:ILE:HG23  | 2:C:108:ILE:CD1  | 2.27                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:478:VAL:HG13  | 2:C:506:ASN:HB3   | 1.79                     | 0.64              |
| 2:C:564:MET:CE    | 2:C:846:LYS:CD    | 2.76                     | 0.64              |
| 2:C:564:MET:CE    | 2:C:846:LYS:HE2   | 2.16                     | 0.64              |
| 3:D:1122:LEU:HD13 | 3:D:1185:GLU:CA   | 2.27                     | 0.64              |
| 3:D:625:TYR:HB3   | 3:D:749:VAL:HG23  | 1.80                     | 0.64              |
| 3:D:95:LEU:HD23   | 3:D:551:ASN:OD1   | 1.98                     | 0.64              |
| 1:G:27:PRO:C      | 1:G:28:LEU:HD23   | 2.17                     | 0.64              |
| 1:G:58:ILE:HB     | 1:G:61:VAL:HB     | 1.78                     | 0.64              |
| 2:H:1017:THR:O    | 2:H:1018:GLN:HB2  | 1.96                     | 0.64              |
| 2:H:191:PHE:CE2   | 2:H:192:PRO:O     | 2.49                     | 0.64              |
| 2:H:169:GLY:HA2   | 2:H:263:ASP:HB3   | 1.78                     | 0.64              |
| 3:I:86:ARG:O      | 3:I:87:ARG:CZ     | 2.45                     | 0.64              |
| 2:M:524:VAL:CG1   | 2:M:528:GLU:HB2   | 2.26                     | 0.64              |
| 2:M:911:GLU:OE1   | 3:N:951:ILE:HD13  | 1.93                     | 0.64              |
| 2:M:73:LEU:HB2    | 2:M:93:PRO:O      | 1.98                     | 0.64              |
| 3:N:800:LYS:HD2   | 3:N:804:LEU:HB3   | 1.78                     | 0.64              |
| 3:N:817:GLU:HG3   | 3:N:839:LEU:HD23  | 1.78                     | 0.64              |
| 7:X:6:LYS:HB3     | 7:X:75:LEU:HD11   | 1.79                     | 0.64              |
| 3:D:1312:LEU:CD1  | 3:D:1327:ARG:HH21 | 2.10                     | 0.64              |
| 1:G:206:THR:HG23  | 1:G:208:LEU:H     | 1.62                     | 0.64              |
| 2:H:1036:GLU:HG3  | 3:I:707:THR:OG1   | 1.97                     | 0.64              |
| 2:H:317:VAL:N     | 2:H:318:PRO:CD    | 2.60                     | 0.64              |
| 2:H:171:TRP:HH2   | 2:H:417:GLY:O     | 1.78                     | 0.64              |
| 2:H:496:ILE:HD12  | 2:H:496:ILE:N     | 2.12                     | 0.64              |
| 2:H:6:PHE:CZ      | 2:H:917:LEU:HD11  | 2.33                     | 0.64              |
| 3:I:134:VAL:O     | 3:I:454:ALA:HB1   | 1.97                     | 0.64              |
| 2:H:678:PRO:CG    | 3:I:947:ILE:HD11  | 2.27                     | 0.64              |
| 4:J:27:ALA:HA     | 4:J:30:LEU:HD12   | 1.78                     | 0.64              |
| 4:J:38:THR:OG1    | 4:J:39:VAL:N      | 2.28                     | 0.64              |
| 1:L:152:PRO:HG2   | 3:N:857:ILE:HD11  | 1.79                     | 0.64              |
| 2:M:440:PRO:HB2   | 3:N:1074:SER:OG   | 1.97                     | 0.64              |
| 3:N:956:ILE:HD11  | 3:N:1062:ARG:HG3  | 1.78                     | 0.64              |
| 3:I:780:LYS:NZ    | 7:Y:38:GLU:HB3    | 2.13                     | 0.64              |
| 1:A:58:ILE:CD1    | 1:A:140:MET:HB3   | 2.23                     | 0.64              |
| 1:A:49:PRO:HB3    | 1:A:148:VAL:HG22  | 1.80                     | 0.64              |
| 1:B:20:TYR:HD2    | 1:B:21:GLY:N      | 1.95                     | 0.64              |
| 3:D:355:VAL:CG2   | 3:D:367:ILE:HG23  | 2.28                     | 0.64              |
| 2:C:987:ILE:HD11  | 3:D:946:GLY:CA    | 2.28                     | 0.64              |
| 2:H:196:LEU:HD23  | 2:H:200:LEU:CD1   | 2.22                     | 0.64              |
| 2:H:329:GLY:HA3   | 2:H:489:THR:HG23  | 1.79                     | 0.64              |
| 3:I:17:LYS:HG2    | 3:I:21:TRP:NE1    | 2.12                     | 0.64              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:I:660:LYS:HZ1   | 3:I:660:LYS:HA   | 1.61                     | 0.64              |
| 2:M:140:ILE:HD13  | 2:M:331:ARG:CZ   | 2.27                     | 0.64              |
| 2:M:313:LEU:HD13  | 2:M:321:GLU:HG3  | 1.79                     | 0.64              |
| 2:M:317:VAL:HG13  | 2:M:320:HIS:CD2  | 2.33                     | 0.64              |
| 2:M:80:GLN:HG3    | 2:M:90:TYR:HE2   | 1.60                     | 0.64              |
| 2:M:862:PRO:HB3   | 2:M:929:ARG:HH22 | 1.63                     | 0.64              |
| 3:N:102:ILE:HD13  | 3:N:102:ILE:O    | 1.98                     | 0.64              |
| 3:N:1107:VAL:HG23 | 3:N:1219:GLU:O   | 1.98                     | 0.64              |
| 2:C:498:GLN:HE21  | 2:C:498:GLN:HA   | 1.63                     | 0.64              |
| 3:D:638:LYS:HA    | 3:D:932:ASP:OD1  | 1.97                     | 0.64              |
| 1:G:20:TYR:HD2    | 1:G:21:GLY:N     | 1.95                     | 0.64              |
| 2:H:129:ILE:HD11  | 2:H:386:PHE:HD2  | 1.62                     | 0.64              |
| 2:H:148:PHE:CE1   | 2:H:309:TYR:CD1  | 2.86                     | 0.64              |
| 2:H:862:PRO:HB3   | 2:H:929:ARG:HH22 | 1.63                     | 0.64              |
| 2:H:964:LYS:O     | 2:H:968:LEU:HG   | 1.97                     | 0.64              |
| 3:I:785:ILE:H     | 3:I:785:ILE:CD1  | 2.01                     | 0.64              |
| 2:M:170:PRO:HD3   | 2:M:263:ASP:CB   | 2.11                     | 0.64              |
| 2:M:257:VAL:HG12  | 2:M:263:ASP:OD2  | 1.98                     | 0.64              |
| 2:M:258:TYR:CE2   | 2:M:290:LEU:HD11 | 2.32                     | 0.64              |
| 3:N:411:THR:HG23  | 3:N:436:GLU:HA   | 1.80                     | 0.64              |
| 3:N:89:ARG:O      | 3:N:521:PRO:HG3  | 1.97                     | 0.64              |
| 2:C:101:ILE:HA    | 2:C:108:ILE:HG12 | 1.80                     | 0.64              |
| 2:C:976:ASP:CB    | 2:C:979:THR:HG22 | 2.26                     | 0.64              |
| 3:D:166:GLN:HG2   | 3:D:396:VAL:CG1  | 2.24                     | 0.64              |
| 3:D:52:PRO:C      | 3:D:86:ARG:HD3   | 2.18                     | 0.64              |
| 1:F:171:PHE:O     | 1:F:173:PRO:HD3  | 1.97                     | 0.64              |
| 1:G:112:ARG:HG3   | 1:G:125:PRO:CA   | 2.28                     | 0.64              |
| 1:G:80:LEU:HG     | 3:I:844:ALA:CB   | 2.27                     | 0.64              |
| 2:H:569:VAL:HG12  | 2:H:996:LYS:O    | 1.98                     | 0.64              |
| 2:H:64:LEU:CB     | 2:H:359:MET:HG3  | 2.25                     | 0.64              |
| 3:I:1123:PHE:CE2  | 3:I:1184:GLN:HG3 | 2.33                     | 0.64              |
| 2:M:565:GLN:HE21  | 2:M:842:ARG:CG   | 2.04                     | 0.64              |
| 3:N:178:LEU:N     | 3:N:178:LEU:HD12 | 2.11                     | 0.64              |
| 2:C:140:ILE:CD1   | 2:C:412:ALA:HA   | 2.27                     | 0.64              |
| 2:C:697:ARG:HG3   | 2:C:699:PHE:CD1  | 2.32                     | 0.64              |
| 2:C:957:LYS:CD    | 2:C:961:GLU:HB3  | 2.26                     | 0.64              |
| 3:D:166:GLN:CG    | 3:D:396:VAL:HG12 | 2.21                     | 0.64              |
| 3:D:554:LEU:O     | 3:D:558:LEU:HG   | 1.98                     | 0.64              |
| 1:B:187:GLY:CA    | 3:D:685:ASP:HB3  | 2.21                     | 0.64              |
| 1:F:49:PRO:HB3    | 1:F:148:VAL:HG22 | 1.80                     | 0.64              |
| 3:I:1107:VAL:HG12 | 3:I:1217:ILE:HA  | 1.80                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:111:LYS:HD3   | 3:I:1448:THR:HG22 | 1.79                     | 0.64              |
| 1:G:80:LEU:CG     | 3:I:844:ALA:HA    | 2.27                     | 0.64              |
| 1:L:74:ASP:CB     | 3:N:872:ARG:NH2   | 2.54                     | 0.64              |
| 2:M:100:LEU:C     | 2:M:108:ILE:HG23  | 2.18                     | 0.64              |
| 2:M:144:PRO:HB3   | 2:M:164:PRO:HA    | 1.79                     | 0.64              |
| 2:M:217:LEU:HD12  | 2:M:311:PHE:CB    | 2.27                     | 0.64              |
| 2:M:500:ASN:OD1   | 3:N:1067:VAL:HG23 | 1.98                     | 0.64              |
| 3:N:161:LEU:HA    | 3:N:397:LYS:HZ2   | 1.63                     | 0.64              |
| 3:N:191:LEU:O     | 3:N:192:ALA:HB2   | 1.97                     | 0.64              |
| 3:N:638:LYS:HA    | 3:N:932:ASP:OD1   | 1.97                     | 0.64              |
| 2:C:224:GLU:HB3   | 2:C:228:ALA:N     | 2.13                     | 0.64              |
| 2:C:964:LYS:O     | 2:C:968:LEU:HG    | 1.97                     | 0.64              |
| 2:C:987:ILE:HD11  | 3:D:946:GLY:HA2   | 1.80                     | 0.64              |
| 3:D:1146:GLY:HA3  | 3:D:1207:TYR:HB3  | 1.80                     | 0.64              |
| 3:D:1231:GLU:HB3  | 3:D:1232:PRO:HD3  | 1.79                     | 0.64              |
| 3:D:367:ILE:HB    | 3:D:377:VAL:CG1   | 2.28                     | 0.64              |
| 2:H:342:ASP:O     | 2:H:346:VAL:HG23  | 1.98                     | 0.64              |
| 3:I:1216:SER:HB3  | 4:J:15:SER:OG     | 1.98                     | 0.64              |
| 3:I:826:PRO:O     | 3:I:829:VAL:HG23  | 1.97                     | 0.64              |
| 1:K:171:PHE:O     | 1:K:173:PRO:HD3   | 1.97                     | 0.64              |
| 2:M:216:GLU:OE2   | 2:M:219:GLN:NE2   | 2.31                     | 0.64              |
| 2:M:184:MET:SD    | 2:M:303:PHE:CE2   | 2.88                     | 0.64              |
| 2:M:325:ILE:CD1   | 2:M:325:ILE:H     | 2.08                     | 0.64              |
| 1:K:46:SER:HB3    | 2:M:856:GLU:HG2   | 1.78                     | 0.64              |
| 2:M:554:ASP:HB2   | 2:M:880:MET:HB2   | 1.80                     | 0.64              |
| 2:M:964:LYS:O     | 2:M:968:LEU:HG    | 1.97                     | 0.64              |
| 2:M:1093:GLN:OE1  | 3:N:21:TRP:CE3    | 2.51                     | 0.64              |
| 3:N:358:GLY:HA2   | 3:N:385:VAL:O     | 1.98                     | 0.64              |
| 2:M:1004:LYS:CD   | 3:N:744:GLN:NE2   | 2.57                     | 0.64              |
| 4:O:54:LEU:HA     | 4:O:58:PRO:HG2    | 1.80                     | 0.64              |
| 7:Y:88:VAL:HG13   | 7:Y:103:GLN:HB2   | 1.79                     | 0.64              |
| 7:Y:19:LEU:HD21   | 7:Y:23:ARG:HH21   | 1.62                     | 0.64              |
| 3:D:795:VAL:HG23  | 3:D:879:ARG:HH12  | 1.63                     | 0.63              |
| 4:E:35:PHE:C      | 4:E:36:LYS:HZ3    | 2.00                     | 0.63              |
| 3:I:115:LEU:HD23  | 3:I:115:LEU:C     | 2.18                     | 0.63              |
| 3:I:1317:ASP:OD1  | 3:I:1318:TYR:N    | 2.31                     | 0.63              |
| 2:M:343:GLN:O     | 2:M:346:VAL:HB    | 1.98                     | 0.63              |
| 2:M:583:LEU:O     | 2:M:587:VAL:HG23  | 1.99                     | 0.63              |
| 3:N:1099:VAL:O    | 3:N:1103:HIS:HB3  | 1.98                     | 0.63              |
| 3:N:1114:THR:HG21 | 3:N:1195:GLN:HB3  | 1.79                     | 0.63              |
| 3:N:1317:ASP:OD1  | 3:N:1318:TYR:N    | 2.30                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:169:TYR:CZ    | 3:N:198:ARG:HG3   | 2.32                     | 0.63              |
| 3:N:50:PHE:CE2    | 3:N:522:PRO:CG    | 2.81                     | 0.63              |
| 3:N:711:LEU:HD12  | 3:N:778:LEU:HD23  | 1.79                     | 0.63              |
| 7:Z:55:LYS:O      | 7:Z:59:GLU:HG3    | 1.98                     | 0.63              |
| 2:C:1030:GLN:HE21 | 3:D:628:ARG:HD3   | 1.63                     | 0.63              |
| 2:C:224:GLU:OE1   | 2:C:224:GLU:HA    | 1.98                     | 0.63              |
| 2:C:276:LYS:O     | 2:C:280:LYS:HB2   | 1.98                     | 0.63              |
| 3:D:984:THR:HG22  | 3:D:987:GLU:HG3   | 1.79                     | 0.63              |
| 2:H:122:THR:HG22  | 2:H:124:ASP:H     | 1.63                     | 0.63              |
| 2:H:571:LEU:HD21  | 2:H:700:TYR:HA    | 1.80                     | 0.63              |
| 3:I:1161:GLU:CG   | 3:I:1164:ARG:HB2  | 2.28                     | 0.63              |
| 3:I:127:LEU:C     | 3:I:127:LEU:HD12  | 2.18                     | 0.63              |
| 3:I:860:LEU:HD22  | 3:I:878:GLY:HA2   | 1.79                     | 0.63              |
| 1:K:42:ARG:NH1    | 1:L:34:VAL:CB     | 2.54                     | 0.63              |
| 2:M:122:THR:HG22  | 2:M:124:ASP:H     | 1.63                     | 0.63              |
| 2:M:284:ARG:HG2   | 2:M:285:LEU:H     | 1.62                     | 0.63              |
| 2:M:503:LEU:HD23  | 2:M:507:ARG:C     | 2.18                     | 0.63              |
| 3:N:758:GLU:HB3   | 4:O:20:THR:HG21   | 1.81                     | 0.63              |
| 3:N:894:LYS:O     | 3:N:898:GLU:HG3   | 1.97                     | 0.63              |
| 7:Y:139:SER:HB3   | 7:Y:148:GLU:CD    | 2.18                     | 0.63              |
| 2:C:1015:LEU:N    | 2:C:1015:LEU:HD12 | 2.13                     | 0.63              |
| 2:C:1092:LEU:O    | 2:C:1097:LEU:O    | 2.16                     | 0.63              |
| 2:C:113:VAL:HG21  | 2:C:373:VAL:HG21  | 1.80                     | 0.63              |
| 2:C:717:LEU:HB3   | 2:C:761:PHE:CG    | 2.33                     | 0.63              |
| 2:C:794:PRO:HG2   | 2:C:1025:ALA:O    | 1.98                     | 0.63              |
| 2:C:80:GLN:HA     | 2:C:90:TYR:HD2    | 1.63                     | 0.63              |
| 2:C:862:PRO:HB3   | 2:C:929:ARG:HH22  | 1.62                     | 0.63              |
| 3:D:142:LEU:HB3   | 3:D:145:VAL:C     | 2.18                     | 0.63              |
| 2:H:512:ARG:CG    | 2:H:523:ILE:HD11  | 2.28                     | 0.63              |
| 2:H:589:ARG:HG3   | 2:H:596:TYR:CE2   | 2.33                     | 0.63              |
| 3:I:1231:GLU:HB3  | 3:I:1232:PRO:HD3  | 1.78                     | 0.63              |
| 3:I:414:ARG:HB3   | 3:I:450:TYR:HE1   | 1.63                     | 0.63              |
| 3:I:50:PHE:CE2    | 3:I:522:PRO:HD2   | 2.33                     | 0.63              |
| 3:I:650:LEU:HD13  | 3:I:688:TRP:CZ3   | 2.32                     | 0.63              |
| 3:I:50:PHE:O      | 3:I:89:ARG:CB     | 2.45                     | 0.63              |
| 3:I:969:ARG:HG3   | 3:I:970:LYS:H     | 1.62                     | 0.63              |
| 4:J:25:LYS:CA     | 4:J:28:GLN:HG3    | 2.27                     | 0.63              |
| 2:M:1112:PHE:CD2  | 2:M:1112:PHE:O    | 2.51                     | 0.63              |
| 2:M:73:LEU:HD12   | 2:M:73:LEU:C      | 2.19                     | 0.63              |
| 3:N:115:LEU:C     | 3:N:115:LEU:HD23  | 2.19                     | 0.63              |
| 3:N:1312:LEU:CD1  | 3:N:1327:ARG:HH21 | 2.10                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1465:ASN:HD21 | 3:N:1470:ARG:NH2  | 1.96                     | 0.63              |
| 4:O:64:ALA:O      | 4:O:68:LEU:HD13   | 1.98                     | 0.63              |
| 3:I:991:GLN:NE2   | 7:Y:112:VAL:HG21  | 2.13                     | 0.63              |
| 1:B:25:LEU:O      | 1:B:28:LEU:HD21   | 1.98                     | 0.63              |
| 2:C:115:LEU:HA    | 2:C:375:SER:HG    | 1.63                     | 0.63              |
| 2:C:512:ARG:CG    | 2:C:523:ILE:HD11  | 2.29                     | 0.63              |
| 2:C:876:VAL:O     | 2:C:879:ARG:O     | 2.17                     | 0.63              |
| 3:D:115:LEU:HD23  | 3:D:115:LEU:C     | 2.19                     | 0.63              |
| 3:D:133:ILE:CG2   | 3:D:134:VAL:N     | 2.61                     | 0.63              |
| 3:D:51:GLY:C      | 3:D:86:ARG:CD     | 2.67                     | 0.63              |
| 3:D:881:LEU:CD1   | 3:D:885:ILE:HD11  | 2.29                     | 0.63              |
| 1:G:86:VAL:HG12   | 1:G:124:ASN:HD22  | 1.63                     | 0.63              |
| 2:H:1043:TYR:CE1  | 3:I:710:ARG:O     | 2.52                     | 0.63              |
| 2:H:182:VAL:O     | 2:H:193:LEU:CD1   | 2.47                     | 0.63              |
| 2:H:211:LEU:HD11  | 2:H:311:PHE:CD1   | 2.34                     | 0.63              |
| 2:H:464:LEU:HG    | 2:H:464:LEU:O     | 1.99                     | 0.63              |
| 3:I:179:VAL:HG13  | 3:I:183:GLU:HB3   | 1.79                     | 0.63              |
| 3:I:711:LEU:HD12  | 3:I:778:LEU:HD23  | 1.79                     | 0.63              |
| 3:N:1083:ASP:O    | 3:N:1087:ARG:HB3  | 1.99                     | 0.63              |
| 3:N:86:ARG:NE     | 3:N:523:ASP:CG    | 2.51                     | 0.63              |
| 1:A:11:PHE:HE1    | 1:A:23:PHE:HB3    | 1.63                     | 0.63              |
| 2:C:897:LEU:HD21  | 2:C:921:ALA:HA    | 1.81                     | 0.63              |
| 3:D:1078:ARG:CG   | 3:D:1078:ARG:HH11 | 2.12                     | 0.63              |
| 3:D:1148:VAL:HG13 | 3:D:1163:GLY:O    | 1.99                     | 0.63              |
| 3:D:1421:LEU:O    | 3:D:1421:LEU:HG   | 1.97                     | 0.63              |
| 3:D:189:GLN:O     | 3:D:196:VAL:HG13  | 1.99                     | 0.63              |
| 3:D:650:LEU:HD13  | 3:D:688:TRP:CZ3   | 2.32                     | 0.63              |
| 3:D:677:LEU:CD2   | 3:D:683:ILE:HD13  | 2.28                     | 0.63              |
| 1:F:58:ILE:CD1    | 1:F:140:MET:HB3   | 2.23                     | 0.63              |
| 2:H:1092:LEU:O    | 2:H:1097:LEU:O    | 2.16                     | 0.63              |
| 2:H:512:ARG:HD3   | 2:H:523:ILE:HG13  | 1.80                     | 0.63              |
| 3:I:794:GLN:HG2   | 3:I:1017:PHE:HE2  | 1.62                     | 0.63              |
| 3:I:1397:LYS:HZ1  | 3:I:1432:LYS:HZ2  | 1.47                     | 0.63              |
| 3:I:1493:LYS:O    | 3:I:1497:GLU:HG2  | 1.97                     | 0.63              |
| 3:I:40:GLU:CA     | 3:I:40:GLU:OE1    | 2.42                     | 0.63              |
| 3:I:800:LYS:CE    | 3:I:804:LEU:HD22  | 2.28                     | 0.63              |
| 4:J:26:ARG:HH11   | 4:J:73:LEU:HD21   | 1.63                     | 0.63              |
| 2:M:266:ARG:NH1   | 2:M:288:ARG:NH2   | 2.47                     | 0.63              |
| 3:N:1286:THR:HG22 | 3:N:1287:GLU:H    | 1.63                     | 0.63              |
| 3:N:133:ILE:HG22  | 3:N:134:VAL:N     | 2.12                     | 0.63              |
| 3:N:171:LEU:HD23  | 3:N:172:PRO:N     | 2.14                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:211:VAL:HG12  | 3:N:213:VAL:HG23  | 1.79                     | 0.63              |
| 6:Q:12:G:H2'      | 6:Q:13:G:H8       | 1.62                     | 0.63              |
| 2:C:361:MET:CE    | 3:I:1317:ASP:HB2  | 2.28                     | 0.63              |
| 3:D:158:TYR:CD1   | 3:D:162:ARG:HB2   | 2.33                     | 0.63              |
| 3:D:646:LYS:HG3   | 3:D:647:ARG:H     | 1.64                     | 0.63              |
| 2:C:1086:ARG:CD   | 3:D:88:TYR:CE1    | 2.78                     | 0.63              |
| 1:F:123:MET:O     | 1:F:125:PRO:HD3   | 1.99                     | 0.63              |
| 2:H:182:VAL:HG12  | 2:H:193:LEU:CG    | 2.27                     | 0.63              |
| 2:H:861:LEU:CG    | 2:H:862:PRO:HD2   | 2.25                     | 0.63              |
| 3:I:1262:LEU:HB3  | 3:I:1352:ILE:HD11 | 1.81                     | 0.63              |
| 3:I:12:LEU:HD21   | 3:I:104:PHE:CZ    | 2.30                     | 0.63              |
| 3:I:127:LEU:HD22  | 3:I:134:VAL:HG13  | 1.81                     | 0.63              |
| 3:I:1397:LYS:HZ3  | 3:I:1432:LYS:HZ3  | 1.46                     | 0.63              |
| 3:I:407:VAL:HG22  | 3:I:408:GLU:N     | 2.09                     | 0.63              |
| 3:I:41:ARG:HD2    | 3:I:41:ARG:O      | 1.97                     | 0.63              |
| 3:I:141:ILE:HG13  | 3:I:448:GLU:HG3   | 1.79                     | 0.63              |
| 3:I:465:LEU:HD11  | 3:I:509:PRO:O     | 1.99                     | 0.63              |
| 3:I:796:ARG:HD3   | 3:I:1017:PHE:CE1  | 2.33                     | 0.63              |
| 2:M:498:GLN:OE1   | 3:N:1068:LEU:CD1  | 2.47                     | 0.63              |
| 2:M:512:ARG:CG    | 2:M:523:ILE:HD11  | 2.29                     | 0.63              |
| 2:M:675:ALA:HB2   | 2:M:867:VAL:HG11  | 1.81                     | 0.63              |
| 2:M:794:PRO:HG2   | 2:M:1025:ALA:O    | 1.98                     | 0.63              |
| 2:M:850:ALA:HA    | 3:N:632:VAL:HG13  | 1.80                     | 0.63              |
| 2:M:861:LEU:HG    | 2:M:862:PRO:CD    | 2.26                     | 0.63              |
| 3:N:1288:GLU:O    | 3:N:1307:LYS:HG2  | 1.99                     | 0.63              |
| 3:N:456:MET:HE1   | 3:N:568:ARG:NH2   | 2.14                     | 0.63              |
| 2:C:1088:LEU:HD21 | 3:D:614:PHE:CE1   | 2.33                     | 0.63              |
| 2:C:21:ILE:HD12   | 2:C:21:ILE:N      | 2.07                     | 0.63              |
| 2:C:274:ARG:HD2   | 2:C:285:LEU:HD22  | 1.81                     | 0.63              |
| 3:D:660:LYS:HZ1   | 3:D:660:LYS:HA    | 1.62                     | 0.63              |
| 2:H:258:TYR:CE2   | 2:H:290:LEU:HD21  | 2.34                     | 0.63              |
| 3:I:1312:LEU:CD1  | 3:I:1327:ARG:HH21 | 2.10                     | 0.63              |
| 3:I:1421:LEU:HG   | 3:I:1421:LEU:O    | 1.98                     | 0.63              |
| 2:M:195:LEU:HD21  | 2:M:238:LEU:HG    | 1.79                     | 0.63              |
| 2:M:408:ARG:NH2   | 2:M:455:LEU:HD11  | 2.13                     | 0.63              |
| 3:N:1094:LEU:HG   | 3:N:1098:LEU:HD22 | 1.81                     | 0.63              |
| 3:N:1258:ARG:HH21 | 3:N:1351:GLU:CG   | 2.11                     | 0.63              |
| 3:N:1472:ILE:O    | 3:N:1477:GLY:HA3  | 1.99                     | 0.63              |
| 3:N:13:ALA:HB1    | 3:N:18:ILE:HD11   | 1.81                     | 0.63              |
| 1:A:42:ARG:HH12   | 1:B:34:VAL:HG11   | 1.64                     | 0.63              |
| 2:C:409:ARG:HA    | 2:C:454:SER:HA    | 1.81                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:512:ARG:HD3   | 2:C:523:ILE:HG13  | 1.80                     | 0.63              |
| 2:C:840:ALA:HB2   | 2:C:846:LYS:HA    | 1.80                     | 0.63              |
| 3:D:168:THR:CG2   | 3:D:169:TYR:N     | 2.62                     | 0.63              |
| 3:D:736:PHE:O     | 3:D:738:ALA:N     | 2.32                     | 0.63              |
| 1:G:132:LEU:HD11  | 1:G:138:LEU:HD13  | 1.81                     | 0.63              |
| 2:H:571:LEU:HD11  | 2:H:700:TYR:HA    | 1.81                     | 0.63              |
| 3:I:1078:ARG:HH11 | 3:I:1078:ARG:CG   | 2.12                     | 0.63              |
| 3:I:1434:TRP:CZ3  | 3:I:1457:ASP:HB2  | 2.34                     | 0.63              |
| 3:I:646:LYS:HG3   | 3:I:647:ARG:H     | 1.64                     | 0.63              |
| 3:I:678:GLU:HG3   | 3:I:679:ARG:HG3   | 1.81                     | 0.63              |
| 3:I:984:THR:HG22  | 3:I:987:GLU:HG3   | 1.80                     | 0.63              |
| 1:K:49:PRO:HB3    | 1:K:148:VAL:HG22  | 1.80                     | 0.63              |
| 1:L:94:LEU:HD11   | 1:L:119:ASP:HB2   | 1.79                     | 0.63              |
| 2:M:1092:LEU:O    | 2:M:1097:LEU:O    | 2.16                     | 0.63              |
| 3:N:1231:GLU:HB3  | 3:N:1232:PRO:HD3  | 1.79                     | 0.63              |
| 3:N:501:ALA:HB1   | 3:N:1452:ILE:HG22 | 1.79                     | 0.63              |
| 3:N:881:LEU:CD1   | 3:N:885:ILE:HD11  | 2.29                     | 0.63              |
| 1:A:158:ILE:HD12  | 1:A:158:ILE:H     | 1.64                     | 0.63              |
| 2:C:1035:MET:HB3  | 2:C:1036:GLU:OE1  | 1.99                     | 0.63              |
| 2:C:1092:LEU:CD1  | 2:C:1099:VAL:HG21 | 2.14                     | 0.63              |
| 2:C:48:PHE:O      | 2:C:52:PHE:HB2    | 1.99                     | 0.63              |
| 3:D:1109:GLU:CG   | 3:D:1201:CYS:HB2  | 2.29                     | 0.63              |
| 3:D:1286:THR:O    | 3:D:1287:GLU:HB2  | 1.99                     | 0.63              |
| 3:D:1495:ILE:CD1  | 4:E:88:GLU:HG3    | 2.29                     | 0.63              |
| 3:D:163:TYR:O     | 2:H:209:ARG:CZ    | 2.47                     | 0.63              |
| 3:D:520:LEU:HD11  | 3:D:524:LEU:HD22  | 1.81                     | 0.63              |
| 3:D:711:LEU:HD12  | 3:D:778:LEU:HD23  | 1.79                     | 0.63              |
| 2:H:840:ALA:HB2   | 2:H:846:LYS:HA    | 1.80                     | 0.63              |
| 3:I:1209:LEU:HD11 | 4:J:16:LYS:HD2    | 1.79                     | 0.63              |
| 3:I:414:ARG:HB3   | 3:I:450:TYR:CE1   | 2.34                     | 0.63              |
| 3:I:620:GLY:O     | 3:I:621:LYS:NZ    | 2.30                     | 0.63              |
| 4:J:47:LYS:HA     | 4:J:54:LEU:HB3    | 1.81                     | 0.63              |
| 3:N:1109:GLU:HG2  | 3:N:1201:CYS:CA   | 2.28                     | 0.63              |
| 3:N:11:ALA:HB1    | 3:N:507:ASN:HD22  | 1.64                     | 0.63              |
| 7:X:17:GLN:O      | 7:X:21:ARG:HD3    | 1.98                     | 0.63              |
| 1:B:26:GLU:HB2    | 1:B:27:PRO:HA     | 1.81                     | 0.62              |
| 2:C:861:LEU:CG    | 2:C:862:PRO:HD2   | 2.25                     | 0.62              |
| 3:D:123:LEU:HD21  | 3:D:151:GLN:NE2   | 2.14                     | 0.62              |
| 2:H:154:ARG:NH1   | 2:H:178:PRO:HD2   | 2.13                     | 0.62              |
| 2:H:474:VAL:HG23  | 2:H:478:VAL:C     | 2.19                     | 0.62              |
| 2:H:666:LEU:HD12  | 2:H:667:ALA:N     | 2.14                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:25:LEU:O      | 1:L:28:LEU:HD21   | 1.98                     | 0.62              |
| 2:M:199:VAL:HG11  | 2:M:235:LEU:HG    | 1.79                     | 0.62              |
| 2:M:260:LEU:C     | 2:M:260:LEU:HD23  | 2.18                     | 0.62              |
| 2:M:666:LEU:HD12  | 2:M:667:ALA:N     | 2.13                     | 0.62              |
| 2:M:730:SER:O     | 2:M:734:LEU:HD13  | 1.99                     | 0.62              |
| 2:M:876:VAL:O     | 2:M:879:ARG:O     | 2.17                     | 0.62              |
| 3:N:1105:ILE:N    | 3:N:1105:ILE:HD12 | 2.14                     | 0.62              |
| 3:N:1256:LEU:C    | 3:N:1260:ILE:HG13 | 2.18                     | 0.62              |
| 3:N:179:VAL:HA    | 3:N:183:GLU:OE2   | 1.99                     | 0.62              |
| 1:L:65:PHE:CD1    | 3:N:813:LEU:HD22  | 2.33                     | 0.62              |
| 3:D:1487:VAL:HG11 | 3:D:1492:LEU:HD23 | 1.81                     | 0.62              |
| 3:D:51:GLY:C      | 3:D:86:ARG:NE     | 2.52                     | 0.62              |
| 3:D:93:ILE:HD13   | 3:D:547:LEU:HD23  | 1.81                     | 0.62              |
| 3:D:800:LYS:HZ2   | 3:D:804:LEU:HD22  | 1.64                     | 0.62              |
| 3:D:789:LEU:HD13  | 3:D:911:LEU:HD21  | 1.81                     | 0.62              |
| 2:H:1032:PHE:O    | 2:H:1033:GLY:O    | 2.16                     | 0.62              |
| 2:H:1058:ASP:OD2  | 2:H:1083:GLU:HB2  | 1.98                     | 0.62              |
| 2:H:159:ILE:O     | 2:H:159:ILE:HD12  | 1.99                     | 0.62              |
| 2:H:316:GLY:C     | 2:H:318:PRO:CD    | 2.68                     | 0.62              |
| 2:H:516:ARG:HE    | 3:I:1068:LEU:HD13 | 1.62                     | 0.62              |
| 1:F:46:SER:HB3    | 2:H:856:GLU:HG2   | 1.80                     | 0.62              |
| 3:I:600:LEU:HD12  | 3:I:600:LEU:H     | 1.64                     | 0.62              |
| 3:I:789:LEU:HD13  | 3:I:911:LEU:HD21  | 1.81                     | 0.62              |
| 1:K:31:GLY:N      | 1:K:193:ASP:OD1   | 2.26                     | 0.62              |
| 1:L:79:ILE:HD12   | 1:L:167:VAL:HG13  | 1.81                     | 0.62              |
| 2:M:462:ASP:HB3   | 2:M:468:ARG:HD2   | 1.80                     | 0.62              |
| 3:N:996:TRP:CE2   | 3:N:1056:PRO:HG2  | 2.33                     | 0.62              |
| 3:N:1109:GLU:OE1  | 3:N:1201:CYS:HB2  | 1.99                     | 0.62              |
| 3:N:1330:ILE:N    | 3:N:1330:ILE:HD12 | 2.14                     | 0.62              |
| 3:N:1462:LEU:O    | 3:N:1466:VAL:HG23 | 1.98                     | 0.62              |
| 3:N:1033:GLN:NE2  | 7:Z:54:GLU:OE2    | 2.32                     | 0.62              |
| 1:B:101:LEU:C     | 1:B:101:LEU:HD23  | 2.20                     | 0.62              |
| 2:C:253:ALA:O     | 2:C:257:VAL:HG23  | 1.99                     | 0.62              |
| 2:C:557:ARG:HG2   | 2:C:881:ASN:ND2   | 2.13                     | 0.62              |
| 2:C:676:ILE:O     | 2:C:676:ILE:HG23  | 2.00                     | 0.62              |
| 3:D:547:LEU:CD1   | 3:D:578:VAL:HG22  | 2.29                     | 0.62              |
| 2:H:408:ARG:NH2   | 2:H:455:LEU:HD11  | 2.12                     | 0.62              |
| 2:H:1086:ARG:NE   | 3:I:88:TYR:HE2    | 1.97                     | 0.62              |
| 2:M:127:PHE:CD1   | 2:M:136:ILE:HD13  | 2.34                     | 0.62              |
| 2:M:391:LEU:O     | 2:M:391:LEU:HD23  | 1.99                     | 0.62              |
| 3:N:1041:LEU:HD12 | 3:N:1058:ARG:O    | 1.99                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1421:LEU:HG   | 3:N:1421:LEU:O    | 1.98                     | 0.62              |
| 3:N:465:LEU:HD11  | 3:N:509:PRO:O     | 1.99                     | 0.62              |
| 3:D:1359:GLN:O    | 7:X:37:MET:SD     | 2.56                     | 0.62              |
| 7:Y:155:HIS:O     | 7:Y:156:GLY:C     | 2.38                     | 0.62              |
| 2:C:1005:MET:SD   | 3:D:724:GLN:OE1   | 2.57                     | 0.62              |
| 2:C:101:ILE:HD13  | 2:C:108:ILE:HG23  | 1.81                     | 0.62              |
| 2:C:197:LEU:HA    | 2:C:200:LEU:HD12  | 1.80                     | 0.62              |
| 2:C:503:LEU:HD23  | 2:C:507:ARG:O     | 1.99                     | 0.62              |
| 2:C:73:LEU:C      | 2:C:73:LEU:HD12   | 2.19                     | 0.62              |
| 2:C:939:ARG:CA    | 2:C:939:ARG:HE    | 2.06                     | 0.62              |
| 3:D:1495:ILE:HD13 | 4:E:88:GLU:HG3    | 1.80                     | 0.62              |
| 3:D:152:LEU:CD2   | 3:D:152:LEU:H     | 2.13                     | 0.62              |
| 3:D:50:PHE:CD1    | 3:D:522:PRO:HG2   | 2.34                     | 0.62              |
| 3:D:561:GLY:O     | 3:D:563:PRO:HD2   | 2.00                     | 0.62              |
| 3:D:767:HIS:HA    | 3:D:924:MET:SD    | 2.39                     | 0.62              |
| 3:D:868:TYR:CE1   | 3:D:869:MET:HG3   | 2.34                     | 0.62              |
| 1:F:102:LYS:HD3   | 1:F:139:ASN:HD21  | 1.64                     | 0.62              |
| 3:I:1114:THR:O    | 3:I:1114:THR:HG23 | 1.99                     | 0.62              |
| 3:I:152:LEU:N     | 3:I:152:LEU:HD23  | 2.15                     | 0.62              |
| 3:I:618:LEU:HD13  | 3:I:1463:LYS:HE2  | 1.80                     | 0.62              |
| 1:K:123:MET:O     | 1:K:125:PRO:HD3   | 1.99                     | 0.62              |
| 2:M:512:ARG:HD3   | 2:M:523:ILE:HG13  | 1.80                     | 0.62              |
| 2:M:1046:ALA:HB2  | 3:N:1476:THR:CB   | 2.29                     | 0.62              |
| 3:N:171:LEU:HA    | 3:N:195:VAL:HG21  | 1.80                     | 0.62              |
| 3:N:868:TYR:CE1   | 3:N:869:MET:HG3   | 2.34                     | 0.62              |
| 5:R:17:DG:H2'     | 5:R:18:DC:C6      | 2.34                     | 0.62              |
| 2:C:217:LEU:O     | 2:C:219:GLN:N     | 2.31                     | 0.62              |
| 3:D:1366:LYS:O    | 3:D:1369:GLU:HB2  | 1.99                     | 0.62              |
| 3:D:210:ARG:HB3   | 3:D:389:GLU:HG3   | 1.81                     | 0.62              |
| 4:E:35:PHE:C      | 4:E:36:LYS:HE2    | 2.19                     | 0.62              |
| 2:H:660:ALA:O     | 2:H:667:ALA:HB3   | 2.00                     | 0.62              |
| 3:I:1041:LEU:HD12 | 3:I:1058:ARG:O    | 1.99                     | 0.62              |
| 3:I:202:VAL:HG11  | 3:I:445:ARG:HH21  | 1.64                     | 0.62              |
| 4:J:51:LEU:HG     | 4:J:53:GLY:H      | 1.62                     | 0.62              |
| 1:L:101:LEU:HD23  | 1:L:101:LEU:C     | 2.20                     | 0.62              |
| 1:L:12:THR:OG1    | 1:L:24:VAL:HB     | 1.99                     | 0.62              |
| 2:M:516:ARG:HG3   | 3:N:1068:LEU:CD1  | 2.30                     | 0.62              |
| 3:N:1252:ILE:HG13 | 3:N:1253:THR:H    | 1.64                     | 0.62              |
| 3:N:650:LEU:HD13  | 3:N:688:TRP:CZ3   | 2.31                     | 0.62              |
| 4:O:54:LEU:HG     | 4:O:58:PRO:HG2    | 1.80                     | 0.62              |
| 1:B:102:LYS:HB2   | 1:B:139:ASN:OD1   | 1.99                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:497:ALA:HA    | 2:C:515:ALA:HA    | 1.82                     | 0.62              |
| 3:D:1047:LYS:HB3  | 3:D:1048:PRO:HD2  | 1.81                     | 0.62              |
| 3:D:108:VAL:HB    | 3:D:109:PRO:CD    | 2.29                     | 0.62              |
| 3:D:116:LEU:O     | 3:D:117:ASP:CB    | 2.47                     | 0.62              |
| 3:D:1147:ARG:HB3  | 3:D:1188:VAL:CG2  | 2.29                     | 0.62              |
| 3:D:1330:ILE:HD12 | 3:D:1330:ILE:N    | 2.15                     | 0.62              |
| 3:D:465:LEU:HD11  | 3:D:509:PRO:O     | 1.99                     | 0.62              |
| 3:D:54:LYS:CD     | 3:D:55:ASP:H      | 2.12                     | 0.62              |
| 2:H:794:PRO:CD    | 2:H:1024:LYS:O    | 2.47                     | 0.62              |
| 2:H:263:ASP:HB2   | 2:H:264:PRO:HD3   | 1.81                     | 0.62              |
| 3:I:1047:LYS:HB3  | 3:I:1048:PRO:HD2  | 1.80                     | 0.62              |
| 3:I:111:LYS:HD3   | 3:I:1448:THR:CG2  | 2.29                     | 0.62              |
| 3:I:1487:VAL:HG12 | 3:I:1488:ASP:N    | 2.14                     | 0.62              |
| 3:I:838:ARG:HB3   | 3:I:865:THR:CG2   | 2.30                     | 0.62              |
| 1:K:42:ARG:HH12   | 1:L:34:VAL:CG1    | 2.12                     | 0.62              |
| 1:K:64:GLU:OE1    | 2:M:830:LYS:HE2   | 2.00                     | 0.62              |
| 1:L:34:VAL:HG11   | 2:M:978:ARG:HB3   | 1.82                     | 0.62              |
| 2:M:683:ASN:HB2   | 2:M:872:ASN:HB2   | 1.81                     | 0.62              |
| 3:N:736:PHE:O     | 3:N:738:ALA:N     | 2.32                     | 0.62              |
| 1:A:31:GLY:H      | 1:A:193:ASP:CG    | 2.02                     | 0.62              |
| 1:B:115:LEU:O     | 1:B:115:LEU:HD12  | 1.99                     | 0.62              |
| 2:C:124:ASP:HB2   | 2:C:407:LYS:NZ    | 2.15                     | 0.62              |
| 2:C:212:GLY:C     | 2:C:214:TYR:H     | 2.01                     | 0.62              |
| 2:C:216:GLU:HG3   | 2:C:216:GLU:O     | 2.00                     | 0.62              |
| 3:D:1114:THR:O    | 3:D:1114:THR:HG23 | 2.00                     | 0.62              |
| 3:D:1145:TYR:O    | 3:D:1147:ARG:HG2  | 2.00                     | 0.62              |
| 3:D:1114:THR:HG22 | 3:D:1195:GLN:HB3  | 1.81                     | 0.62              |
| 3:D:1262:LEU:HB3  | 3:D:1352:ILE:HD11 | 1.81                     | 0.62              |
| 3:D:408:GLU:HG3   | 3:D:409:VAL:H     | 1.64                     | 0.62              |
| 1:G:226:SER:O     | 1:G:228:PRO:HD3   | 1.99                     | 0.62              |
| 2:H:22:GLN:HB3    | 2:H:121:MET:HE1   | 1.81                     | 0.62              |
| 3:I:1330:ILE:N    | 3:I:1330:ILE:HD12 | 2.14                     | 0.62              |
| 3:I:133:ILE:HD12  | 3:I:158:TYR:CD2   | 2.34                     | 0.62              |
| 3:I:142:LEU:HD23  | 3:I:146:PRO:CA    | 2.28                     | 0.62              |
| 2:M:1038:TRP:HA   | 2:M:1041:GLU:HG3  | 1.82                     | 0.62              |
| 2:M:660:ALA:CB    | 2:M:667:ALA:O     | 2.37                     | 0.62              |
| 2:M:432:ARG:HH12  | 3:N:1047:LYS:HG2  | 1.65                     | 0.62              |
| 3:N:1047:LYS:HB3  | 3:N:1048:PRO:HD2  | 1.80                     | 0.62              |
| 3:N:205:TYR:HD1   | 3:N:390:PRO:CB    | 2.13                     | 0.62              |
| 7:X:99:ARG:HG3    | 7:X:99:ARG:HH11   | 1.63                     | 0.62              |
| 3:N:783:ARG:NE    | 7:Z:41:ASP:OD2    | 2.31                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:185:ARG:CZ    | 3:D:692:GLU:CG    | 2.72                     | 0.62              |
| 1:B:54:THR:HG22   | 1:B:156:HIS:CE1   | 2.34                     | 0.62              |
| 2:C:479:VAL:HG22  | 2:C:506:ASN:HA    | 1.81                     | 0.62              |
| 3:D:1372:VAL:HA   | 3:D:1375:MET:HE2  | 1.82                     | 0.62              |
| 3:D:406:ASP:O     | 3:D:422:ALA:HB1   | 1.99                     | 0.62              |
| 2:H:140:ILE:CD1   | 2:H:412:ALA:HA    | 2.28                     | 0.62              |
| 2:H:447:ALA:O     | 2:H:448:ASN:HB2   | 2.00                     | 0.62              |
| 3:I:202:VAL:HG11  | 3:I:445:ARG:NE    | 2.14                     | 0.62              |
| 3:I:881:LEU:CD1   | 3:I:885:ILE:HD11  | 2.29                     | 0.62              |
| 1:K:224:TYR:CD1   | 1:L:9:PRO:HD2     | 2.34                     | 0.62              |
| 2:M:1012:PRO:HD2  | 2:M:1026:GLN:HB2  | 1.82                     | 0.62              |
| 2:M:536:PRO:HB3   | 2:M:906:PHE:HD1   | 1.65                     | 0.62              |
| 2:M:600:ASP:OD1   | 2:M:650:ARG:HA    | 2.00                     | 0.62              |
| 2:M:693:GLU:OE1   | 2:M:696:LYS:HD2   | 2.00                     | 0.62              |
| 2:M:759:THR:HB    | 2:M:785:VAL:CG2   | 2.29                     | 0.62              |
| 3:N:141:ILE:CG1   | 3:N:448:GLU:CD    | 2.66                     | 0.62              |
| 3:N:456:MET:SD    | 3:N:568:ARG:NE    | 2.73                     | 0.62              |
| 1:A:123:MET:O     | 1:A:125:PRO:HD3   | 1.99                     | 0.62              |
| 1:B:12:THR:OG1    | 1:B:24:VAL:HB     | 1.99                     | 0.62              |
| 2:C:508:ILE:CD1   | 2:C:526:PRO:HB3   | 2.30                     | 0.62              |
| 3:D:1112:CYS:HB2  | 3:D:1195:GLN:CG   | 2.24                     | 0.62              |
| 3:D:482:LYS:HE2   | 3:D:1388:ARG:HH22 | 1.64                     | 0.62              |
| 3:D:758:GLU:HA    | 4:E:20:THR:CG2    | 2.29                     | 0.62              |
| 2:H:242:LEU:O     | 2:H:243:ARG:CB    | 2.46                     | 0.62              |
| 2:H:327:HIS:CE1   | 2:H:489:THR:HA    | 2.35                     | 0.62              |
| 3:I:171:LEU:HB2   | 3:I:391:ALA:O     | 2.00                     | 0.62              |
| 3:I:546:ARG:HH12  | 3:I:550:ARG:NH2   | 1.97                     | 0.62              |
| 3:I:642:CYS:HB3   | 3:I:716:PHE:CB    | 2.29                     | 0.62              |
| 3:I:754:PHE:HZ    | 4:J:21:VAL:HG13   | 1.65                     | 0.62              |
| 2:M:111:ASP:HB3   | 2:M:369:PRO:HG3   | 1.80                     | 0.62              |
| 2:M:154:ARG:NH1   | 2:M:178:PRO:CD    | 2.62                     | 0.62              |
| 2:M:284:ARG:HG2   | 2:M:285:LEU:N     | 2.15                     | 0.62              |
| 2:M:680:ASP:O     | 3:N:939:PHE:HB3   | 2.00                     | 0.62              |
| 3:N:957:PRO:CG    | 3:N:1007:VAL:HA   | 2.30                     | 0.62              |
| 3:N:1155:VAL:HG12 | 3:N:1177:ALA:HB1  | 1.82                     | 0.62              |
| 3:N:131:LYS:O     | 3:N:133:ILE:N     | 2.32                     | 0.62              |
| 3:N:646:LYS:HG3   | 3:N:647:ARG:H     | 1.64                     | 0.62              |
| 1:G:134:GLU:HG3   | 3:N:821:VAL:HG12  | 1.82                     | 0.62              |
| 7:Z:155:HIS:O     | 7:Z:156:GLY:C     | 2.38                     | 0.62              |
| 1:G:73:GLU:HG3    | 1:G:130:ALA:HA    | 1.80                     | 0.62              |
| 2:H:293:PHE:N     | 2:H:293:PHE:CD1   | 2.65                     | 0.62              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:H:703:ILE:N     | 2:H:703:ILE:HD12 | 2.14                     | 0.62              |
| 3:I:1007:VAL:HG11 | 3:I:1039:CYS:HB2 | 1.81                     | 0.62              |
| 3:I:204:LEU:CB    | 3:I:394:LEU:HG   | 2.21                     | 0.62              |
| 3:I:555:LYS:HA    | 3:I:558:LEU:CD1  | 2.29                     | 0.62              |
| 2:M:261:ILE:N     | 2:M:261:ILE:HD12 | 2.14                     | 0.62              |
| 2:M:443:THR:HG21  | 3:N:1078:ARG:HD2 | 1.82                     | 0.62              |
| 2:M:44:ILE:HG23   | 2:M:344:PHE:CE1  | 2.35                     | 0.62              |
| 2:M:56:GLU:CD     | 2:M:56:GLU:C     | 2.59                     | 0.62              |
| 3:N:102:ILE:HD12  | 3:N:586:ARG:HG3  | 1.81                     | 0.62              |
| 3:N:1156:LEU:HD13 | 3:N:1176:LYS:HE3 | 1.81                     | 0.62              |
| 2:M:1046:ALA:CB   | 3:N:1476:THR:OG1 | 2.47                     | 0.62              |
| 3:N:171:LEU:HD23  | 3:N:172:PRO:O    | 1.99                     | 0.62              |
| 3:N:39:PRO:HG2    | 3:N:47:GLU:OE2   | 2.00                     | 0.62              |
| 7:Z:84:GLY:HA2    | 7:Z:130:LEU:HD12 | 1.80                     | 0.62              |
| 1:A:156:HIS:CD2   | 1:A:157:GLY:N    | 2.66                     | 0.61              |
| 1:A:189:ARG:HH11  | 1:A:189:ARG:CG   | 2.13                     | 0.61              |
| 2:C:307:LEU:HD11  | 2:C:311:PHE:CE2  | 2.34                     | 0.61              |
| 2:C:412:ALA:HB1   | 2:C:419:THR:HG21 | 1.82                     | 0.61              |
| 2:C:690:ILE:HG13  | 2:C:694:LEU:HD12 | 1.82                     | 0.61              |
| 3:D:1168:MET:CE   | 3:D:1171:VAL:HB  | 2.30                     | 0.61              |
| 3:D:1433:SER:OG   | 3:D:1457:ASP:OD2 | 2.18                     | 0.61              |
| 3:D:13:ALA:HB1    | 3:D:18:ILE:HD11  | 1.81                     | 0.61              |
| 3:D:47:GLU:O      | 3:D:51:GLY:CA    | 2.48                     | 0.61              |
| 2:H:443:THR:HG21  | 3:I:1078:ARG:NE  | 2.15                     | 0.61              |
| 3:I:457:GLY:O     | 3:I:459:GLU:N    | 2.33                     | 0.61              |
| 3:I:736:PHE:O     | 3:I:738:ALA:N    | 2.32                     | 0.61              |
| 2:M:794:PRO:CG    | 2:M:1025:ALA:HA  | 2.29                     | 0.61              |
| 2:M:1061:GLU:HB2  | 3:N:84:ILE:HD13  | 1.80                     | 0.61              |
| 2:M:580:MET:HB3   | 2:M:584:GLU:CD   | 2.21                     | 0.61              |
| 3:N:1366:LYS:O    | 3:N:1369:GLU:HB2 | 1.99                     | 0.61              |
| 3:N:398:ALA:HB2   | 3:N:447:VAL:HG12 | 1.80                     | 0.61              |
| 3:N:841:TYR:HB2   | 3:N:864:VAL:CG1  | 2.30                     | 0.61              |
| 7:Y:89:VAL:HG12   | 7:Y:91:LEU:CD2   | 2.29                     | 0.61              |
| 3:D:642:CYS:HB3   | 3:D:716:PHE:CB   | 2.29                     | 0.61              |
| 3:D:656:PHE:HB3   | 3:D:694:VAL:HG11 | 1.82                     | 0.61              |
| 3:D:834:THR:HB    | 3:D:838:ARG:HB2  | 1.82                     | 0.61              |
| 3:D:850:LEU:HD12  | 3:D:850:LEU:H    | 1.65                     | 0.61              |
| 1:F:73:GLU:HB2    | 1:F:78:ILE:CD1   | 2.29                     | 0.61              |
| 2:H:40:GLU:HG2    | 2:H:42:VAL:HG22  | 1.83                     | 0.61              |
| 2:H:676:ILE:O     | 2:H:676:ILE:HG23 | 1.99                     | 0.61              |
| 3:I:1107:VAL:CG1  | 3:I:1217:ILE:HA  | 2.29                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:202:VAL:HB    | 3:I:396:VAL:HG22  | 1.82                     | 0.61              |
| 3:I:205:TYR:HA    | 3:I:392:SER:O     | 2.00                     | 0.61              |
| 3:I:841:TYR:HB2   | 3:I:864:VAL:CG1   | 2.30                     | 0.61              |
| 1:L:133:GLU:HG3   | 1:L:134:GLU:N     | 2.14                     | 0.61              |
| 2:M:64:LEU:HD22   | 2:M:359:MET:CB    | 2.29                     | 0.61              |
| 3:N:1078:ARG:CG   | 3:N:1078:ARG:HH11 | 2.12                     | 0.61              |
| 3:N:389:GLU:N     | 3:N:390:PRO:HD3   | 2.15                     | 0.61              |
| 3:N:519:VAL:HA    | 3:N:544:TYR:OH    | 2.00                     | 0.61              |
| 3:N:581:LEU:CD2   | 3:N:581:LEU:H     | 2.14                     | 0.61              |
| 3:N:642:CYS:HB3   | 3:N:716:PHE:CB    | 2.29                     | 0.61              |
| 3:N:860:LEU:HD23  | 3:N:877:PRO:HB2   | 1.82                     | 0.61              |
| 4:O:59:ASN:OD1    | 4:O:61:VAL:HG22   | 1.99                     | 0.61              |
| 2:C:1081:VAL:HG21 | 2:C:1111:ILE:HG23 | 1.82                     | 0.61              |
| 2:C:260:LEU:HB3   | 2:C:293:PHE:CE2   | 2.35                     | 0.61              |
| 2:C:408:ARG:HH21  | 2:C:455:LEU:HD12  | 1.64                     | 0.61              |
| 3:D:1041:LEU:HD12 | 3:D:1058:ARG:O    | 2.00                     | 0.61              |
| 3:D:1257:PRO:HA   | 3:D:1260:ILE:HD12 | 1.82                     | 0.61              |
| 3:D:1261:GLU:O    | 3:D:1264:GLU:O    | 2.18                     | 0.61              |
| 2:H:17:PRO:HB2    | 2:H:20:GLU:HB3    | 1.82                     | 0.61              |
| 2:H:808:ARG:O     | 2:H:810:ASP:N     | 2.34                     | 0.61              |
| 3:I:477:LEU:HD11  | 3:I:495:ARG:HG2   | 1.83                     | 0.61              |
| 1:L:32:PHE:HA     | 1:L:35:THR:OG1    | 2.00                     | 0.61              |
| 2:M:334:ARG:HG2   | 2:M:338:GLU:OE1   | 2.01                     | 0.61              |
| 2:M:56:GLU:HG2    | 2:M:356:ARG:HG3   | 1.82                     | 0.61              |
| 3:N:1262:LEU:HB3  | 3:N:1352:ILE:HD11 | 1.81                     | 0.61              |
| 3:N:1273:VAL:O    | 3:N:1273:VAL:HG23 | 2.00                     | 0.61              |
| 3:N:692:GLU:OE1   | 3:N:720:LEU:HD13  | 2.00                     | 0.61              |
| 3:N:785:ILE:CD1   | 3:N:785:ILE:H     | 2.01                     | 0.61              |
| 3:N:864:VAL:HG12  | 3:N:865:THR:H     | 1.65                     | 0.61              |
| 2:M:889:HIS:CD2   | 3:N:951:ILE:HG22  | 2.34                     | 0.61              |
| 4:O:54:LEU:O      | 4:O:54:LEU:HD23   | 1.99                     | 0.61              |
| 3:D:1359:GLN:O    | 7:X:37:MET:CE     | 2.48                     | 0.61              |
| 2:C:99:GLN:HA     | 2:C:109:LYS:O     | 1.99                     | 0.61              |
| 2:C:498:GLN:OE1   | 3:D:1067:VAL:HB   | 2.00                     | 0.61              |
| 3:D:30:GLU:HA     | 3:D:30:GLU:OE1    | 2.00                     | 0.61              |
| 3:D:580:ALA:HA    | 3:D:584:ASN:OD1   | 2.00                     | 0.61              |
| 1:B:185:ARG:HD3   | 3:D:692:GLU:OE2   | 2.01                     | 0.61              |
| 3:D:841:TYR:HB2   | 3:D:864:VAL:CG1   | 2.30                     | 0.61              |
| 1:G:101:LEU:C     | 1:G:101:LEU:HD23  | 2.20                     | 0.61              |
| 2:H:292:ARG:HB2   | 2:H:299:LYS:HE2   | 1.81                     | 0.61              |
| 2:H:876:VAL:O     | 2:H:879:ARG:O     | 2.17                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:875:THR:HG22  | 3:I:879:ARG:HB2   | 1.83                     | 0.61              |
| 2:M:840:ALA:HB2   | 2:M:846:LYS:HA    | 1.80                     | 0.61              |
| 3:N:1251:ASP:O    | 3:N:1252:ILE:HB   | 2.00                     | 0.61              |
| 3:N:1252:ILE:HG13 | 3:N:1253:THR:N    | 2.14                     | 0.61              |
| 3:N:1281:VAL:HG21 | 3:N:1313:VAL:CG2  | 2.29                     | 0.61              |
| 3:N:350:HIS:HD2   | 3:N:371:ILE:HG12  | 1.65                     | 0.61              |
| 3:N:656:PHE:HB3   | 3:N:694:VAL:HG11  | 1.82                     | 0.61              |
| 3:N:789:LEU:HD13  | 3:N:911:LEU:HD21  | 1.82                     | 0.61              |
| 3:N:826:PRO:HD2   | 3:N:829:VAL:HG22  | 1.82                     | 0.61              |
| 7:Y:55:LYS:O      | 7:Y:59:GLU:HG3    | 2.00                     | 0.61              |
| 1:B:55:SER:HA     | 1:B:167:VAL:HG23  | 1.81                     | 0.61              |
| 2:C:263:ASP:HB2   | 2:C:264:PRO:HD3   | 1.83                     | 0.61              |
| 2:C:297:GLU:HG2   | 2:C:298:PHE:N     | 2.16                     | 0.61              |
| 2:C:585:GLU:OE2   | 2:C:589:ARG:HD2   | 2.00                     | 0.61              |
| 2:C:662:GLU:CD    | 2:C:662:GLU:O     | 2.39                     | 0.61              |
| 3:D:802:ALA:O     | 3:D:803:GLY:O     | 2.18                     | 0.61              |
| 1:G:188:GLN:HG2   | 3:I:685:ASP:OD1   | 2.00                     | 0.61              |
| 1:G:26:GLU:HB2    | 1:G:27:PRO:HA     | 1.81                     | 0.61              |
| 2:H:73:LEU:C      | 2:H:73:LEU:HD12   | 2.21                     | 0.61              |
| 2:H:897:LEU:HD21  | 2:H:921:ALA:HA    | 1.81                     | 0.61              |
| 3:I:118:LEU:O     | 3:I:120:ALA:N     | 2.34                     | 0.61              |
| 3:I:1257:PRO:HA   | 3:I:1260:ILE:CD1  | 2.27                     | 0.61              |
| 3:I:137:PRO:HD3   | 3:I:453:ASP:HB2   | 1.82                     | 0.61              |
| 3:I:405:ASP:N     | 3:I:423:ASP:OD1   | 2.33                     | 0.61              |
| 3:I:481:MET:HE2   | 3:I:493:ARG:HA    | 1.83                     | 0.61              |
| 3:I:581:LEU:CD2   | 3:I:581:LEU:H     | 2.13                     | 0.61              |
| 3:I:868:TYR:CE1   | 3:I:869:MET:HG3   | 2.34                     | 0.61              |
| 4:J:69:LEU:HD23   | 4:J:70:THR:HG22   | 1.82                     | 0.61              |
| 1:L:56:VAL:O      | 1:L:165:ILE:HD13  | 2.01                     | 0.61              |
| 1:K:42:ARG:NH2    | 1:L:31:GLY:O      | 2.33                     | 0.61              |
| 3:N:30:GLU:HA     | 3:N:30:GLU:OE1    | 2.00                     | 0.61              |
| 2:C:170:PRO:HD3   | 2:C:263:ASP:HB3   | 1.80                     | 0.61              |
| 2:C:660:ALA:O     | 2:C:667:ALA:HB3   | 2.00                     | 0.61              |
| 2:C:81:ASP:HA     | 2:C:84:ARG:HH11   | 1.64                     | 0.61              |
| 2:C:92:ALA:HB2    | 2:C:120:LEU:HD11  | 1.83                     | 0.61              |
| 3:D:1102:THR:CA   | 3:D:1105:ILE:HD13 | 2.28                     | 0.61              |
| 3:D:683:ILE:O     | 3:D:683:ILE:HG22  | 1.99                     | 0.61              |
| 1:G:12:THR:OG1    | 1:G:24:VAL:HB     | 1.99                     | 0.61              |
| 2:H:188:LYS:HB2   | 2:H:188:LYS:HZ3   | 1.62                     | 0.61              |
| 2:H:191:PHE:CD2   | 2:H:192:PRO:O     | 2.54                     | 0.61              |
| 2:H:343:GLN:O     | 2:H:346:VAL:HB    | 2.01                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:662:GLU:O     | 2:H:662:GLU:CD    | 2.39                     | 0.61              |
| 2:H:675:ALA:HB2   | 2:H:867:VAL:HG11  | 1.81                     | 0.61              |
| 3:I:957:PRO:CG    | 3:I:1007:VAL:HA   | 2.31                     | 0.61              |
| 3:I:1112:CYS:HB2  | 3:I:1195:GLN:CG   | 2.28                     | 0.61              |
| 3:I:1122:LEU:CD1  | 3:I:1186:VAL:HG23 | 2.30                     | 0.61              |
| 3:I:139:GLY:HA3   | 3:I:162:ARG:NH2   | 2.15                     | 0.61              |
| 3:I:202:VAL:O     | 3:I:396:VAL:N     | 2.32                     | 0.61              |
| 4:J:28:GLN:HB3    | 4:J:32:ARG:HH12   | 1.66                     | 0.61              |
| 3:I:693:GLU:HG3   | 4:J:48:MET:HE1    | 1.81                     | 0.61              |
| 2:M:759:THR:HB    | 2:M:785:VAL:HG22  | 1.81                     | 0.61              |
| 3:N:1003:VAL:HG11 | 3:N:1041:LEU:CD2  | 2.31                     | 0.61              |
| 3:N:956:ILE:HD13  | 3:N:1062:ARG:HH21 | 1.66                     | 0.61              |
| 3:N:154:THR:HG23  | 3:N:157:GLU:HB2   | 1.83                     | 0.61              |
| 4:O:6:ILE:HD11    | 4:O:10:PHE:CE1    | 2.36                     | 0.61              |
| 3:I:1359:GLN:O    | 7:Y:37:MET:HE1    | 1.99                     | 0.61              |
| 2:C:1032:PHE:O    | 2:C:1033:GLY:O    | 2.18                     | 0.61              |
| 3:D:1291:SER:HB2  | 3:D:1293:PHE:HE1  | 1.64                     | 0.61              |
| 3:D:159:ARG:HH12  | 2:H:218:VAL:HB    | 1.66                     | 0.61              |
| 3:D:554:LEU:HD22  | 3:D:574:LEU:HD22  | 1.82                     | 0.61              |
| 3:D:704:ARG:CB    | 3:D:736:PHE:HB3   | 2.31                     | 0.61              |
| 3:D:922:LEU:N     | 3:D:922:LEU:HD23  | 2.15                     | 0.61              |
| 1:F:156:HIS:CD2   | 1:F:157:GLY:N     | 2.66                     | 0.61              |
| 2:H:30:LEU:HB3    | 2:H:44:ILE:HG13   | 1.82                     | 0.61              |
| 2:H:19:THR:HG23   | 2:H:404:LEU:HD11  | 1.81                     | 0.61              |
| 3:I:182:GLY:CA    | 3:I:441:ARG:HH11  | 2.13                     | 0.61              |
| 3:I:615:ARG:HD2   | 3:I:619:LEU:HD21  | 1.82                     | 0.61              |
| 2:M:673:LEU:HD22  | 2:M:867:VAL:HG12  | 1.83                     | 0.61              |
| 3:N:1353:GLN:O    | 3:N:1357:ARG:HG3  | 2.00                     | 0.61              |
| 3:N:181:ASP:O     | 3:N:204:LEU:HA    | 1.99                     | 0.61              |
| 3:N:477:LEU:HD11  | 3:N:495:ARG:HG2   | 1.82                     | 0.61              |
| 3:N:520:LEU:HD11  | 3:N:524:LEU:HD22  | 1.81                     | 0.61              |
| 3:N:567:ILE:O     | 3:N:571:LYS:HG2   | 2.01                     | 0.61              |
| 3:N:922:LEU:N     | 3:N:922:LEU:HD23  | 2.16                     | 0.61              |
| 7:X:139:SER:CB    | 7:X:148:GLU:HG3   | 2.30                     | 0.61              |
| 7:Z:89:VAL:CG1    | 7:Z:151:VAL:HG13  | 2.31                     | 0.61              |
| 1:A:206:THR:HG22  | 1:A:209:GLU:HG3   | 1.83                     | 0.61              |
| 1:B:57:TYR:CE2    | 1:B:161:ARG:HG2   | 2.36                     | 0.61              |
| 2:C:1035:MET:HA   | 2:C:1038:TRP:CE3  | 2.35                     | 0.61              |
| 2:C:108:ILE:HG22  | 2:C:109:LYS:N     | 2.15                     | 0.61              |
| 2:C:342:ASP:O     | 2:C:345:ARG:HG2   | 2.01                     | 0.61              |
| 2:C:451:LEU:C     | 2:C:452:ILE:HD12  | 2.21                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:544:THR:O     | 2:C:547:ILE:CD1   | 2.49                     | 0.61              |
| 3:D:1041:LEU:HD12 | 3:D:1058:ARG:C    | 2.21                     | 0.61              |
| 3:D:1121:PRO:HB2  | 3:D:1135:ARG:NH1  | 1.98                     | 0.61              |
| 3:D:1123:PHE:CZ   | 3:D:1178:ALA:HB1  | 2.35                     | 0.61              |
| 3:D:1273:VAL:HG21 | 3:D:1305:LEU:HD21 | 1.81                     | 0.61              |
| 3:D:457:GLY:O     | 3:D:459:GLU:N     | 2.33                     | 0.61              |
| 4:E:41:GLU:OE1    | 4:E:42:PRO:HD3    | 2.01                     | 0.61              |
| 1:F:158:ILE:HD12  | 1:F:158:ILE:H     | 1.64                     | 0.61              |
| 2:H:418:LEU:HD12  | 2:H:418:LEU:N     | 2.16                     | 0.61              |
| 3:I:123:LEU:HD11  | 3:I:152:LEU:HD21  | 1.82                     | 0.61              |
| 3:I:847:ASP:O     | 3:I:851:LEU:HG    | 2.01                     | 0.61              |
| 1:L:102:LYS:HZ1   | 1:L:137:ARG:HH12  | 1.47                     | 0.61              |
| 1:L:26:GLU:HB2    | 1:L:27:PRO:HA     | 1.81                     | 0.61              |
| 2:M:195:LEU:O     | 2:M:198:ARG:HB2   | 2.00                     | 0.61              |
| 2:M:109:LYS:NZ    | 2:M:367:LEU:C     | 2.54                     | 0.61              |
| 2:M:451:LEU:C     | 2:M:452:ILE:HD12  | 2.21                     | 0.61              |
| 2:M:544:THR:O     | 2:M:547:ILE:CD1   | 2.49                     | 0.61              |
| 2:M:676:ILE:O     | 2:M:676:ILE:HG23  | 2.00                     | 0.61              |
| 2:M:808:ARG:O     | 2:M:810:ASP:N     | 2.34                     | 0.61              |
| 3:N:957:PRO:HG2   | 3:N:1007:VAL:HA   | 1.83                     | 0.61              |
| 3:N:1066:THR:CG2  | 3:N:1069:GLU:HB2  | 2.26                     | 0.61              |
| 3:N:432:TYR:CD2   | 3:N:450:TYR:HE2   | 2.17                     | 0.61              |
| 3:N:997:THR:HG21  | 7:Z:61:ARG:NH1    | 2.15                     | 0.61              |
| 2:C:666:LEU:HD12  | 2:C:667:ALA:N     | 2.14                     | 0.61              |
| 2:C:808:ARG:O     | 2:C:810:ASP:N     | 2.34                     | 0.61              |
| 3:D:801:GLY:O     | 3:D:802:ALA:HB2   | 1.99                     | 0.61              |
| 3:D:826:PRO:HD2   | 3:D:829:VAL:HG22  | 1.82                     | 0.61              |
| 2:H:544:THR:O     | 2:H:547:ILE:CD1   | 2.49                     | 0.61              |
| 2:H:9:ILE:O       | 2:H:9:ILE:HG13    | 2.01                     | 0.61              |
| 3:I:1041:LEU:HD12 | 3:I:1058:ARG:C    | 2.21                     | 0.61              |
| 3:I:704:ARG:CB    | 3:I:736:PHE:HB3   | 2.31                     | 0.61              |
| 2:M:577:PRO:HG3   | 2:M:993:PHE:CE1   | 2.35                     | 0.61              |
| 3:N:1041:LEU:HD12 | 3:N:1058:ARG:C    | 2.21                     | 0.61              |
| 3:N:1112:CYS:HB2  | 3:N:1195:GLN:CG   | 2.31                     | 0.61              |
| 3:N:133:ILE:HG23  | 3:N:455:ARG:O     | 1.99                     | 0.61              |
| 3:N:617:ASN:HD22  | 3:N:1466:VAL:HG12 | 1.65                     | 0.61              |
| 3:N:168:THR:HG22  | 3:N:170:PRO:CD    | 2.29                     | 0.61              |
| 3:N:203:ALA:HB1   | 3:N:393:ILE:CG2   | 2.30                     | 0.61              |
| 3:N:907:GLU:HG2   | 3:N:909:ASN:H     | 1.66                     | 0.61              |
| 6:U:14:C:H2'      | 6:U:15:G:C8       | 2.35                     | 0.61              |
| 7:Y:7:LEU:HA      | 7:Y:109:GLU:OE2   | 2.01                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1065:ALA:HB1  | 2:C:1077:PRO:CG   | 2.18                     | 0.61              |
| 2:C:144:PRO:O     | 2:C:276:LYS:NZ    | 2.34                     | 0.61              |
| 2:C:199:VAL:HG13  | 2:C:235:LEU:HG    | 1.82                     | 0.61              |
| 2:C:430:VAL:O     | 2:C:430:VAL:HG13  | 2.01                     | 0.61              |
| 2:C:697:ARG:HD2   | 2:C:699:PHE:CE1   | 2.36                     | 0.61              |
| 3:D:152:LEU:HD23  | 3:D:152:LEU:N     | 2.10                     | 0.61              |
| 2:C:1084:SER:HB3  | 3:D:617:ASN:OD1   | 2.00                     | 0.61              |
| 3:D:762:GLN:NE2   | 4:E:20:THR:CG2    | 2.42                     | 0.61              |
| 1:G:52:ALA:HB2    | 1:G:170:VAL:C     | 2.22                     | 0.61              |
| 2:H:126:SER:HB3   | 2:H:395:LYS:HZ1   | 1.66                     | 0.61              |
| 2:H:272:ALA:HA    | 2:H:464:LEU:HD22  | 1.82                     | 0.61              |
| 3:I:1353:GLN:O    | 3:I:1357:ARG:HG3  | 2.01                     | 0.61              |
| 3:I:1397:LYS:HZ1  | 3:I:1432:LYS:NZ   | 1.99                     | 0.61              |
| 3:I:1487:VAL:HG12 | 3:I:1488:ASP:H    | 1.65                     | 0.61              |
| 3:I:679:ARG:HB2   | 3:I:682:ASP:OD1   | 2.01                     | 0.61              |
| 3:I:684:LYS:O     | 3:I:687:VAL:HG23  | 2.01                     | 0.61              |
| 3:I:864:VAL:HG12  | 3:I:865:THR:H     | 1.65                     | 0.61              |
| 3:I:907:GLU:HG2   | 3:I:909:ASN:H     | 1.66                     | 0.61              |
| 3:I:956:ILE:HD11  | 3:I:1062:ARG:CB   | 2.31                     | 0.61              |
| 1:K:80:LEU:HD23   | 1:K:81:ASN:N      | 2.16                     | 0.61              |
| 1:L:52:ALA:HB2    | 1:L:170:VAL:C     | 2.22                     | 0.61              |
| 3:N:1025:GLN:NE2  | 3:N:1025:GLN:HA   | 2.16                     | 0.61              |
| 7:Y:11:GLY:HA3    | 7:Y:109:GLU:OE1   | 2.01                     | 0.61              |
| 1:B:132:LEU:HD21  | 1:B:138:LEU:CB    | 2.30                     | 0.60              |
| 2:C:1081:VAL:CB   | 2:C:1111:ILE:HG22 | 2.30                     | 0.60              |
| 2:C:91:GLN:HA     | 2:C:119:PRO:HA    | 1.83                     | 0.60              |
| 2:C:202:TYR:HB3   | 2:C:207:LEU:HD12  | 1.81                     | 0.60              |
| 2:C:300:ASP:OD2   | 2:C:303:PHE:HB2   | 2.00                     | 0.60              |
| 3:D:1264:GLU:HG2  | 3:D:1266:ARG:HH21 | 1.66                     | 0.60              |
| 3:D:654:LYS:HB3   | 3:D:655:PRO:CD    | 2.29                     | 0.60              |
| 3:D:957:PRO:CG    | 3:D:1007:VAL:HA   | 2.31                     | 0.60              |
| 3:D:988:ARG:O     | 3:D:992:ILE:HG13  | 2.01                     | 0.60              |
| 4:E:24:ALA:O      | 4:E:27:ALA:N      | 2.34                     | 0.60              |
| 2:H:1105:LYS:HZ1  | 2:H:1107:ASN:HB2  | 1.63                     | 0.60              |
| 2:H:313:LEU:CB    | 2:H:320:HIS:HE1   | 2.14                     | 0.60              |
| 2:H:54:ILE:CG2    | 2:H:54:ILE:O      | 2.50                     | 0.60              |
| 2:H:682:TYR:CE1   | 2:H:851:LYS:HD3   | 2.36                     | 0.60              |
| 3:I:198:ARG:HH11  | 3:I:198:ARG:HG3   | 1.66                     | 0.60              |
| 3:I:23:TYR:O      | 3:I:49:ILE:CG2    | 2.49                     | 0.60              |
| 3:I:567:ILE:O     | 3:I:571:LYS:HG2   | 2.01                     | 0.60              |
| 2:H:1070:ILE:HG21 | 3:I:655:PRO:HB2   | 1.81                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:850:LEU:H    | 3:I:850:LEU:HD12  | 1.65                     | 0.60              |
| 1:K:206:THR:HG22 | 1:K:209:GLU:HG3   | 1.83                     | 0.60              |
| 1:L:86:VAL:HG13  | 1:L:124:ASN:HB2   | 1.83                     | 0.60              |
| 2:M:184:MET:HB2  | 2:M:193:LEU:CG    | 2.31                     | 0.60              |
| 2:M:63:GLY:N     | 2:M:103:LYS:CG    | 2.63                     | 0.60              |
| 2:M:690:ILE:HG13 | 2:M:694:LEU:HD12  | 1.82                     | 0.60              |
| 7:Y:14:ARG:HB3   | 7:Y:14:ARG:HH11   | 1.64                     | 0.60              |
| 2:C:101:ILE:HG23 | 2:C:108:ILE:CG1   | 2.31                     | 0.60              |
| 2:C:146:VAL:HB   | 2:C:281:LEU:HD21  | 1.82                     | 0.60              |
| 3:D:1273:VAL:O   | 3:D:1273:VAL:HG23 | 2.00                     | 0.60              |
| 3:D:458:ALA:HB2  | 3:D:575:GLN:HE22  | 1.66                     | 0.60              |
| 1:F:189:ARG:CG   | 1:F:189:ARG:HH11  | 2.13                     | 0.60              |
| 1:F:206:THR:HG22 | 1:F:209:GLU:HG3   | 1.83                     | 0.60              |
| 2:H:1095:LEU:HB2 | 3:I:101:HIS:HE1   | 1.66                     | 0.60              |
| 3:D:564:GLU:H    | 2:H:223:ASP:HA    | 1.66                     | 0.60              |
| 2:H:430:VAL:HG13 | 2:H:430:VAL:O     | 2.01                     | 0.60              |
| 2:H:580:MET:HB3  | 2:H:584:GLU:CD    | 2.21                     | 0.60              |
| 2:H:939:ARG:HE   | 2:H:939:ARG:CA    | 2.06                     | 0.60              |
| 3:I:1018:ASN:HB3 | 3:I:1021:TYR:HB3  | 1.83                     | 0.60              |
| 3:I:1264:GLU:HG2 | 3:I:1266:ARG:HH21 | 1.66                     | 0.60              |
| 3:I:561:GLY:C    | 3:I:563:PRO:HD3   | 2.20                     | 0.60              |
| 3:I:615:ARG:CG   | 3:I:619:LEU:HD21  | 2.31                     | 0.60              |
| 3:I:692:GLU:OE1  | 3:I:720:LEU:HD13  | 2.01                     | 0.60              |
| 2:M:143:SER:O    | 2:M:147:TYR:OH    | 2.19                     | 0.60              |
| 2:M:282:GLY:C    | 2:M:283:ILE:HG12  | 2.20                     | 0.60              |
| 2:M:333:ILE:N    | 2:M:333:ILE:CD1   | 2.65                     | 0.60              |
| 2:M:660:ALA:O    | 2:M:667:ALA:HB3   | 2.00                     | 0.60              |
| 2:M:662:GLU:CD   | 2:M:662:GLU:O     | 2.39                     | 0.60              |
| 2:M:897:LEU:HD21 | 2:M:921:ALA:HA    | 1.81                     | 0.60              |
| 3:N:675:ARG:NH1  | 3:N:679:ARG:HH11  | 1.99                     | 0.60              |
| 3:N:785:ILE:HD12 | 3:N:785:ILE:N     | 2.03                     | 0.60              |
| 3:N:850:LEU:H    | 3:N:850:LEU:HD12  | 1.65                     | 0.60              |
| 7:Z:17:GLN:O     | 7:Z:21:ARG:HD3    | 2.01                     | 0.60              |
| 1:B:52:ALA:HB2   | 1:B:170:VAL:C     | 2.21                     | 0.60              |
| 2:C:22:GLN:HB3   | 2:C:121:MET:CE    | 2.31                     | 0.60              |
| 2:C:307:LEU:HD12 | 2:C:310:LEU:HB3   | 1.82                     | 0.60              |
| 2:C:473:ARG:NE   | 2:C:531:PHE:CZ    | 2.69                     | 0.60              |
| 2:C:52:PHE:CG    | 2:C:68:PHE:HB2    | 2.36                     | 0.60              |
| 2:C:571:LEU:HD11 | 2:C:700:TYR:HA    | 1.83                     | 0.60              |
| 3:D:152:LEU:CD2  | 3:D:152:LEU:N     | 2.64                     | 0.60              |
| 2:H:18:LEU:CD1   | 2:H:586:ARG:NH1   | 2.65                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:212:GLY:C     | 2:H:214:TYR:H     | 2.04                     | 0.60              |
| 2:H:571:LEU:CD1   | 2:H:701:THR:N     | 2.65                     | 0.60              |
| 2:H:690:ILE:HG13  | 2:H:694:LEU:HD12  | 1.82                     | 0.60              |
| 2:H:697:ARG:HB2   | 2:H:699:PHE:HD1   | 1.67                     | 0.60              |
| 3:I:1205:TYR:HD2  | 3:I:1215:VAL:HG21 | 1.67                     | 0.60              |
| 3:I:1366:LYS:O    | 3:I:1369:GLU:HB2  | 2.00                     | 0.60              |
| 3:I:656:PHE:HB3   | 3:I:694:VAL:HG11  | 1.82                     | 0.60              |
| 1:L:170:VAL:HG11  | 3:N:848:GLU:OE2   | 2.01                     | 0.60              |
| 2:M:127:PHE:O     | 2:M:133:ASP:HA    | 2.01                     | 0.60              |
| 2:M:185:LYS:HG2   | 2:M:190:LYS:HG3   | 1.83                     | 0.60              |
| 2:M:666:LEU:HD12  | 2:M:667:ALA:H     | 1.65                     | 0.60              |
| 2:M:966:LEU:HD21  | 2:M:986:PRO:CG    | 2.32                     | 0.60              |
| 3:N:1388:ARG:NH1  | 3:N:1388:ARG:HA   | 2.16                     | 0.60              |
| 3:N:153:LEU:CD1   | 3:N:158:TYR:HB2   | 2.31                     | 0.60              |
| 3:N:1486:VAL:HG12 | 4:O:22:VAL:HG13   | 1.84                     | 0.60              |
| 5:R:18:DC:H2'     | 5:R:19:DC:C6      | 2.36                     | 0.60              |
| 3:N:991:GLN:OE1   | 7:Z:111:ASN:HA    | 2.01                     | 0.60              |
| 2:C:9:ILE:HG12    | 2:C:907:ASP:OD2   | 2.01                     | 0.60              |
| 3:D:160:GLU:CG    | 3:D:165:LYS:HE3   | 2.31                     | 0.60              |
| 3:D:677:LEU:HD23  | 3:D:683:ILE:HD13  | 1.79                     | 0.60              |
| 1:G:62:LEU:CD1    | 1:G:63:HIS:H      | 2.11                     | 0.60              |
| 2:H:794:PRO:HG2   | 2:H:1025:ALA:C    | 2.21                     | 0.60              |
| 2:H:204:GLN:NE2   | 2:H:228:ALA:CB    | 2.64                     | 0.60              |
| 2:H:52:PHE:HZ     | 2:H:98:LEU:HB3    | 1.67                     | 0.60              |
| 2:H:861:LEU:HG    | 2:H:862:PRO:CD    | 2.26                     | 0.60              |
| 2:H:94:LEU:HD12   | 2:H:95:TYR:N      | 2.16                     | 0.60              |
| 3:I:1273:VAL:O    | 3:I:1273:VAL:HG23 | 2.00                     | 0.60              |
| 3:I:729:HIS:CE1   | 3:I:731:LEU:HB2   | 2.36                     | 0.60              |
| 3:I:947:ILE:CD1   | 3:I:947:ILE:O     | 2.46                     | 0.60              |
| 1:K:31:GLY:H      | 1:K:193:ASP:CG    | 2.05                     | 0.60              |
| 2:M:235:LEU:CD1   | 2:M:298:PHE:CZ    | 2.81                     | 0.60              |
| 2:M:654:LEU:CD2   | 2:M:654:LEU:H     | 2.13                     | 0.60              |
| 3:N:179:VAL:HG13  | 3:N:183:GLU:CG    | 2.31                     | 0.60              |
| 3:N:400:VAL:HG22  | 3:N:443:VAL:HG21  | 1.82                     | 0.60              |
| 3:N:704:ARG:CB    | 3:N:736:PHE:HB3   | 2.31                     | 0.60              |
| 3:N:847:ASP:O     | 3:N:851:LEU:HG    | 2.01                     | 0.60              |
| 3:N:982:PHE:HB3   | 7:Z:119:ILE:HD12  | 1.83                     | 0.60              |
| 3:D:477:LEU:HD11  | 3:D:495:ARG:HG2   | 1.83                     | 0.60              |
| 3:D:847:ASP:O     | 3:D:851:LEU:HG    | 2.02                     | 0.60              |
| 2:H:333:ILE:HD12  | 2:H:333:ILE:N     | 2.16                     | 0.60              |
| 2:H:679:PHE:CE2   | 2:H:853:LEU:HD21  | 2.37                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:860:LEU:HD23  | 3:I:877:PRO:HB2   | 1.82                     | 0.60              |
| 1:K:156:HIS:CD2   | 1:K:157:GLY:N     | 2.66                     | 0.60              |
| 1:K:158:ILE:HD12  | 1:K:158:ILE:H     | 1.64                     | 0.60              |
| 2:M:1034:GLU:OE2  | 3:N:1096:ARG:NH1  | 2.35                     | 0.60              |
| 2:M:100:LEU:O     | 2:M:108:ILE:HA    | 2.01                     | 0.60              |
| 2:M:254:VAL:C     | 2:M:257:VAL:HG23  | 2.21                     | 0.60              |
| 2:M:904:PRO:HD2   | 2:M:908:GLY:HA2   | 1.82                     | 0.60              |
| 3:N:770:LEU:HB2   | 3:N:1210:SER:O    | 2.00                     | 0.60              |
| 3:N:908:LYS:HB2   | 3:N:1027:GLY:HA3  | 1.83                     | 0.60              |
| 1:A:9:PRO:HB2     | 1:B:224:TYR:HB3   | 1.84                     | 0.60              |
| 2:C:580:MET:HB3   | 2:C:584:GLU:CD    | 2.21                     | 0.60              |
| 2:C:706:GLU:HG2   | 2:C:708:TYR:CZ    | 2.36                     | 0.60              |
| 2:C:98:LEU:H      | 2:C:98:LEU:HD12   | 1.66                     | 0.60              |
| 2:C:449:ILE:HG21  | 3:D:1082:ALA:HA   | 1.84                     | 0.60              |
| 3:D:1137:ARG:O    | 3:D:1141:GLU:HG3  | 2.01                     | 0.60              |
| 3:D:1149:LEU:HD23 | 3:D:1187:PRO:O    | 2.00                     | 0.60              |
| 3:D:1102:THR:HG21 | 3:D:1371:VAL:HG22 | 1.83                     | 0.60              |
| 3:D:792:ILE:O     | 3:D:878:GLY:HA3   | 2.01                     | 0.60              |
| 3:D:907:GLU:HG2   | 3:D:909:ASN:H     | 1.66                     | 0.60              |
| 2:H:660:ALA:CB    | 2:H:667:ALA:O     | 2.37                     | 0.60              |
| 2:H:705:ILE:HG23  | 2:H:827:VAL:O     | 2.02                     | 0.60              |
| 3:I:108:VAL:HB    | 3:I:109:PRO:CD    | 2.29                     | 0.60              |
| 3:I:1114:THR:HG22 | 3:I:1195:GLN:HB3  | 1.83                     | 0.60              |
| 3:I:119:SER:HB2   | 3:I:123:LEU:N     | 2.17                     | 0.60              |
| 3:I:1397:LYS:NZ   | 3:I:1432:LYS:HZ3  | 2.00                     | 0.60              |
| 3:I:1441:GLN:HG2  | 3:I:1442:ASN:N    | 2.16                     | 0.60              |
| 3:I:792:ILE:O     | 3:I:878:GLY:HA3   | 2.01                     | 0.60              |
| 3:I:922:LEU:N     | 3:I:922:LEU:HD23  | 2.16                     | 0.60              |
| 2:M:458:TYR:CD1   | 2:M:458:TYR:N     | 2.70                     | 0.60              |
| 2:M:674:VAL:HG12  | 2:M:990:GLY:O     | 2.01                     | 0.60              |
| 3:N:1149:LEU:HG   | 3:N:1166:LEU:CD2  | 2.32                     | 0.60              |
| 3:N:792:ILE:O     | 3:N:878:GLY:HA3   | 2.01                     | 0.60              |
| 3:N:838:ARG:HB3   | 3:N:865:THR:CG2   | 2.30                     | 0.60              |
| 7:Z:102:VAL:HG11  | 7:Z:125:MET:HE1   | 1.83                     | 0.60              |
| 1:B:59:GLU:OE2    | 1:B:139:ASN:HB3   | 2.02                     | 0.60              |
| 1:B:92:PRO:HA     | 1:B:146:ARG:NH1   | 2.17                     | 0.60              |
| 2:C:207:LEU:HD22  | 2:C:221:LEU:CD2   | 2.32                     | 0.60              |
| 2:C:269:LEU:HD23  | 2:C:270:GLY:N     | 2.16                     | 0.60              |
| 2:C:904:PRO:HD2   | 2:C:908:GLY:HA2   | 1.82                     | 0.60              |
| 2:C:675:ALA:CA    | 2:C:989:VAL:HG12  | 2.28                     | 0.60              |
| 3:D:1353:GLN:O    | 3:D:1357:ARG:HG3  | 2.00                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1043:TYR:CE2  | 3:D:710:ARG:HD2   | 2.36                     | 0.60              |
| 3:D:692:GLU:OE1   | 3:D:720:LEU:HD13  | 2.00                     | 0.60              |
| 3:D:729:HIS:CE1   | 3:D:731:LEU:HB2   | 2.36                     | 0.60              |
| 3:D:864:VAL:HG12  | 3:D:865:THR:H     | 1.65                     | 0.60              |
| 1:F:150:TYR:HE2   | 1:F:152:PRO:HG3   | 1.67                     | 0.60              |
| 1:G:42:ARG:CZ     | 1:G:42:ARG:HB3    | 2.31                     | 0.60              |
| 2:H:666:LEU:HD12  | 2:H:667:ALA:H     | 1.66                     | 0.60              |
| 2:H:904:PRO:HD2   | 2:H:908:GLY:HA2   | 1.83                     | 0.60              |
| 2:H:966:LEU:HD21  | 2:H:986:PRO:CG    | 2.32                     | 0.60              |
| 3:I:957:PRO:HG2   | 3:I:1007:VAL:HA   | 1.84                     | 0.60              |
| 3:I:143:ASN:CB    | 3:I:161:LEU:HD11  | 2.31                     | 0.60              |
| 3:I:30:GLU:OE1    | 3:I:30:GLU:HA     | 2.00                     | 0.60              |
| 3:I:204:LEU:O     | 3:I:394:LEU:N     | 2.34                     | 0.60              |
| 3:I:834:THR:HB    | 3:I:838:ARG:HB2   | 1.82                     | 0.60              |
| 3:I:885:ILE:HD13  | 3:I:885:ILE:N     | 2.16                     | 0.60              |
| 1:K:39:PRO:HG3    | 1:L:39:PRO:CG     | 2.31                     | 0.60              |
| 2:M:1035:MET:HA   | 2:M:1038:TRP:CE3  | 2.36                     | 0.60              |
| 2:M:144:PRO:O     | 2:M:276:LYS:NZ    | 2.34                     | 0.60              |
| 2:M:188:LYS:CG    | 2:M:188:LYS:O     | 2.47                     | 0.60              |
| 2:M:657:ASP:OD1   | 2:M:661:SER:O     | 2.20                     | 0.60              |
| 2:M:939:ARG:CA    | 2:M:939:ARG:HE    | 2.06                     | 0.60              |
| 3:N:1264:GLU:HG2  | 3:N:1266:ARG:HH21 | 1.66                     | 0.60              |
| 3:N:1280:VAL:HA   | 3:N:1318:TYR:HA   | 1.83                     | 0.60              |
| 3:N:729:HIS:CE1   | 3:N:731:LEU:HB2   | 2.36                     | 0.60              |
| 3:N:907:GLU:HG2   | 3:N:908:LYS:N     | 2.17                     | 0.60              |
| 2:C:15:LEU:HD12   | 2:C:15:LEU:N      | 2.16                     | 0.60              |
| 2:C:63:GLY:N      | 2:C:103:LYS:HD3   | 2.17                     | 0.60              |
| 2:C:683:ASN:HA    | 2:C:687:ALA:HB3   | 1.83                     | 0.60              |
| 3:D:1107:VAL:HG23 | 3:D:1219:GLU:O    | 2.02                     | 0.60              |
| 3:D:977:ALA:CB    | 3:D:983:LEU:HD21  | 2.31                     | 0.60              |
| 3:D:758:GLU:HA    | 4:E:20:THR:HG21   | 1.83                     | 0.60              |
| 3:I:615:ARG:HE    | 3:I:619:LEU:HD21  | 1.66                     | 0.60              |
| 2:H:1043:TYR:HE1  | 3:I:710:ARG:O     | 1.85                     | 0.60              |
| 2:M:129:ILE:CD1   | 2:M:129:ILE:N     | 2.65                     | 0.60              |
| 3:N:1025:GLN:HE21 | 3:N:1025:GLN:CA   | 2.14                     | 0.60              |
| 3:N:124:GLU:O     | 3:N:127:LEU:HD12  | 2.01                     | 0.60              |
| 3:N:50:PHE:CZ     | 3:N:522:PRO:HG3   | 2.37                     | 0.60              |
| 2:M:946:ARG:NH1   | 3:N:796:ARG:HH22  | 1.99                     | 0.60              |
| 2:M:1086:ARG:CZ   | 3:N:88:TYR:CE1    | 2.84                     | 0.60              |
| 2:M:1044:GLY:HA3  | 4:O:17:TYR:CE1    | 2.37                     | 0.60              |
| 1:A:34:VAL:HG11   | 1:B:42:ARG:HH21   | 1.66                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:243:ARG:HB2  | 2:C:244:PRO:HD3   | 1.84                     | 0.60              |
| 2:C:302:VAL:C    | 2:C:305:PRO:HD2   | 2.21                     | 0.60              |
| 2:C:47:ALA:O     | 2:C:348:LEU:HD23  | 2.02                     | 0.60              |
| 3:D:1105:ILE:HB  | 3:D:1222:GLY:CA   | 2.31                     | 0.60              |
| 3:D:179:VAL:CG1  | 3:D:183:GLU:HB3   | 2.32                     | 0.60              |
| 3:D:452:ILE:H    | 3:D:452:ILE:HD13  | 1.66                     | 0.60              |
| 3:D:544:TYR:CE2  | 3:D:581:LEU:HD12  | 2.37                     | 0.60              |
| 3:D:860:LEU:HD23 | 3:D:877:PRO:HB2   | 1.82                     | 0.60              |
| 4:E:43:GLU:O     | 4:E:44:GLU:HB2    | 2.01                     | 0.60              |
| 2:H:1102:LEU:HB2 | 3:I:7:LYS:O       | 2.01                     | 0.60              |
| 2:H:304:LEU:HG   | 2:H:305:PRO:CD    | 2.25                     | 0.60              |
| 2:H:376:ARG:HB3  | 2:H:377:PRO:HD3   | 1.84                     | 0.60              |
| 2:H:458:TYR:CD1  | 2:H:458:TYR:N     | 2.70                     | 0.60              |
| 3:I:615:ARG:HG3  | 3:I:619:LEU:HD21  | 1.83                     | 0.60              |
| 3:I:826:PRO:HD2  | 3:I:829:VAL:HG22  | 1.82                     | 0.60              |
| 1:G:74:ASP:N     | 1:L:162:ILE:HD13  | 2.17                     | 0.60              |
| 2:M:157:ARG:CZ   | 2:M:314:THR:HG23  | 2.31                     | 0.60              |
| 2:M:395:LYS:O    | 2:M:397:GLU:HG3   | 2.01                     | 0.60              |
| 2:M:988:VAL:HG11 | 3:N:949:ILE:O     | 2.02                     | 0.60              |
| 3:N:108:VAL:HB   | 3:N:109:PRO:CD    | 2.29                     | 0.60              |
| 3:N:1235:GLN:NE2 | 7:Z:43:TYR:HE1    | 2.00                     | 0.60              |
| 3:N:372:ASP:C    | 3:N:374:GLU:H     | 2.05                     | 0.60              |
| 2:M:987:ILE:HD11 | 3:N:946:GLY:CA    | 2.32                     | 0.60              |
| 3:I:997:THR:CG2  | 7:Y:61:ARG:NH1    | 2.63                     | 0.60              |
| 1:B:190:THR:CB   | 3:D:722:GLU:OE1   | 2.49                     | 0.60              |
| 2:C:1033:GLY:O   | 2:C:1037:VAL:HG23 | 2.02                     | 0.60              |
| 3:D:25:GLU:HB2   | 3:D:92:HIS:CE1    | 2.37                     | 0.60              |
| 3:D:814:ALA:HB1  | 3:D:818:ARG:HE    | 1.67                     | 0.60              |
| 3:D:838:ARG:HB3  | 3:D:865:THR:CG2   | 2.29                     | 0.60              |
| 3:D:907:GLU:HG2  | 3:D:908:LYS:N     | 2.17                     | 0.60              |
| 4:E:19:LEU:O     | 4:E:23:VAL:HG23   | 2.02                     | 0.60              |
| 2:H:52:PHE:O     | 2:H:54:ILE:N      | 2.35                     | 0.60              |
| 2:H:657:ASP:OD1  | 2:H:661:SER:O     | 2.20                     | 0.60              |
| 2:H:6:PHE:CE2    | 2:H:917:LEU:HD11  | 2.37                     | 0.60              |
| 3:I:1040:GLY:O   | 3:I:1060:SER:HB3  | 2.02                     | 0.60              |
| 3:I:984:THR:CG2  | 3:I:987:GLU:H     | 2.14                     | 0.60              |
| 2:M:129:ILE:CG1  | 2:M:134:ARG:CD    | 2.79                     | 0.60              |
| 2:M:236:ILE:H    | 2:M:236:ILE:CD1   | 2.15                     | 0.60              |
| 4:O:51:LEU:HD12  | 4:O:53:GLY:N      | 2.17                     | 0.60              |
| 2:C:1034:GLU:HG3 | 2:C:1038:TRP:CZ2  | 2.37                     | 0.59              |
| 3:D:1031:ASN:OD1 | 3:D:1033:GLN:HB3  | 2.02                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1422:MET:CE   | 3:D:1427:SER:HA   | 2.32                     | 0.59              |
| 3:D:191:LEU:HD12  | 3:D:195:VAL:HG12  | 1.83                     | 0.59              |
| 2:H:260:LEU:HD23  | 2:H:261:ILE:N     | 2.17                     | 0.59              |
| 2:H:313:LEU:CG    | 2:H:320:HIS:ND1   | 2.60                     | 0.59              |
| 3:I:1047:LYS:NZ   | 3:I:1053:PHE:HA   | 2.17                     | 0.59              |
| 3:I:1071:PHE:O    | 3:I:1074:SER:HB3  | 2.02                     | 0.59              |
| 3:I:25:GLU:HB2    | 3:I:92:HIS:CE1    | 2.37                     | 0.59              |
| 2:H:1008:ARG:NH1  | 3:I:624:ASP:OD1   | 2.34                     | 0.59              |
| 3:I:799:LYS:HD3   | 3:I:826:PRO:CG    | 2.32                     | 0.59              |
| 3:I:988:ARG:O     | 3:I:992:ILE:HG13  | 2.01                     | 0.59              |
| 3:I:992:ILE:O     | 3:I:995:LEU:HB3   | 2.02                     | 0.59              |
| 1:K:39:PRO:HG3    | 1:L:39:PRO:HG2    | 1.84                     | 0.59              |
| 1:K:218:LEU:HD23  | 1:L:222:LEU:HD21  | 1.84                     | 0.59              |
| 2:M:516:ARG:CD    | 3:N:1068:LEU:HD22 | 2.32                     | 0.59              |
| 3:N:118:LEU:O     | 3:N:120:ALA:N     | 2.34                     | 0.59              |
| 2:M:1046:ALA:CB   | 3:N:1476:THR:CB   | 2.79                     | 0.59              |
| 3:N:189:GLN:HE22  | 3:N:191:LEU:H     | 1.49                     | 0.59              |
| 3:N:970:LYS:NZ    | 7:Z:113:LEU:HB3   | 2.17                     | 0.59              |
| 3:N:977:ALA:CB    | 3:N:983:LEU:HD21  | 2.31                     | 0.59              |
| 4:O:70:THR:OG1    | 4:O:72:ARG:HG2    | 2.02                     | 0.59              |
| 7:X:26:LEU:HD13   | 7:X:58:ILE:CG2    | 2.32                     | 0.59              |
| 2:C:1014:SER:HB2  | 2:C:1021:LEU:HD13 | 1.83                     | 0.59              |
| 2:C:274:ARG:NH1   | 2:C:274:ARG:HG2   | 2.13                     | 0.59              |
| 2:C:317:VAL:HG12  | 2:C:317:VAL:O     | 2.01                     | 0.59              |
| 3:D:1037:GLN:OE1  | 3:D:1042:ARG:NH1  | 2.35                     | 0.59              |
| 3:D:1040:GLY:O    | 3:D:1060:SER:HB3  | 2.02                     | 0.59              |
| 3:D:875:THR:HG22  | 3:D:879:ARG:HB2   | 1.83                     | 0.59              |
| 3:D:992:ILE:O     | 3:D:995:LEU:HB3   | 2.03                     | 0.59              |
| 3:I:991:GLN:HE22  | 7:Y:112:VAL:HG21  | 1.65                     | 0.59              |
| 2:M:683:ASN:HA    | 2:M:687:ALA:HB3   | 1.83                     | 0.59              |
| 3:N:1283:ILE:HG22 | 3:N:1284:GLU:N    | 2.17                     | 0.59              |
| 2:C:257:VAL:HG12  | 2:C:263:ASP:CG    | 2.22                     | 0.59              |
| 2:C:332:ARG:NH1   | 2:C:464:LEU:HD21  | 2.17                     | 0.59              |
| 3:D:1047:LYS:NZ   | 3:D:1053:PHE:HA   | 2.17                     | 0.59              |
| 3:D:1463:LYS:O    | 3:D:1466:VAL:HB   | 2.01                     | 0.59              |
| 3:D:1489:GLN:O    | 3:D:1493:LYS:HG3  | 2.02                     | 0.59              |
| 3:D:972:LEU:O     | 3:D:976:GLN:HG3   | 2.02                     | 0.59              |
| 3:D:984:THR:CG2   | 3:D:987:GLU:H     | 2.14                     | 0.59              |
| 2:H:12:VAL:HG13   | 2:H:13:ILE:H      | 1.65                     | 0.59              |
| 2:H:292:ARG:CG    | 2:H:299:LYS:HB3   | 2.27                     | 0.59              |
| 2:H:442:GLU:OE2   | 2:H:543:ASN:HB3   | 2.02                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:H:564:MET:HE2   | 2:H:846:LYS:HD2  | 1.84                     | 0.59              |
| 2:H:80:GLN:HG3    | 2:H:90:TYR:CE2   | 2.37                     | 0.59              |
| 3:I:131:LYS:CA    | 3:I:568:ARG:HD2  | 2.31                     | 0.59              |
| 2:M:274:ARG:NH2   | 2:M:278:GLU:OE2  | 2.36                     | 0.59              |
| 2:M:557:ARG:NH1   | 2:M:560:MET:CG   | 2.65                     | 0.59              |
| 3:N:100:ALA:CB    | 3:N:128:TYR:OH   | 2.51                     | 0.59              |
| 3:N:972:LEU:O     | 3:N:976:GLN:HG3  | 2.02                     | 0.59              |
| 7:X:81:GLU:O      | 7:X:154:ILE:CD1  | 2.48                     | 0.59              |
| 2:C:458:TYR:CD1   | 2:C:458:TYR:N    | 2.70                     | 0.59              |
| 2:C:585:GLU:O     | 2:C:588:VAL:HG22 | 2.02                     | 0.59              |
| 3:D:171:LEU:HD23  | 3:D:172:PRO:CD   | 2.33                     | 0.59              |
| 3:D:171:LEU:HB3   | 3:D:391:ALA:O    | 2.01                     | 0.59              |
| 1:B:190:THR:HB    | 3:D:722:GLU:OE1  | 2.02                     | 0.59              |
| 1:G:211:LEU:O     | 1:G:215:VAL:HG13 | 2.02                     | 0.59              |
| 2:H:1052:MET:SD   | 3:I:623:VAL:CG2  | 2.91                     | 0.59              |
| 3:I:1288:GLU:HG2  | 3:I:1307:LYS:NZ  | 2.17                     | 0.59              |
| 3:I:972:LEU:O     | 3:I:976:GLN:HG3  | 2.02                     | 0.59              |
| 2:M:118:ILE:HD12  | 2:M:118:ILE:C    | 2.23                     | 0.59              |
| 2:M:267:TYR:CB    | 2:M:272:ALA:HB1  | 2.26                     | 0.59              |
| 2:M:376:ARG:HB3   | 2:M:377:PRO:HD3  | 1.84                     | 0.59              |
| 2:M:966:LEU:HD21  | 2:M:986:PRO:HG3  | 1.85                     | 0.59              |
| 2:M:1098:ASP:N    | 3:N:11:ALA:O     | 2.34                     | 0.59              |
| 3:N:814:ALA:HB1   | 3:N:818:ARG:HE   | 1.67                     | 0.59              |
| 3:N:988:ARG:O     | 3:N:992:ILE:HG13 | 2.01                     | 0.59              |
| 3:N:992:ILE:O     | 3:N:995:LEU:HB3  | 2.02                     | 0.59              |
| 7:X:115:THR:HB    | 7:X:116:PRO:CD   | 2.32                     | 0.59              |
| 7:X:32:ILE:O      | 7:X:36:LEU:HG    | 2.03                     | 0.59              |
| 3:N:1359:GLN:NE2  | 7:Z:52:LYS:HD3   | 2.17                     | 0.59              |
| 2:C:603:VAL:HG13  | 2:C:613:VAL:CG1  | 2.32                     | 0.59              |
| 3:D:584:ASN:ND2   | 3:D:590:PRO:HG2  | 2.16                     | 0.59              |
| 2:H:486:MET:HG3   | 2:H:490:GLU:HB2  | 1.84                     | 0.59              |
| 2:H:500:ASN:ND2   | 2:H:500:ASN:N    | 2.45                     | 0.59              |
| 2:H:1004:LYS:CD   | 3:I:744:GLN:HE22 | 2.07                     | 0.59              |
| 3:I:977:ALA:CB    | 3:I:983:LEU:HD21 | 2.31                     | 0.59              |
| 1:K:102:LYS:HD3   | 1:K:139:ASN:HD21 | 1.64                     | 0.59              |
| 2:M:1095:LEU:HD11 | 2:M:1097:LEU:CB  | 2.28                     | 0.59              |
| 2:M:442:GLU:OE2   | 2:M:543:ASN:HB3  | 2.02                     | 0.59              |
| 3:N:1040:GLY:O    | 3:N:1060:SER:HB3 | 2.02                     | 0.59              |
| 1:A:54:THR:HG22   | 1:A:158:ILE:HD13 | 1.83                     | 0.59              |
| 2:C:405:ARG:NH2   | 2:C:566:THR:HG21 | 2.17                     | 0.59              |
| 3:D:1018:ASN:HB3  | 3:D:1021:TYR:HB3 | 1.83                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1255:GLY:O    | 3:D:1259:VAL:HG23 | 2.02                     | 0.59              |
| 3:D:126:VAL:O     | 3:D:132:TYR:HD2   | 1.86                     | 0.59              |
| 2:H:126:SER:HB3   | 2:H:395:LYS:NZ    | 2.17                     | 0.59              |
| 2:H:474:VAL:HG13  | 2:H:529:VAL:O     | 2.02                     | 0.59              |
| 2:H:654:LEU:H     | 2:H:654:LEU:CD2   | 2.13                     | 0.59              |
| 3:I:127:LEU:CD1   | 3:I:457:GLY:HA2   | 2.32                     | 0.59              |
| 3:I:520:LEU:CD1   | 3:I:524:LEU:HD22  | 2.14                     | 0.59              |
| 2:M:154:ARG:HH12  | 2:M:178:PRO:CD    | 2.15                     | 0.59              |
| 3:N:1205:TYR:HD2  | 3:N:1215:VAL:HG21 | 1.66                     | 0.59              |
| 3:N:397:LYS:O     | 3:N:397:LYS:HG3   | 2.01                     | 0.59              |
| 2:M:1031:ARG:NH2  | 3:N:621:LYS:NZ    | 2.50                     | 0.59              |
| 3:N:806:PHE:HE1   | 3:N:813:LEU:HB3   | 1.67                     | 0.59              |
| 3:N:983:LEU:N     | 3:N:983:LEU:HD23  | 2.18                     | 0.59              |
| 7:X:16:MET:CE     | 7:X:69:LEU:HD13   | 2.33                     | 0.59              |
| 2:C:129:ILE:N     | 2:C:129:ILE:HD12  | 2.17                     | 0.59              |
| 2:C:380:ALA:O     | 2:C:384:GLU:HB2   | 2.03                     | 0.59              |
| 2:C:557:ARG:NH1   | 2:C:560:MET:CG    | 2.64                     | 0.59              |
| 3:D:101:HIS:ND1   | 3:D:103:TRP:HB2   | 2.17                     | 0.59              |
| 3:D:10:ILE:HG13   | 3:D:1434:TRP:CZ2  | 2.36                     | 0.59              |
| 3:D:1101:VAL:CG1  | 3:D:1424:VAL:HG23 | 2.32                     | 0.59              |
| 3:D:1225:ALA:O    | 3:D:1229:ILE:HG13 | 2.03                     | 0.59              |
| 3:D:205:TYR:HD1   | 3:D:390:PRO:CG    | 2.16                     | 0.59              |
| 3:D:407:VAL:HG22  | 3:D:408:GLU:N     | 2.10                     | 0.59              |
| 3:D:853:VAL:HG22  | 3:D:858:VAL:HG23  | 1.84                     | 0.59              |
| 1:F:54:THR:HG22   | 1:F:158:ILE:HD13  | 1.83                     | 0.59              |
| 2:H:363:SER:HB2   | 2:H:366:SER:CB    | 2.31                     | 0.59              |
| 3:I:1122:LEU:HD11 | 3:I:1186:VAL:CG2  | 2.29                     | 0.59              |
| 3:I:1288:GLU:O    | 3:I:1307:LYS:HE2  | 2.03                     | 0.59              |
| 3:I:1216:SER:CB   | 4:J:16:LYS:H      | 2.15                     | 0.59              |
| 2:M:142:ARG:NE    | 2:M:325:ILE:CG2   | 2.66                     | 0.59              |
| 2:M:157:ARG:NH1   | 2:M:314:THR:HG21  | 2.17                     | 0.59              |
| 2:M:18:LEU:N      | 2:M:18:LEU:HD12   | 2.16                     | 0.59              |
| 2:M:204:GLN:NE2   | 2:M:228:ALA:HB1   | 2.17                     | 0.59              |
| 2:M:212:GLY:C     | 2:M:214:TYR:H     | 2.06                     | 0.59              |
| 3:N:1018:ASN:HB3  | 3:N:1021:TYR:HB3  | 1.83                     | 0.59              |
| 3:N:119:SER:HB2   | 3:N:123:LEU:N     | 2.17                     | 0.59              |
| 3:N:179:VAL:HG22  | 3:N:183:GLU:OE2   | 2.02                     | 0.59              |
| 3:N:351:MET:HG3   | 3:N:370:ALA:HB2   | 1.83                     | 0.59              |
| 3:N:137:PRO:CG    | 3:N:453:ASP:HB2   | 2.31                     | 0.59              |
| 3:N:834:THR:HB    | 3:N:838:ARG:HB2   | 1.82                     | 0.59              |
| 3:N:875:THR:HG22  | 3:N:879:ARG:HB2   | 1.83                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:T:18:DC:H2"     | 5:T:19:DC:C5'    | 2.27                     | 0.59              |
| 1:B:185:ARG:NH1   | 3:D:692:GLU:HB3  | 2.18                     | 0.59              |
| 2:C:1091:GLU:OE2  | 3:D:613:ARG:HG3  | 2.03                     | 0.59              |
| 2:C:953:VAL:HG11  | 2:C:962:GLN:HB3  | 1.85                     | 0.59              |
| 3:D:208:PRO:HG3   | 3:D:353:VAL:CG1  | 2.33                     | 0.59              |
| 3:D:983:LEU:N     | 3:D:983:LEU:HD23 | 2.18                     | 0.59              |
| 1:F:42:ARG:HH12   | 1:G:34:VAL:CG1   | 2.16                     | 0.59              |
| 1:G:133:GLU:HG3   | 1:G:134:GLU:N    | 2.16                     | 0.59              |
| 2:H:313:LEU:HB3   | 2:H:320:HIS:HE1  | 1.68                     | 0.59              |
| 2:H:571:LEU:CD1   | 2:H:701:THR:H    | 2.16                     | 0.59              |
| 3:I:131:LYS:NZ    | 3:I:133:ILE:HD11 | 2.18                     | 0.59              |
| 3:I:814:ALA:HB1   | 3:I:818:ARG:NH2  | 2.17                     | 0.59              |
| 2:M:1059:ASP:OD1  | 2:M:1062:GLY:N   | 2.34                     | 0.59              |
| 2:M:200:LEU:HD13  | 2:M:300:ASP:CG   | 2.22                     | 0.59              |
| 3:N:1442:ASN:HD21 | 3:N:1444:THR:HB  | 1.66                     | 0.59              |
| 3:N:853:VAL:HG22  | 3:N:858:VAL:HG23 | 1.84                     | 0.59              |
| 3:N:885:ILE:N     | 3:N:885:ILE:HD13 | 2.16                     | 0.59              |
| 3:N:25:GLU:HB2    | 3:N:92:HIS:CE1   | 2.37                     | 0.59              |
| 4:O:59:ASN:HD21   | 4:O:61:VAL:CG2   | 2.16                     | 0.59              |
| 7:Z:102:VAL:HG13  | 7:Z:119:ILE:HG12 | 1.84                     | 0.59              |
| 2:C:657:ASP:OD1   | 2:C:661:SER:O    | 2.20                     | 0.59              |
| 2:C:577:PRO:HG3   | 2:C:993:PHE:CE1  | 2.37                     | 0.59              |
| 3:D:1147:ARG:O    | 3:D:1165:TYR:HA  | 2.02                     | 0.59              |
| 3:D:160:GLU:OE1   | 3:D:161:LEU:HG   | 2.03                     | 0.59              |
| 3:D:171:LEU:CD2   | 3:D:175:VAL:HB   | 2.32                     | 0.59              |
| 3:D:206:ARG:CD    | 3:D:394:LEU:HD21 | 2.31                     | 0.59              |
| 3:D:480:GLU:O     | 3:D:484:PRO:HG2  | 2.01                     | 0.59              |
| 3:D:800:LYS:HD2   | 3:D:804:LEU:HD13 | 1.85                     | 0.59              |
| 1:G:102:LYS:HG3   | 1:G:139:ASN:HB2  | 1.85                     | 0.59              |
| 3:D:170:PRO:CD    | 2:H:318:PRO:HB3  | 2.28                     | 0.59              |
| 2:H:557:ARG:NH1   | 2:H:560:MET:CG   | 2.64                     | 0.59              |
| 2:H:851:LYS:HG2   | 2:H:853:LEU:HD12 | 1.85                     | 0.59              |
| 3:I:1233:GLY:HA2  | 3:I:1236:LEU:HG  | 1.85                     | 0.59              |
| 3:I:525:ARG:HD3   | 3:I:525:ARG:H    | 1.67                     | 0.59              |
| 3:I:907:GLU:HG2   | 3:I:908:LYS:N    | 2.17                     | 0.59              |
| 3:I:963:TYR:CD2   | 3:I:1002:LYS:HD3 | 2.38                     | 0.59              |
| 1:L:211:LEU:O     | 1:L:215:VAL:HG13 | 2.02                     | 0.59              |
| 2:M:272:ALA:HA    | 2:M:464:LEU:CD2  | 2.33                     | 0.59              |
| 2:M:662:GLU:O     | 2:M:663:ASN:HB2  | 2.03                     | 0.59              |
| 3:N:1152:GLU:CG   | 3:N:1161:GLU:HA  | 2.31                     | 0.59              |
| 7:Z:5:VAL:HB      | 7:Z:72:ALA:HA    | 1.84                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:319:GLY:O    | 2:C:321:GLU:OE2   | 2.21                     | 0.59              |
| 2:C:64:LEU:HD22  | 2:C:359:MET:CG    | 2.33                     | 0.59              |
| 2:C:496:ILE:HA   | 2:C:531:PHE:O     | 2.02                     | 0.59              |
| 2:C:442:GLU:OE2  | 2:C:543:ASN:HB3   | 2.02                     | 0.59              |
| 2:C:666:LEU:HD12 | 2:C:667:ALA:H     | 1.66                     | 0.59              |
| 3:D:173:PRO:HB3  | 2:H:279:GLU:OE1   | 2.03                     | 0.59              |
| 3:D:347:VAL:HG22 | 3:D:368:VAL:HG11  | 1.83                     | 0.59              |
| 3:D:365:ASP:O    | 3:D:379:ALA:HB3   | 2.03                     | 0.59              |
| 3:D:403:PHE:CD2  | 3:D:444:VAL:HG23  | 2.36                     | 0.59              |
| 2:H:292:ARG:HD2  | 2:H:299:LYS:HE2   | 1.85                     | 0.59              |
| 2:H:683:ASN:HA   | 2:H:687:ALA:HB3   | 1.83                     | 0.59              |
| 2:H:697:ARG:HB2  | 2:H:699:PHE:CD1   | 2.37                     | 0.59              |
| 3:I:996:TRP:CE2  | 3:I:1056:PRO:HG2  | 2.37                     | 0.59              |
| 4:J:54:LEU:HA    | 4:J:58:PRO:CG     | 2.33                     | 0.59              |
| 2:M:111:ASP:OD2  | 2:M:369:PRO:CG    | 2.50                     | 0.59              |
| 2:M:254:VAL:O    | 2:M:257:VAL:HG23  | 2.02                     | 0.59              |
| 2:M:141:HIS:O    | 2:M:331:ARG:HA    | 2.02                     | 0.59              |
| 2:M:415:PRO:HB2  | 2:M:418:LEU:CD1   | 2.33                     | 0.59              |
| 2:M:707:ARG:HG3  | 2:M:826:TYR:CD1   | 2.38                     | 0.59              |
| 3:N:1258:ARG:NH2 | 3:N:1262:LEU:HD11 | 2.17                     | 0.59              |
| 3:N:23:TYR:O     | 3:N:49:ILE:HG23   | 2.03                     | 0.59              |
| 6:U:15:G:C2'     | 6:U:16:G:H5'      | 2.32                     | 0.59              |
| 7:Y:139:SER:HB3  | 7:Y:148:GLU:CG    | 2.33                     | 0.59              |
| 2:C:1012:PRO:HD2 | 2:C:1026:GLN:CB   | 2.33                     | 0.58              |
| 2:C:500:ASN:ND2  | 2:C:500:ASN:N     | 2.51                     | 0.58              |
| 2:C:80:GLN:OE1   | 2:C:90:TYR:CE2    | 2.56                     | 0.58              |
| 2:C:966:LEU:HD21 | 2:C:986:PRO:CG    | 2.32                     | 0.58              |
| 3:D:102:ILE:CD1  | 3:D:106:LYS:HB2   | 2.34                     | 0.58              |
| 3:D:139:GLY:CA   | 3:D:162:ARG:NH2   | 2.53                     | 0.58              |
| 1:F:75:VAL:O     | 1:F:79:ILE:HG12   | 2.03                     | 0.58              |
| 2:H:1086:ARG:CZ  | 3:I:88:TYR:CZ     | 2.85                     | 0.58              |
| 2:H:305:PRO:HG3  | 2:H:308:ARG:HH21  | 1.68                     | 0.58              |
| 2:H:351:LEU:HD12 | 2:H:374:ASN:HD22  | 1.68                     | 0.58              |
| 2:H:360:LEU:H    | 2:H:360:LEU:HD23  | 1.68                     | 0.58              |
| 2:H:553:ASP:OD1  | 2:H:843:HIS:ND1   | 2.33                     | 0.58              |
| 2:H:662:GLU:O    | 2:H:663:ASN:HB2   | 2.03                     | 0.58              |
| 2:H:906:PHE:CD1  | 3:I:1067:VAL:HG13 | 2.38                     | 0.58              |
| 3:I:153:LEU:CD1  | 3:I:158:TYR:HB2   | 2.32                     | 0.58              |
| 1:L:124:ASN:N    | 1:L:125:PRO:HD3   | 2.18                     | 0.58              |
| 2:M:312:ALA:HB1  | 2:M:318:PRO:HG2   | 1.84                     | 0.58              |
| 3:N:1037:GLN:OE1 | 3:N:1042:ARG:NH1  | 2.35                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:101:HIS:ND1   | 3:N:103:TRP:HB2   | 2.17                     | 0.58              |
| 3:N:1047:LYS:NZ   | 3:N:1053:PHE:HA   | 2.17                     | 0.58              |
| 3:N:1189:ARG:HH11 | 3:N:1189:ARG:HG3  | 1.68                     | 0.58              |
| 3:N:368:VAL:HB    | 3:N:377:VAL:CG2   | 2.33                     | 0.58              |
| 3:N:205:TYR:CD1   | 3:N:390:PRO:HB3   | 2.38                     | 0.58              |
| 1:A:102:LYS:HD3   | 1:A:139:ASN:HD21  | 1.64                     | 0.58              |
| 2:C:175:GLU:O     | 2:C:183:SER:N     | 2.36                     | 0.58              |
| 2:C:338:GLU:HA    | 2:C:341:THR:HG22  | 1.85                     | 0.58              |
| 3:D:1264:GLU:O    | 3:D:1266:ARG:HG3  | 2.03                     | 0.58              |
| 3:D:881:LEU:HD11  | 3:D:885:ILE:HD11  | 1.85                     | 0.58              |
| 3:D:889:ALA:HB1   | 3:D:930:LEU:HA    | 1.86                     | 0.58              |
| 2:H:99:GLN:HA     | 2:H:109:LYS:O     | 2.03                     | 0.58              |
| 2:H:498:GLN:O     | 2:H:501:THR:HG23  | 2.02                     | 0.58              |
| 2:H:6:PHE:HB2     | 2:H:909:ALA:HA    | 1.85                     | 0.58              |
| 2:H:516:ARG:NE    | 3:I:1068:LEU:HD22 | 2.18                     | 0.58              |
| 2:H:1097:LEU:HD21 | 3:I:1447:LEU:HB3  | 1.85                     | 0.58              |
| 1:L:188:GLN:HG2   | 3:N:685:ASP:OD1   | 2.02                     | 0.58              |
| 2:M:173:ASP:O     | 2:M:174:LEU:HD23  | 2.02                     | 0.58              |
| 2:M:430:VAL:HG13  | 2:M:430:VAL:O     | 2.01                     | 0.58              |
| 2:M:564:MET:SD    | 2:M:846:LYS:CD    | 2.89                     | 0.58              |
| 2:M:9:ILE:HG12    | 2:M:907:ASP:OD2   | 2.01                     | 0.58              |
| 3:N:1292:VAL:CG2  | 3:N:1311:LEU:HD13 | 2.33                     | 0.58              |
| 3:N:148:GLU:HG2   | 3:N:151:GLN:CB    | 2.33                     | 0.58              |
| 3:N:211:VAL:HG12  | 3:N:211:VAL:O     | 2.02                     | 0.58              |
| 3:N:881:LEU:HD11  | 3:N:885:ILE:HD11  | 1.85                     | 0.58              |
| 7:Y:84:GLY:HA2    | 7:Y:130:LEU:CD1   | 2.32                     | 0.58              |
| 3:D:1293:PHE:HZ   | 3:D:1302:GLU:OE1  | 1.86                     | 0.58              |
| 3:D:1435:LEU:HB2  | 3:D:1457:ASP:OD2  | 2.03                     | 0.58              |
| 3:D:139:GLY:H     | 3:D:147:VAL:HG21  | 1.66                     | 0.58              |
| 3:D:355:VAL:HG21  | 3:D:367:ILE:HG23  | 1.85                     | 0.58              |
| 4:E:73:LEU:N      | 4:E:73:LEU:HD12   | 2.18                     | 0.58              |
| 2:H:185:LYS:HG2   | 2:H:189:ARG:O     | 2.02                     | 0.58              |
| 2:H:174:LEU:HD12  | 2:H:306:THR:HG22  | 1.84                     | 0.58              |
| 3:I:1264:GLU:O    | 3:I:1266:ARG:HG3  | 2.04                     | 0.58              |
| 3:I:1463:LYS:O    | 3:I:1466:VAL:HB   | 2.03                     | 0.58              |
| 3:I:411:THR:HG23  | 3:I:436:GLU:HA    | 1.85                     | 0.58              |
| 1:K:25:LEU:HD22   | 1:L:225:PHE:HE2   | 1.60                     | 0.58              |
| 2:M:184:MET:HB3   | 2:M:191:PHE:CE1   | 2.39                     | 0.58              |
| 2:M:204:GLN:CD    | 2:M:228:ALA:HB1   | 2.24                     | 0.58              |
| 3:N:1225:ALA:O    | 3:N:1229:ILE:HG13 | 2.03                     | 0.58              |
| 3:N:140:ALA:HB3   | 3:N:432:TYR:CE1   | 2.38                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:515:GLU:HG3   | 3:N:516:ALA:N     | 2.19                     | 0.58              |
| 3:N:563:PRO:O     | 3:N:567:ILE:HG12  | 2.03                     | 0.58              |
| 3:N:789:LEU:HD13  | 3:N:934:LEU:HD22  | 1.86                     | 0.58              |
| 3:N:812:ALA:O     | 3:N:816:HIS:HB2   | 2.03                     | 0.58              |
| 3:N:984:THR:CG2   | 3:N:987:GLU:H     | 2.14                     | 0.58              |
| 1:A:151:VAL:HB    | 1:A:169:ALA:HB3   | 1.86                     | 0.58              |
| 2:C:1045:ALA:HB1  | 2:C:1048:THR:HB   | 1.83                     | 0.58              |
| 2:C:226:VAL:HG13  | 2:C:227:PHE:CD1   | 2.37                     | 0.58              |
| 2:C:939:ARG:HD3   | 2:C:982:PRO:HD3   | 1.86                     | 0.58              |
| 3:D:1156:LEU:CD1  | 3:D:1176:LYS:HE3  | 2.33                     | 0.58              |
| 3:D:1253:THR:O    | 3:D:1258:ARG:HD3  | 2.04                     | 0.58              |
| 3:D:1287:GLU:OE1  | 3:D:1287:GLU:HA   | 2.04                     | 0.58              |
| 3:D:1481:VAL:HG13 | 4:E:18:ARG:HD3    | 1.86                     | 0.58              |
| 2:H:36:PRO:C      | 2:H:39:ARG:HG3    | 2.21                     | 0.58              |
| 1:F:175:ARG:HH22  | 2:H:697:ARG:NH2   | 2.01                     | 0.58              |
| 3:I:1189:ARG:HG3  | 3:I:1189:ARG:HH11 | 1.68                     | 0.58              |
| 3:I:654:LYS:HB3   | 3:I:655:PRO:CD    | 2.29                     | 0.58              |
| 1:K:151:VAL:HB    | 1:K:169:ALA:HB3   | 1.86                     | 0.58              |
| 1:K:54:THR:HG22   | 1:K:158:ILE:HD13  | 1.83                     | 0.58              |
| 2:M:627:ARG:O     | 2:M:638:ASP:HB3   | 2.03                     | 0.58              |
| 7:Y:11:GLY:O      | 7:Y:15:LEU:HG     | 2.04                     | 0.58              |
| 1:B:102:LYS:HG3   | 1:B:139:ASN:HB2   | 1.86                     | 0.58              |
| 2:C:50:GLU:HG2    | 2:C:51:THR:HG23   | 1.86                     | 0.58              |
| 2:C:872:ASN:ND2   | 2:C:874:LEU:HB2   | 2.19                     | 0.58              |
| 3:D:1425:THR:O    | 3:D:1429:LEU:HD13 | 2.02                     | 0.58              |
| 3:D:209:ARG:HB3   | 3:D:389:GLU:CB    | 2.33                     | 0.58              |
| 3:D:484:PRO:HB3   | 3:D:488:ARG:NE    | 2.17                     | 0.58              |
| 3:D:115:LEU:HD12  | 3:D:502:PHE:HE1   | 1.68                     | 0.58              |
| 3:D:728:LEU:HD12  | 3:D:729:HIS:N     | 2.19                     | 0.58              |
| 2:H:1078:GLU:HA   | 2:H:1078:GLU:OE1  | 2.04                     | 0.58              |
| 2:H:12:VAL:HG22   | 2:H:13:ILE:CG2    | 2.33                     | 0.58              |
| 2:H:304:LEU:N     | 2:H:304:LEU:HD23  | 2.18                     | 0.58              |
| 2:H:332:ARG:HG3   | 2:H:464:LEU:O     | 2.03                     | 0.58              |
| 2:H:572:ILE:CG2   | 2:H:703:ILE:HD11  | 2.32                     | 0.58              |
| 2:H:879:ARG:CZ    | 7:Y:42:ASP:HB2    | 2.33                     | 0.58              |
| 3:I:1037:GLN:OE1  | 3:I:1042:ARG:NH1  | 2.35                     | 0.58              |
| 3:I:1225:ALA:O    | 3:I:1229:ILE:HG13 | 2.03                     | 0.58              |
| 3:I:1481:VAL:CG1  | 4:J:18:ARG:HD3    | 2.33                     | 0.58              |
| 3:I:853:VAL:HG22  | 3:I:858:VAL:HG23  | 1.85                     | 0.58              |
| 3:I:889:ALA:HB1   | 3:I:930:LEU:HA    | 1.86                     | 0.58              |
| 1:K:150:TYR:HE2   | 1:K:152:PRO:HG3   | 1.67                     | 0.58              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:18:LEU:H      | 2:M:18:LEU:CD1   | 2.15                     | 0.58              |
| 2:M:690:ILE:HG23  | 2:M:852:ILE:HA   | 1.85                     | 0.58              |
| 3:N:1041:LEU:HD12 | 3:N:1058:ARG:HA  | 1.86                     | 0.58              |
| 3:N:728:LEU:HD12  | 3:N:729:HIS:N    | 2.18                     | 0.58              |
| 7:Y:6:LYS:O       | 7:Y:106:SER:HB2  | 2.03                     | 0.58              |
| 1:A:221:HIS:HA    | 1:A:224:TYR:HD2  | 1.69                     | 0.58              |
| 2:C:127:PHE:CD1   | 2:C:136:ILE:HD13 | 2.39                     | 0.58              |
| 2:C:242:LEU:HD11  | 2:C:254:VAL:HB   | 1.86                     | 0.58              |
| 2:C:442:GLU:HG2   | 2:C:454:SER:OG   | 2.03                     | 0.58              |
| 2:C:469:THR:OG1   | 2:C:470:PRO:HD2  | 2.04                     | 0.58              |
| 2:C:5:ARG:HB3     | 2:C:902:ILE:HB   | 1.85                     | 0.58              |
| 3:D:208:PRO:HG3   | 3:D:353:VAL:HG13 | 1.84                     | 0.58              |
| 3:D:515:GLU:HG3   | 3:D:516:ALA:N    | 2.18                     | 0.58              |
| 2:C:1070:ILE:HG21 | 3:D:655:PRO:HB2  | 1.86                     | 0.58              |
| 3:D:899:LEU:HD12  | 3:D:900:ILE:CG2  | 2.34                     | 0.58              |
| 1:G:36:LEU:O      | 1:G:39:PRO:HD2   | 2.04                     | 0.58              |
| 3:I:1109:GLU:CG   | 3:I:1201:CYS:HB2 | 2.33                     | 0.58              |
| 1:G:185:ARG:NH1   | 3:I:692:GLU:CG   | 2.66                     | 0.58              |
| 3:I:983:LEU:HD23  | 3:I:983:LEU:N    | 2.18                     | 0.58              |
| 1:K:79:ILE:HG13   | 1:K:80:LEU:H     | 1.68                     | 0.58              |
| 1:L:115:LEU:HD12  | 1:L:116:PRO:O    | 2.03                     | 0.58              |
| 1:L:39:PRO:O      | 1:L:43:ILE:HG12  | 2.02                     | 0.58              |
| 2:M:437:ARG:NH2   | 2:M:488:ALA:CA   | 2.64                     | 0.58              |
| 2:M:508:ILE:HG22  | 2:M:509:ALA:N    | 2.18                     | 0.58              |
| 3:N:178:LEU:HD11  | 3:N:191:LEU:CA   | 2.33                     | 0.58              |
| 3:N:189:GLN:HE21  | 3:N:190:GLU:H    | 1.51                     | 0.58              |
| 3:N:204:LEU:HD12  | 3:N:205:TYR:H    | 1.69                     | 0.58              |
| 3:N:805:GLU:O     | 3:N:809:PRO:HD2  | 2.03                     | 0.58              |
| 7:Y:31:LYS:O      | 7:Y:35:GLU:HG2   | 2.04                     | 0.58              |
| 2:C:26:TYR:HB2    | 2:C:121:MET:SD   | 2.44                     | 0.58              |
| 2:C:191:PHE:CZ    | 2:C:196:LEU:HB2  | 2.36                     | 0.58              |
| 2:C:662:GLU:O     | 2:C:663:ASN:HB2  | 2.02                     | 0.58              |
| 2:C:966:LEU:HD21  | 2:C:986:PRO:HG3  | 1.85                     | 0.58              |
| 3:D:1156:LEU:HD13 | 3:D:1176:LYS:HE3 | 1.86                     | 0.58              |
| 3:D:814:ALA:HB1   | 3:D:818:ARG:NH2  | 2.16                     | 0.58              |
| 3:D:884:ARG:HD3   | 3:D:888:GLU:OE2  | 2.04                     | 0.58              |
| 3:D:885:ILE:HD13  | 3:D:885:ILE:N    | 2.16                     | 0.58              |
| 1:F:221:HIS:HA    | 1:F:224:TYR:HD2  | 1.69                     | 0.58              |
| 1:G:59:GLU:HG3    | 1:G:60:ASP:N     | 2.18                     | 0.58              |
| 2:H:224:GLU:HB2   | 2:H:228:ALA:HB2  | 1.86                     | 0.58              |
| 2:H:627:ARG:O     | 2:H:638:ASP:HB3  | 2.04                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:872:ASN:ND2  | 2:H:874:LEU:HB2   | 2.18                     | 0.58              |
| 3:I:1087:ARG:HB2 | 3:I:1237:THR:HG23 | 1.86                     | 0.58              |
| 3:I:515:GLU:HG3  | 3:I:516:ALA:N     | 2.18                     | 0.58              |
| 3:I:18:ILE:HG23  | 3:I:518:PRO:HG3   | 1.85                     | 0.58              |
| 3:I:814:ALA:HB1  | 3:I:818:ARG:HE    | 1.67                     | 0.58              |
| 3:I:885:ILE:HG23 | 3:I:937:TYR:CE1   | 2.39                     | 0.58              |
| 3:N:963:TYR:CD2  | 3:N:1002:LYS:HD3  | 2.38                     | 0.58              |
| 3:N:1264:GLU:O   | 3:N:1266:ARG:HG3  | 2.04                     | 0.58              |
| 3:N:142:LEU:HD22 | 3:N:145:VAL:C     | 2.23                     | 0.58              |
| 2:M:1097:LEU:CD1 | 3:N:1451:ALA:HB2  | 2.23                     | 0.58              |
| 3:N:178:LEU:H    | 3:N:178:LEU:CD1   | 2.10                     | 0.58              |
| 3:N:184:GLU:HA   | 3:N:184:GLU:OE1   | 2.02                     | 0.58              |
| 3:N:165:LYS:NZ   | 3:N:199:LEU:HD22  | 2.18                     | 0.58              |
| 3:N:400:VAL:CG2  | 3:N:443:VAL:HG21  | 2.34                     | 0.58              |
| 3:N:81:THR:HG23  | 3:N:82:LYS:H      | 1.62                     | 0.58              |
| 3:N:889:ALA:HB1  | 3:N:930:LEU:HA    | 1.85                     | 0.58              |
| 3:N:885:ILE:HG23 | 3:N:937:TYR:CE1   | 2.39                     | 0.58              |
| 3:D:970:LYS:HZ2  | 7:X:113:LEU:HD23  | 1.67                     | 0.58              |
| 1:B:70:GLY:O     | 1:B:132:LEU:HA    | 2.03                     | 0.58              |
| 2:C:1090:LYS:HE3 | 3:D:90:MET:SD     | 2.43                     | 0.58              |
| 2:C:140:ILE:HD11 | 2:C:412:ALA:CA    | 2.33                     | 0.58              |
| 3:D:1189:ARG:HG3 | 3:D:1189:ARG:HH11 | 1.68                     | 0.58              |
| 3:D:470:LEU:N    | 3:D:470:LEU:HD23  | 2.18                     | 0.58              |
| 2:C:984:GLU:CG   | 3:D:944:THR:O     | 2.51                     | 0.58              |
| 3:D:957:PRO:HG2  | 3:D:1007:VAL:HA   | 1.84                     | 0.58              |
| 2:H:224:GLU:HB3  | 2:H:228:ALA:HB2   | 1.85                     | 0.58              |
| 3:I:1148:VAL:O   | 3:I:1188:VAL:HG23 | 2.03                     | 0.58              |
| 3:I:136:ASP:HB3  | 3:I:137:PRO:CD    | 2.23                     | 0.58              |
| 3:I:205:TYR:HD1  | 3:I:390:PRO:HB3   | 1.68                     | 0.58              |
| 3:I:470:LEU:HD23 | 3:I:470:LEU:N     | 2.18                     | 0.58              |
| 3:I:702:LEU:O    | 3:I:713:ILE:HG23  | 2.04                     | 0.58              |
| 3:I:899:LEU:HD12 | 3:I:900:ILE:CG2   | 2.34                     | 0.58              |
| 2:H:1090:LYS:NZ  | 3:I:90:MET:SD     | 2.74                     | 0.58              |
| 2:M:333:ILE:HG12 | 2:M:410:ILE:HD11  | 1.85                     | 0.58              |
| 2:M:442:GLU:HG2  | 2:M:454:SER:OG    | 2.03                     | 0.58              |
| 2:M:836:GLY:HA3  | 2:M:1001:VAL:CG2  | 2.28                     | 0.58              |
| 3:N:126:VAL:HG12 | 3:N:132:TYR:HB2   | 1.84                     | 0.58              |
| 3:N:879:ARG:HH21 | 3:N:903:ASP:C     | 2.07                     | 0.58              |
| 7:Y:128:ALA:HB2  | 7:Y:140:LEU:HD11  | 1.86                     | 0.58              |
| 1:A:150:TYR:HE2  | 1:A:152:PRO:HG3   | 1.67                     | 0.58              |
| 1:A:218:LEU:O    | 1:A:222:LEU:HD13  | 2.04                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:261:ILE:CD1   | 2:C:262:ALA:H     | 2.17                     | 0.58              |
| 2:C:263:ASP:O     | 2:C:264:PRO:O     | 2.22                     | 0.58              |
| 2:C:937:ASP:O     | 2:C:941:VAL:HG23  | 2.04                     | 0.58              |
| 2:C:98:LEU:HD12   | 2:C:111:ASP:O     | 2.04                     | 0.58              |
| 3:D:1071:PHE:O    | 3:D:1074:SER:HB3  | 2.02                     | 0.58              |
| 3:D:885:ILE:HG23  | 3:D:937:TYR:CE1   | 2.39                     | 0.58              |
| 4:E:15:SER:O      | 4:E:18:ARG:HB3    | 2.02                     | 0.58              |
| 2:H:139:GLN:HE22  | 2:H:414:GLY:HA3   | 1.69                     | 0.58              |
| 3:I:638:LYS:HA    | 3:I:932:ASP:OD1   | 2.04                     | 0.58              |
| 2:M:25:SER:O      | 2:M:29:ALA:HB2    | 2.04                     | 0.58              |
| 2:M:273:GLY:HA2   | 2:M:276:LYS:HD2   | 1.84                     | 0.58              |
| 2:M:63:GLY:CA     | 2:M:103:LYS:HG2   | 2.34                     | 0.58              |
| 2:M:691:SER:HB2   | 2:M:858:MET:SD    | 2.44                     | 0.58              |
| 2:M:851:LYS:HG2   | 2:M:853:LEU:HD12  | 1.85                     | 0.58              |
| 2:M:937:ASP:O     | 2:M:941:VAL:HG23  | 2.04                     | 0.58              |
| 3:N:1071:PHE:O    | 3:N:1074:SER:HB3  | 2.02                     | 0.58              |
| 3:N:1468:LEU:HD22 | 3:N:1470:ARG:CB   | 2.29                     | 0.58              |
| 3:N:474:GLU:O     | 3:N:478:LEU:HG    | 2.03                     | 0.58              |
| 3:N:987:GLU:OE1   | 7:Z:120:SER:HB2   | 2.03                     | 0.58              |
| 7:X:127:LYS:C     | 7:X:127:LYS:HD3   | 2.24                     | 0.58              |
| 7:Y:30:THR:HG22   | 7:Y:31:LYS:N      | 2.18                     | 0.58              |
| 7:Z:137:VAL:C     | 7:Z:138:LEU:HD23  | 2.23                     | 0.58              |
| 1:A:213:GLN:O     | 1:A:217:ILE:HG13  | 2.04                     | 0.58              |
| 2:C:101:ILE:HG23  | 2:C:108:ILE:HD11  | 1.84                     | 0.58              |
| 2:C:211:LEU:CD2   | 2:C:221:LEU:HD23  | 2.34                     | 0.58              |
| 2:C:328:LEU:HA    | 2:C:331:ARG:HB2   | 1.84                     | 0.58              |
| 2:C:374:ASN:ND2   | 2:C:374:ASN:N     | 2.51                     | 0.58              |
| 2:C:850:ALA:HA    | 3:D:632:VAL:HG13  | 1.86                     | 0.58              |
| 3:D:789:LEU:HD13  | 3:D:934:LEU:HD22  | 1.86                     | 0.58              |
| 1:F:218:LEU:O     | 1:F:222:LEU:HD13  | 2.04                     | 0.58              |
| 2:H:351:LEU:CD1   | 2:H:374:ASN:HD22  | 2.16                     | 0.58              |
| 2:H:620:LEU:O     | 2:H:620:LEU:HD12  | 2.03                     | 0.58              |
| 3:I:1137:ARG:HG2  | 3:I:1141:GLU:OE1  | 2.04                     | 0.58              |
| 3:I:412:GLY:HA2   | 3:I:434:ARG:HD3   | 1.86                     | 0.58              |
| 3:I:795:VAL:HG22  | 3:I:879:ARG:HH12  | 1.68                     | 0.58              |
| 1:L:71:VAL:HG22   | 1:L:132:LEU:CD1   | 2.34                     | 0.58              |
| 2:M:343:GLN:HE21  | 2:M:346:VAL:HG21  | 1.69                     | 0.58              |
| 2:M:39:ARG:CG     | 2:M:45:GLN:NE2    | 2.67                     | 0.58              |
| 2:M:9:ILE:HD13    | 2:M:907:ASP:HB2   | 1.86                     | 0.58              |
| 3:N:1148:VAL:O    | 3:N:1188:VAL:HG23 | 2.04                     | 0.58              |
| 3:N:87:ARG:HB2    | 3:N:524:LEU:CD1   | 2.33                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:884:ARG:HD3   | 3:N:888:GLU:OE2   | 2.04                     | 0.58              |
| 1:B:211:LEU:O     | 1:B:215:VAL:HG13  | 2.02                     | 0.57              |
| 1:B:42:ARG:NH1    | 1:B:42:ARG:HG2    | 2.17                     | 0.57              |
| 2:C:1098:ASP:N    | 3:D:11:ALA:O      | 2.36                     | 0.57              |
| 2:C:611:ILE:CG1   | 2:C:625:LEU:HD21  | 2.34                     | 0.57              |
| 2:C:834:GLN:HE22  | 3:D:724:GLN:CG    | 2.14                     | 0.57              |
| 2:C:948:GLU:HG2   | 2:C:955:PRO:HG3   | 1.85                     | 0.57              |
| 3:D:1171:VAL:O    | 3:D:1175:ILE:HG13 | 2.04                     | 0.57              |
| 3:D:134:VAL:CG2   | 3:D:455:ARG:O     | 2.51                     | 0.57              |
| 3:D:618:LEU:HD22  | 3:D:1463:LYS:HE2  | 1.85                     | 0.57              |
| 3:D:474:GLU:O     | 3:D:478:LEU:HG    | 2.04                     | 0.57              |
| 3:D:963:TYR:CD2   | 3:D:1002:LYS:HD3  | 2.38                     | 0.57              |
| 1:F:50:GLY:O      | 1:F:146:ARG:HA    | 2.04                     | 0.57              |
| 2:H:1034:GLU:HG3  | 2:H:1038:TRP:CZ2  | 2.38                     | 0.57              |
| 3:I:615:ARG:O     | 3:I:619:LEU:CG    | 2.47                     | 0.57              |
| 2:H:1030:GLN:CD   | 3:I:628:ARG:HD3   | 2.20                     | 0.57              |
| 1:K:50:GLY:O      | 1:K:146:ARG:HA    | 2.04                     | 0.57              |
| 2:M:342:ASP:HA    | 2:M:345:ARG:HD3   | 1.86                     | 0.57              |
| 2:M:391:LEU:C     | 2:M:393:GLN:NE2   | 2.57                     | 0.57              |
| 3:N:1101:VAL:HG12 | 3:N:1428:ALA:HB2  | 1.86                     | 0.57              |
| 3:N:402:PRO:CA    | 3:N:443:VAL:HG23  | 2.33                     | 0.57              |
| 3:N:50:PHE:CE2    | 3:N:522:PRO:CD    | 2.73                     | 0.57              |
| 3:N:55:ASP:O      | 3:N:56:TYR:HB2    | 2.04                     | 0.57              |
| 3:D:706:PRO:CD    | 6:Q:16:G:H21      | 2.12                     | 0.57              |
| 2:C:194:VAL:HG11  | 2:C:221:LEU:O     | 2.04                     | 0.57              |
| 2:C:571:LEU:HD21  | 2:C:700:TYR:HA    | 1.85                     | 0.57              |
| 2:C:675:ALA:HB2   | 2:C:867:VAL:HG11  | 1.86                     | 0.57              |
| 3:D:1021:TYR:CE2  | 3:D:1025:GLN:HG2  | 2.39                     | 0.57              |
| 3:D:563:PRO:CA    | 2:H:223:ASP:HB2   | 2.29                     | 0.57              |
| 2:H:242:LEU:HD13  | 2:H:254:VAL:HG11  | 1.86                     | 0.57              |
| 2:H:442:GLU:HG2   | 2:H:454:SER:OG    | 2.03                     | 0.57              |
| 2:H:680:ASP:O     | 3:I:939:PHE:HB3   | 2.04                     | 0.57              |
| 2:H:939:ARG:HD3   | 2:H:982:PRO:HD3   | 1.86                     | 0.57              |
| 2:H:953:VAL:HG11  | 2:H:962:GLN:HB3   | 1.85                     | 0.57              |
| 3:I:102:ILE:CD1   | 3:I:106:LYS:HB2   | 2.33                     | 0.57              |
| 3:I:1041:LEU:HD12 | 3:I:1058:ARG:HA   | 1.85                     | 0.57              |
| 3:I:1468:LEU:CD1  | 3:I:1470:ARG:HE   | 2.16                     | 0.57              |
| 3:I:728:LEU:HD12  | 3:I:729:HIS:N     | 2.19                     | 0.57              |
| 3:I:812:ALA:O     | 3:I:816:HIS:HB2   | 2.04                     | 0.57              |
| 3:I:879:ARG:HH21  | 3:I:903:ASP:C     | 2.07                     | 0.57              |
| 2:M:1032:PHE:O    | 2:M:1033:GLY:O    | 2.22                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:136:ILE:HD12 | 2:M:136:ILE:N     | 2.20                     | 0.57              |
| 2:M:285:LEU:O    | 2:M:285:LEU:HD23  | 2.04                     | 0.57              |
| 2:M:580:MET:HE2  | 2:M:902:ILE:HG12  | 1.86                     | 0.57              |
| 2:M:953:VAL:HG11 | 2:M:962:GLN:HB3   | 1.86                     | 0.57              |
| 3:N:1171:VAL:O   | 3:N:1175:ILE:HG13 | 2.04                     | 0.57              |
| 3:N:516:ALA:O    | 3:N:518:PRO:HD3   | 2.04                     | 0.57              |
| 3:N:631:ILE:HG12 | 3:N:740:PHE:CE2   | 2.39                     | 0.57              |
| 7:Y:6:LYS:C      | 7:Y:7:LEU:HD23    | 2.25                     | 0.57              |
| 1:B:39:PRO:O     | 1:B:43:ILE:HG12   | 2.05                     | 0.57              |
| 2:C:418:LEU:HD12 | 2:C:418:LEU:N     | 2.18                     | 0.57              |
| 3:D:908:LYS:CB   | 3:D:1027:GLY:HA3  | 2.34                     | 0.57              |
| 3:D:1364:HIS:CE1 | 3:D:1366:LYS:HG3  | 2.39                     | 0.57              |
| 3:D:631:ILE:HG12 | 3:D:740:PHE:CE2   | 2.39                     | 0.57              |
| 2:H:328:LEU:H    | 2:H:433:THR:HG21  | 1.70                     | 0.57              |
| 3:I:1344:VAL:O   | 3:I:1348:LEU:HD13 | 2.04                     | 0.57              |
| 2:H:873:PRO:HB3  | 3:I:949:ILE:CD1   | 2.33                     | 0.57              |
| 1:L:56:VAL:HG13  | 1:L:142:VAL:HG12  | 1.86                     | 0.57              |
| 1:L:38:ASN:O     | 1:L:42:ARG:HG3    | 2.04                     | 0.57              |
| 2:M:160:ALA:HB3  | 2:M:174:LEU:HB2   | 1.85                     | 0.57              |
| 2:M:328:LEU:C    | 2:M:330:ASN:H     | 2.07                     | 0.57              |
| 3:N:1481:VAL:CG1 | 4:O:18:ARG:HD3    | 2.35                     | 0.57              |
| 3:N:55:ASP:OD1   | 3:N:55:ASP:N      | 2.37                     | 0.57              |
| 3:N:705:ALA:HB2  | 6:U:16:G:O2'      | 2.03                     | 0.57              |
| 7:Z:115:THR:HB   | 7:Z:116:PRO:CD    | 2.32                     | 0.57              |
| 2:C:836:GLY:HA3  | 2:C:1001:VAL:HG21 | 1.86                     | 0.57              |
| 2:C:660:ALA:CB   | 2:C:667:ALA:O     | 2.37                     | 0.57              |
| 3:D:111:LYS:CG   | 3:D:1452:ILE:HG12 | 2.35                     | 0.57              |
| 3:D:832:ARG:HA   | 3:D:832:ARG:CZ    | 2.34                     | 0.57              |
| 1:F:31:GLY:H     | 1:F:193:ASP:CG    | 2.07                     | 0.57              |
| 1:F:213:GLN:O    | 1:F:217:ILE:HG13  | 2.04                     | 0.57              |
| 2:H:221:LEU:C    | 2:H:223:ASP:N     | 2.57                     | 0.57              |
| 2:H:948:GLU:HG2  | 2:H:955:PRO:HG3   | 1.85                     | 0.57              |
| 2:H:966:LEU:HD21 | 2:H:986:PRO:HG3   | 1.85                     | 0.57              |
| 3:I:465:LEU:HD22 | 3:I:510:GLU:HA    | 1.86                     | 0.57              |
| 3:I:806:PHE:CE1  | 3:I:813:LEU:HB3   | 2.39                     | 0.57              |
| 1:K:221:HIS:HA   | 1:K:224:TYR:HD2   | 1.69                     | 0.57              |
| 2:M:24:GLU:OE2   | 2:M:27:ARG:HD2    | 2.05                     | 0.57              |
| 2:M:575:GLN:NE2  | 2:M:670:GLN:OE1   | 2.38                     | 0.57              |
| 3:N:153:LEU:HD13 | 3:N:158:TYR:HB2   | 1.85                     | 0.57              |
| 3:N:433:GLY:CA   | 3:N:447:VAL:O     | 2.53                     | 0.57              |
| 2:M:1056:LYS:HB3 | 3:N:623:VAL:HG13  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:832:ARG:HA    | 3:N:832:ARG:CZ    | 2.35                     | 0.57              |
| 3:N:982:PHE:H     | 3:N:982:PHE:HD2   | 1.52                     | 0.57              |
| 4:O:36:LYS:NZ     | 4:O:45:ARG:HH22   | 2.03                     | 0.57              |
| 1:B:197:LEU:HD23  | 1:B:197:LEU:O     | 2.05                     | 0.57              |
| 1:A:215:VAL:HG13  | 1:B:222:LEU:HD22  | 1.84                     | 0.57              |
| 2:C:1008:ARG:HH22 | 2:C:1011:GLY:C    | 2.07                     | 0.57              |
| 2:C:212:GLY:O     | 2:C:214:TYR:N     | 2.38                     | 0.57              |
| 2:C:627:ARG:O     | 2:C:638:ASP:HB3   | 2.03                     | 0.57              |
| 3:D:355:VAL:CG1   | 3:D:359:ALA:HB3   | 2.34                     | 0.57              |
| 3:D:583:ASP:OD2   | 3:D:604:THR:HG21  | 2.04                     | 0.57              |
| 2:H:687:ALA:HB1   | 2:H:850:ALA:HB2   | 1.85                     | 0.57              |
| 3:I:400:VAL:HG12  | 3:I:402:PRO:HD3   | 1.87                     | 0.57              |
| 3:I:832:ARG:HA    | 3:I:832:ARG:CZ    | 2.35                     | 0.57              |
| 3:I:87:ARG:HA     | 3:I:87:ARG:NH1    | 2.19                     | 0.57              |
| 1:K:32:PHE:HZ     | 1:L:47:SER:HB2    | 1.70                     | 0.57              |
| 2:M:1085:PHE:O    | 2:M:1089:VAL:HG23 | 2.05                     | 0.57              |
| 2:M:368:THR:HG22  | 2:M:369:PRO:HD3   | 1.86                     | 0.57              |
| 2:M:94:LEU:HD12   | 2:M:94:LEU:C      | 2.25                     | 0.57              |
| 3:N:1422:MET:CE   | 3:N:1427:SER:HA   | 2.34                     | 0.57              |
| 3:N:156:GLU:O     | 3:N:160:GLU:HB2   | 2.05                     | 0.57              |
| 3:N:387:LEU:CD1   | 3:N:387:LEU:H     | 2.08                     | 0.57              |
| 3:N:433:GLY:HA3   | 3:N:447:VAL:O     | 2.04                     | 0.57              |
| 6:U:15:G:H2'      | 6:U:16:G:H5'      | 1.85                     | 0.57              |
| 1:A:50:GLY:O      | 1:A:146:ARG:HA    | 2.04                     | 0.57              |
| 1:A:68:ILE:O      | 1:A:71:VAL:HB     | 2.03                     | 0.57              |
| 2:C:80:GLN:HA     | 2:C:90:TYR:CD2    | 2.40                     | 0.57              |
| 2:C:9:ILE:HG13    | 2:C:9:ILE:O       | 2.04                     | 0.57              |
| 3:D:1052:THR:HG22 | 7:X:57:ARG:NH1    | 2.11                     | 0.57              |
| 3:D:1109:GLU:HG3  | 3:D:1217:ILE:HD12 | 1.87                     | 0.57              |
| 3:D:1205:TYR:HD2  | 3:D:1215:VAL:HG21 | 1.67                     | 0.57              |
| 3:D:1256:LEU:O    | 3:D:1260:ILE:HG13 | 2.04                     | 0.57              |
| 3:D:1277:ILE:O    | 3:D:1294:VAL:HG11 | 2.04                     | 0.57              |
| 3:D:1291:SER:HB2  | 3:D:1293:PHE:CE1  | 2.39                     | 0.57              |
| 3:D:158:TYR:CE1   | 3:D:162:ARG:HB3   | 2.40                     | 0.57              |
| 3:D:165:LYS:HZ2   | 3:D:199:LEU:HD22  | 1.69                     | 0.57              |
| 3:D:355:VAL:HG13  | 3:D:359:ALA:HB3   | 1.85                     | 0.57              |
| 3:D:516:ALA:O     | 3:D:518:PRO:HD3   | 2.04                     | 0.57              |
| 3:D:608:SER:HB3   | 3:D:1443:THR:OG1  | 2.05                     | 0.57              |
| 3:D:702:LEU:O     | 3:D:713:ILE:HG23  | 2.04                     | 0.57              |
| 1:G:112:ARG:CG    | 1:G:125:PRO:CB    | 2.80                     | 0.57              |
| 2:H:207:LEU:HD22  | 2:H:221:LEU:HD13  | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:52:PHE:CG     | 2:H:68:PHE:HB2    | 2.40                     | 0.57              |
| 2:H:595:LEU:HD23  | 2:H:655:LEU:HB2   | 1.87                     | 0.57              |
| 2:H:516:ARG:HG3   | 3:I:1068:LEU:HD11 | 1.87                     | 0.57              |
| 3:I:1147:ARG:O    | 3:I:1165:TYR:HA   | 2.05                     | 0.57              |
| 3:I:1372:VAL:HA   | 3:I:1375:MET:CE   | 2.34                     | 0.57              |
| 4:J:70:THR:OG1    | 4:J:72:ARG:HG2    | 2.05                     | 0.57              |
| 1:K:213:GLN:O     | 1:K:217:ILE:HG13  | 2.04                     | 0.57              |
| 1:L:85:LEU:HD12   | 1:L:86:VAL:H      | 1.70                     | 0.57              |
| 2:M:1008:ARG:NH1  | 2:M:1010:THR:HA   | 2.19                     | 0.57              |
| 2:M:1043:TYR:CE1  | 3:N:710:ARG:O     | 2.57                     | 0.57              |
| 2:M:332:ARG:C     | 2:M:333:ILE:HD12  | 2.25                     | 0.57              |
| 2:M:367:LEU:CB    | 2:M:371:LYS:HG2   | 2.33                     | 0.57              |
| 2:M:39:ARG:HG2    | 2:M:45:GLN:NE2    | 2.16                     | 0.57              |
| 2:M:83:CYS:SG     | 2:M:90:TYR:CD2    | 2.98                     | 0.57              |
| 2:M:939:ARG:HD3   | 2:M:982:PRO:HD3   | 1.86                     | 0.57              |
| 3:N:1292:VAL:CG2  | 3:N:1305:LEU:HG   | 2.31                     | 0.57              |
| 3:N:1312:LEU:HD11 | 3:N:1327:ARG:HH21 | 1.67                     | 0.57              |
| 3:N:702:LEU:O     | 3:N:713:ILE:HG23  | 2.04                     | 0.57              |
| 3:N:638:LYS:HD3   | 3:N:932:ASP:HB3   | 1.85                     | 0.57              |
| 1:B:62:LEU:CD1    | 1:B:62:LEU:H      | 1.97                     | 0.57              |
| 2:C:1078:GLU:HA   | 2:C:1078:GLU:OE1  | 2.04                     | 0.57              |
| 2:C:172:ILE:HD12  | 2:C:172:ILE:N     | 2.20                     | 0.57              |
| 2:C:36:PRO:HA     | 2:C:39:ARG:CG     | 2.33                     | 0.57              |
| 2:C:578:VAL:HG11  | 2:C:991:GLN:HB3   | 1.85                     | 0.57              |
| 2:H:200:LEU:HD13  | 2:H:300:ASP:OD1   | 2.04                     | 0.57              |
| 2:H:29:ALA:O      | 2:H:43:GLY:HA3    | 2.05                     | 0.57              |
| 2:H:674:VAL:HG12  | 2:H:990:GLY:O     | 2.04                     | 0.57              |
| 3:I:1169:ASP:O    | 3:I:1172:HIS:HB2  | 2.05                     | 0.57              |
| 3:I:1384:PRO:CG   | 3:I:1389:LEU:HB3  | 2.33                     | 0.57              |
| 3:I:1198:TYR:OH   | 3:I:1394:VAL:HG11 | 2.05                     | 0.57              |
| 3:I:884:ARG:HD3   | 3:I:888:GLU:OE2   | 2.04                     | 0.57              |
| 3:I:980:MET:CB    | 3:I:982:PHE:CE2   | 2.88                     | 0.57              |
| 4:J:24:ALA:O      | 4:J:27:ALA:N      | 2.38                     | 0.57              |
| 2:M:1042:ALA:HB2  | 3:N:1223:ILE:CG2  | 2.34                     | 0.57              |
| 2:M:111:ASP:CG    | 2:M:369:PRO:CG    | 2.70                     | 0.57              |
| 2:M:118:ILE:HD12  | 2:M:118:ILE:O     | 2.05                     | 0.57              |
| 2:M:144:PRO:O     | 2:M:276:LYS:HD3   | 2.04                     | 0.57              |
| 2:M:728:HIS:O     | 2:M:729:LEU:HD22  | 2.04                     | 0.57              |
| 3:N:102:ILE:CD1   | 3:N:106:LYS:HB2   | 2.34                     | 0.57              |
| 2:M:1038:TRP:NE1  | 3:N:1099:VAL:HG11 | 2.20                     | 0.57              |
| 3:N:199:LEU:HD23  | 3:N:200:ASP:N     | 2.19                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:206:THR:HG23  | 1:B:208:LEU:N     | 2.20                     | 0.57              |
| 2:C:338:GLU:HA    | 2:C:341:THR:CG2   | 2.35                     | 0.57              |
| 2:C:851:LYS:HG2   | 2:C:853:LEU:HD12  | 1.85                     | 0.57              |
| 3:D:1144:LEU:HD22 | 3:D:1166:LEU:HD11 | 1.87                     | 0.57              |
| 3:D:1283:ILE:HG22 | 3:D:1284:GLU:N    | 2.18                     | 0.57              |
| 3:D:351:MET:HA    | 3:D:370:ALA:HB2   | 1.87                     | 0.57              |
| 3:D:204:LEU:HD13  | 3:D:441:ARG:NH1   | 2.20                     | 0.57              |
| 3:D:481:MET:HE2   | 3:D:493:ARG:HA    | 1.85                     | 0.57              |
| 3:D:129:PHE:CZ    | 3:D:587:ARG:CD    | 2.87                     | 0.57              |
| 3:D:671:LYS:O     | 3:D:675:ARG:HG3   | 2.05                     | 0.57              |
| 2:H:204:GLN:CD    | 2:H:228:ALA:HB1   | 2.25                     | 0.57              |
| 2:H:374:ASN:N     | 2:H:374:ASN:HD22  | 1.99                     | 0.57              |
| 2:H:52:PHE:HB3    | 2:H:53:PRO:HD3    | 1.86                     | 0.57              |
| 2:H:443:THR:HG21  | 3:I:1078:ARG:CD   | 2.35                     | 0.57              |
| 3:I:1106:VAL:CG1  | 3:I:1107:VAL:H    | 2.15                     | 0.57              |
| 3:I:438:ASP:CG    | 3:I:441:ARG:NH2   | 2.58                     | 0.57              |
| 3:I:474:GLU:O     | 3:I:478:LEU:HG    | 2.03                     | 0.57              |
| 3:I:729:HIS:CE1   | 3:I:730:PRO:HG2   | 2.40                     | 0.57              |
| 3:I:631:ILE:HG12  | 3:I:740:PHE:CE2   | 2.39                     | 0.57              |
| 3:I:982:PHE:H     | 3:I:982:PHE:HD2   | 1.52                     | 0.57              |
| 1:K:218:LEU:O     | 1:K:222:LEU:HD13  | 2.04                     | 0.57              |
| 1:L:57:TYR:CD2    | 1:L:161:ARG:HG2   | 2.39                     | 0.57              |
| 2:M:129:ILE:CD1   | 2:M:134:ARG:HB2   | 2.35                     | 0.57              |
| 3:N:1110:ALA:O    | 3:N:1111:ASP:C    | 2.42                     | 0.57              |
| 3:N:138:LYS:H     | 3:N:138:LYS:HD3   | 1.69                     | 0.57              |
| 3:N:625:TYR:HB3   | 3:N:749:VAL:CG2   | 2.30                     | 0.57              |
| 3:N:88:TYR:N      | 3:N:88:TYR:HD2    | 2.01                     | 0.57              |
| 2:H:685:GLU:OE2   | 7:Y:41:ASP:HB2    | 2.05                     | 0.57              |
| 2:C:575:GLN:NE2   | 2:C:670:GLN:OE1   | 2.38                     | 0.57              |
| 2:C:675:ALA:HA    | 2:C:989:VAL:CG1   | 2.29                     | 0.57              |
| 3:D:111:LYS:HG3   | 3:D:1452:ILE:HG12 | 1.87                     | 0.57              |
| 3:D:24:GLY:HA3    | 3:D:49:ILE:HG12   | 1.87                     | 0.57              |
| 3:D:812:ALA:O     | 3:D:816:HIS:HB2   | 2.04                     | 0.57              |
| 2:H:265:ARG:HG2   | 2:H:267:TYR:CD1   | 2.38                     | 0.57              |
| 2:H:309:TYR:O     | 2:H:313:LEU:HD12  | 2.01                     | 0.57              |
| 2:H:579:VAL:HB    | 2:H:890:LEU:HD22  | 1.87                     | 0.57              |
| 2:H:555:ALA:HA    | 3:I:1070:TYR:OH   | 2.04                     | 0.57              |
| 3:I:41:ARG:O      | 3:I:42:ASP:CB     | 2.53                     | 0.57              |
| 3:I:140:ALA:HB3   | 3:I:432:TYR:CE1   | 2.39                     | 0.57              |
| 2:H:1029:GLY:O    | 3:I:622:ARG:NE    | 2.37                     | 0.57              |
| 2:M:186:VAL:O     | 2:M:186:VAL:HG23  | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:22:GLN:NE2    | 2:M:336:VAL:CG2   | 2.68                     | 0.57              |
| 2:M:516:ARG:NH1   | 2:M:521:PRO:HB3   | 2.19                     | 0.57              |
| 3:N:1169:ASP:O    | 3:N:1172:HIS:HB2  | 2.05                     | 0.57              |
| 3:N:1326:THR:CG2  | 3:N:1327:ARG:H    | 2.18                     | 0.57              |
| 3:N:1364:HIS:CE1  | 3:N:1366:LYS:HG3  | 2.39                     | 0.57              |
| 3:N:1498:ALA:HB2  | 4:O:88:GLU:OE1    | 2.05                     | 0.57              |
| 3:N:178:LEU:HD11  | 3:N:191:LEU:HA    | 1.86                     | 0.57              |
| 3:N:167:GLU:OE2   | 3:N:198:ARG:HB2   | 2.04                     | 0.57              |
| 3:N:729:HIS:CE1   | 3:N:730:PRO:HG2   | 2.40                     | 0.57              |
| 7:X:91:LEU:HB3    | 7:X:149:PHE:HB3   | 1.87                     | 0.57              |
| 7:Z:91:LEU:HB3    | 7:Z:149:PHE:HB3   | 1.87                     | 0.57              |
| 1:B:150:TYR:CE1   | 1:B:170:VAL:HG12  | 2.36                     | 0.57              |
| 1:B:71:VAL:HG13   | 1:B:132:LEU:CD1   | 2.35                     | 0.57              |
| 2:C:1085:PHE:O    | 2:C:1089:VAL:HG23 | 2.05                     | 0.57              |
| 2:C:606:VAL:HG21  | 2:C:645:VAL:HG22  | 1.87                     | 0.57              |
| 2:C:897:LEU:HB3   | 2:C:899:GLN:NE2   | 2.20                     | 0.57              |
| 2:C:9:ILE:HD13    | 2:C:907:ASP:HB2   | 1.86                     | 0.57              |
| 3:D:1041:LEU:HD12 | 3:D:1058:ARG:HA   | 1.85                     | 0.57              |
| 3:D:166:GLN:NE2   | 3:D:396:VAL:HG12  | 2.19                     | 0.57              |
| 3:D:538:SER:HB3   | 3:D:541:ASN:HD22  | 1.70                     | 0.57              |
| 3:D:52:PRO:CA     | 3:D:86:ARG:HD3    | 2.35                     | 0.57              |
| 3:D:879:ARG:HH21  | 3:D:903:ASP:C     | 2.07                     | 0.57              |
| 3:D:996:TRP:HE3   | 3:D:999:THR:HG21  | 1.70                     | 0.57              |
| 1:F:151:VAL:HB    | 1:F:169:ALA:HB3   | 1.86                     | 0.57              |
| 1:F:26:GLU:OE2    | 1:F:194:LYS:HE3   | 2.05                     | 0.57              |
| 1:G:197:LEU:HD23  | 1:G:197:LEU:O     | 2.05                     | 0.57              |
| 2:H:12:VAL:HG22   | 2:H:13:ILE:HG22   | 1.87                     | 0.57              |
| 2:H:334:ARG:HG2   | 2:H:338:GLU:OE1   | 2.05                     | 0.57              |
| 2:H:397:GLU:HG2   | 2:H:403:SER:HB3   | 1.87                     | 0.57              |
| 2:H:862:PRO:HG2   | 2:H:925:TYR:OH    | 2.05                     | 0.57              |
| 3:I:1402:ALA:HB2  | 3:I:1415:VAL:CG2  | 2.35                     | 0.57              |
| 3:I:1437:ALA:HB1  | 3:I:1446:VAL:CG2  | 2.34                     | 0.57              |
| 3:I:624:ASP:O     | 3:I:625:TYR:HB2   | 2.04                     | 0.57              |
| 3:I:881:LEU:HD11  | 3:I:885:ILE:HD11  | 1.86                     | 0.57              |
| 3:I:789:LEU:HD13  | 3:I:934:LEU:HD22  | 1.85                     | 0.57              |
| 3:I:696:HIS:NE2   | 4:J:54:LEU:HD11   | 2.20                     | 0.57              |
| 4:J:22:VAL:HG12   | 4:J:68:LEU:HD21   | 1.87                     | 0.57              |
| 2:M:95:TYR:HB3    | 2:M:114:PHE:HA    | 1.87                     | 0.57              |
| 2:M:274:ARG:HD2   | 2:M:285:LEU:HD13  | 1.87                     | 0.57              |
| 2:M:334:ARG:HA    | 2:M:338:GLU:OE2   | 2.04                     | 0.57              |
| 2:M:948:GLU:HG2   | 2:M:955:PRO:HG3   | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:443:THR:HG21  | 3:N:1078:ARG:CD   | 2.35                     | 0.57              |
| 3:N:1344:VAL:O    | 3:N:1348:LEU:HD13 | 2.04                     | 0.57              |
| 3:N:1372:VAL:HA   | 3:N:1375:MET:HE2  | 1.87                     | 0.57              |
| 3:N:1372:VAL:HA   | 3:N:1375:MET:CE   | 2.34                     | 0.57              |
| 3:N:1453:ALA:O    | 3:N:1455:LYS:N    | 2.38                     | 0.57              |
| 3:N:368:VAL:HB    | 3:N:377:VAL:HB    | 1.85                     | 0.57              |
| 3:N:671:LYS:O     | 3:N:675:ARG:CG    | 2.52                     | 0.57              |
| 3:N:899:LEU:HD12  | 3:N:900:ILE:CG2   | 2.34                     | 0.57              |
| 7:X:103:GLN:NE2   | 7:X:105:VAL:HG13  | 2.18                     | 0.57              |
| 7:Z:107:PRO:HA    | 7:Z:120:SER:OG    | 2.04                     | 0.57              |
| 1:B:179:PHE:H     | 1:B:179:PHE:HD2   | 1.53                     | 0.56              |
| 1:B:56:VAL:HG21   | 1:B:82:LEU:CD1    | 2.34                     | 0.56              |
| 2:C:332:ARG:C     | 2:C:333:ILE:HD12  | 2.25                     | 0.56              |
| 2:C:588:VAL:CG1   | 2:C:661:SER:HB3   | 2.35                     | 0.56              |
| 3:D:349:PRO:HB3   | 2:H:274:ARG:CZ    | 2.35                     | 0.56              |
| 3:D:159:ARG:NH2   | 2:H:208:ALA:HB1   | 2.21                     | 0.56              |
| 2:H:564:MET:CE    | 2:H:846:LYS:CD    | 2.82                     | 0.56              |
| 2:H:937:ASP:O     | 2:H:941:VAL:HG23  | 2.04                     | 0.56              |
| 3:I:131:LYS:HB2   | 3:I:568:ARG:NH1   | 2.20                     | 0.56              |
| 2:M:473:ARG:HD3   | 2:M:531:PHE:CZ    | 2.40                     | 0.56              |
| 2:M:579:VAL:HB    | 2:M:890:LEU:HD22  | 1.87                     | 0.56              |
| 2:M:654:LEU:N     | 2:M:654:LEU:HD23  | 2.17                     | 0.56              |
| 2:M:593:ALA:HB1   | 2:M:659:PRO:HD2   | 1.87                     | 0.56              |
| 2:M:872:ASN:ND2   | 2:M:874:LEU:HB2   | 2.19                     | 0.56              |
| 3:N:1280:VAL:HG22 | 3:N:1295:GLU:O    | 2.04                     | 0.56              |
| 3:N:393:ILE:N     | 3:N:393:ILE:HD12  | 2.20                     | 0.56              |
| 3:N:465:LEU:HD22  | 3:N:510:GLU:HA    | 1.86                     | 0.56              |
| 3:N:86:ARG:HD3    | 3:N:523:ASP:OD2   | 2.02                     | 0.56              |
| 3:N:654:LYS:HB3   | 3:N:655:PRO:CD    | 2.29                     | 0.56              |
| 3:N:693:GLU:HA    | 4:O:48:MET:HE1    | 1.87                     | 0.56              |
| 3:N:970:LYS:HZ1   | 7:Z:113:LEU:CA    | 2.15                     | 0.56              |
| 3:N:980:MET:CB    | 3:N:982:PHE:CE2   | 2.88                     | 0.56              |
| 7:Z:5:VAL:HG23    | 7:Z:71:ARG:NH1    | 2.19                     | 0.56              |
| 2:C:742:VAL:HG12  | 2:C:743:VAL:N     | 2.21                     | 0.56              |
| 2:C:77:PRO:HD3    | 2:C:93:PRO:HD3    | 1.86                     | 0.56              |
| 3:D:1094:LEU:HG   | 3:D:1098:LEU:CD1  | 2.35                     | 0.56              |
| 3:D:1235:GLN:HB3  | 7:X:52:LYS:HZ1    | 1.70                     | 0.56              |
| 3:D:574:LEU:O     | 3:D:578:VAL:HG23  | 2.05                     | 0.56              |
| 1:F:31:GLY:N      | 1:F:193:ASP:OD1   | 2.29                     | 0.56              |
| 2:H:1060:ILE:O    | 2:H:1060:ILE:HG13 | 2.04                     | 0.56              |
| 2:H:445:GLU:HG3   | 2:H:560:MET:CE    | 2.34                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:559:LEU:HD23 | 2:H:559:LEU:C     | 2.25                     | 0.56              |
| 3:I:123:LEU:HD12 | 3:I:152:LEU:HD11  | 1.86                     | 0.56              |
| 3:I:671:LYS:O    | 3:I:675:ARG:HG3   | 2.05                     | 0.56              |
| 4:J:59:ASN:HB3   | 4:J:62:THR:OG1    | 2.05                     | 0.56              |
| 2:M:22:GLN:NE2   | 2:M:136:ILE:O     | 2.38                     | 0.56              |
| 2:M:26:TYR:HA    | 2:M:29:ALA:HB3    | 1.88                     | 0.56              |
| 2:M:545:ASN:OD1  | 2:M:905:ILE:HG13  | 2.05                     | 0.56              |
| 1:B:56:VAL:CG2   | 1:B:142:VAL:HG12  | 2.32                     | 0.56              |
| 2:C:342:ASP:HA   | 2:C:345:ARG:HD3   | 1.86                     | 0.56              |
| 2:C:455:LEU:CD1  | 2:C:456:ALA:O     | 2.54                     | 0.56              |
| 3:D:102:ILE:HD12 | 3:D:586:ARG:HG3   | 1.88                     | 0.56              |
| 2:C:443:THR:HG21 | 3:D:1078:ARG:NE   | 2.20                     | 0.56              |
| 3:D:1372:VAL:HA  | 3:D:1375:MET:CE   | 2.34                     | 0.56              |
| 3:D:441:ARG:HB2  | 3:D:443:VAL:HG12  | 1.87                     | 0.56              |
| 3:D:441:ARG:NH1  | 3:D:445:ARG:NH1   | 2.53                     | 0.56              |
| 3:D:520:LEU:HD12 | 3:D:521:PRO:CD    | 2.31                     | 0.56              |
| 3:D:704:ARG:HH12 | 3:D:743:ASP:CG    | 2.09                     | 0.56              |
| 4:E:10:PHE:CE1   | 4:E:16:LYS:HG3    | 2.41                     | 0.56              |
| 2:H:171:TRP:C    | 2:H:172:ILE:HD12  | 2.25                     | 0.56              |
| 2:H:313:LEU:CG   | 2:H:320:HIS:HE1   | 2.12                     | 0.56              |
| 3:I:1171:VAL:O   | 3:I:1175:ILE:HG13 | 2.04                     | 0.56              |
| 3:I:970:LYS:HG2  | 3:I:995:LEU:HD13  | 1.87                     | 0.56              |
| 4:J:40:LEU:O     | 4:J:40:LEU:HD12   | 2.06                     | 0.56              |
| 1:K:117:VAL:HG12 | 1:K:120:VAL:HG12  | 1.88                     | 0.56              |
| 1:K:35:THR:HG23  | 1:L:39:PRO:HA     | 1.87                     | 0.56              |
| 2:M:317:VAL:CG1  | 2:M:320:HIS:CE1   | 2.85                     | 0.56              |
| 2:M:565:GLN:NE2  | 2:M:842:ARG:CG    | 2.61                     | 0.56              |
| 3:N:546:ARG:HG2  | 3:N:546:ARG:NH1   | 2.20                     | 0.56              |
| 3:N:970:LYS:HZ3  | 7:Z:113:LEU:HD23  | 0.74                     | 0.56              |
| 3:N:996:TRP:HA   | 3:N:999:THR:HG22  | 1.87                     | 0.56              |
| 4:O:37:ASN:HD22  | 4:O:37:ASN:N      | 2.02                     | 0.56              |
| 4:O:47:LYS:N     | 4:O:54:LEU:HD13   | 2.19                     | 0.56              |
| 7:Y:7:LEU:CD2    | 7:Y:72:ALA:HB1    | 2.32                     | 0.56              |
| 1:A:115:LEU:HD12 | 1:A:116:PRO:HD2   | 1.87                     | 0.56              |
| 2:C:1084:SER:O   | 2:C:1087:VAL:HG12 | 2.06                     | 0.56              |
| 2:C:73:LEU:CD2   | 2:C:118:ILE:HD11  | 2.36                     | 0.56              |
| 2:C:285:LEU:HD21 | 2:C:287:GLY:O     | 2.05                     | 0.56              |
| 3:D:1344:VAL:O   | 3:D:1348:LEU:HD13 | 2.04                     | 0.56              |
| 3:D:165:LYS:HD2  | 3:D:165:LYS:O     | 2.05                     | 0.56              |
| 3:D:180:LYS:HG2  | 3:D:183:GLU:OE1   | 2.04                     | 0.56              |
| 3:D:452:ILE:CD1  | 3:D:452:ILE:N     | 2.68                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:267:TYR:CE2   | 2:H:289:THR:HG23  | 2.40                     | 0.56              |
| 2:H:455:LEU:CD1   | 2:H:456:ALA:O     | 2.54                     | 0.56              |
| 2:H:516:ARG:NH1   | 2:H:521:PRO:HB3   | 2.20                     | 0.56              |
| 2:H:742:VAL:HG12  | 2:H:743:VAL:N     | 2.20                     | 0.56              |
| 2:H:2:GLU:O       | 2:H:899:GLN:CB    | 2.53                     | 0.56              |
| 3:I:1109:GLU:HG2  | 3:I:1201:CYS:HB2  | 1.86                     | 0.56              |
| 3:I:1209:LEU:HD21 | 4:J:16:LYS:HZ1    | 1.69                     | 0.56              |
| 3:I:1299:PHE:HD2  | 3:I:1299:PHE:H    | 1.53                     | 0.56              |
| 3:I:1422:MET:CE   | 3:I:1427:SER:HA   | 2.35                     | 0.56              |
| 3:I:1485:GLN:NE2  | 4:J:80:VAL:H      | 2.03                     | 0.56              |
| 1:L:79:ILE:HD12   | 1:L:83:LYS:HE2    | 1.87                     | 0.56              |
| 2:M:140:ILE:HD11  | 2:M:331:ARG:NH2   | 2.11                     | 0.56              |
| 2:M:140:ILE:HD13  | 2:M:331:ARG:NE    | 2.20                     | 0.56              |
| 2:M:175:GLU:O     | 2:M:183:SER:N     | 2.36                     | 0.56              |
| 2:M:52:PHE:CE1    | 2:M:67:ASP:C      | 2.79                     | 0.56              |
| 3:N:676:MET:O     | 3:N:680:GLN:HB2   | 2.03                     | 0.56              |
| 2:C:267:TYR:OH    | 2:C:289:THR:HG22  | 2.05                     | 0.56              |
| 2:C:332:ARG:CZ    | 2:C:464:LEU:HG    | 2.35                     | 0.56              |
| 2:C:50:GLU:HG2    | 2:C:51:THR:N      | 2.20                     | 0.56              |
| 3:D:550:ARG:HD3   | 3:D:573:MET:HB3   | 1.88                     | 0.56              |
| 2:H:1088:LEU:HD21 | 3:I:614:PHE:CE1   | 2.39                     | 0.56              |
| 2:H:139:GLN:HB3   | 2:H:334:ARG:HD3   | 1.87                     | 0.56              |
| 2:H:139:GLN:OE1   | 2:H:334:ARG:NH1   | 2.35                     | 0.56              |
| 2:H:178:PRO:O     | 2:H:180:GLY:N     | 2.37                     | 0.56              |
| 2:H:253:ALA:O     | 2:H:256:TYR:HB3   | 2.06                     | 0.56              |
| 2:H:722:ILE:HG23  | 2:H:722:ILE:O     | 2.06                     | 0.56              |
| 2:H:580:MET:HE2   | 2:H:902:ILE:HG12  | 1.87                     | 0.56              |
| 3:I:1140:ILE:CG2  | 3:I:1144:LEU:HD12 | 2.35                     | 0.56              |
| 3:I:1364:HIS:CE1  | 3:I:1366:LYS:HG3  | 2.39                     | 0.56              |
| 3:I:521:PRO:HD2   | 3:I:524:LEU:HD13  | 1.87                     | 0.56              |
| 3:I:50:PHE:HA     | 3:I:89:ARG:HG2    | 1.86                     | 0.56              |
| 4:J:37:ASN:ND2    | 4:J:37:ASN:N      | 2.53                     | 0.56              |
| 1:K:66:SER:O      | 1:K:75:VAL:HG23   | 2.05                     | 0.56              |
| 1:L:197:LEU:HD23  | 1:L:197:LEU:O     | 2.05                     | 0.56              |
| 1:L:206:THR:HG23  | 1:L:208:LEU:N     | 2.20                     | 0.56              |
| 2:M:1054:THR:O    | 2:M:1056:LYS:N    | 2.38                     | 0.56              |
| 2:M:1063:ARG:HD2  | 2:M:1063:ARG:O    | 2.06                     | 0.56              |
| 2:M:115:LEU:CD2   | 2:M:115:LEU:N     | 2.65                     | 0.56              |
| 2:M:279:GLU:HG3   | 2:M:280:LYS:N     | 2.20                     | 0.56              |
| 2:M:559:LEU:C     | 2:M:559:LEU:HD23  | 2.26                     | 0.56              |
| 2:M:689:VAL:HB    | 2:M:870:ILE:CG1   | 2.28                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:579:VAL:CG1   | 2:M:887:GLU:HG3   | 2.31                     | 0.56              |
| 2:M:52:PHE:CE2    | 2:M:98:LEU:HG     | 2.40                     | 0.56              |
| 3:N:179:VAL:HG13  | 3:N:183:GLU:HB3   | 1.88                     | 0.56              |
| 3:N:26:VAL:HG23   | 3:N:93:ILE:HG12   | 1.86                     | 0.56              |
| 3:N:432:TYR:HB3   | 3:N:450:TYR:CB    | 2.36                     | 0.56              |
| 4:O:85:LEU:HD23   | 4:O:85:LEU:C      | 2.26                     | 0.56              |
| 7:Y:103:GLN:HE21  | 7:Y:105:VAL:CG1   | 2.19                     | 0.56              |
| 7:Z:89:VAL:HG22   | 7:Z:154:ILE:HG23  | 1.88                     | 0.56              |
| 3:N:783:ARG:CZ    | 7:Z:41:ASP:CB     | 2.78                     | 0.56              |
| 2:C:1095:LEU:HD11 | 2:C:1097:LEU:CB   | 2.28                     | 0.56              |
| 2:C:654:LEU:HD13  | 2:C:663:ASN:C     | 2.26                     | 0.56              |
| 3:D:118:LEU:O     | 3:D:119:SER:C     | 2.43                     | 0.56              |
| 3:D:1443:THR:O    | 3:D:1447:LEU:HD13 | 2.05                     | 0.56              |
| 2:C:1097:LEU:HD11 | 3:D:1451:ALA:HA   | 1.87                     | 0.56              |
| 3:D:685:ASP:O     | 3:D:689:ASP:N     | 2.35                     | 0.56              |
| 3:D:632:VAL:HG23  | 3:D:725:SER:HB2   | 1.87                     | 0.56              |
| 3:D:731:LEU:HD22  | 3:D:779:ALA:O     | 2.05                     | 0.56              |
| 2:C:680:ASP:O     | 3:D:939:PHE:HB3   | 2.05                     | 0.56              |
| 4:E:37:ASN:HD22   | 4:E:37:ASN:N      | 2.03                     | 0.56              |
| 1:F:117:VAL:HG12  | 1:F:120:VAL:HG12  | 1.88                     | 0.56              |
| 1:G:48:ILE:HD12   | 1:G:48:ILE:N      | 2.20                     | 0.56              |
| 2:H:266:ARG:HA    | 2:H:288:ARG:CD    | 2.18                     | 0.56              |
| 2:H:31:GLN:NE2    | 2:H:71:TYR:OH     | 2.38                     | 0.56              |
| 2:H:88:LEU:HD13   | 2:H:89:THR:H      | 1.69                     | 0.56              |
| 3:I:137:PRO:CD    | 3:I:453:ASP:HB2   | 2.36                     | 0.56              |
| 3:I:421:LEU:HB2   | 3:I:427:VAL:HG12  | 1.87                     | 0.56              |
| 3:I:564:GLU:C     | 3:I:566:ILE:N     | 2.57                     | 0.56              |
| 3:I:639:LEU:HD12  | 3:I:640:HIS:N     | 2.20                     | 0.56              |
| 4:J:26:ARG:NH1    | 4:J:73:LEU:HD21   | 2.19                     | 0.56              |
| 3:N:111:LYS:HD3   | 3:N:1448:THR:CG2  | 2.35                     | 0.56              |
| 3:N:1493:LYS:HA   | 3:N:1493:LYS:NZ   | 2.21                     | 0.56              |
| 3:N:454:ALA:O     | 3:N:455:ARG:HG2   | 2.06                     | 0.56              |
| 3:N:798:GLU:HG2   | 3:N:799:LYS:H     | 1.69                     | 0.56              |
| 4:O:6:ILE:HD11    | 4:O:10:PHE:CE2    | 2.40                     | 0.56              |
| 5:R:21:DC:N3      | 6:S:10:G:O6       | 2.38                     | 0.56              |
| 3:I:743:ASP:OD1   | 6:S:16:G:O3'      | 2.24                     | 0.56              |
| 7:X:7:LEU:HD13    | 7:X:15:LEU:HD12   | 1.85                     | 0.56              |
| 2:C:516:ARG:NH1   | 2:C:521:PRO:HB3   | 2.19                     | 0.56              |
| 2:C:524:VAL:HG12  | 2:C:525:SER:H     | 1.69                     | 0.56              |
| 3:D:1102:THR:HA   | 3:D:1105:ILE:CD1  | 2.34                     | 0.56              |
| 3:D:168:THR:CG2   | 3:D:169:TYR:H     | 2.16                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:911:LEU:O     | 3:D:915:VAL:HG23  | 2.06                     | 0.56              |
| 3:D:970:LYS:HG2   | 3:D:995:LEU:HD13  | 1.87                     | 0.56              |
| 2:H:1048:THR:HG21 | 3:I:763:MET:HE3   | 1.87                     | 0.56              |
| 2:H:298:PHE:CD1   | 2:H:298:PHE:N     | 2.73                     | 0.56              |
| 2:H:794:PRO:HG2   | 2:H:1025:ALA:CA   | 2.34                     | 0.56              |
| 3:I:606:ILE:HG13  | 3:I:613:ARG:CG    | 2.35                     | 0.56              |
| 2:M:742:VAL:HG12  | 2:M:743:VAL:N     | 2.20                     | 0.56              |
| 2:M:79:PRO:CG     | 2:M:82:GLU:HG3    | 2.35                     | 0.56              |
| 2:M:831:ARG:HH12  | 2:M:1002:GLU:CB   | 2.19                     | 0.56              |
| 2:M:578:VAL:HG11  | 2:M:991:GLN:HB3   | 1.87                     | 0.56              |
| 3:N:127:LEU:HD23  | 3:N:134:VAL:CG1   | 2.36                     | 0.56              |
| 3:N:639:LEU:HD12  | 3:N:640:HIS:N     | 2.21                     | 0.56              |
| 7:Z:58:ILE:HG22   | 7:Z:62:ILE:HD13   | 1.86                     | 0.56              |
| 1:A:42:ARG:NH2    | 1:B:31:GLY:O      | 2.38                     | 0.56              |
| 2:C:224:GLU:HB3   | 2:C:228:ALA:H     | 1.70                     | 0.56              |
| 2:C:503:LEU:HD23  | 2:C:507:ARG:C     | 2.26                     | 0.56              |
| 2:C:559:LEU:C     | 2:C:559:LEU:HD23  | 2.26                     | 0.56              |
| 2:C:862:PRO:HG2   | 2:C:925:TYR:OH    | 2.05                     | 0.56              |
| 3:D:1007:VAL:HG11 | 3:D:1039:CYS:HB2  | 1.86                     | 0.56              |
| 3:D:1083:ASP:O    | 3:D:1087:ARG:HB3  | 2.05                     | 0.56              |
| 3:D:1487:VAL:HG12 | 3:D:1488:ASP:N    | 2.20                     | 0.56              |
| 3:D:165:LYS:HZ1   | 3:D:199:LEU:HD22  | 1.70                     | 0.56              |
| 3:D:729:HIS:CE1   | 3:D:730:PRO:HG2   | 2.40                     | 0.56              |
| 1:B:152:PRO:HG3   | 3:D:857:ILE:HG13  | 1.88                     | 0.56              |
| 4:E:18:ARG:O      | 4:E:22:VAL:HG23   | 2.06                     | 0.56              |
| 1:G:177:VAL:HG12  | 1:G:199:ILE:HD12  | 1.88                     | 0.56              |
| 1:G:48:ILE:HD12   | 1:G:48:ILE:H      | 1.70                     | 0.56              |
| 2:H:1095:LEU:HD11 | 2:H:1097:LEU:HD23 | 1.88                     | 0.56              |
| 2:H:328:LEU:HB2   | 2:H:488:ALA:CB    | 2.36                     | 0.56              |
| 2:H:897:LEU:HD21  | 2:H:921:ALA:CA    | 2.36                     | 0.56              |
| 3:I:1161:GLU:OE2  | 3:I:1164:ARG:CD   | 2.50                     | 0.56              |
| 3:I:1166:LEU:N    | 3:I:1166:LEU:HD23 | 2.21                     | 0.56              |
| 3:I:516:ALA:O     | 3:I:518:PRO:HD3   | 2.05                     | 0.56              |
| 3:I:520:LEU:HD12  | 3:I:521:PRO:HD2   | 1.87                     | 0.56              |
| 3:I:705:ALA:HB1   | 3:I:706:PRO:HD3   | 1.88                     | 0.56              |
| 2:M:1043:TYR:CD2  | 3:N:710:ARG:HD2   | 2.40                     | 0.56              |
| 2:M:1097:LEU:CD1  | 3:N:1451:ALA:CB   | 2.83                     | 0.56              |
| 2:M:1095:LEU:HD11 | 2:M:1097:LEU:HD23 | 1.87                     | 0.56              |
| 2:M:976:ASP:HB3   | 2:M:979:THR:HG22  | 1.88                     | 0.56              |
| 3:N:1402:ALA:HB2  | 3:N:1415:VAL:CG2  | 2.35                     | 0.56              |
| 3:N:215:TYR:HE2   | 3:N:343:LYS:HB2   | 1.70                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:470:LEU:N     | 3:N:470:LEU:HD23  | 2.18                     | 0.56              |
| 3:N:678:GLU:OE1   | 3:N:679:ARG:N     | 2.39                     | 0.56              |
| 3:N:731:LEU:HD22  | 3:N:779:ALA:O     | 2.05                     | 0.56              |
| 3:N:87:ARG:HB2    | 3:N:524:LEU:HD11  | 1.87                     | 0.56              |
| 7:Y:91:LEU:HD11   | 7:Y:129:LEU:HD21  | 1.88                     | 0.56              |
| 7:Z:89:VAL:HG12   | 7:Z:90:GLU:N      | 2.19                     | 0.56              |
| 1:B:92:PRO:HA     | 1:B:146:ARG:HH12  | 1.70                     | 0.56              |
| 1:B:20:TYR:CD2    | 1:B:21:GLY:N      | 2.74                     | 0.56              |
| 2:C:136:ILE:CD1   | 2:C:136:ILE:N     | 2.68                     | 0.56              |
| 2:C:139:GLN:HB3   | 2:C:334:ARG:HB2   | 1.88                     | 0.56              |
| 2:C:64:LEU:CB     | 2:C:359:MET:HG3   | 2.35                     | 0.56              |
| 3:D:1168:MET:HA   | 3:D:1168:MET:HE3  | 1.87                     | 0.56              |
| 3:D:119:SER:CB    | 3:D:123:LEU:H     | 2.18                     | 0.56              |
| 3:D:1468:LEU:CD2  | 3:D:1470:ARG:HD3  | 2.36                     | 0.56              |
| 3:D:160:GLU:HG2   | 3:D:165:LYS:HB2   | 1.85                     | 0.56              |
| 3:D:158:TYR:CE1   | 3:D:162:ARG:CB    | 2.89                     | 0.56              |
| 3:D:26:VAL:HG23   | 3:D:93:ILE:HG12   | 1.86                     | 0.56              |
| 3:D:638:LYS:HD3   | 3:D:932:ASP:HB3   | 1.87                     | 0.56              |
| 3:D:980:MET:CB    | 3:D:982:PHE:CE2   | 2.88                     | 0.56              |
| 2:H:1095:LEU:HD11 | 2:H:1097:LEU:CB   | 2.28                     | 0.56              |
| 2:H:313:LEU:HB3   | 2:H:320:HIS:CE1   | 2.41                     | 0.56              |
| 3:I:1140:ILE:HG22 | 3:I:1144:LEU:HD12 | 1.86                     | 0.56              |
| 3:I:1111:ASP:CG   | 3:I:1203:LYS:HD2  | 2.26                     | 0.56              |
| 3:I:26:VAL:HG23   | 3:I:93:ILE:HG12   | 1.86                     | 0.56              |
| 3:I:18:ILE:CG2    | 3:I:518:PRO:HG3   | 2.36                     | 0.56              |
| 3:I:862:ASP:O     | 3:I:877:PRO:HD3   | 2.06                     | 0.56              |
| 1:K:42:ARG:NH1    | 1:L:34:VAL:CG1    | 2.69                     | 0.56              |
| 2:M:1078:GLU:HA   | 2:M:1078:GLU:OE1  | 2.04                     | 0.56              |
| 2:M:30:LEU:C      | 2:M:30:LEU:HD12   | 2.20                     | 0.56              |
| 2:M:500:ASN:HD22  | 2:M:500:ASN:N     | 2.02                     | 0.56              |
| 2:M:544:THR:O     | 2:M:547:ILE:HD13  | 2.06                     | 0.56              |
| 2:M:701:THR:HG23  | 2:M:832:LYS:HA    | 1.88                     | 0.56              |
| 3:N:1487:VAL:HG12 | 3:N:1488:ASP:H    | 1.69                     | 0.56              |
| 3:N:421:LEU:HB2   | 3:N:427:VAL:HG12  | 1.87                     | 0.56              |
| 3:N:141:ILE:HG13  | 3:N:448:GLU:OE2   | 2.06                     | 0.56              |
| 7:Z:78:GLY:O      | 7:Z:156:GLY:HA2   | 2.06                     | 0.56              |
| 7:Z:83:ILE:HG13   | 7:Z:154:ILE:HD13  | 1.87                     | 0.56              |
| 1:B:57:TYR:HE1    | 1:B:163:ASN:HD21  | 1.54                     | 0.56              |
| 2:C:292:ARG:CG    | 2:C:299:LYS:HB3   | 2.35                     | 0.56              |
| 2:C:196:LEU:HD22  | 2:C:303:PHE:CD2   | 2.39                     | 0.56              |
| 3:D:1408:ILE:HD12 | 3:D:1408:ILE:N    | 2.21                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:160:GLU:HG3   | 3:D:165:LYS:HE3   | 1.88                     | 0.56              |
| 3:D:408:GLU:OE2   | 3:D:409:VAL:HG23  | 2.06                     | 0.56              |
| 3:D:996:TRP:HA    | 3:D:999:THR:HG22  | 1.87                     | 0.56              |
| 1:F:107:LYS:NZ    | 1:F:113:ASP:OD2   | 2.37                     | 0.56              |
| 1:G:20:TYR:CD2    | 1:G:21:GLY:N      | 2.74                     | 0.56              |
| 2:H:22:GLN:HB3    | 2:H:121:MET:CE    | 2.36                     | 0.56              |
| 2:H:332:ARG:C     | 2:H:333:ILE:HD12  | 2.27                     | 0.56              |
| 2:H:480:THR:HB    | 2:H:482:GLU:H     | 1.71                     | 0.56              |
| 2:H:575:GLN:NE2   | 2:H:670:GLN:OE1   | 2.38                     | 0.56              |
| 3:I:638:LYS:HD3   | 3:I:932:ASP:HB3   | 1.87                     | 0.56              |
| 4:J:33:HIS:CG     | 4:J:89:MET:HG2    | 2.40                     | 0.56              |
| 1:L:177:VAL:HG12  | 1:L:199:ILE:HD12  | 1.88                     | 0.56              |
| 2:M:1042:ALA:HB2  | 3:N:1223:ILE:HG21 | 1.87                     | 0.56              |
| 2:M:12:VAL:HG21   | 2:M:472:ARG:HH11  | 1.70                     | 0.56              |
| 2:M:111:ASP:HB2   | 2:M:369:PRO:HG2   | 1.78                     | 0.56              |
| 2:M:36:PRO:HG2    | 2:M:70:GLU:HG2    | 1.87                     | 0.56              |
| 2:M:806:LEU:HD13  | 2:M:813:VAL:HG21  | 1.88                     | 0.56              |
| 2:M:897:LEU:HD22  | 2:M:920:GLN:HG2   | 1.88                     | 0.56              |
| 3:N:167:GLU:CD    | 3:N:198:ARG:HB2   | 2.26                     | 0.56              |
| 3:N:180:LYS:HZ1   | 3:N:386:HIS:HA    | 1.71                     | 0.56              |
| 3:N:501:ALA:HB3   | 3:N:1452:ILE:CG2  | 2.36                     | 0.56              |
| 7:Y:120:SER:O     | 7:Y:123:SER:HB3   | 2.06                     | 0.56              |
| 1:A:117:VAL:HG12  | 1:A:120:VAL:HG12  | 1.88                     | 0.56              |
| 1:B:76:VAL:O      | 1:B:79:ILE:HG13   | 2.06                     | 0.56              |
| 2:C:806:LEU:HD13  | 2:C:813:VAL:HG21  | 1.88                     | 0.56              |
| 3:D:1234:THR:HB   | 3:D:1235:GLN:OE1  | 2.06                     | 0.56              |
| 3:D:1312:LEU:HD11 | 3:D:1327:ARG:HH21 | 1.68                     | 0.56              |
| 3:D:1402:ALA:HB2  | 3:D:1415:VAL:CG2  | 2.35                     | 0.56              |
| 3:D:165:LYS:HD3   | 3:D:167:GLU:CB    | 2.25                     | 0.56              |
| 3:D:36:THR:C      | 3:D:38:LYS:N      | 2.59                     | 0.56              |
| 3:D:465:LEU:HD22  | 3:D:510:GLU:HA    | 1.86                     | 0.56              |
| 3:D:639:LEU:HD12  | 3:D:640:HIS:N     | 2.21                     | 0.56              |
| 3:D:862:ASP:O     | 3:D:877:PRO:HD3   | 2.06                     | 0.56              |
| 3:D:86:ARG:CB     | 3:D:523:ASP:OD2   | 2.54                     | 0.56              |
| 3:D:982:PHE:CE1   | 7:X:100:LEU:CD2   | 2.87                     | 0.56              |
| 1:G:137:ARG:HH11  | 1:G:137:ARG:HB3   | 1.71                     | 0.56              |
| 2:H:1071:ILE:HD12 | 3:I:670:VAL:HG11  | 1.88                     | 0.56              |
| 2:H:185:LYS:CD    | 2:H:190:LYS:CG    | 2.80                     | 0.56              |
| 2:H:295:ASP:O     | 2:H:297:GLU:N     | 2.38                     | 0.56              |
| 2:H:437:ARG:NH1   | 2:H:491:GLU:OE2   | 2.37                     | 0.56              |
| 2:H:54:ILE:O      | 2:H:54:ILE:HG23   | 2.05                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:J:25:LYS:O     | 4:J:29:GLN:HG3    | 2.05                     | 0.56              |
| 3:I:696:HIS:CD2  | 4:J:58:PRO:CB     | 2.89                     | 0.56              |
| 1:L:102:LYS:NZ   | 1:L:137:ARG:NH1   | 2.54                     | 0.56              |
| 1:L:20:TYR:CD2   | 1:L:21:GLY:N      | 2.74                     | 0.56              |
| 2:M:524:VAL:CG1  | 2:M:525:SER:N     | 2.69                     | 0.56              |
| 2:M:654:LEU:HD13 | 2:M:663:ASN:C     | 2.27                     | 0.56              |
| 2:M:707:ARG:HG3  | 2:M:826:TYR:HE1   | 1.67                     | 0.56              |
| 3:N:127:LEU:HD12 | 3:N:127:LEU:H     | 1.71                     | 0.56              |
| 3:N:185:VAL:HG12 | 3:N:186:VAL:N     | 2.21                     | 0.56              |
| 3:N:355:VAL:CG2  | 3:N:367:ILE:HG23  | 2.36                     | 0.56              |
| 3:N:538:SER:O    | 3:N:540:LEU:N     | 2.39                     | 0.56              |
| 7:Y:17:GLN:O     | 7:Y:21:ARG:HD3    | 2.06                     | 0.56              |
| 1:B:177:VAL:HG12 | 1:B:199:ILE:HD12  | 1.87                     | 0.55              |
| 1:B:85:LEU:HD12  | 1:B:124:ASN:HB3   | 1.88                     | 0.55              |
| 2:C:496:ILE:HD12 | 2:C:496:ILE:N     | 2.21                     | 0.55              |
| 2:C:571:LEU:HD11 | 2:C:701:THR:H     | 1.70                     | 0.55              |
| 1:A:198:ARG:NH2  | 2:C:934:PHE:CD1   | 2.74                     | 0.55              |
| 3:D:1472:ILE:O   | 3:D:1477:GLY:HA3  | 2.06                     | 0.55              |
| 3:D:347:VAL:HG13 | 3:D:351:MET:HB2   | 1.88                     | 0.55              |
| 3:D:490:ALA:O    | 3:D:493:ARG:HG3   | 2.06                     | 0.55              |
| 1:G:179:PHE:HD2  | 1:G:179:PHE:H     | 1.53                     | 0.55              |
| 1:G:197:LEU:HD21 | 1:G:199:ILE:HD11  | 1.88                     | 0.55              |
| 2:H:170:PRO:HD3  | 2:H:263:ASP:OD1   | 2.06                     | 0.55              |
| 2:H:690:ILE:HG23 | 2:H:852:ILE:HA    | 1.88                     | 0.55              |
| 2:H:578:VAL:HG11 | 2:H:991:GLN:HB3   | 1.88                     | 0.55              |
| 3:I:1491:THR:O   | 3:I:1494:ALA:HB3  | 2.06                     | 0.55              |
| 3:I:606:ILE:HG13 | 3:I:613:ARG:HG3   | 1.87                     | 0.55              |
| 2:M:1088:LEU:CD2 | 2:M:1092:LEU:HD12 | 2.33                     | 0.55              |
| 3:N:348:GLN:H    | 3:N:351:MET:HE2   | 1.71                     | 0.55              |
| 3:N:862:ASP:O    | 3:N:877:PRO:HD3   | 2.06                     | 0.55              |
| 7:Y:89:VAL:HG12  | 7:Y:91:LEU:HD21   | 1.85                     | 0.55              |
| 2:C:1036:GLU:O   | 2:C:1039:ALA:HB3  | 2.06                     | 0.55              |
| 2:C:221:LEU:HD12 | 2:C:222:MET:CA    | 2.37                     | 0.55              |
| 3:D:149:LYS:CE   | 3:D:149:LYS:H     | 2.18                     | 0.55              |
| 3:D:33:ASN:ND2   | 3:D:35:ARG:NH2    | 2.53                     | 0.55              |
| 4:E:30:LEU:O     | 4:E:35:PHE:HA     | 2.06                     | 0.55              |
| 1:F:115:LEU:HD12 | 1:F:116:PRO:HD2   | 1.87                     | 0.55              |
| 2:H:252:LYS:O    | 2:H:255:ALA:N     | 2.36                     | 0.55              |
| 2:H:456:ALA:HB3  | 2:H:459:ALA:HB2   | 1.88                     | 0.55              |
| 3:I:401:TYR:OH   | 3:I:430:ASP:HB2   | 2.06                     | 0.55              |
| 2:M:181:VAL:HG12 | 2:M:223:ASP:OD2   | 2.07                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:290:LEU:O     | 2:M:290:LEU:HD12  | 2.06                     | 0.55              |
| 2:M:441:VAL:HG12  | 2:M:559:LEU:HA    | 1.88                     | 0.55              |
| 2:M:496:ILE:N     | 2:M:496:ILE:CD1   | 2.69                     | 0.55              |
| 2:M:606:VAL:HG22  | 2:M:645:VAL:HG13  | 1.88                     | 0.55              |
| 2:M:862:PRO:HG2   | 2:M:925:TYR:OH    | 2.05                     | 0.55              |
| 3:N:1136:LYS:O    | 3:N:1140:ILE:HG13 | 2.06                     | 0.55              |
| 3:N:1408:ILE:HD12 | 3:N:1408:ILE:N    | 2.21                     | 0.55              |
| 3:N:156:GLU:HB2   | 3:N:157:GLU:OE2   | 2.06                     | 0.55              |
| 3:N:456:MET:SD    | 3:N:568:ARG:NH2   | 2.79                     | 0.55              |
| 3:N:590:PRO:O     | 3:N:600:LEU:HD12  | 2.05                     | 0.55              |
| 3:N:800:LYS:HD3   | 3:N:830:ALA:O     | 2.06                     | 0.55              |
| 3:N:762:GLN:HE21  | 4:O:20:THR:CB     | 2.18                     | 0.55              |
| 7:X:90:GLU:HA     | 7:X:100:LEU:O     | 2.06                     | 0.55              |
| 1:A:107:LYS:NZ    | 1:A:113:ASP:OD2   | 2.37                     | 0.55              |
| 1:B:45:LEU:HD11   | 1:B:177:VAL:HG22  | 1.87                     | 0.55              |
| 2:C:12:VAL:HB     | 2:C:472:ARG:NH1   | 2.22                     | 0.55              |
| 2:C:383:ARG:HB2   | 2:C:383:ARG:NH1   | 2.06                     | 0.55              |
| 2:C:553:ASP:OD1   | 2:C:843:HIS:ND1   | 2.37                     | 0.55              |
| 2:C:690:ILE:HG23  | 2:C:852:ILE:HA    | 1.87                     | 0.55              |
| 2:C:679:PHE:CE2   | 2:C:853:LEU:HD21  | 2.41                     | 0.55              |
| 3:D:1286:THR:HG22 | 3:D:1287:GLU:N    | 2.16                     | 0.55              |
| 3:D:134:VAL:O     | 3:D:454:ALA:CB    | 2.49                     | 0.55              |
| 3:D:553:ARG:HD2   | 3:D:570:GLU:OE1   | 2.07                     | 0.55              |
| 3:D:704:ARG:HH22  | 6:Q:16:G:HO2'     | 1.53                     | 0.55              |
| 3:D:702:LEU:O     | 3:D:713:ILE:HA    | 2.07                     | 0.55              |
| 3:D:882:PHE:O     | 3:D:886:VAL:HG23  | 2.07                     | 0.55              |
| 1:G:206:THR:HG23  | 1:G:208:LEU:N     | 2.20                     | 0.55              |
| 2:H:242:LEU:HD11  | 2:H:254:VAL:HG11  | 1.87                     | 0.55              |
| 2:H:332:ARG:HD2   | 2:H:464:LEU:HG    | 1.89                     | 0.55              |
| 2:H:441:VAL:HG12  | 2:H:559:LEU:HA    | 1.88                     | 0.55              |
| 3:I:1123:PHE:CE2  | 3:I:1184:GLN:HA   | 2.40                     | 0.55              |
| 3:I:119:SER:O     | 3:I:121:THR:N     | 2.40                     | 0.55              |
| 3:I:1460:ILE:O    | 3:I:1460:ILE:HD12 | 2.06                     | 0.55              |
| 3:I:24:GLY:HA3    | 3:I:49:ILE:HG12   | 1.89                     | 0.55              |
| 3:I:550:ARG:NH1   | 3:I:573:MET:HB3   | 2.20                     | 0.55              |
| 3:I:956:ILE:CD1   | 3:I:1062:ARG:HG3  | 2.36                     | 0.55              |
| 2:H:1075:ASP:HB2  | 4:J:31:LEU:HD13   | 1.88                     | 0.55              |
| 1:K:115:LEU:HD12  | 1:K:116:PRO:HD2   | 1.87                     | 0.55              |
| 2:M:162:ILE:HG22  | 2:M:172:ILE:HD13  | 1.88                     | 0.55              |
| 2:M:431:HIS:H     | 2:M:434:HIS:CE1   | 2.24                     | 0.55              |
| 2:M:272:ALA:HA    | 2:M:464:LEU:HD21  | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:86:LYS:HD2    | 2:M:813:VAL:HB    | 1.88                     | 0.55              |
| 2:M:540:PHE:HZ    | 3:N:1070:TYR:HD1  | 1.54                     | 0.55              |
| 3:N:1329:ALA:C    | 3:N:1330:ILE:HD12 | 2.26                     | 0.55              |
| 3:N:189:GLN:NE2   | 3:N:191:LEU:H     | 2.03                     | 0.55              |
| 3:N:470:LEU:HD12  | 3:N:503:LEU:CD2   | 2.37                     | 0.55              |
| 3:N:93:ILE:HG12   | 3:N:548:ILE:HD11  | 1.89                     | 0.55              |
| 3:N:704:ARG:HH12  | 3:N:743:ASP:CG    | 2.08                     | 0.55              |
| 2:H:685:GLU:HG2   | 7:Y:41:ASP:OD1    | 1.99                     | 0.55              |
| 1:A:86:VAL:HG13   | 1:A:86:VAL:O      | 2.07                     | 0.55              |
| 2:C:363:SER:OG    | 2:C:366:SER:HB2   | 2.07                     | 0.55              |
| 3:D:1329:ALA:C    | 3:D:1330:ILE:HD12 | 2.26                     | 0.55              |
| 3:D:705:ALA:HB1   | 3:D:706:PRO:HD3   | 1.88                     | 0.55              |
| 3:D:802:ALA:O     | 3:D:803:GLY:C     | 2.44                     | 0.55              |
| 1:F:222:LEU:HD21  | 1:G:218:LEU:HD23  | 1.88                     | 0.55              |
| 2:H:1084:SER:O    | 2:H:1087:VAL:HG12 | 2.06                     | 0.55              |
| 2:H:654:LEU:HD13  | 2:H:663:ASN:C     | 2.26                     | 0.55              |
| 2:H:728:HIS:O     | 2:H:729:LEU:HB3   | 2.06                     | 0.55              |
| 2:H:850:ALA:HA    | 3:I:632:VAL:HG11  | 1.88                     | 0.55              |
| 3:I:1442:ASN:HD21 | 3:I:1444:THR:HB   | 1.71                     | 0.55              |
| 3:I:202:VAL:HG11  | 3:I:445:ARG:NH2   | 2.21                     | 0.55              |
| 3:I:177:ALA:N     | 3:I:390:PRO:HD3   | 2.16                     | 0.55              |
| 3:I:47:GLU:O      | 3:I:51:GLY:N      | 2.38                     | 0.55              |
| 3:I:615:ARG:HG3   | 3:I:619:LEU:CD1   | 2.37                     | 0.55              |
| 3:I:704:ARG:HH12  | 3:I:743:ASP:CG    | 2.09                     | 0.55              |
| 3:I:632:VAL:HG23  | 3:I:725:SER:HB2   | 1.87                     | 0.55              |
| 1:K:33:GLY:O      | 1:K:195:LEU:HD13  | 2.06                     | 0.55              |
| 1:L:102:LYS:HG3   | 1:L:139:ASN:HB2   | 1.87                     | 0.55              |
| 1:L:52:ALA:HB2    | 1:L:170:VAL:O     | 2.06                     | 0.55              |
| 2:M:1084:SER:O    | 2:M:1087:VAL:HG12 | 2.06                     | 0.55              |
| 2:M:1086:ARG:HD3  | 3:N:88:TYR:CD2    | 2.41                     | 0.55              |
| 2:M:158:TYR:O     | 2:M:310:LEU:HD11  | 2.06                     | 0.55              |
| 2:M:455:LEU:CD1   | 2:M:456:ALA:O     | 2.54                     | 0.55              |
| 2:M:524:VAL:HG12  | 2:M:525:SER:H     | 1.69                     | 0.55              |
| 2:M:726:ILE:HG13  | 2:M:734:LEU:HD11  | 1.88                     | 0.55              |
| 2:M:834:GLN:NE2   | 3:N:724:GLN:CG    | 2.61                     | 0.55              |
| 3:N:1189:ARG:HB3  | 3:N:1204:CYS:HA   | 1.89                     | 0.55              |
| 3:N:350:HIS:CD2   | 3:N:371:ILE:HG12  | 2.41                     | 0.55              |
| 3:N:699:VAL:HG22  | 3:N:756:GLN:OE1   | 2.06                     | 0.55              |
| 3:N:980:MET:HB3   | 3:N:982:PHE:HE2   | 1.72                     | 0.55              |
| 3:N:982:PHE:HB2   | 3:N:983:LEU:HD23  | 1.88                     | 0.55              |
| 4:O:6:ILE:O       | 4:O:6:ILE:HD12    | 2.07                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:Y:90:GLU:HA     | 7:Y:100:LEU:O     | 2.06                     | 0.55              |
| 1:B:124:ASN:ND2   | 1:B:127:LEU:HD22  | 2.21                     | 0.55              |
| 1:B:59:GLU:HG3    | 1:B:60:ASP:H      | 1.71                     | 0.55              |
| 2:C:221:LEU:C     | 2:C:221:LEU:HD12  | 2.26                     | 0.55              |
| 2:C:202:TYR:OH    | 2:C:304:LEU:HD22  | 2.07                     | 0.55              |
| 2:C:897:LEU:HD21  | 2:C:921:ALA:CA    | 2.36                     | 0.55              |
| 3:D:1047:LYS:HZ1  | 3:D:1053:PHE:HA   | 1.71                     | 0.55              |
| 3:D:1209:LEU:HD22 | 3:D:1211:MET:CB   | 2.36                     | 0.55              |
| 3:D:1301:LYS:HG3  | 3:D:1303:TYR:CZ   | 2.42                     | 0.55              |
| 3:D:1282:ARG:HD2  | 3:D:1315:ASP:HB3  | 1.87                     | 0.55              |
| 3:D:614:PHE:CE2   | 3:D:1438:ALA:HB1  | 2.42                     | 0.55              |
| 3:D:942:SER:O     | 3:D:947:ILE:HD11  | 2.06                     | 0.55              |
| 2:H:39:ARG:O      | 2:H:39:ARG:HD2    | 2.07                     | 0.55              |
| 2:H:976:ASP:HB3   | 2:H:979:THR:HG22  | 1.88                     | 0.55              |
| 3:I:731:LEU:HD22  | 3:I:779:ALA:O     | 2.05                     | 0.55              |
| 3:I:911:LEU:O     | 3:I:915:VAL:HG23  | 2.06                     | 0.55              |
| 1:L:179:PHE:HD2   | 1:L:179:PHE:H     | 1.54                     | 0.55              |
| 2:M:212:GLY:O     | 2:M:214:TYR:N     | 2.40                     | 0.55              |
| 2:M:64:LEU:HB2    | 2:M:359:MET:CG    | 2.36                     | 0.55              |
| 3:N:141:ILE:O     | 3:N:162:ARG:NH2   | 2.39                     | 0.55              |
| 3:N:796:ARG:HB2   | 3:N:828:LYS:HD3   | 1.89                     | 0.55              |
| 3:N:911:LEU:O     | 3:N:915:VAL:HG23  | 2.06                     | 0.55              |
| 7:X:26:LEU:HD13   | 7:X:58:ILE:HG22   | 1.88                     | 0.55              |
| 2:C:1095:LEU:HB2  | 3:D:101:HIS:CE1   | 2.41                     | 0.55              |
| 2:C:391:LEU:O     | 2:C:391:LEU:HD23  | 2.07                     | 0.55              |
| 2:C:433:THR:HG21  | 2:C:488:ALA:HB1   | 1.87                     | 0.55              |
| 2:C:11:GLU:CD     | 2:C:537:LYS:HZ2   | 2.09                     | 0.55              |
| 2:C:544:THR:O     | 2:C:547:ILE:HD13  | 2.06                     | 0.55              |
| 3:D:1152:GLU:HG3  | 3:D:1161:GLU:HA   | 1.88                     | 0.55              |
| 3:D:729:HIS:CE1   | 3:D:731:LEU:H     | 2.24                     | 0.55              |
| 3:D:982:PHE:HD2   | 3:D:982:PHE:H     | 1.53                     | 0.55              |
| 1:G:112:ARG:NH1   | 1:G:126:ASP:N     | 2.55                     | 0.55              |
| 2:H:1034:GLU:OE1  | 3:I:1096:ARG:NH2  | 2.35                     | 0.55              |
| 2:H:1085:PHE:O    | 2:H:1089:VAL:HG23 | 2.05                     | 0.55              |
| 2:H:139:GLN:HE22  | 2:H:415:PRO:CD    | 2.19                     | 0.55              |
| 2:H:332:ARG:HE    | 2:H:464:LEU:CD1   | 2.20                     | 0.55              |
| 2:H:468:ARG:HB3   | 2:H:485:TYR:HB3   | 1.87                     | 0.55              |
| 2:H:498:GLN:HE21  | 2:H:498:GLN:HA    | 1.71                     | 0.55              |
| 2:H:544:THR:O     | 2:H:547:ILE:HD13  | 2.06                     | 0.55              |
| 3:I:191:LEU:HD22  | 3:I:393:ILE:HG21  | 1.87                     | 0.55              |
| 3:I:729:HIS:CE1   | 3:I:731:LEU:H     | 2.24                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:780:LYS:HZ1   | 7:Y:38:GLU:HB3    | 1.70                     | 0.55              |
| 2:M:140:ILE:HD13  | 2:M:331:ARG:HE    | 1.71                     | 0.55              |
| 3:N:705:ALA:HB1   | 3:N:706:PRO:HD3   | 1.88                     | 0.55              |
| 3:N:729:HIS:CE1   | 3:N:731:LEU:H     | 2.24                     | 0.55              |
| 3:N:84:ILE:HG13   | 3:N:85:VAL:N      | 2.21                     | 0.55              |
| 3:N:970:LYS:HG2   | 3:N:995:LEU:HD13  | 1.87                     | 0.55              |
| 2:C:415:PRO:HB2   | 2:C:418:LEU:HD13  | 1.88                     | 0.55              |
| 2:C:976:ASP:HB3   | 2:C:979:THR:HG22  | 1.88                     | 0.55              |
| 2:C:987:ILE:HD12  | 3:D:948:THR:HG23  | 1.88                     | 0.55              |
| 3:D:1110:ALA:O    | 3:D:1111:ASP:C    | 2.45                     | 0.55              |
| 3:D:804:LEU:CD2   | 3:D:804:LEU:N     | 2.70                     | 0.55              |
| 1:F:35:THR:HG21   | 1:G:43:ILE:HD11   | 1.88                     | 0.55              |
| 1:G:56:VAL:HG12   | 1:G:57:TYR:N      | 2.22                     | 0.55              |
| 3:I:1258:ARG:HH21 | 3:I:1262:LEU:HD11 | 1.70                     | 0.55              |
| 3:I:1329:ALA:C    | 3:I:1330:ILE:HD12 | 2.26                     | 0.55              |
| 3:I:15:PRO:HB3    | 3:I:515:GLU:OE1   | 2.06                     | 0.55              |
| 3:I:17:LYS:CG     | 3:I:21:TRP:HE1    | 2.20                     | 0.55              |
| 3:I:400:VAL:HG13  | 3:I:443:VAL:CG2   | 2.36                     | 0.55              |
| 3:I:470:LEU:HD12  | 3:I:503:LEU:CD2   | 2.37                     | 0.55              |
| 3:I:563:PRO:O     | 3:I:566:ILE:N     | 2.36                     | 0.55              |
| 3:I:636:GLN:HG2   | 3:I:637:LEU:N     | 2.22                     | 0.55              |
| 3:I:702:LEU:O     | 3:I:713:ILE:HA    | 2.07                     | 0.55              |
| 3:I:956:ILE:HD11  | 3:I:1062:ARG:HB3  | 1.89                     | 0.55              |
| 3:I:982:PHE:HB2   | 3:I:983:LEU:HD23  | 1.88                     | 0.55              |
| 2:M:1029:GLY:O    | 3:N:622:ARG:HG2   | 2.06                     | 0.55              |
| 2:M:192:PRO:O     | 2:M:195:LEU:HB3   | 2.06                     | 0.55              |
| 2:M:206:THR:HG23  | 2:M:207:LEU:N     | 2.22                     | 0.55              |
| 2:M:221:LEU:C     | 2:M:223:ASP:N     | 2.53                     | 0.55              |
| 2:M:433:THR:CG2   | 2:M:488:ALA:HB1   | 2.37                     | 0.55              |
| 2:M:39:ARG:CD     | 2:M:45:GLN:NE2    | 2.59                     | 0.55              |
| 2:M:75:GLU:OE1    | 2:M:75:GLU:HA     | 2.06                     | 0.55              |
| 3:N:119:SER:H     | 3:N:123:LEU:CD2   | 2.20                     | 0.55              |
| 3:N:1205:TYR:CZ   | 3:N:1366:LYS:HD3  | 2.42                     | 0.55              |
| 3:N:17:LYS:CG     | 3:N:21:TRP:HE1    | 2.20                     | 0.55              |
| 3:N:780:LYS:HZ3   | 7:Z:38:GLU:HB3    | 1.70                     | 0.55              |
| 1:A:34:VAL:CG1    | 1:B:42:ARG:HH21   | 2.19                     | 0.55              |
| 1:B:44:LEU:CA     | 1:B:48:ILE:HD13   | 2.35                     | 0.55              |
| 2:C:64:LEU:HD12   | 2:C:100:LEU:HD11  | 1.89                     | 0.55              |
| 2:C:165:LEU:HB3   | 2:C:265:ARG:NH1   | 2.20                     | 0.55              |
| 2:C:47:ALA:HB1    | 2:C:345:ARG:HB3   | 1.89                     | 0.55              |
| 2:C:717:LEU:HD13  | 2:C:761:PHE:HD2   | 1.70                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1189:ARG:HB3  | 3:D:1204:CYS:HA   | 1.89                     | 0.55              |
| 1:F:221:HIS:NE2   | 1:G:32:PHE:CD2    | 2.75                     | 0.55              |
| 2:H:205:GLU:OE2   | 2:H:206:THR:HG22  | 2.06                     | 0.55              |
| 2:H:18:LEU:HD11   | 2:H:586:ARG:NH1   | 2.21                     | 0.55              |
| 3:I:1108:ARG:HD3  | 3:I:1108:ARG:N    | 2.21                     | 0.55              |
| 3:I:1150:ALA:HB3  | 3:I:1187:PRO:HB2  | 1.89                     | 0.55              |
| 1:G:80:LEU:HD23   | 3:I:867:ARG:HG3   | 1.89                     | 0.55              |
| 1:K:58:ILE:HG21   | 1:K:68:ILE:HD11   | 1.89                     | 0.55              |
| 2:M:1006:HIS:CD2  | 2:M:1027:PHE:HB3  | 2.42                     | 0.55              |
| 2:M:500:ASN:OD1   | 3:N:1067:VAL:CG2  | 2.55                     | 0.55              |
| 2:M:810:ASP:HB3   | 2:M:813:VAL:HG12  | 1.89                     | 0.55              |
| 3:N:1107:VAL:HG13 | 3:N:1200:VAL:O    | 2.07                     | 0.55              |
| 3:N:1149:LEU:HG   | 3:N:1166:LEU:HD22 | 1.88                     | 0.55              |
| 3:N:1388:ARG:HH11 | 3:N:1388:ARG:HA   | 1.69                     | 0.55              |
| 3:N:205:TYR:O     | 3:N:205:TYR:CD2   | 2.60                     | 0.55              |
| 3:N:632:VAL:HG23  | 3:N:725:SER:HB2   | 1.87                     | 0.55              |
| 3:N:660:LYS:NZ    | 3:N:660:LYS:HA    | 2.22                     | 0.55              |
| 3:N:1486:VAL:CG1  | 4:O:22:VAL:HG13   | 2.37                     | 0.55              |
| 5:T:18:DC:C2'     | 5:T:19:DC:H5'     | 2.28                     | 0.55              |
| 1:A:56:VAL:CG1    | 1:A:142:VAL:HG12  | 2.27                     | 0.55              |
| 1:B:79:ILE:HD12   | 1:B:83:LYS:HE3    | 1.89                     | 0.55              |
| 3:D:1053:PHE:CZ   | 3:D:1072:ILE:HD12 | 2.42                     | 0.55              |
| 3:D:1205:TYR:CZ   | 3:D:1366:LYS:HD3  | 2.42                     | 0.55              |
| 3:D:181:ASP:O     | 3:D:205:TYR:N     | 2.40                     | 0.55              |
| 3:D:190:GLU:HG2   | 3:D:196:VAL:CG2   | 2.36                     | 0.55              |
| 3:D:457:GLY:O     | 3:D:460:ALA:N     | 2.39                     | 0.55              |
| 4:E:54:LEU:HA     | 4:E:58:PRO:CG     | 2.36                     | 0.55              |
| 1:G:74:ASP:HB2    | 3:I:872:ARG:HH21  | 1.71                     | 0.55              |
| 2:H:1037:VAL:O    | 2:H:1041:GLU:HG3  | 2.06                     | 0.55              |
| 2:H:162:ILE:HB    | 2:H:172:ILE:HB    | 1.87                     | 0.55              |
| 2:H:351:LEU:CD1   | 2:H:374:ASN:ND2   | 2.68                     | 0.55              |
| 2:H:524:VAL:CG1   | 2:H:525:SER:N     | 2.69                     | 0.55              |
| 2:H:71:TYR:HD2    | 2:H:71:TYR:H      | 1.53                     | 0.55              |
| 2:H:948:GLU:CD    | 2:H:955:PRO:HA    | 2.27                     | 0.55              |
| 3:I:660:LYS:NZ    | 3:I:660:LYS:HA    | 2.22                     | 0.55              |
| 3:I:800:LYS:HG3   | 3:I:829:VAL:CG1   | 2.37                     | 0.55              |
| 2:M:327:HIS:O     | 2:M:330:ASN:N     | 2.35                     | 0.55              |
| 2:M:897:LEU:HD21  | 2:M:921:ALA:CA    | 2.36                     | 0.55              |
| 2:M:948:GLU:CD    | 2:M:955:PRO:HA    | 2.28                     | 0.55              |
| 3:N:1205:TYR:CE2  | 3:N:1366:LYS:HD3  | 2.42                     | 0.55              |
| 3:N:1209:LEU:HD21 | 4:O:16:LYS:HZ1    | 1.68                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1380:GLU:HB2  | 3:N:1420:LEU:HD11 | 1.89                     | 0.55              |
| 3:N:1460:ILE:O    | 3:N:1460:ILE:HD12 | 2.07                     | 0.55              |
| 3:N:355:VAL:HG11  | 3:N:385:VAL:HG21  | 1.89                     | 0.55              |
| 3:N:814:ALA:HB1   | 3:N:818:ARG:NH2   | 2.17                     | 0.55              |
| 3:N:948:THR:C     | 3:N:949:ILE:HD12  | 2.27                     | 0.55              |
| 7:Y:115:THR:OG1   | 7:Y:116:PRO:HD3   | 2.06                     | 0.55              |
| 1:A:23:PHE:HE2    | 1:A:199:ILE:HD12  | 1.72                     | 0.55              |
| 1:A:35:THR:HG21   | 1:B:43:ILE:CG1    | 2.36                     | 0.55              |
| 1:A:39:PRO:HG3    | 1:B:39:PRO:HG3    | 1.88                     | 0.55              |
| 1:B:42:ARG:CG     | 1:B:42:ARG:HH11   | 2.19                     | 0.55              |
| 1:B:58:ILE:CD1    | 1:B:58:ILE:N      | 2.70                     | 0.55              |
| 2:C:441:VAL:HG12  | 2:C:559:LEU:HA    | 1.88                     | 0.55              |
| 2:C:571:LEU:CD1   | 2:C:701:THR:N     | 2.69                     | 0.55              |
| 3:D:1426:LYS:HA   | 3:D:1429:LEU:HD22 | 1.89                     | 0.55              |
| 3:D:584:ASN:CG    | 3:D:590:PRO:HG2   | 2.27                     | 0.55              |
| 3:D:699:VAL:HG22  | 3:D:756:GLN:OE1   | 2.06                     | 0.55              |
| 2:H:1043:TYR:HE2  | 3:I:768:ASN:ND2   | 2.04                     | 0.55              |
| 2:H:165:LEU:HA    | 2:H:166:PRO:O     | 2.07                     | 0.55              |
| 3:D:159:ARG:HD2   | 2:H:222:MET:HE1   | 1.89                     | 0.55              |
| 3:I:1118:ILE:HG13 | 3:I:1192:LEU:HD12 | 1.88                     | 0.55              |
| 3:I:1205:TYR:CE2  | 3:I:1366:LYS:HD3  | 2.42                     | 0.55              |
| 3:I:1408:ILE:HD12 | 3:I:1408:ILE:N    | 2.21                     | 0.55              |
| 2:H:1009:SER:HB3  | 3:I:651:GLU:O     | 2.07                     | 0.55              |
| 3:I:789:LEU:CD1   | 3:I:911:LEU:HD21  | 2.37                     | 0.55              |
| 2:M:200:LEU:CD2   | 2:M:300:ASP:CG    | 2.72                     | 0.55              |
| 2:M:549:PHE:CD2   | 2:M:886:LEU:HB3   | 2.42                     | 0.55              |
| 3:N:1097:LYS:O    | 3:N:1100:ASP:HB2  | 2.07                     | 0.55              |
| 3:N:1463:LYS:O    | 3:N:1466:VAL:HB   | 2.07                     | 0.55              |
| 3:N:1468:LEU:HD23 | 3:N:1468:LEU:O    | 2.07                     | 0.55              |
| 2:M:1046:ALA:HB2  | 3:N:1476:THR:HB   | 1.89                     | 0.55              |
| 2:M:1046:ALA:HB2  | 3:N:1476:THR:OG1  | 2.05                     | 0.55              |
| 3:N:348:GLN:HB2   | 3:N:351:MET:SD    | 2.47                     | 0.55              |
| 3:N:808:THR:OG1   | 3:N:809:PRO:HD3   | 2.07                     | 0.55              |
| 7:X:7:LEU:CD2     | 7:X:109:GLU:HB2   | 2.36                     | 0.55              |
| 7:Z:90:GLU:HA     | 7:Z:100:LEU:O     | 2.07                     | 0.55              |
| 1:B:56:VAL:HG12   | 1:B:57:TYR:N      | 2.22                     | 0.54              |
| 2:C:162:ILE:HB    | 2:C:172:ILE:HB    | 1.89                     | 0.54              |
| 2:C:22:GLN:HB3    | 2:C:121:MET:HE1   | 1.88                     | 0.54              |
| 2:C:31:GLN:HG2    | 2:C:34:VAL:HG23   | 1.88                     | 0.54              |
| 3:D:418:GLY:O     | 3:D:428:LYS:HD2   | 2.07                     | 0.54              |
| 3:D:636:GLN:HG2   | 3:D:637:LEU:N     | 2.22                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:804:LEU:HB3   | 3:D:830:ALA:O     | 2.07                     | 0.54              |
| 3:D:982:PHE:HB2   | 3:D:983:LEU:HD23  | 1.88                     | 0.54              |
| 2:H:178:PRO:C     | 2:H:180:GLY:H     | 2.10                     | 0.54              |
| 2:H:368:THR:HG22  | 2:H:369:PRO:HD3   | 1.89                     | 0.54              |
| 2:H:547:ILE:HD12  | 2:H:547:ILE:N     | 2.22                     | 0.54              |
| 2:H:54:ILE:HG22   | 2:H:66:LEU:N      | 2.16                     | 0.54              |
| 3:I:1466:VAL:HG12 | 3:I:1467:ILE:N    | 2.22                     | 0.54              |
| 3:I:204:LEU:O     | 3:I:393:ILE:HG23  | 2.08                     | 0.54              |
| 3:I:882:PHE:O     | 3:I:886:VAL:HG23  | 2.07                     | 0.54              |
| 3:I:996:TRP:HA    | 3:I:999:THR:HG22  | 1.87                     | 0.54              |
| 4:J:37:ASN:HD22   | 4:J:37:ASN:H      | 1.53                     | 0.54              |
| 1:L:56:VAL:HG12   | 1:L:57:TYR:N      | 2.22                     | 0.54              |
| 2:M:1014:SER:HB3  | 2:M:1019:GLN:H    | 1.71                     | 0.54              |
| 2:M:302:VAL:O     | 2:M:305:PRO:HD2   | 2.06                     | 0.54              |
| 2:M:500:ASN:N     | 2:M:500:ASN:ND2   | 2.54                     | 0.54              |
| 2:M:547:ILE:N     | 2:M:547:ILE:HD12  | 2.23                     | 0.54              |
| 3:N:1053:PHE:CE1  | 3:N:1072:ILE:HG23 | 2.42                     | 0.54              |
| 3:N:186:VAL:HA    | 3:N:200:ASP:OD2   | 2.07                     | 0.54              |
| 3:N:394:LEU:HD23  | 3:N:394:LEU:N     | 2.22                     | 0.54              |
| 3:N:433:GLY:HA3   | 3:N:446:VAL:HG12  | 1.87                     | 0.54              |
| 3:N:636:GLN:HG2   | 3:N:637:LEU:N     | 2.22                     | 0.54              |
| 3:N:86:ARG:NE     | 3:N:523:ASP:OD1   | 2.40                     | 0.54              |
| 3:N:875:THR:CG2   | 3:N:879:ARG:HB2   | 2.38                     | 0.54              |
| 1:B:153:ALA:HA    | 1:B:156:HIS:NE2   | 2.21                     | 0.54              |
| 1:B:74:ASP:CB     | 3:D:872:ARG:NH2   | 2.58                     | 0.54              |
| 2:C:1036:GLU:OE1  | 2:C:1036:GLU:N    | 2.41                     | 0.54              |
| 2:C:1041:GLU:OE1  | 3:D:1462:LEU:HB3  | 2.08                     | 0.54              |
| 2:C:165:LEU:HB2   | 2:C:265:ARG:HH12  | 1.69                     | 0.54              |
| 2:C:437:ARG:HG2   | 2:C:467:ILE:O     | 2.07                     | 0.54              |
| 2:C:606:VAL:CG2   | 2:C:645:VAL:HG22  | 2.36                     | 0.54              |
| 3:D:160:GLU:O     | 3:D:165:LYS:N     | 2.41                     | 0.54              |
| 3:D:181:ASP:HA    | 3:D:205:TYR:HB3   | 1.88                     | 0.54              |
| 3:D:441:ARG:HD2   | 3:D:445:ARG:HH22  | 1.72                     | 0.54              |
| 3:D:398:ALA:CB    | 3:D:447:VAL:HA    | 2.35                     | 0.54              |
| 3:D:584:ASN:OD1   | 3:D:590:PRO:HG2   | 2.08                     | 0.54              |
| 3:D:866:VAL:HG11  | 3:D:880:ILE:CD1   | 2.38                     | 0.54              |
| 1:F:18:ARG:HH11   | 1:F:123:MET:CE    | 2.20                     | 0.54              |
| 2:H:122:THR:HG22  | 2:H:123:GLU:N     | 2.23                     | 0.54              |
| 2:H:218:VAL:CG1   | 2:H:222:MET:HG3   | 2.37                     | 0.54              |
| 2:H:512:ARG:HG2   | 2:H:523:ILE:HD11  | 1.89                     | 0.54              |
| 3:I:997:THR:HG21  | 7:Y:61:ARG:HH22   | 1.70                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:571:LEU:HD11  | 2:M:701:THR:H     | 1.70                     | 0.54              |
| 2:M:689:VAL:HG11  | 2:M:853:LEU:HD22  | 1.89                     | 0.54              |
| 3:N:1166:LEU:N    | 3:N:1166:LEU:HD23 | 2.21                     | 0.54              |
| 3:N:1118:ILE:HD11 | 3:N:1193:THR:HG23 | 1.88                     | 0.54              |
| 3:N:1434:TRP:CE3  | 3:N:1455:LYS:HB3  | 2.42                     | 0.54              |
| 3:N:205:TYR:HD1   | 3:N:390:PRO:CG    | 2.20                     | 0.54              |
| 3:N:700:VAL:HG22  | 3:N:718:PRO:HG3   | 1.89                     | 0.54              |
| 7:X:62:ILE:CG2    | 7:X:63:ASP:N      | 2.71                     | 0.54              |
| 1:B:165:ILE:H     | 1:B:165:ILE:HD13  | 1.70                     | 0.54              |
| 1:B:197:LEU:HD21  | 1:B:199:ILE:HD11  | 1.88                     | 0.54              |
| 1:B:80:LEU:HG     | 3:D:844:ALA:CA    | 2.37                     | 0.54              |
| 2:C:292:ARG:HD2   | 2:C:299:LYS:NZ    | 2.22                     | 0.54              |
| 2:C:547:ILE:HD12  | 2:C:547:ILE:N     | 2.23                     | 0.54              |
| 2:C:604:ALA:HB3   | 2:C:612:VAL:O     | 2.07                     | 0.54              |
| 2:C:890:LEU:HD21  | 2:C:901:TYR:CD1   | 2.43                     | 0.54              |
| 2:C:948:GLU:CD    | 2:C:955:PRO:HA    | 2.27                     | 0.54              |
| 3:D:116:LEU:HD13  | 3:D:118:LEU:HD12  | 1.89                     | 0.54              |
| 3:D:660:LYS:NZ    | 3:D:660:LYS:HA    | 2.22                     | 0.54              |
| 1:G:165:ILE:N     | 1:G:165:ILE:CD1   | 2.66                     | 0.54              |
| 2:H:1112:PHE:HB3  | 3:I:88:TYR:CD1    | 2.42                     | 0.54              |
| 2:H:279:GLU:HG3   | 2:H:280:LYS:N     | 2.21                     | 0.54              |
| 2:H:367:LEU:HD12  | 2:H:367:LEU:O     | 2.07                     | 0.54              |
| 3:I:1053:PHE:CE1  | 3:I:1072:ILE:HG23 | 2.42                     | 0.54              |
| 3:I:1109:GLU:HG3  | 3:I:1217:ILE:CD1  | 2.36                     | 0.54              |
| 3:I:1372:VAL:HA   | 3:I:1375:MET:HE2  | 1.90                     | 0.54              |
| 3:I:185:VAL:HG13  | 3:I:189:GLN:NE2   | 2.22                     | 0.54              |
| 2:M:188:LYS:HZ2   | 2:M:188:LYS:HA    | 1.73                     | 0.54              |
| 2:M:230:ARG:HH11  | 2:M:230:ARG:HG2   | 1.72                     | 0.54              |
| 2:M:668:LEU:CD1   | 2:M:668:LEU:N     | 2.66                     | 0.54              |
| 2:M:701:THR:HA    | 2:M:831:ARG:O     | 2.08                     | 0.54              |
| 3:N:1053:PHE:CZ   | 3:N:1072:ILE:HD12 | 2.42                     | 0.54              |
| 3:N:119:SER:O     | 3:N:121:THR:N     | 2.40                     | 0.54              |
| 3:N:1221:VAL:CG1  | 3:N:1370:ILE:HD13 | 2.37                     | 0.54              |
| 3:N:367:ILE:HG22  | 3:N:368:VAL:HG23  | 1.90                     | 0.54              |
| 1:L:190:THR:OG1   | 3:N:722:GLU:OE1   | 2.25                     | 0.54              |
| 1:A:58:ILE:HG21   | 1:A:68:ILE:HD11   | 1.89                     | 0.54              |
| 1:B:86:VAL:HG13   | 1:B:86:VAL:O      | 2.07                     | 0.54              |
| 2:C:1095:LEU:HD11 | 2:C:1097:LEU:HD23 | 1.88                     | 0.54              |
| 2:C:224:GLU:O     | 2:C:228:ALA:HB3   | 2.08                     | 0.54              |
| 2:C:512:ARG:HG2   | 2:C:523:ILE:HD11  | 1.90                     | 0.54              |
| 3:D:1053:PHE:CE1  | 3:D:1072:ILE:HG23 | 2.43                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:789:LEU:CD1   | 3:D:911:LEU:HD21  | 2.37                     | 0.54              |
| 1:F:67:THR:CG2    | 2:H:627:ARG:NH2   | 2.71                     | 0.54              |
| 1:F:58:ILE:HG21   | 1:F:68:ILE:HD11   | 1.89                     | 0.54              |
| 2:H:1056:LYS:HD3  | 3:I:623:VAL:HG13  | 1.87                     | 0.54              |
| 2:H:258:TYR:CZ    | 2:H:290:LEU:HD21  | 2.42                     | 0.54              |
| 2:H:654:LEU:N     | 2:H:654:LEU:HD23  | 2.17                     | 0.54              |
| 3:I:160:GLU:CA    | 3:I:165:LYS:HB2   | 2.36                     | 0.54              |
| 3:I:510:GLU:HB2   | 3:I:511:TRP:CZ3   | 2.43                     | 0.54              |
| 3:I:875:THR:CG2   | 3:I:879:ARG:HB2   | 2.37                     | 0.54              |
| 2:M:657:ASP:CG    | 2:M:662:GLU:HA    | 2.28                     | 0.54              |
| 3:N:1029:ARG:CA   | 3:N:1029:ARG:HH11 | 2.19                     | 0.54              |
| 3:N:1109:GLU:HG2  | 3:N:1202:GLN:N    | 2.20                     | 0.54              |
| 3:N:186:VAL:HG12  | 3:N:187:LYS:H     | 1.71                     | 0.54              |
| 4:O:10:PHE:CE2    | 4:O:19:LEU:HD23   | 2.42                     | 0.54              |
| 5:R:20:DG:H22     | 6:S:11:C:N4       | 2.03                     | 0.54              |
| 1:A:19:GLU:CD     | 1:A:19:GLU:H      | 2.10                     | 0.54              |
| 2:C:1081:VAL:HG13 | 2:C:1085:PHE:CB   | 2.38                     | 0.54              |
| 2:C:175:GLU:O     | 2:C:183:SER:HB3   | 2.06                     | 0.54              |
| 2:C:368:THR:HB    | 2:C:369:PRO:CD    | 2.38                     | 0.54              |
| 2:C:683:ASN:HB2   | 2:C:872:ASN:HB2   | 1.89                     | 0.54              |
| 2:C:555:ALA:HA    | 3:D:1070:TYR:OH   | 2.06                     | 0.54              |
| 3:D:1109:GLU:HG2  | 3:D:1201:CYS:CA   | 2.38                     | 0.54              |
| 3:D:434:ARG:HB3   | 3:D:447:VAL:CG2   | 2.38                     | 0.54              |
| 3:D:481:MET:CE    | 3:D:496:LEU:HD23  | 2.38                     | 0.54              |
| 2:H:63:GLY:HA3    | 2:H:103:LYS:CE    | 2.37                     | 0.54              |
| 2:H:91:GLN:HA     | 2:H:119:PRO:HA    | 1.90                     | 0.54              |
| 2:H:185:LYS:HG2   | 2:H:190:LYS:HA    | 1.90                     | 0.54              |
| 2:H:431:HIS:H     | 2:H:434:HIS:CE1   | 2.25                     | 0.54              |
| 2:H:545:ASN:HA    | 2:H:905:ILE:HD11  | 1.90                     | 0.54              |
| 3:I:1221:VAL:CG1  | 3:I:1370:ILE:HD13 | 2.38                     | 0.54              |
| 3:I:1283:ILE:HG22 | 3:I:1284:GLU:N    | 2.22                     | 0.54              |
| 3:I:699:VAL:HG22  | 3:I:756:GLN:OE1   | 2.06                     | 0.54              |
| 4:J:6:ILE:O       | 4:J:9:LEU:HB2     | 2.07                     | 0.54              |
| 2:M:456:ALA:HB3   | 2:M:459:ALA:HB2   | 1.89                     | 0.54              |
| 3:N:702:LEU:O     | 3:N:713:ILE:HA    | 2.07                     | 0.54              |
| 3:N:766:ALA:HB1   | 4:O:2:ALA:HB2     | 1.89                     | 0.54              |
| 3:N:1216:SER:CB   | 4:O:16:LYS:H      | 2.21                     | 0.54              |
| 4:O:36:LYS:HZ1    | 4:O:45:ARG:HH22   | 1.56                     | 0.54              |
| 2:C:1017:THR:O    | 2:C:1018:GLN:HB2  | 2.07                     | 0.54              |
| 2:C:431:HIS:H     | 2:C:434:HIS:CE1   | 2.25                     | 0.54              |
| 2:C:456:ALA:HB3   | 2:C:459:ALA:HB2   | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:523:ILE:HG23  | 2:C:523:ILE:O     | 2.08                     | 0.54              |
| 2:C:524:VAL:CG1   | 2:C:525:SER:N     | 2.69                     | 0.54              |
| 2:C:657:ASP:CG    | 2:C:662:GLU:HA    | 2.28                     | 0.54              |
| 3:D:1326:THR:CG2  | 3:D:1327:ARG:H    | 2.18                     | 0.54              |
| 3:D:1401:GLU:CD   | 3:D:1415:VAL:HG11 | 2.28                     | 0.54              |
| 3:D:470:LEU:HD12  | 3:D:503:LEU:CD2   | 2.37                     | 0.54              |
| 3:D:52:PRO:N      | 3:D:86:ARG:CD     | 2.71                     | 0.54              |
| 3:D:1481:VAL:CG1  | 4:E:18:ARG:HA     | 2.21                     | 0.54              |
| 4:E:47:LYS:HA     | 4:E:54:LEU:CB     | 2.38                     | 0.54              |
| 2:H:897:LEU:HB3   | 2:H:899:GLN:NE2   | 2.20                     | 0.54              |
| 2:H:890:LEU:HD21  | 2:H:901:TYR:CD1   | 2.43                     | 0.54              |
| 3:I:101:HIS:ND1   | 3:I:103:TRP:HB2   | 2.17                     | 0.54              |
| 3:I:1053:PHE:CZ   | 3:I:1072:ILE:HD12 | 2.42                     | 0.54              |
| 3:I:122:GLU:O     | 3:I:126:VAL:HG23  | 2.08                     | 0.54              |
| 3:I:1326:THR:CG2  | 3:I:1327:ARG:H    | 2.18                     | 0.54              |
| 3:I:540:LEU:H     | 3:I:540:LEU:HD12  | 1.73                     | 0.54              |
| 3:I:541:ASN:O     | 3:I:545:ARG:HG3   | 2.08                     | 0.54              |
| 3:I:697:GLY:C     | 4:J:59:ASN:HD22   | 2.10                     | 0.54              |
| 3:I:809:PRO:O     | 3:I:812:ALA:HB3   | 2.07                     | 0.54              |
| 1:K:56:VAL:CG1    | 1:K:142:VAL:HG12  | 2.27                     | 0.54              |
| 1:K:221:HIS:HA    | 1:K:224:TYR:CD2   | 2.43                     | 0.54              |
| 2:M:958:THR:HG23  | 2:M:961:GLU:HG2   | 1.89                     | 0.54              |
| 3:N:1401:GLU:CD   | 3:N:1415:VAL:HG11 | 2.28                     | 0.54              |
| 3:N:179:VAL:CG1   | 3:N:183:GLU:HB3   | 2.37                     | 0.54              |
| 3:N:787:LEU:HD21  | 3:N:947:ILE:HD13  | 1.90                     | 0.54              |
| 2:H:879:ARG:NH2   | 7:Y:42:ASP:CG     | 2.61                     | 0.54              |
| 3:N:1358:ALA:O    | 7:Z:55:LYS:NZ     | 2.40                     | 0.54              |
| 3:D:1352:ILE:O    | 3:D:1355:VAL:HG23 | 2.08                     | 0.54              |
| 3:D:700:VAL:HG22  | 3:D:718:PRO:HG3   | 1.89                     | 0.54              |
| 3:D:87:ARG:O      | 3:D:524:LEU:HD11  | 2.07                     | 0.54              |
| 4:E:61:VAL:HG23   | 4:E:62:THR:N      | 2.22                     | 0.54              |
| 2:H:1015:LEU:N    | 2:H:1015:LEU:CD1  | 2.71                     | 0.54              |
| 2:H:810:ASP:HB3   | 2:H:813:VAL:HG12  | 1.89                     | 0.54              |
| 2:H:957:LYS:O     | 2:H:962:GLN:NE2   | 2.25                     | 0.54              |
| 3:I:1205:TYR:CZ   | 3:I:1366:LYS:HD3  | 2.42                     | 0.54              |
| 3:I:138:LYS:HD3   | 3:I:138:LYS:N     | 2.19                     | 0.54              |
| 3:I:1395:LEU:HD23 | 3:I:1395:LEU:C    | 2.27                     | 0.54              |
| 3:I:1380:GLU:HB2  | 3:I:1420:LEU:HD11 | 1.89                     | 0.54              |
| 3:I:796:ARG:NH2   | 3:I:859:ASP:OD1   | 2.41                     | 0.54              |
| 3:I:866:VAL:HG11  | 3:I:880:ILE:CD1   | 2.38                     | 0.54              |
| 4:J:25:LYS:HA     | 4:J:28:GLN:CG     | 2.36                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:132:LEU:HD23  | 1:L:136:GLY:O     | 2.08                     | 0.54              |
| 1:L:197:LEU:HD21  | 1:L:199:ILE:HD11  | 1.88                     | 0.54              |
| 2:M:199:VAL:HG13  | 2:M:235:LEU:HD12  | 1.88                     | 0.54              |
| 2:M:603:VAL:HG22  | 2:M:613:VAL:HG12  | 1.90                     | 0.54              |
| 2:M:625:LEU:HB3   | 2:M:639:GLN:HB2   | 1.90                     | 0.54              |
| 2:M:443:THR:HG21  | 3:N:1078:ARG:NE   | 2.23                     | 0.54              |
| 3:N:789:LEU:CD1   | 3:N:911:LEU:HD21  | 2.37                     | 0.54              |
| 7:Y:115:THR:HB    | 7:Y:116:PRO:HD3   | 1.90                     | 0.54              |
| 1:B:16:GLN:HE21   | 1:B:16:GLN:HA     | 1.73                     | 0.54              |
| 2:C:81:ASP:N      | 2:C:84:ARG:NH1    | 2.56                     | 0.54              |
| 2:C:878:SER:OG    | 3:D:1029:ARG:CZ   | 2.56                     | 0.54              |
| 3:D:1122:LEU:HD12 | 3:D:1122:LEU:N    | 2.23                     | 0.54              |
| 3:D:1161:GLU:HG2  | 3:D:1164:ARG:HB2  | 1.90                     | 0.54              |
| 3:D:1095:THR:HG23 | 3:D:1230:GLY:HA3  | 1.90                     | 0.54              |
| 3:D:1205:TYR:CE2  | 3:D:1366:LYS:HD3  | 2.42                     | 0.54              |
| 3:D:1437:ALA:HB3  | 3:D:1446:VAL:CG1  | 2.38                     | 0.54              |
| 3:D:176:ASP:HB3   | 3:D:389:GLU:CG    | 2.26                     | 0.54              |
| 3:D:376:GLU:O     | 3:D:378:ILE:HG13  | 2.07                     | 0.54              |
| 3:D:590:PRO:O     | 3:D:600:LEU:HD12  | 2.08                     | 0.54              |
| 1:G:38:ASN:O      | 1:G:42:ARG:HG3    | 2.08                     | 0.54              |
| 2:H:1099:VAL:HG22 | 3:I:10:ILE:HG13   | 1.90                     | 0.54              |
| 2:H:140:ILE:HD12  | 2:H:140:ILE:O     | 2.07                     | 0.54              |
| 2:H:148:PHE:CZ    | 2:H:309:TYR:HB3   | 2.42                     | 0.54              |
| 2:H:806:LEU:HD13  | 2:H:813:VAL:HG21  | 1.89                     | 0.54              |
| 2:H:958:THR:HG23  | 2:H:961:GLU:HG2   | 1.89                     | 0.54              |
| 3:I:1112:CYS:SG   | 3:I:1112:CYS:O    | 2.65                     | 0.54              |
| 3:I:111:LYS:CD    | 3:I:1448:THR:HG22 | 2.38                     | 0.54              |
| 3:I:119:SER:H     | 3:I:123:LEU:CD2   | 2.20                     | 0.54              |
| 3:I:137:PRO:HB2   | 3:I:138:LYS:HD3   | 1.89                     | 0.54              |
| 3:I:179:VAL:HG21  | 3:I:189:GLN:NE2   | 2.23                     | 0.54              |
| 3:I:99:ALA:O      | 3:I:514:LEU:HB2   | 2.08                     | 0.54              |
| 2:H:1071:ILE:HG23 | 3:I:670:VAL:HG11  | 1.89                     | 0.54              |
| 3:I:700:VAL:HG22  | 3:I:718:PRO:HG3   | 1.88                     | 0.54              |
| 1:K:86:VAL:HG13   | 1:K:86:VAL:O      | 2.07                     | 0.54              |
| 1:L:55:SER:OG     | 1:L:158:ILE:HB    | 2.07                     | 0.54              |
| 1:L:88:ARG:HD2    | 1:L:123:MET:CE    | 2.38                     | 0.54              |
| 2:M:188:LYS:O     | 2:M:189:ARG:NE    | 2.26                     | 0.54              |
| 2:M:28:ARG:HG2    | 2:M:42:VAL:HG21   | 1.90                     | 0.54              |
| 2:M:398:THR:O     | 2:M:570:PRO:HD3   | 2.08                     | 0.54              |
| 2:M:897:LEU:HB3   | 2:M:899:GLN:NE2   | 2.21                     | 0.54              |
| 3:N:1114:THR:HG23 | 3:N:1114:THR:O    | 2.08                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:132:TYR:H     | 3:N:132:TYR:HD1   | 1.54                     | 0.54              |
| 3:N:157:GLU:N     | 3:N:157:GLU:OE2   | 2.40                     | 0.54              |
| 3:N:481:MET:CE    | 3:N:496:LEU:HD23  | 2.38                     | 0.54              |
| 3:N:813:LEU:HD12  | 3:N:814:ALA:CA    | 2.38                     | 0.54              |
| 1:B:156:HIS:ND1   | 1:B:158:ILE:HG12  | 2.22                     | 0.54              |
| 2:C:1044:GLY:HA2  | 3:D:1475:GLY:HA3  | 1.89                     | 0.54              |
| 2:C:269:LEU:HD23  | 2:C:269:LEU:C     | 2.29                     | 0.54              |
| 2:C:74:GLY:O      | 2:C:76:PRO:HD3    | 2.08                     | 0.54              |
| 2:C:997:LEU:O     | 2:C:999:HIS:N     | 2.41                     | 0.54              |
| 3:D:1311:LEU:HD23 | 3:D:1311:LEU:H    | 1.73                     | 0.54              |
| 3:D:875:THR:CG2   | 3:D:879:ARG:HB2   | 2.37                     | 0.54              |
| 1:G:16:GLN:HE21   | 1:G:16:GLN:HA     | 1.73                     | 0.54              |
| 2:H:523:ILE:O     | 2:H:523:ILE:HG23  | 2.07                     | 0.54              |
| 2:H:6:PHE:CD1     | 2:H:6:PHE:N       | 2.75                     | 0.54              |
| 2:H:516:ARG:NE    | 3:I:1068:LEU:HD13 | 2.22                     | 0.54              |
| 3:I:133:ILE:HG22  | 3:I:134:VAL:H     | 1.72                     | 0.54              |
| 3:I:1352:ILE:O    | 3:I:1355:VAL:HG23 | 2.08                     | 0.54              |
| 3:I:141:ILE:HG22  | 3:I:162:ARG:NH1   | 2.23                     | 0.54              |
| 1:G:190:THR:OG1   | 3:I:722:GLU:OE1   | 2.26                     | 0.54              |
| 1:K:107:LYS:NZ    | 1:K:113:ASP:OD2   | 2.37                     | 0.54              |
| 1:L:58:ILE:N      | 1:L:58:ILE:CD1    | 2.68                     | 0.54              |
| 2:M:1111:ILE:O    | 2:M:1112:PHE:C    | 2.46                     | 0.54              |
| 2:M:274:ARG:HG3   | 2:M:285:LEU:HB3   | 1.89                     | 0.54              |
| 2:M:39:ARG:NE     | 2:M:45:GLN:HE21   | 1.88                     | 0.54              |
| 2:M:523:ILE:HG23  | 2:M:523:ILE:O     | 2.07                     | 0.54              |
| 2:M:586:ARG:NH1   | 2:M:590:ASP:OD2   | 2.41                     | 0.54              |
| 2:M:697:ARG:O     | 2:M:698:ASP:HB2   | 2.08                     | 0.54              |
| 3:N:996:TRP:CD1   | 3:N:1056:PRO:HG2  | 2.40                     | 0.54              |
| 3:N:356:PRO:HG2   | 3:N:359:ALA:CB    | 2.33                     | 0.54              |
| 3:N:407:VAL:HA    | 3:N:422:ALA:CB    | 2.37                     | 0.54              |
| 2:C:185:LYS:HD2   | 2:C:190:LYS:HE2   | 1.90                     | 0.54              |
| 3:D:1221:VAL:CG1  | 3:D:1370:ILE:HD13 | 2.38                     | 0.54              |
| 3:D:1326:THR:CG2  | 3:D:1327:ARG:N    | 2.71                     | 0.54              |
| 3:D:348:GLN:HB2   | 3:D:351:MET:SD    | 2.48                     | 0.54              |
| 3:D:506:GLY:O     | 3:D:507:ASN:C     | 2.46                     | 0.54              |
| 4:E:79:LEU:HG     | 4:E:80:VAL:HG23   | 1.89                     | 0.54              |
| 1:G:23:PHE:O      | 1:G:196:THR:HA    | 2.08                     | 0.54              |
| 2:H:182:VAL:C     | 2:H:193:LEU:CD1   | 2.75                     | 0.54              |
| 3:D:562:ALA:O     | 2:H:223:ASP:O     | 2.25                     | 0.54              |
| 3:D:207:PHE:CE2   | 2:H:284:ARG:HB2   | 2.42                     | 0.54              |
| 2:H:897:LEU:HD22  | 2:H:920:GLN:HG2   | 1.88                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:107:ASP:O    | 3:I:108:VAL:C     | 2.46                     | 0.54              |
| 3:I:1098:LEU:CD2 | 3:I:1229:ILE:HB   | 2.37                     | 0.54              |
| 3:I:788:GLY:O    | 3:I:792:ILE:HG22  | 2.09                     | 0.54              |
| 3:I:835:SER:H    | 3:I:838:ARG:CD    | 2.21                     | 0.54              |
| 2:M:150:PRO:HA   | 2:M:158:TYR:HB3   | 1.90                     | 0.54              |
| 2:M:16:PRO:O     | 2:M:18:LEU:HD12   | 2.07                     | 0.54              |
| 2:M:195:LEU:CD2  | 2:M:238:LEU:HG    | 2.38                     | 0.54              |
| 2:M:140:ILE:CG2  | 2:M:333:ILE:HG13  | 2.38                     | 0.54              |
| 2:M:588:VAL:CG1  | 2:M:661:SER:HB3   | 2.39                     | 0.54              |
| 2:M:957:LYS:O    | 2:M:962:GLN:NE2   | 2.26                     | 0.54              |
| 2:M:676:ILE:HG23 | 2:M:988:VAL:HG13  | 1.84                     | 0.54              |
| 3:N:185:VAL:CG1  | 3:N:186:VAL:N     | 2.71                     | 0.54              |
| 3:N:866:VAL:HG11 | 3:N:880:ILE:CD1   | 2.38                     | 0.54              |
| 7:Y:89:VAL:HG12  | 7:Y:90:GLU:N      | 2.23                     | 0.54              |
| 1:A:124:ASN:ND2  | 1:A:127:LEU:HD22  | 2.22                     | 0.53              |
| 1:A:221:HIS:HA   | 1:A:224:TYR:CD2   | 2.43                     | 0.53              |
| 1:B:74:ASP:CG    | 3:D:872:ARG:NH2   | 2.61                     | 0.53              |
| 2:C:1044:GLY:HA3 | 4:E:17:TYR:HE1    | 1.71                     | 0.53              |
| 2:C:158:TYR:CD1  | 2:C:158:TYR:N     | 2.70                     | 0.53              |
| 2:C:182:VAL:CB   | 2:C:193:LEU:HB3   | 2.38                     | 0.53              |
| 2:C:487:THR:HB   | 2:C:490:GLU:HG3   | 1.89                     | 0.53              |
| 2:C:582:GLY:C    | 2:C:583:LEU:HD12  | 2.29                     | 0.53              |
| 2:C:897:LEU:HD22 | 2:C:920:GLN:HG2   | 1.88                     | 0.53              |
| 3:D:788:GLY:O    | 3:D:792:ILE:HG22  | 2.08                     | 0.53              |
| 1:G:185:ARG:CD   | 3:I:692:GLU:CG    | 2.85                     | 0.53              |
| 2:H:1092:LEU:CD1 | 2:H:1099:VAL:HG21 | 2.14                     | 0.53              |
| 2:H:678:PRO:O    | 3:I:943:THR:HA    | 2.07                     | 0.53              |
| 2:H:830:LYS:HD2  | 2:H:832:LYS:HE3   | 1.89                     | 0.53              |
| 3:I:1326:THR:CG2 | 3:I:1327:ARG:N    | 2.71                     | 0.53              |
| 3:I:177:ALA:H    | 3:I:390:PRO:CD    | 2.20                     | 0.53              |
| 3:I:396:VAL:HG21 | 3:I:445:ARG:HD3   | 1.89                     | 0.53              |
| 3:I:481:MET:CE   | 3:I:496:LEU:HD23  | 2.38                     | 0.53              |
| 3:I:506:GLY:O    | 3:I:507:ASN:C     | 2.46                     | 0.53              |
| 1:L:102:LYS:NZ   | 1:L:137:ARG:HH12  | 2.05                     | 0.53              |
| 2:M:114:PHE:CG   | 2:M:114:PHE:O     | 2.60                     | 0.53              |
| 2:M:757:GLY:HA2  | 2:M:789:SER:OG    | 2.08                     | 0.53              |
| 2:M:678:PRO:HG3  | 2:M:873:PRO:HD2   | 1.90                     | 0.53              |
| 3:N:1108:ARG:HG2 | 3:N:1108:ARG:O    | 2.07                     | 0.53              |
| 3:N:1352:ILE:O   | 3:N:1355:VAL:HG23 | 2.08                     | 0.53              |
| 3:N:171:LEU:CD2  | 3:N:172:PRO:O     | 2.55                     | 0.53              |
| 3:N:882:PHE:O    | 3:N:886:VAL:HG23  | 2.07                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:X:105:VAL:HB    | 7:X:109:GLU:HB3   | 1.90                     | 0.53              |
| 2:C:1088:LEU:CD2  | 2:C:1092:LEU:HD12 | 2.34                     | 0.53              |
| 2:C:473:ARG:CB    | 2:C:531:PHE:CE1   | 2.88                     | 0.53              |
| 2:C:654:LEU:CD2   | 2:C:654:LEU:H     | 2.13                     | 0.53              |
| 2:C:81:ASP:N      | 2:C:84:ARG:HH12   | 2.07                     | 0.53              |
| 2:C:879:ARG:HH21  | 7:X:42:ASP:CG     | 1.80                     | 0.53              |
| 3:D:107:ASP:O     | 3:D:108:VAL:C     | 2.46                     | 0.53              |
| 3:D:1120:VAL:HG23 | 3:D:1188:VAL:CG1  | 2.38                     | 0.53              |
| 3:D:1128:VAL:O    | 3:D:1129:THR:HB   | 2.08                     | 0.53              |
| 4:E:52:GLU:N      | 4:E:52:GLU:CD     | 2.62                     | 0.53              |
| 1:F:221:HIS:HA    | 1:F:224:TYR:CD2   | 2.43                     | 0.53              |
| 2:H:108:ILE:HG22  | 2:H:109:LYS:N     | 2.23                     | 0.53              |
| 2:H:165:LEU:HB3   | 2:H:265:ARG:NH1   | 2.23                     | 0.53              |
| 3:I:198:ARG:NH1   | 3:I:198:ARG:HG3   | 2.23                     | 0.53              |
| 3:I:766:ALA:HB1   | 4:J:2:ALA:HB2     | 1.90                     | 0.53              |
| 1:G:170:VAL:CG1   | 3:I:848:GLU:OE2   | 2.49                     | 0.53              |
| 1:K:104:GLU:OE1   | 1:K:137:ARG:HG2   | 2.09                     | 0.53              |
| 1:K:36:LEU:C      | 1:K:39:PRO:HD2    | 2.28                     | 0.53              |
| 2:M:1070:ILE:CG2  | 3:N:656:PHE:CD1   | 2.91                     | 0.53              |
| 2:M:97:ARG:CD     | 2:M:97:ARG:N      | 2.71                     | 0.53              |
| 3:N:501:ALA:HB1   | 3:N:1453:ALA:HB2  | 1.90                     | 0.53              |
| 3:N:810:GLU:C     | 3:N:812:ALA:H     | 2.11                     | 0.53              |
| 7:Y:84:GLY:HA2    | 7:Y:130:LEU:HD11  | 1.89                     | 0.53              |
| 2:C:1047:HIS:HA   | 2:C:1050:GLN:HB3  | 1.90                     | 0.53              |
| 2:C:279:GLU:HG3   | 2:C:280:LYS:N     | 2.22                     | 0.53              |
| 2:C:328:LEU:HD22  | 2:C:433:THR:O     | 2.08                     | 0.53              |
| 2:C:725:ASP:O     | 2:C:727:PRO:HD3   | 2.08                     | 0.53              |
| 3:D:608:SER:HA    | 3:D:1443:THR:HG21 | 1.90                     | 0.53              |
| 2:C:1075:ASP:OD1  | 4:E:31:LEU:HD11   | 2.07                     | 0.53              |
| 1:F:104:GLU:OE1   | 1:F:137:ARG:HG2   | 2.09                     | 0.53              |
| 1:F:86:VAL:HG13   | 1:F:86:VAL:O      | 2.07                     | 0.53              |
| 1:G:58:ILE:N      | 1:G:58:ILE:HD12   | 2.23                     | 0.53              |
| 2:H:151:ASP:CG    | 2:H:152:PRO:CD    | 2.76                     | 0.53              |
| 2:H:18:LEU:N      | 2:H:18:LEU:HD12   | 2.20                     | 0.53              |
| 2:H:261:ILE:HD12  | 2:H:262:ALA:H     | 1.70                     | 0.53              |
| 2:H:360:LEU:N     | 2:H:360:LEU:HD23  | 2.23                     | 0.53              |
| 2:H:368:THR:HG22  | 2:H:369:PRO:CD    | 2.39                     | 0.53              |
| 2:H:516:ARG:CZ    | 3:I:1068:LEU:HD22 | 2.38                     | 0.53              |
| 3:I:1209:LEU:HD23 | 3:I:1210:SER:N    | 2.24                     | 0.53              |
| 3:I:1280:VAL:O    | 3:I:1294:VAL:HA   | 2.08                     | 0.53              |
| 3:I:1295:GLU:CB   | 3:I:1300:SER:HB3  | 2.37                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1096:ALA:HB1  | 3:I:12:LEU:HD22   | 1.90                     | 0.53              |
| 3:I:1401:GLU:CD   | 3:I:1415:VAL:HG11 | 2.28                     | 0.53              |
| 3:I:9:ARG:HG3     | 3:I:1456:LYS:HG2  | 1.90                     | 0.53              |
| 3:I:182:GLY:HA3   | 3:I:441:ARG:HD3   | 1.89                     | 0.53              |
| 3:I:521:PRO:HB2   | 3:I:524:LEU:CD1   | 2.38                     | 0.53              |
| 3:I:813:LEU:HD12  | 3:I:814:ALA:CA    | 2.38                     | 0.53              |
| 3:I:86:ARG:O      | 3:I:87:ARG:NE     | 2.40                     | 0.53              |
| 2:M:249:LYS:O     | 2:M:251:ASP:N     | 2.41                     | 0.53              |
| 2:M:36:PRO:O      | 2:M:39:ARG:CB     | 2.56                     | 0.53              |
| 2:M:437:ARG:HG2   | 2:M:467:ILE:O     | 2.06                     | 0.53              |
| 2:M:572:ILE:HD11  | 2:M:698:ASP:O     | 2.08                     | 0.53              |
| 3:N:1209:LEU:HD23 | 3:N:1210:SER:N    | 2.24                     | 0.53              |
| 3:N:129:PHE:N     | 3:N:129:PHE:CD1   | 2.77                     | 0.53              |
| 3:N:520:LEU:HD12  | 3:N:521:PRO:CD    | 2.31                     | 0.53              |
| 3:N:788:GLY:O     | 3:N:792:ILE:HG22  | 2.09                     | 0.53              |
| 3:N:87:ARG:HB3    | 3:N:523:ASP:HB2   | 1.89                     | 0.53              |
| 2:M:1086:ARG:NH1  | 3:N:88:TYR:CG     | 2.76                     | 0.53              |
| 7:Y:57:ARG:O      | 7:Y:61:ARG:HD3    | 2.08                     | 0.53              |
| 2:C:170:PRO:HD3   | 2:C:263:ASP:CG    | 2.28                     | 0.53              |
| 2:C:338:GLU:CA    | 2:C:341:THR:HG22  | 2.39                     | 0.53              |
| 2:C:361:MET:HE1   | 3:I:1317:ASP:HB2  | 1.91                     | 0.53              |
| 3:D:1008:PHE:HE2  | 3:D:1035:ILE:HG21 | 1.74                     | 0.53              |
| 3:D:1380:GLU:HB2  | 3:D:1420:LEU:HD11 | 1.89                     | 0.53              |
| 3:D:804:LEU:CB    | 3:D:830:ALA:O     | 2.56                     | 0.53              |
| 2:H:300:ASP:OD2   | 2:H:303:PHE:HB2   | 2.09                     | 0.53              |
| 2:H:571:LEU:HD11  | 2:H:700:TYR:CA    | 2.37                     | 0.53              |
| 2:H:834:GLN:HE22  | 3:I:724:GLN:CG    | 2.14                     | 0.53              |
| 3:I:1105:ILE:N    | 3:I:1105:ILE:HD12 | 2.22                     | 0.53              |
| 2:M:1081:VAL:HG13 | 2:M:1085:PHE:CB   | 2.38                     | 0.53              |
| 2:M:122:THR:HG22  | 2:M:123:GLU:N     | 2.23                     | 0.53              |
| 2:M:333:ILE:CD1   | 2:M:467:ILE:HG13  | 2.38                     | 0.53              |
| 2:M:63:GLY:HA2    | 2:M:359:MET:CE    | 2.38                     | 0.53              |
| 2:M:577:PRO:HG3   | 2:M:993:PHE:CD1   | 2.43                     | 0.53              |
| 2:M:870:ILE:HD13  | 2:M:870:ILE:N     | 2.24                     | 0.53              |
| 3:N:543:LEU:CD2   | 3:N:580:ALA:HB1   | 2.37                     | 0.53              |
| 4:O:30:LEU:O      | 4:O:35:PHE:HA     | 2.08                     | 0.53              |
| 1:A:32:PHE:HZ     | 1:B:47:SER:HB2    | 1.73                     | 0.53              |
| 1:B:38:ASN:CB     | 1:B:39:PRO:HD3    | 2.37                     | 0.53              |
| 2:C:292:ARG:CB    | 2:C:299:LYS:HE2   | 2.37                     | 0.53              |
| 2:C:378:LEU:O     | 2:C:381:ALA:HB3   | 2.08                     | 0.53              |
| 3:D:1111:ASP:CG   | 3:D:1203:LYS:HD2  | 2.29                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:42:ARG:CG     | 1:G:42:ARG:NH1    | 2.68                     | 0.53              |
| 3:I:547:LEU:HD11  | 3:I:578:VAL:CG2   | 2.38                     | 0.53              |
| 3:I:606:ILE:HD11  | 3:I:613:ARG:NE    | 2.22                     | 0.53              |
| 3:I:87:ARG:HH11   | 3:I:87:ARG:HA     | 1.73                     | 0.53              |
| 1:L:16:GLN:HA     | 1:L:16:GLN:HE21   | 1.73                     | 0.53              |
| 2:M:1082:PRO:HG2  | 3:N:1469:GLY:HA3  | 1.89                     | 0.53              |
| 2:M:278:GLU:HA    | 2:M:283:ILE:O     | 2.08                     | 0.53              |
| 3:N:1007:VAL:HG11 | 3:N:1039:CYS:CB   | 2.36                     | 0.53              |
| 3:N:135:LEU:HD23  | 3:N:136:ASP:N     | 2.24                     | 0.53              |
| 3:N:199:LEU:HD23  | 3:N:200:ASP:O     | 2.08                     | 0.53              |
| 3:N:432:TYR:HB3   | 3:N:450:TYR:CG    | 2.43                     | 0.53              |
| 3:N:996:TRP:HE3   | 3:N:999:THR:HG21  | 1.70                     | 0.53              |
| 5:P:20:DG:C2      | 5:P:21:DC:N4      | 2.77                     | 0.53              |
| 7:X:90:GLU:O      | 7:X:152:VAL:HB    | 2.08                     | 0.53              |
| 1:B:23:PHE:O      | 1:B:196:THR:HA    | 2.09                     | 0.53              |
| 2:C:269:LEU:HG    | 2:C:287:GLY:O     | 2.09                     | 0.53              |
| 2:C:264:PRO:HB3   | 2:C:289:THR:HG21  | 1.90                     | 0.53              |
| 2:C:455:LEU:HD12  | 2:C:456:ALA:O     | 2.09                     | 0.53              |
| 2:C:625:LEU:HB3   | 2:C:639:GLN:HB2   | 1.90                     | 0.53              |
| 2:C:603:VAL:HG23  | 2:C:647:GLN:O     | 2.09                     | 0.53              |
| 2:C:654:LEU:CD1   | 2:C:663:ASN:C     | 2.77                     | 0.53              |
| 2:C:810:ASP:HB3   | 2:C:813:VAL:HG12  | 1.90                     | 0.53              |
| 3:D:1018:ASN:O    | 3:D:1022:VAL:HG23 | 2.08                     | 0.53              |
| 3:D:1066:THR:HG23 | 3:D:1069:GLU:H    | 1.74                     | 0.53              |
| 3:D:1144:LEU:HD21 | 3:D:1186:VAL:HG11 | 1.90                     | 0.53              |
| 3:D:1146:GLY:CA   | 3:D:1207:TYR:HB3  | 2.36                     | 0.53              |
| 3:D:1208:ASP:O    | 3:D:1215:VAL:CG2  | 2.57                     | 0.53              |
| 3:D:664:LYS:O     | 3:D:666:ILE:N     | 2.42                     | 0.53              |
| 3:D:813:LEU:HD12  | 3:D:814:ALA:CA    | 2.38                     | 0.53              |
| 2:H:212:GLY:O     | 2:H:214:TYR:N     | 2.42                     | 0.53              |
| 2:H:300:ASP:CG    | 2:H:300:ASP:O     | 2.44                     | 0.53              |
| 2:H:722:ILE:HD13  | 2:H:722:ILE:O     | 2.08                     | 0.53              |
| 2:H:870:ILE:HD13  | 2:H:870:ILE:N     | 2.24                     | 0.53              |
| 2:H:997:LEU:O     | 2:H:999:HIS:N     | 2.40                     | 0.53              |
| 2:H:99:GLN:HE21   | 2:H:101:ILE:CD1   | 2.16                     | 0.53              |
| 3:I:143:ASN:OD1   | 3:I:161:LEU:HD21  | 2.08                     | 0.53              |
| 3:I:407:VAL:CG2   | 3:I:408:GLU:H     | 2.11                     | 0.53              |
| 3:I:789:LEU:CD1   | 3:I:934:LEU:HD22  | 2.39                     | 0.53              |
| 3:I:996:TRP:HE3   | 3:I:999:THR:HG21  | 1.70                     | 0.53              |
| 1:L:16:GLN:HA     | 1:L:16:GLN:NE2    | 2.24                     | 0.53              |
| 2:M:438:ILE:HD11  | 2:M:467:ILE:HD12  | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:582:GLY:C     | 2:M:583:LEU:HD12  | 2.29                     | 0.53              |
| 2:M:611:ILE:CD1   | 2:M:625:LEU:HD21  | 2.38                     | 0.53              |
| 2:M:754:ILE:N     | 2:M:754:ILE:CD1   | 2.71                     | 0.53              |
| 2:M:890:LEU:HD21  | 2:M:901:TYR:CD1   | 2.43                     | 0.53              |
| 3:N:14:SER:O      | 3:N:18:ILE:HG12   | 2.09                     | 0.53              |
| 7:X:39:SER:OG     | 7:X:40:SER:N      | 2.40                     | 0.53              |
| 2:C:212:GLY:C     | 2:C:214:TYR:N     | 2.62                     | 0.53              |
| 2:C:284:ARG:HG2   | 2:C:285:LEU:N     | 2.22                     | 0.53              |
| 2:C:717:LEU:HD13  | 2:C:761:PHE:CD2   | 2.44                     | 0.53              |
| 3:D:706:PRO:CG    | 6:Q:16:G:N2       | 2.72                     | 0.53              |
| 2:H:325:ILE:HD12  | 2:H:325:ILE:H     | 1.74                     | 0.53              |
| 2:H:401:LEU:HD13  | 2:H:587:VAL:HG11  | 1.91                     | 0.53              |
| 2:H:592:LEU:HD23  | 2:H:592:LEU:N     | 2.23                     | 0.53              |
| 2:H:850:ALA:HA    | 3:I:632:VAL:HG13  | 1.90                     | 0.53              |
| 2:H:95:TYR:HD2    | 2:H:114:PHE:HB3   | 1.74                     | 0.53              |
| 2:H:975:TYR:HA    | 2:H:982:PRO:HA    | 1.91                     | 0.53              |
| 3:I:1283:ILE:HG22 | 3:I:1284:GLU:H    | 1.74                     | 0.53              |
| 3:I:457:GLY:O     | 3:I:460:ALA:N     | 2.39                     | 0.53              |
| 3:I:39:PRO:CB     | 3:I:45:PHE:HB2    | 2.38                     | 0.53              |
| 3:I:704:ARG:HB2   | 3:I:736:PHE:HB3   | 1.91                     | 0.53              |
| 1:L:141:GLU:OE2   | 1:L:161:ARG:HD3   | 2.09                     | 0.53              |
| 2:M:836:GLY:CA    | 2:M:1001:VAL:HG21 | 2.31                     | 0.53              |
| 2:M:139:GLN:HE22  | 2:M:415:PRO:HD3   | 1.74                     | 0.53              |
| 2:M:304:LEU:HG    | 2:M:305:PRO:CD    | 2.38                     | 0.53              |
| 2:M:893:ALA:HB2   | 2:M:918:LEU:HD12  | 1.90                     | 0.53              |
| 3:N:1465:ASN:HD21 | 3:N:1470:ARG:CZ   | 2.21                     | 0.53              |
| 3:N:115:LEU:CD1   | 3:N:502:PHE:CE1   | 2.92                     | 0.53              |
| 2:M:1030:GLN:CD   | 3:N:628:ARG:HD3   | 2.27                     | 0.53              |
| 3:N:835:SER:H     | 3:N:838:ARG:CD    | 2.21                     | 0.53              |
| 2:M:1061:GLU:OE1  | 3:N:84:ILE:CD1    | 2.56                     | 0.53              |
| 7:X:120:SER:HB2   | 7:X:123:SER:HB2   | 1.91                     | 0.53              |
| 7:Y:57:ARG:CB     | 7:Y:57:ARG:HH21   | 2.21                     | 0.53              |
| 2:C:140:ILE:HG23  | 2:C:410:ILE:HG21  | 1.90                     | 0.53              |
| 2:C:839:LEU:HD23  | 2:C:839:LEU:N     | 2.24                     | 0.53              |
| 3:D:1101:VAL:CG2  | 3:D:1424:VAL:HG23 | 2.38                     | 0.53              |
| 3:D:1235:GLN:HB3  | 7:X:52:LYS:NZ     | 2.23                     | 0.53              |
| 3:D:1286:THR:CG2  | 3:D:1287:GLU:H    | 2.17                     | 0.53              |
| 3:D:789:LEU:CD1   | 3:D:934:LEU:HD22  | 2.39                     | 0.53              |
| 1:F:25:LEU:CD2    | 1:F:28:LEU:HD11   | 2.38                     | 0.53              |
| 2:H:1014:SER:CB   | 2:H:1021:LEU:HD13 | 2.32                     | 0.53              |
| 2:H:657:ASP:CG    | 2:H:662:GLU:HA    | 2.28                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:794:GLN:CG    | 3:I:1017:PHE:HE2  | 2.21                     | 0.53              |
| 3:I:1275:SER:HB2  | 3:I:1294:VAL:HG21 | 1.90                     | 0.53              |
| 1:L:102:LYS:HZ1   | 1:L:137:ARG:NH1   | 2.07                     | 0.53              |
| 1:L:79:ILE:HG13   | 1:L:80:LEU:N      | 2.23                     | 0.53              |
| 2:M:189:ARG:HE    | 2:M:189:ARG:HA    | 1.72                     | 0.53              |
| 2:M:197:LEU:HD12  | 2:M:207:LEU:HD11  | 1.91                     | 0.53              |
| 2:M:206:THR:HG23  | 2:M:207:LEU:H     | 1.74                     | 0.53              |
| 2:M:274:ARG:CB    | 2:M:285:LEU:HD13  | 2.35                     | 0.53              |
| 2:M:682:TYR:CE1   | 2:M:851:LYS:HD3   | 2.44                     | 0.53              |
| 2:M:6:PHE:CD1     | 2:M:6:PHE:N       | 2.76                     | 0.53              |
| 3:N:1018:ASN:O    | 3:N:1022:VAL:HG23 | 2.08                     | 0.53              |
| 3:N:142:LEU:HD13  | 3:N:144:GLY:C     | 2.28                     | 0.53              |
| 3:N:1487:VAL:CG1  | 3:N:1488:ASP:N    | 2.71                     | 0.53              |
| 3:N:50:PHE:CD1    | 3:N:522:PRO:HG3   | 2.41                     | 0.53              |
| 3:N:102:ILE:CD1   | 3:N:586:ARG:HG3   | 2.39                     | 0.53              |
| 3:N:799:LYS:O     | 3:N:826:PRO:HG2   | 2.09                     | 0.53              |
| 4:O:15:SER:O      | 4:O:18:ARG:HB3    | 2.09                     | 0.53              |
| 4:O:18:ARG:O      | 4:O:22:VAL:HG23   | 2.09                     | 0.53              |
| 7:Y:74:ILE:HD12   | 7:Y:75:LEU:N      | 2.22                     | 0.53              |
| 7:Z:120:SER:O     | 7:Z:123:SER:HB2   | 2.09                     | 0.53              |
| 1:A:91:ASN:HD22   | 1:A:93:SER:HB2    | 1.74                     | 0.53              |
| 1:B:65:PHE:CD1    | 1:B:65:PHE:N      | 2.77                     | 0.53              |
| 2:C:1046:ALA:CB   | 3:D:1476:THR:HB   | 2.39                     | 0.53              |
| 2:C:135:VAL:C     | 2:C:136:ILE:HD12  | 2.29                     | 0.53              |
| 2:C:170:PRO:HD3   | 2:C:263:ASP:OD1   | 2.08                     | 0.53              |
| 2:C:328:LEU:HD13  | 2:C:433:THR:HB    | 1.90                     | 0.53              |
| 2:C:668:LEU:CD1   | 2:C:668:LEU:N     | 2.66                     | 0.53              |
| 1:A:46:SER:HB3    | 2:C:856:GLU:HG2   | 1.89                     | 0.53              |
| 2:C:870:ILE:N     | 2:C:870:ILE:HD13  | 2.24                     | 0.53              |
| 3:D:1098:LEU:HD23 | 3:D:1229:ILE:HB   | 1.90                     | 0.53              |
| 3:D:1434:TRP:CZ3  | 3:D:1457:ASP:HB2  | 2.44                     | 0.53              |
| 3:D:1487:VAL:HG12 | 3:D:1488:ASP:H    | 1.74                     | 0.53              |
| 3:D:1491:THR:O    | 3:D:1494:ALA:HB3  | 2.09                     | 0.53              |
| 1:G:76:VAL:HB     | 3:I:872:ARG:CZ    | 2.36                     | 0.53              |
| 2:H:1004:LYS:HD2  | 3:I:744:GLN:CD    | 2.22                     | 0.53              |
| 2:H:455:LEU:HD12  | 2:H:456:ALA:O     | 2.09                     | 0.53              |
| 2:H:625:LEU:HB3   | 2:H:639:GLN:HB2   | 1.90                     | 0.53              |
| 2:H:654:LEU:CD1   | 2:H:663:ASN:C     | 2.77                     | 0.53              |
| 2:H:859:PRO:HB2   | 2:H:867:VAL:HG21  | 1.91                     | 0.53              |
| 2:H:893:ALA:HB2   | 2:H:918:LEU:HD12  | 1.90                     | 0.53              |
| 2:H:877:PRO:HG3   | 3:I:1023:MET:SD   | 2.48                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1401:GLU:OE2  | 3:I:1415:VAL:HG21 | 2.09                     | 0.53              |
| 3:I:465:LEU:CD1   | 3:I:510:GLU:HA    | 2.36                     | 0.53              |
| 3:I:520:LEU:CD1   | 3:I:521:PRO:HD2   | 2.39                     | 0.53              |
| 3:I:701:LEU:HD12  | 3:I:701:LEU:N     | 2.24                     | 0.53              |
| 3:I:93:ILE:HD11   | 3:I:519:VAL:HG22  | 1.91                     | 0.53              |
| 3:I:1476:THR:CG2  | 4:J:21:VAL:HG22   | 2.35                     | 0.53              |
| 2:M:17:PRO:HB2    | 2:M:20:GLU:HB3    | 1.91                     | 0.53              |
| 2:M:211:LEU:CD2   | 2:M:221:LEU:CD2   | 2.84                     | 0.53              |
| 2:M:374:ASN:O     | 2:M:377:PRO:HD2   | 2.09                     | 0.53              |
| 3:N:1438:ALA:O    | 3:N:1443:THR:HG22 | 2.09                     | 0.53              |
| 3:N:506:GLY:O     | 3:N:507:ASN:C     | 2.46                     | 0.53              |
| 3:N:50:PHE:CE1    | 3:N:522:PRO:HG3   | 2.44                     | 0.53              |
| 1:A:9:PRO:HB3     | 1:A:25:LEU:CD1    | 2.38                     | 0.53              |
| 1:A:36:LEU:C      | 1:A:39:PRO:HD2    | 2.28                     | 0.53              |
| 2:C:1081:VAL:HG11 | 2:C:1111:ILE:HG21 | 1.90                     | 0.53              |
| 2:C:565:GLN:NE2   | 2:C:842:ARG:CG    | 2.68                     | 0.53              |
| 3:D:1197:ARG:HB3  | 3:D:1396:GLU:OE2  | 2.09                     | 0.53              |
| 3:D:1434:TRP:NE1  | 3:D:1435:LEU:HD12 | 2.24                     | 0.53              |
| 3:D:1466:VAL:HG12 | 3:D:1467:ILE:HD13 | 1.91                     | 0.53              |
| 3:D:168:THR:HG22  | 3:D:170:PRO:HD3   | 1.91                     | 0.53              |
| 3:D:479:GLU:O     | 3:D:483:HIS:ND1   | 2.38                     | 0.53              |
| 3:D:787:LEU:HD12  | 3:D:787:LEU:O     | 2.09                     | 0.53              |
| 3:D:827:ILE:HG22  | 3:D:827:ILE:O     | 2.09                     | 0.53              |
| 3:D:804:LEU:HB2   | 3:D:831:GLY:HA2   | 1.90                     | 0.53              |
| 3:D:835:SER:H     | 3:D:838:ARG:CD    | 2.21                     | 0.53              |
| 4:E:48:MET:N      | 4:E:54:LEU:HB2    | 2.24                     | 0.53              |
| 3:D:696:HIS:NE2   | 4:E:54:LEU:HD11   | 2.24                     | 0.53              |
| 2:H:16:PRO:O      | 2:H:18:LEU:HD12   | 2.09                     | 0.53              |
| 3:I:1031:ASN:OD1  | 3:I:1034:GLN:HG3  | 2.08                     | 0.53              |
| 3:I:1087:ARG:HB2  | 3:I:1237:THR:CG2  | 2.39                     | 0.53              |
| 3:I:1312:LEU:HD11 | 3:I:1327:ARG:HH21 | 1.67                     | 0.53              |
| 3:I:1225:ALA:HB2  | 3:I:1370:ILE:HD12 | 1.91                     | 0.53              |
| 3:I:192:ALA:HB1   | 3:I:193:PRO:HD2   | 1.91                     | 0.53              |
| 3:I:639:LEU:N     | 3:I:729:HIS:CD2   | 2.77                     | 0.53              |
| 3:I:980:MET:HB3   | 3:I:982:PHE:HE2   | 1.72                     | 0.53              |
| 2:M:157:ARG:HD3   | 2:M:314:THR:HG1   | 1.69                     | 0.53              |
| 2:M:64:LEU:HB2    | 2:M:359:MET:HG3   | 1.91                     | 0.53              |
| 2:M:139:GLN:HG3   | 2:M:411:SER:O     | 2.08                     | 0.53              |
| 2:M:455:LEU:HD12  | 2:M:456:ALA:O     | 2.09                     | 0.53              |
| 2:M:512:ARG:HG2   | 2:M:523:ILE:HD11  | 1.89                     | 0.53              |
| 2:M:606:VAL:CG2   | 2:M:645:VAL:HG22  | 2.39                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:1033:GLN:OE1 | 3:N:1033:GLN:HA   | 2.08                     | 0.53              |
| 3:N:1288:GLU:HA  | 3:N:1307:LYS:HD3  | 1.90                     | 0.53              |
| 3:N:176:ASP:HB2  | 3:N:389:GLU:HG2   | 1.89                     | 0.53              |
| 3:N:32:ILE:HG12  | 3:N:39:PRO:HA     | 1.91                     | 0.53              |
| 3:N:510:GLU:HB2  | 3:N:511:TRP:CZ3   | 2.43                     | 0.53              |
| 2:M:1052:MET:SD  | 3:N:623:VAL:HG21  | 2.49                     | 0.53              |
| 2:M:1071:ILE:O   | 3:N:659:LYS:HD3   | 2.08                     | 0.53              |
| 3:N:787:LEU:O    | 3:N:787:LEU:HD12  | 2.09                     | 0.53              |
| 3:N:767:HIS:HA   | 3:N:924:MET:SD    | 2.49                     | 0.53              |
| 1:B:73:GLU:OE1   | 1:B:131:THR:N     | 2.43                     | 0.52              |
| 2:C:170:PRO:HD3  | 2:C:263:ASP:CB    | 2.38                     | 0.52              |
| 2:C:500:ASN:HD22 | 2:C:500:ASN:N     | 2.05                     | 0.52              |
| 2:C:516:ARG:HG3  | 3:D:1068:LEU:HD13 | 1.90                     | 0.52              |
| 3:D:15:PRO:O     | 3:D:19:ARG:HG2    | 2.09                     | 0.52              |
| 3:D:484:PRO:HB2  | 3:D:488:ARG:HG3   | 1.91                     | 0.52              |
| 3:D:510:GLU:HB2  | 3:D:511:TRP:CZ3   | 2.43                     | 0.52              |
| 3:D:701:LEU:N    | 3:D:701:LEU:HD12  | 2.24                     | 0.52              |
| 4:E:31:LEU:HB3   | 4:E:35:PHE:CE1    | 2.44                     | 0.52              |
| 1:F:18:ARG:HH22  | 1:F:88:ARG:NH2    | 2.06                     | 0.52              |
| 1:F:91:ASN:HD22  | 1:F:93:SER:HB2    | 1.74                     | 0.52              |
| 1:G:190:THR:N    | 3:I:722:GLU:OE1   | 2.39                     | 0.52              |
| 2:H:1047:HIS:HA  | 2:H:1050:GLN:HB3  | 1.91                     | 0.52              |
| 2:H:92:ALA:N     | 2:H:118:ILE:O     | 2.38                     | 0.52              |
| 2:H:516:ARG:HH11 | 2:H:521:PRO:HB3   | 1.74                     | 0.52              |
| 2:H:582:GLY:C    | 2:H:583:LEU:HD12  | 2.28                     | 0.52              |
| 2:H:579:VAL:CG1  | 2:H:887:GLU:HG3   | 2.37                     | 0.52              |
| 3:I:1256:LEU:CG  | 3:I:1260:ILE:HD11 | 2.34                     | 0.52              |
| 3:I:134:VAL:CG2  | 3:I:460:ALA:CB    | 2.84                     | 0.52              |
| 1:K:156:HIS:CD2  | 1:K:158:ILE:HD12  | 2.44                     | 0.52              |
| 2:M:191:PHE:CZ   | 2:M:196:LEU:HD12  | 2.43                     | 0.52              |
| 3:N:1084:THR:HB  | 3:N:1087:ARG:NH1  | 2.24                     | 0.52              |
| 3:N:356:PRO:CB   | 3:N:441:ARG:HA    | 2.39                     | 0.52              |
| 3:N:36:THR:C     | 3:N:38:LYS:N      | 2.59                     | 0.52              |
| 4:O:49:GLN:N     | 4:O:49:GLN:CD     | 2.61                     | 0.52              |
| 2:C:879:ARG:NE   | 7:X:42:ASP:OD1    | 2.40                     | 0.52              |
| 1:A:208:LEU:HD23 | 1:A:212:ASN:OD1   | 2.09                     | 0.52              |
| 1:B:133:GLU:HG3  | 1:B:134:GLU:N     | 2.19                     | 0.52              |
| 1:B:74:ASP:O     | 1:B:78:ILE:HG13   | 2.10                     | 0.52              |
| 2:C:54:ILE:HD11  | 2:C:356:ARG:HG3   | 1.90                     | 0.52              |
| 2:C:893:ALA:HB2  | 2:C:918:LEU:HD12  | 1.91                     | 0.52              |
| 3:D:794:GLN:HG2  | 3:D:1017:PHE:HE2  | 1.73                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1256:LEU:O    | 3:D:1259:VAL:N    | 2.42                     | 0.52              |
| 3:D:1484:THR:HG21 | 4:E:22:VAL:HG22   | 1.90                     | 0.52              |
| 3:D:50:PHE:CD1    | 3:D:522:PRO:CG    | 2.92                     | 0.52              |
| 3:D:638:LYS:HD3   | 3:D:932:ASP:CG    | 2.30                     | 0.52              |
| 3:D:729:HIS:CG    | 3:D:730:PRO:HD2   | 2.44                     | 0.52              |
| 3:D:918:ALA:HB3   | 3:D:927:THR:HG23  | 1.91                     | 0.52              |
| 1:F:56:VAL:CG1    | 1:F:142:VAL:HG12  | 2.27                     | 0.52              |
| 1:F:208:LEU:HD23  | 1:F:212:ASN:OD1   | 2.09                     | 0.52              |
| 2:H:352:ALA:HA    | 2:H:355:VAL:CG1   | 2.40                     | 0.52              |
| 2:H:839:LEU:N     | 2:H:839:LEU:HD23  | 2.25                     | 0.52              |
| 4:J:19:LEU:O      | 4:J:23:VAL:HG23   | 2.09                     | 0.52              |
| 2:M:295:ASP:C     | 2:M:297:GLU:H     | 2.13                     | 0.52              |
| 2:M:478:VAL:HA    | 2:M:506:ASN:O     | 2.09                     | 0.52              |
| 3:N:10:ILE:HG13   | 3:N:1434:TRP:CZ2  | 2.44                     | 0.52              |
| 3:N:1197:ARG:HB3  | 3:N:1396:GLU:OE2  | 2.09                     | 0.52              |
| 3:N:141:ILE:HD13  | 3:N:142:LEU:CA    | 2.39                     | 0.52              |
| 3:N:729:HIS:CG    | 3:N:730:PRO:HD2   | 2.44                     | 0.52              |
| 1:A:156:HIS:CD2   | 1:A:158:ILE:HD12  | 2.44                     | 0.52              |
| 1:B:79:ILE:HD12   | 1:B:83:LYS:CE     | 2.39                     | 0.52              |
| 2:C:975:TYR:HA    | 2:C:982:PRO:HA    | 1.91                     | 0.52              |
| 3:D:1352:ILE:HG21 | 3:D:1368:ILE:HD12 | 1.91                     | 0.52              |
| 3:D:162:ARG:CG    | 3:D:452:ILE:HG13  | 2.31                     | 0.52              |
| 3:D:553:ARG:HH12  | 3:D:573:MET:HE2   | 1.75                     | 0.52              |
| 3:D:809:PRO:CB    | 3:D:812:ALA:HB2   | 2.25                     | 0.52              |
| 4:E:19:LEU:HD12   | 4:E:23:VAL:HG23   | 1.90                     | 0.52              |
| 1:G:112:ARG:HG3   | 1:G:125:PRO:HA    | 1.92                     | 0.52              |
| 2:H:1049:LEU:O    | 2:H:1053:LEU:HG   | 2.09                     | 0.52              |
| 2:H:182:VAL:CB    | 2:H:193:LEU:HD22  | 2.38                     | 0.52              |
| 3:I:1026:SER:C    | 3:I:1028:ALA:N    | 2.63                     | 0.52              |
| 3:I:1197:ARG:HB3  | 3:I:1396:GLU:OE2  | 2.09                     | 0.52              |
| 3:I:1272:ALA:CA   | 3:I:1326:THR:HB   | 2.39                     | 0.52              |
| 3:I:1442:ASN:O    | 3:I:1446:VAL:HG23 | 2.09                     | 0.52              |
| 3:I:617:ASN:ND2   | 3:I:1467:ILE:O    | 2.42                     | 0.52              |
| 3:I:525:ARG:HD3   | 3:I:525:ARG:N     | 2.23                     | 0.52              |
| 3:I:664:LYS:O     | 3:I:666:ILE:N     | 2.42                     | 0.52              |
| 1:K:124:ASN:ND2   | 1:K:127:LEU:HD22  | 2.23                     | 0.52              |
| 1:K:208:LEU:HD23  | 1:K:212:ASN:OD1   | 2.08                     | 0.52              |
| 2:M:113:VAL:HG11  | 2:M:373:VAL:HB    | 1.91                     | 0.52              |
| 2:M:471:TYR:CE1   | 2:M:496:ILE:HG12  | 2.44                     | 0.52              |
| 2:M:611:ILE:CG1   | 2:M:625:LEU:HD21  | 2.39                     | 0.52              |
| 2:M:654:LEU:CD1   | 2:M:663:ASN:C     | 2.77                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:728:HIS:O     | 2:M:729:LEU:CD2   | 2.57                     | 0.52              |
| 2:M:975:TYR:HA    | 2:M:982:PRO:HA    | 1.91                     | 0.52              |
| 2:M:98:LEU:N      | 2:M:98:LEU:CD1    | 2.72                     | 0.52              |
| 2:M:398:THR:HG21  | 2:M:998:TYR:HB2   | 1.91                     | 0.52              |
| 2:M:906:PHE:CE1   | 3:N:1067:VAL:HG13 | 2.44                     | 0.52              |
| 3:N:107:ASP:O     | 3:N:108:VAL:C     | 2.46                     | 0.52              |
| 3:N:150:ARG:HB2   | 3:N:150:ARG:HH11  | 1.74                     | 0.52              |
| 3:N:152:LEU:O     | 3:N:152:LEU:HD23  | 2.09                     | 0.52              |
| 3:N:99:ALA:HA     | 3:N:575:GLN:NE2   | 2.23                     | 0.52              |
| 3:N:632:VAL:CG2   | 3:N:725:SER:HB2   | 2.40                     | 0.52              |
| 3:N:87:ARG:HD2    | 3:N:88:TYR:HE2    | 1.74                     | 0.52              |
| 3:N:1481:VAL:HG22 | 4:O:18:ARG:NH2    | 2.24                     | 0.52              |
| 7:Y:75:LEU:HD12   | 7:Y:75:LEU:N      | 2.24                     | 0.52              |
| 7:Z:85:LEU:HD21   | 7:Z:121:ASP:HB2   | 1.90                     | 0.52              |
| 2:C:1050:GLN:CD   | 2:C:1079:PRO:HG2  | 2.29                     | 0.52              |
| 2:C:602:GLU:HG3   | 2:C:603:VAL:H     | 1.75                     | 0.52              |
| 2:C:687:ALA:HB1   | 2:C:850:ALA:HB2   | 1.90                     | 0.52              |
| 2:C:564:MET:HE2   | 2:C:846:LYS:CD    | 2.38                     | 0.52              |
| 3:D:704:ARG:HB2   | 3:D:736:PHE:HB3   | 1.91                     | 0.52              |
| 1:F:124:ASN:ND2   | 1:F:127:LEU:HD22  | 2.23                     | 0.52              |
| 1:F:91:ASN:ND2    | 1:F:93:SER:H      | 2.07                     | 0.52              |
| 1:G:16:GLN:HA     | 1:G:16:GLN:NE2    | 2.24                     | 0.52              |
| 3:I:1101:VAL:CG2  | 3:I:1424:VAL:HG23 | 2.39                     | 0.52              |
| 3:I:1109:GLU:HG2  | 3:I:1201:CYS:CB   | 2.39                     | 0.52              |
| 3:I:1352:ILE:HG21 | 3:I:1368:ILE:HD12 | 1.91                     | 0.52              |
| 3:I:151:GLN:C     | 3:I:152:LEU:HD23  | 2.30                     | 0.52              |
| 3:I:15:PRO:O      | 3:I:19:ARG:HG2    | 2.09                     | 0.52              |
| 3:I:800:LYS:HE2   | 3:I:804:LEU:HD22  | 1.91                     | 0.52              |
| 3:I:853:VAL:HG13  | 3:I:858:VAL:O     | 2.10                     | 0.52              |
| 1:L:73:GLU:OE1    | 1:L:130:ALA:HA    | 2.10                     | 0.52              |
| 2:M:184:MET:HB2   | 2:M:193:LEU:CD2   | 2.39                     | 0.52              |
| 2:M:376:ARG:CB    | 2:M:377:PRO:HD3   | 2.40                     | 0.52              |
| 2:M:461:VAL:HG13  | 2:M:465:GLY:O     | 2.09                     | 0.52              |
| 2:M:585:GLU:O     | 2:M:588:VAL:HG22  | 2.10                     | 0.52              |
| 2:M:616:GLU:OE1   | 2:M:616:GLU:HA    | 2.09                     | 0.52              |
| 2:M:839:LEU:N     | 2:M:839:LEU:HD23  | 2.25                     | 0.52              |
| 3:N:827:ILE:HG22  | 3:N:827:ILE:O     | 2.09                     | 0.52              |
| 3:N:918:ALA:HB3   | 3:N:927:THR:HG23  | 1.91                     | 0.52              |
| 3:N:789:LEU:CD1   | 3:N:934:LEU:HD22  | 2.39                     | 0.52              |
| 3:D:1434:TRP:CZ3  | 3:D:1457:ASP:N    | 2.78                     | 0.52              |
| 1:F:40:LEU:HA     | 1:F:43:ILE:HD12   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:109:VAL:CG2   | 1:G:132:LEU:HD13  | 2.40                     | 0.52              |
| 1:G:161:ARG:HB2   | 1:G:164:ALA:HB2   | 1.92                     | 0.52              |
| 1:F:13:VAL:O      | 1:G:230:ALA:HA    | 2.09                     | 0.52              |
| 2:H:172:ILE:N     | 2:H:172:ILE:CD1   | 2.72                     | 0.52              |
| 2:H:212:GLY:C     | 2:H:214:TYR:N     | 2.63                     | 0.52              |
| 2:H:249:LYS:O     | 2:H:251:ASP:N     | 2.43                     | 0.52              |
| 2:H:469:THR:HG23  | 2:H:470:PRO:CD    | 2.37                     | 0.52              |
| 2:H:524:VAL:HG12  | 2:H:525:SER:H     | 1.70                     | 0.52              |
| 3:I:957:PRO:CG    | 3:I:1007:VAL:HG22 | 2.39                     | 0.52              |
| 3:I:1018:ASN:O    | 3:I:1022:VAL:HG23 | 2.08                     | 0.52              |
| 3:I:104:PHE:O     | 3:I:112:ILE:HG22  | 2.10                     | 0.52              |
| 3:I:1099:VAL:O    | 3:I:1103:HIS:HB3  | 2.08                     | 0.52              |
| 3:I:923:GLY:O     | 3:I:927:THR:OG1   | 2.28                     | 0.52              |
| 3:I:729:HIS:HE2   | 3:I:935:LYS:HD3   | 1.73                     | 0.52              |
| 1:K:91:ASN:ND2    | 1:K:93:SER:H      | 2.07                     | 0.52              |
| 2:M:212:GLY:C     | 2:M:214:TYR:N     | 2.63                     | 0.52              |
| 2:M:21:ILE:HD12   | 2:M:21:ILE:N      | 2.14                     | 0.52              |
| 2:M:254:VAL:HA    | 2:M:257:VAL:CG2   | 2.39                     | 0.52              |
| 2:M:258:TYR:CZ    | 2:M:290:LEU:HD11  | 2.44                     | 0.52              |
| 3:N:1401:GLU:OE2  | 3:N:1415:VAL:HG21 | 2.09                     | 0.52              |
| 3:N:639:LEU:N     | 3:N:729:HIS:CD2   | 2.78                     | 0.52              |
| 3:N:704:ARG:HB2   | 3:N:736:PHE:HB3   | 1.91                     | 0.52              |
| 5:T:19:DC:O2      | 6:U:12:G:O6       | 2.28                     | 0.52              |
| 3:I:997:THR:CG2   | 7:Y:61:ARG:HH12   | 2.22                     | 0.52              |
| 1:A:74:ASP:OD1    | 1:A:77:GLU:HB2    | 2.09                     | 0.52              |
| 2:C:170:PRO:HG2   | 2:C:258:TYR:HD1   | 1.66                     | 0.52              |
| 3:D:1173:LEU:HD12 | 3:D:1176:LYS:NZ   | 2.24                     | 0.52              |
| 3:D:14:SER:O      | 3:D:18:ILE:HG12   | 2.09                     | 0.52              |
| 3:D:639:LEU:N     | 3:D:729:HIS:CD2   | 2.78                     | 0.52              |
| 1:F:85:LEU:HA     | 1:F:124:ASN:ND2   | 2.25                     | 0.52              |
| 2:H:115:LEU:HA    | 2:H:375:SER:CB    | 2.38                     | 0.52              |
| 2:H:139:GLN:NE2   | 2:H:414:GLY:HA3   | 2.24                     | 0.52              |
| 2:H:439:CYS:HB2   | 2:H:541:SER:HB2   | 1.92                     | 0.52              |
| 3:I:1031:ASN:HB3  | 3:I:1034:GLN:OE1  | 2.09                     | 0.52              |
| 3:I:1292:VAL:HG23 | 3:I:1305:LEU:HG   | 1.92                     | 0.52              |
| 3:I:1295:GLU:OE2  | 3:I:1295:GLU:N    | 2.41                     | 0.52              |
| 2:H:834:GLN:NE2   | 3:I:724:GLN:HG3   | 2.15                     | 0.52              |
| 3:I:729:HIS:CG    | 3:I:730:PRO:HD2   | 2.44                     | 0.52              |
| 2:H:679:PHE:C     | 3:I:943:THR:HG22  | 2.29                     | 0.52              |
| 1:K:31:GLY:O      | 1:K:34:VAL:HG13   | 2.10                     | 0.52              |
| 2:M:516:ARG:NE    | 3:N:1068:LEU:HD13 | 2.22                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:668:LEU:H     | 2:M:668:LEU:HD12  | 1.73                     | 0.52              |
| 1:K:38:ASN:HB2    | 2:M:980:GLY:HA3   | 1.92                     | 0.52              |
| 3:N:1173:LEU:HD12 | 3:N:1176:LYS:NZ   | 2.25                     | 0.52              |
| 3:N:1150:ALA:HB3  | 3:N:1187:PRO:HB2  | 1.92                     | 0.52              |
| 3:N:1272:ALA:CA   | 3:N:1326:THR:HB   | 2.39                     | 0.52              |
| 1:A:104:GLU:OE1   | 1:A:137:ARG:HG2   | 2.09                     | 0.52              |
| 1:A:58:ILE:HG21   | 1:A:68:ILE:CD1    | 2.40                     | 0.52              |
| 1:B:16:GLN:NE2    | 1:B:16:GLN:HA     | 2.24                     | 0.52              |
| 1:B:176:ARG:HG3   | 1:B:200:TRP:CE3   | 2.44                     | 0.52              |
| 2:C:182:VAL:HG11  | 2:C:193:LEU:HB2   | 1.91                     | 0.52              |
| 2:C:202:TYR:CZ    | 2:C:304:LEU:HD22  | 2.43                     | 0.52              |
| 2:C:336:VAL:HA    | 2:C:339:LEU:HD12  | 1.91                     | 0.52              |
| 2:C:516:ARG:HH11  | 2:C:521:PRO:HB3   | 1.74                     | 0.52              |
| 2:C:906:PHE:CE1   | 3:D:1067:VAL:HA   | 2.45                     | 0.52              |
| 2:C:958:THR:HG23  | 2:C:961:GLU:HG2   | 1.89                     | 0.52              |
| 3:D:11:ALA:HB1    | 3:D:507:ASN:ND2   | 2.25                     | 0.52              |
| 3:D:123:LEU:O     | 3:D:126:VAL:HB    | 2.09                     | 0.52              |
| 3:D:1272:ALA:CA   | 3:D:1326:THR:HB   | 2.39                     | 0.52              |
| 3:D:1225:ALA:HB2  | 3:D:1370:ILE:HD12 | 1.91                     | 0.52              |
| 3:D:166:GLN:HB2   | 2:H:210:GLU:OE2   | 2.10                     | 0.52              |
| 3:D:957:PRO:HG2   | 3:D:1007:VAL:CG2  | 2.40                     | 0.52              |
| 1:F:20:TYR:HE2    | 1:F:198:ARG:HB2   | 1.75                     | 0.52              |
| 2:H:170:PRO:CD    | 2:H:263:ASP:CB    | 2.74                     | 0.52              |
| 2:H:224:GLU:HB3   | 2:H:228:ALA:CB    | 2.39                     | 0.52              |
| 2:H:437:ARG:CG    | 2:H:467:ILE:HG22  | 2.40                     | 0.52              |
| 3:I:1066:THR:HG23 | 3:I:1069:GLU:H    | 1.73                     | 0.52              |
| 3:I:1149:LEU:HG   | 3:I:1166:LEU:CD2  | 2.39                     | 0.52              |
| 3:I:1112:CYS:HB3  | 3:I:1201:CYS:SG   | 2.49                     | 0.52              |
| 3:I:496:LEU:HD12  | 3:I:496:LEU:O     | 2.10                     | 0.52              |
| 3:I:996:TRP:HA    | 3:I:999:THR:CG2   | 2.40                     | 0.52              |
| 2:M:1083:GLU:HG3  | 3:N:87:ARG:NH1    | 2.25                     | 0.52              |
| 2:M:1092:LEU:CD1  | 2:M:1099:VAL:HG21 | 2.14                     | 0.52              |
| 2:M:139:GLN:HE22  | 2:M:415:PRO:CD    | 2.22                     | 0.52              |
| 2:M:111:ASP:OD2   | 2:M:369:PRO:HG2   | 2.06                     | 0.52              |
| 2:M:439:CYS:HB2   | 2:M:541:SER:HB2   | 1.91                     | 0.52              |
| 2:M:553:ASP:OD2   | 2:M:883:GLY:N     | 2.40                     | 0.52              |
| 2:M:75:GLU:O      | 2:M:93:PRO:HD3    | 2.10                     | 0.52              |
| 3:N:794:GLN:HG2   | 3:N:1017:PHE:HE2  | 1.73                     | 0.52              |
| 3:N:1326:THR:CG2  | 3:N:1327:ARG:N    | 2.71                     | 0.52              |
| 3:N:15:PRO:O      | 3:N:19:ARG:HG2    | 2.09                     | 0.52              |
| 3:N:215:TYR:CE2   | 3:N:343:LYS:HB2   | 2.44                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:371:ILE:HG13 | 3:N:372:ASP:N     | 2.24                     | 0.52              |
| 3:N:683:ILE:HG21 | 3:N:688:TRP:CE2   | 2.45                     | 0.52              |
| 3:N:701:LEU:N    | 3:N:701:LEU:HD12  | 2.24                     | 0.52              |
| 3:N:826:PRO:HD2  | 3:N:829:VAL:CG2   | 2.40                     | 0.52              |
| 4:O:59:ASN:ND2   | 4:O:62:THR:OG1    | 2.43                     | 0.52              |
| 6:U:15:G:O2'     | 6:U:16:G:H5'      | 2.10                     | 0.52              |
| 7:Z:102:VAL:CG1  | 7:Z:103:GLN:N     | 2.73                     | 0.52              |
| 1:A:40:LEU:HA    | 1:A:43:ILE:HD12   | 1.92                     | 0.52              |
| 1:B:80:LEU:HD12  | 1:B:83:LYS:HE3    | 1.90                     | 0.52              |
| 2:C:115:LEU:HA   | 2:C:375:SER:CB    | 2.39                     | 0.52              |
| 2:C:154:ARG:NH2  | 2:C:178:PRO:HD3   | 2.24                     | 0.52              |
| 2:C:879:ARG:CZ   | 7:X:42:ASP:HB2    | 2.39                     | 0.52              |
| 3:D:116:LEU:CD1  | 3:D:461:ILE:HG23  | 2.40                     | 0.52              |
| 3:D:820:GLU:CB   | 3:D:836:VAL:HG21  | 2.40                     | 0.52              |
| 3:D:853:VAL:HG13 | 3:D:858:VAL:O     | 2.10                     | 0.52              |
| 2:H:1056:LYS:CD  | 3:I:623:VAL:HG13  | 2.38                     | 0.52              |
| 2:H:474:VAL:HG13 | 2:H:474:VAL:O     | 2.10                     | 0.52              |
| 2:H:726:ILE:HG12 | 2:H:734:LEU:HD21  | 1.92                     | 0.52              |
| 3:I:1189:ARG:NH1 | 3:I:1189:ARG:HG3  | 2.25                     | 0.52              |
| 3:I:139:GLY:O    | 3:I:162:ARG:NH2   | 2.34                     | 0.52              |
| 3:I:203:ALA:HA   | 3:I:395:VAL:HA    | 1.92                     | 0.52              |
| 3:I:205:TYR:HA   | 3:I:393:ILE:HA    | 1.92                     | 0.52              |
| 4:J:30:LEU:O     | 4:J:35:PHE:HA     | 2.08                     | 0.52              |
| 1:K:117:VAL:HB   | 1:K:120:VAL:HG13  | 1.92                     | 0.52              |
| 1:K:183:ASP:OD1  | 1:K:183:ASP:N     | 2.30                     | 0.52              |
| 2:M:178:PRO:O    | 2:M:180:GLY:N     | 2.43                     | 0.52              |
| 2:M:657:ASP:CG   | 2:M:663:ASN:H     | 2.13                     | 0.52              |
| 2:M:78:PHE:HB3   | 2:M:79:PRO:CD     | 2.35                     | 0.52              |
| 2:M:430:VAL:HG13 | 3:N:1075:HIS:HD1  | 1.74                     | 0.52              |
| 3:N:111:LYS:HD3  | 3:N:1448:THR:HG22 | 1.91                     | 0.52              |
| 3:N:1189:ARG:NH1 | 3:N:1189:ARG:HG3  | 2.24                     | 0.52              |
| 3:N:191:LEU:HD13 | 3:N:393:ILE:HB    | 1.92                     | 0.52              |
| 7:Y:19:LEU:O     | 7:Y:23:ARG:HG3    | 2.10                     | 0.52              |
| 2:C:249:LYS:O    | 2:C:250:ARG:C     | 2.48                     | 0.52              |
| 2:C:442:GLU:CG   | 2:C:454:SER:HB2   | 2.40                     | 0.52              |
| 3:D:1132:LEU:N   | 3:D:1132:LEU:HD12 | 2.24                     | 0.52              |
| 3:D:781:PRO:HB2  | 3:D:786:ILE:CD1   | 2.40                     | 0.52              |
| 2:H:140:ILE:HD11 | 2:H:412:ALA:CA    | 2.35                     | 0.52              |
| 2:H:186:VAL:HG23 | 2:H:186:VAL:O     | 2.09                     | 0.52              |
| 2:H:290:LEU:HB3  | 2:H:302:VAL:CG1   | 2.24                     | 0.52              |
| 2:H:304:LEU:CD2  | 2:H:305:PRO:HD3   | 2.39                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:H:383:ARG:HH11  | 2:H:383:ARG:CB   | 2.18                     | 0.52              |
| 2:H:657:ASP:CG    | 2:H:663:ASN:H    | 2.14                     | 0.52              |
| 2:H:516:ARG:HG3   | 3:I:1068:LEU:CD1 | 2.40                     | 0.52              |
| 3:I:1146:GLY:CA   | 3:I:1207:TYR:HB2 | 2.40                     | 0.52              |
| 3:I:1173:LEU:HD12 | 3:I:1176:LYS:NZ  | 2.25                     | 0.52              |
| 3:I:787:LEU:HD12  | 3:I:787:LEU:O    | 2.09                     | 0.52              |
| 3:I:918:ALA:HB3   | 3:I:927:THR:HG23 | 1.91                     | 0.52              |
| 1:K:40:LEU:HA     | 1:K:43:ILE:HD12  | 1.91                     | 0.52              |
| 1:L:122:ILE:HD12  | 1:L:122:ILE:N    | 2.25                     | 0.52              |
| 1:L:176:ARG:HG3   | 1:L:200:TRP:CE3  | 2.45                     | 0.52              |
| 2:M:252:LYS:O     | 2:M:255:ALA:N    | 2.39                     | 0.52              |
| 2:M:516:ARG:HH11  | 2:M:521:PRO:HB3  | 1.74                     | 0.52              |
| 2:M:97:ARG:C      | 2:M:98:LEU:HD12  | 2.30                     | 0.52              |
| 3:N:1496:GLU:HA   | 3:N:1499:ARG:CZ  | 2.39                     | 0.52              |
| 3:N:372:ASP:C     | 3:N:374:GLU:N    | 2.63                     | 0.52              |
| 3:N:84:ILE:O      | 3:N:87:ARG:HG3   | 2.10                     | 0.52              |
| 4:O:38:THR:OG1    | 4:O:39:VAL:N     | 2.42                     | 0.52              |
| 1:A:91:ASN:ND2    | 1:A:93:SER:H     | 2.07                     | 0.52              |
| 2:C:1019:GLN:CD   | 3:D:621:LYS:HD2  | 2.30                     | 0.52              |
| 2:C:1043:TYR:CD2  | 3:D:710:ARG:HD2  | 2.45                     | 0.52              |
| 2:C:345:ARG:HA    | 2:C:348:LEU:HB2  | 1.92                     | 0.52              |
| 2:C:601:GLY:HA2   | 2:C:616:GLU:HG2  | 1.92                     | 0.52              |
| 2:C:897:LEU:HD11  | 2:C:917:LEU:O    | 2.10                     | 0.52              |
| 3:D:1168:MET:HA   | 3:D:1168:MET:CE  | 2.38                     | 0.52              |
| 3:D:1109:GLU:HG3  | 3:D:1217:ILE:CD1 | 2.40                     | 0.52              |
| 3:D:50:PHE:CB     | 3:D:522:PRO:HG2  | 2.40                     | 0.52              |
| 3:D:996:TRP:HA    | 3:D:999:THR:CG2  | 2.40                     | 0.52              |
| 1:F:156:HIS:CD2   | 1:F:158:ILE:HD12 | 2.44                     | 0.52              |
| 1:F:20:TYR:HD2    | 1:F:21:GLY:H     | 1.56                     | 0.52              |
| 2:H:1081:VAL:HG13 | 2:H:1085:PHE:CB  | 2.38                     | 0.52              |
| 2:H:165:LEU:HG    | 2:H:166:PRO:HA   | 1.92                     | 0.52              |
| 2:H:359:MET:O     | 2:H:359:MET:SD   | 2.69                     | 0.52              |
| 3:I:1001:GLU:OE2  | 7:Y:25:ARG:NH2   | 2.42                     | 0.52              |
| 3:I:1098:LEU:HD23 | 3:I:1229:ILE:HB  | 1.91                     | 0.52              |
| 3:I:686:GLU:HA    | 3:I:689:ASP:OD2  | 2.10                     | 0.52              |
| 3:I:632:VAL:CG2   | 3:I:725:SER:HB2  | 2.39                     | 0.52              |
| 4:J:9:LEU:HB3     | 4:J:19:LEU:CD2   | 2.40                     | 0.52              |
| 1:L:146:ARG:O     | 1:L:146:ARG:HG3  | 2.10                     | 0.52              |
| 2:M:102:HIS:O     | 2:M:104:ASP:O    | 2.28                     | 0.52              |
| 2:M:21:ILE:CD1    | 2:M:21:ILE:H     | 2.10                     | 0.52              |
| 2:M:157:ARG:CD    | 2:M:314:THR:OG1  | 2.45                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:501:THR:HG22 | 2:M:513:VAL:HG13  | 1.92                     | 0.52              |
| 2:M:84:ARG:NE    | 2:M:133:ASP:OD2   | 2.41                     | 0.52              |
| 3:N:1438:ALA:N   | 3:N:1446:VAL:HG11 | 2.25                     | 0.52              |
| 3:N:1493:LYS:O   | 3:N:1497:GLU:HG3  | 2.09                     | 0.52              |
| 3:N:414:ARG:HB3  | 3:N:450:TYR:CE1   | 2.46                     | 0.52              |
| 3:N:607:LEU:HD23 | 3:N:613:ARG:HB2   | 1.91                     | 0.52              |
| 1:A:189:ARG:NH1  | 1:A:189:ARG:CG    | 2.72                     | 0.51              |
| 2:C:524:VAL:HG13 | 2:C:528:GLU:OE1   | 2.10                     | 0.51              |
| 2:C:997:LEU:C    | 2:C:999:HIS:N     | 2.64                     | 0.51              |
| 3:D:1105:ILE:N   | 3:D:1105:ILE:CD1  | 2.72                     | 0.51              |
| 3:D:1122:LEU:CD1 | 3:D:1122:LEU:N    | 2.73                     | 0.51              |
| 3:D:1189:ARG:HG3 | 3:D:1189:ARG:NH1  | 2.25                     | 0.51              |
| 3:D:133:ILE:CG2  | 3:D:134:VAL:H     | 2.23                     | 0.51              |
| 3:D:623:VAL:HG12 | 3:D:624:ASP:O     | 2.10                     | 0.51              |
| 1:F:99:LEU:HB3   | 1:F:114:PHE:CD2   | 2.45                     | 0.51              |
| 1:F:117:VAL:HB   | 1:F:120:VAL:HG13  | 1.92                     | 0.51              |
| 1:F:12:THR:OG1   | 1:F:24:VAL:HB     | 2.09                     | 0.51              |
| 2:H:351:LEU:HD12 | 2:H:374:ASN:HD21  | 1.74                     | 0.51              |
| 2:H:50:GLU:HG2   | 2:H:51:THR:N      | 2.25                     | 0.51              |
| 1:F:198:ARG:NH2  | 2:H:934:PHE:CD1   | 2.78                     | 0.51              |
| 3:I:1110:ALA:O   | 3:I:1111:ASP:C    | 2.48                     | 0.51              |
| 3:I:1156:LEU:CD1 | 3:I:1176:LYS:HE3  | 2.40                     | 0.51              |
| 3:I:543:LEU:HD21 | 3:I:600:LEU:CB    | 2.38                     | 0.51              |
| 4:J:41:GLU:O     | 4:J:42:PRO:O      | 2.28                     | 0.51              |
| 1:K:58:ILE:HG21  | 1:K:68:ILE:CD1    | 2.40                     | 0.51              |
| 1:L:59:GLU:HG3   | 1:L:60:ASP:N      | 2.21                     | 0.51              |
| 2:M:207:LEU:HD22 | 2:M:221:LEU:CD1   | 2.39                     | 0.51              |
| 2:M:202:TYR:CZ   | 2:M:304:LEU:HD23  | 2.44                     | 0.51              |
| 2:M:861:LEU:HD23 | 2:M:863:ASP:N     | 2.23                     | 0.51              |
| 2:M:859:PRO:HB2  | 2:M:867:VAL:HG21  | 1.91                     | 0.51              |
| 3:N:465:LEU:CD1  | 3:N:510:GLU:HA    | 2.36                     | 0.51              |
| 2:C:278:GLU:HA   | 2:C:283:ILE:O     | 2.10                     | 0.51              |
| 2:C:881:ASN:O    | 2:C:884:GLN:HG3   | 2.11                     | 0.51              |
| 2:C:577:PRO:HG3  | 2:C:993:PHE:CZ    | 2.45                     | 0.51              |
| 3:D:1114:THR:CG2 | 3:D:1114:THR:O    | 2.58                     | 0.51              |
| 3:D:1206:GLY:HA3 | 3:D:1366:LYS:HZ3  | 1.76                     | 0.51              |
| 3:D:632:VAL:CG2  | 3:D:725:SER:HB2   | 2.39                     | 0.51              |
| 3:D:826:PRO:HD2  | 3:D:829:VAL:CG2   | 2.40                     | 0.51              |
| 3:D:950:GLY:O    | 3:D:953:ASP:HB2   | 2.10                     | 0.51              |
| 4:E:47:LYS:O     | 4:E:54:LEU:HD12   | 2.11                     | 0.51              |
| 1:G:176:ARG:HG3  | 1:G:200:TRP:CE3   | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:101:ILE:CD1   | 2:H:108:ILE:HG23  | 2.39                     | 0.51              |
| 2:H:278:GLU:HA    | 2:H:283:ILE:O     | 2.10                     | 0.51              |
| 2:H:435:TYR:O     | 2:H:437:ARG:HD2   | 2.11                     | 0.51              |
| 2:H:524:VAL:HG13  | 2:H:528:GLU:OE1   | 2.10                     | 0.51              |
| 3:I:141:ILE:HD11  | 3:I:448:GLU:OE2   | 2.10                     | 0.51              |
| 3:I:190:GLU:HG2   | 3:I:196:VAL:HG22  | 1.92                     | 0.51              |
| 3:I:87:ARG:CG     | 3:I:523:ASP:CB    | 2.76                     | 0.51              |
| 1:L:23:PHE:O      | 1:L:196:THR:HA    | 2.08                     | 0.51              |
| 2:M:214:TYR:HD1   | 2:M:215:GLY:N     | 2.09                     | 0.51              |
| 2:M:897:LEU:CD2   | 2:M:920:GLN:HG2   | 2.40                     | 0.51              |
| 3:N:1066:THR:HG23 | 3:N:1069:GLU:H    | 1.74                     | 0.51              |
| 2:M:447:ALA:HA    | 3:N:1085:ALA:HB1  | 1.92                     | 0.51              |
| 3:N:1283:ILE:HG22 | 3:N:1284:GLU:H    | 1.75                     | 0.51              |
| 3:N:1492:LEU:HD12 | 3:N:1493:LYS:CE   | 2.40                     | 0.51              |
| 3:N:853:VAL:HG13  | 3:N:858:VAL:O     | 2.10                     | 0.51              |
| 1:B:101:LEU:HD12  | 1:B:114:PHE:N     | 2.25                     | 0.51              |
| 2:C:1030:GLN:HE21 | 3:D:628:ARG:CD    | 2.23                     | 0.51              |
| 2:C:501:THR:CG2   | 2:C:513:VAL:CG1   | 2.88                     | 0.51              |
| 2:C:473:ARG:CA    | 2:C:531:PHE:CD1   | 2.92                     | 0.51              |
| 2:C:654:LEU:HD23  | 2:C:654:LEU:N     | 2.17                     | 0.51              |
| 2:C:668:LEU:HD12  | 2:C:668:LEU:H     | 1.73                     | 0.51              |
| 2:C:679:PHE:HB2   | 2:C:683:ASN:ND2   | 2.23                     | 0.51              |
| 2:C:861:LEU:HA    | 2:C:974:LEU:HD12  | 1.92                     | 0.51              |
| 2:C:98:LEU:HD21   | 2:C:113:VAL:CG2   | 2.39                     | 0.51              |
| 3:D:136:ASP:CG    | 3:D:137:PRO:N     | 2.63                     | 0.51              |
| 3:D:1393:GLN:OE1  | 3:D:1397:LYS:HD2  | 2.10                     | 0.51              |
| 3:D:1401:GLU:OE2  | 3:D:1415:VAL:HG21 | 2.10                     | 0.51              |
| 3:D:923:GLY:O     | 3:D:927:THR:OG1   | 2.28                     | 0.51              |
| 3:D:980:MET:HB3   | 3:D:982:PHE:HE2   | 1.72                     | 0.51              |
| 1:F:58:ILE:HG21   | 1:F:68:ILE:CD1    | 2.40                     | 0.51              |
| 1:G:52:ALA:HB2    | 1:G:170:VAL:O     | 2.10                     | 0.51              |
| 2:H:294:GLU:CG    | 2:H:295:ASP:OD2   | 2.58                     | 0.51              |
| 2:H:328:LEU:N     | 2:H:328:LEU:CD1   | 2.72                     | 0.51              |
| 2:H:997:LEU:HD22  | 2:H:997:LEU:N     | 2.26                     | 0.51              |
| 3:I:705:ALA:CB    | 3:I:706:PRO:CD    | 2.89                     | 0.51              |
| 3:I:820:GLU:CB    | 3:I:836:VAL:HG21  | 2.40                     | 0.51              |
| 4:J:54:LEU:HD23   | 4:J:58:PRO:CG     | 2.41                     | 0.51              |
| 2:M:143:SER:HB3   | 2:M:332:ARG:HB2   | 1.92                     | 0.51              |
| 2:M:317:VAL:O     | 2:M:317:VAL:HG12  | 2.11                     | 0.51              |
| 2:M:435:TYR:O     | 2:M:437:ARG:HD2   | 2.10                     | 0.51              |
| 2:M:685:GLU:OE2   | 3:N:783:ARG:HD2   | 2.09                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1155:VAL:HG12 | 3:N:1177:ALA:CB   | 2.39                     | 0.51              |
| 3:N:165:LYS:HZ2   | 3:N:199:LEU:HB3   | 1.75                     | 0.51              |
| 3:N:204:LEU:O     | 3:N:393:ILE:HG23  | 2.11                     | 0.51              |
| 3:N:496:LEU:O     | 3:N:496:LEU:HD12  | 2.10                     | 0.51              |
| 6:U:14:C:H2'      | 6:U:15:G:H8       | 1.75                     | 0.51              |
| 7:Y:90:GLU:O      | 7:Y:91:LEU:HD23   | 2.10                     | 0.51              |
| 7:Z:128:ALA:HB2   | 7:Z:140:LEU:HD11  | 1.91                     | 0.51              |
| 2:C:186:VAL:O     | 2:C:186:VAL:HG23  | 2.10                     | 0.51              |
| 2:C:249:LYS:O     | 2:C:251:ASP:N     | 2.44                     | 0.51              |
| 2:C:327:HIS:CE1   | 2:C:433:THR:HG21  | 2.45                     | 0.51              |
| 2:C:344:PHE:CZ    | 2:C:378:LEU:HD21  | 2.45                     | 0.51              |
| 3:D:805:GLU:O     | 3:D:809:PRO:HD2   | 2.09                     | 0.51              |
| 1:F:101:LEU:HG    | 1:F:102:LYS:N     | 2.25                     | 0.51              |
| 1:G:48:ILE:CD1    | 1:G:48:ILE:H      | 2.23                     | 0.51              |
| 2:H:15:LEU:O      | 2:H:586:ARG:NH2   | 2.44                     | 0.51              |
| 2:H:31:GLN:OE1    | 2:H:39:ARG:HA     | 2.11                     | 0.51              |
| 2:H:474:VAL:HG11  | 2:H:529:VAL:HG12  | 1.91                     | 0.51              |
| 3:I:1256:LEU:HB3  | 3:I:1257:PRO:CD   | 2.36                     | 0.51              |
| 3:I:1381:VAL:O    | 3:I:1389:LEU:O    | 2.28                     | 0.51              |
| 3:I:614:PHE:CE2   | 3:I:1438:ALA:HB1  | 2.46                     | 0.51              |
| 3:I:477:LEU:HD22  | 3:I:492:ALA:CB    | 2.40                     | 0.51              |
| 3:I:610:LYS:O     | 3:I:615:ARG:HG2   | 2.09                     | 0.51              |
| 3:I:95:LEU:HD21   | 3:I:574:LEU:HD11  | 1.93                     | 0.51              |
| 1:L:110:LYS:HD3   | 1:L:126:ASP:HA    | 1.93                     | 0.51              |
| 2:M:263:ASP:CB    | 2:M:264:PRO:HD3   | 2.26                     | 0.51              |
| 2:M:878:SER:HB3   | 3:N:1029:ARG:CZ   | 2.40                     | 0.51              |
| 2:M:997:LEU:O     | 2:M:999:HIS:N     | 2.41                     | 0.51              |
| 3:N:1225:ALA:HB2  | 3:N:1370:ILE:HD12 | 1.91                     | 0.51              |
| 3:N:1252:ILE:CG1  | 3:N:1253:THR:H    | 2.23                     | 0.51              |
| 3:N:1356:TYR:HD2  | 3:N:1361:VAL:HG11 | 1.76                     | 0.51              |
| 3:N:1352:ILE:HG21 | 3:N:1368:ILE:HD12 | 1.91                     | 0.51              |
| 3:N:1496:GLU:HB2  | 3:N:1499:ARG:NH2  | 2.24                     | 0.51              |
| 3:N:186:VAL:HG12  | 3:N:187:LYS:N     | 2.25                     | 0.51              |
| 3:N:205:TYR:CD1   | 3:N:390:PRO:HG3   | 2.45                     | 0.51              |
| 3:N:918:ALA:CB    | 3:N:927:THR:HG23  | 2.41                     | 0.51              |
| 3:N:996:TRP:HA    | 3:N:999:THR:CG2   | 2.40                     | 0.51              |
| 3:D:1001:GLU:OE2  | 7:X:25:ARG:NH2    | 2.43                     | 0.51              |
| 7:Y:64:SER:O      | 7:Y:68:ILE:HG12   | 2.10                     | 0.51              |
| 3:N:1235:GLN:HG3  | 7:Z:43:TYR:OH     | 2.11                     | 0.51              |
| 1:B:52:ALA:HB1    | 1:B:170:VAL:H     | 1.76                     | 0.51              |
| 2:C:1097:LEU:HD13 | 3:D:1451:ALA:HB1  | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1099:VAL:HG22 | 3:D:10:ILE:CD1    | 2.41                     | 0.51              |
| 2:C:71:TYR:O      | 2:C:71:TYR:CD1    | 2.63                     | 0.51              |
| 3:D:1106:VAL:HG12 | 3:D:1107:VAL:N    | 2.25                     | 0.51              |
| 3:D:1198:TYR:HE1  | 3:D:1432:LYS:HZ1  | 1.58                     | 0.51              |
| 3:D:368:VAL:HB    | 3:D:377:VAL:CB    | 2.40                     | 0.51              |
| 3:D:496:LEU:O     | 3:D:496:LEU:HD12  | 2.10                     | 0.51              |
| 1:F:88:ARG:HH12   | 1:F:90:LEU:HD11   | 1.76                     | 0.51              |
| 1:G:83:LYS:HD3    | 3:I:844:ALA:CB    | 2.39                     | 0.51              |
| 2:H:1088:LEU:CD2  | 2:H:1092:LEU:HD12 | 2.34                     | 0.51              |
| 2:H:295:ASP:C     | 2:H:297:GLU:H     | 2.14                     | 0.51              |
| 2:H:64:LEU:HD13   | 2:H:359:MET:HG2   | 1.92                     | 0.51              |
| 2:H:374:ASN:N     | 2:H:374:ASN:ND2   | 2.59                     | 0.51              |
| 2:H:838:LYS:HD3   | 2:H:846:LYS:HZ3   | 1.75                     | 0.51              |
| 3:I:1465:ASN:ND2  | 3:I:1470:ARG:NH2  | 2.46                     | 0.51              |
| 3:I:26:VAL:HG21   | 3:I:519:VAL:HG21  | 1.93                     | 0.51              |
| 3:I:827:ILE:HG22  | 3:I:827:ILE:O     | 2.10                     | 0.51              |
| 2:M:462:ASP:HB2   | 2:M:468:ARG:HH11  | 1.74                     | 0.51              |
| 2:M:897:LEU:HD11  | 2:M:917:LEU:O     | 2.10                     | 0.51              |
| 3:N:1109:GLU:HG3  | 3:N:1217:ILE:CD1  | 2.41                     | 0.51              |
| 3:N:172:PRO:HD3   | 3:N:195:VAL:HG23  | 1.91                     | 0.51              |
| 3:N:611:GLN:O     | 3:N:611:GLN:HG3   | 2.10                     | 0.51              |
| 3:N:660:LYS:HA    | 3:N:660:LYS:HZ1   | 1.76                     | 0.51              |
| 4:O:18:ARG:HH21   | 4:O:18:ARG:CB     | 2.17                     | 0.51              |
| 4:O:26:ARG:NH1    | 4:O:73:LEU:HD23   | 2.26                     | 0.51              |
| 4:O:27:ALA:HA     | 4:O:30:LEU:HD12   | 1.91                     | 0.51              |
| 4:O:54:LEU:CD2    | 4:O:54:LEU:O      | 2.59                     | 0.51              |
| 2:C:1038:TRP:CE2  | 3:D:1099:VAL:HG11 | 2.46                     | 0.51              |
| 2:C:107:LEU:O     | 2:C:108:ILE:HG13  | 2.10                     | 0.51              |
| 2:C:252:LYS:O     | 2:C:255:ALA:N     | 2.39                     | 0.51              |
| 2:C:274:ARG:O     | 2:C:277:ALA:HB3   | 2.10                     | 0.51              |
| 2:C:859:PRO:HB2   | 2:C:867:VAL:HG21  | 1.91                     | 0.51              |
| 2:C:939:ARG:NE    | 2:C:939:ARG:HA    | 2.14                     | 0.51              |
| 3:D:1437:ALA:HB1  | 3:D:1446:VAL:CG2  | 2.40                     | 0.51              |
| 3:D:1493:LYS:O    | 3:D:1497:GLU:HG2  | 2.09                     | 0.51              |
| 3:D:400:VAL:O     | 3:D:400:VAL:HG13  | 2.09                     | 0.51              |
| 3:D:426:LYS:HE3   | 3:D:427:VAL:HG23  | 1.91                     | 0.51              |
| 2:H:1081:VAL:HG12 | 2:H:1085:PHE:HB3  | 1.93                     | 0.51              |
| 2:H:115:LEU:HA    | 2:H:375:SER:OG    | 2.10                     | 0.51              |
| 2:H:115:LEU:HD12  | 2:H:378:LEU:CD2   | 2.41                     | 0.51              |
| 2:H:376:ARG:CB    | 2:H:377:PRO:HD3   | 2.40                     | 0.51              |
| 2:H:332:ARG:HE    | 2:H:464:LEU:HD12  | 1.76                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:679:PHE:C     | 3:I:943:THR:CG2   | 2.79                     | 0.51              |
| 3:I:593:ASN:HD22  | 3:I:594:PRO:HD2   | 1.76                     | 0.51              |
| 3:I:804:LEU:HB3   | 3:I:830:ALA:O     | 2.10                     | 0.51              |
| 1:K:91:ASN:HD22   | 1:K:93:SER:HB2    | 1.75                     | 0.51              |
| 1:L:34:VAL:HG22   | 1:L:181:VAL:HG21  | 1.92                     | 0.51              |
| 1:L:173:PRO:O     | 1:L:201:THR:CG2   | 2.59                     | 0.51              |
| 1:L:62:LEU:CD1    | 1:L:63:HIS:H      | 2.24                     | 0.51              |
| 2:M:26:TYR:O      | 2:M:29:ALA:HB3    | 2.09                     | 0.51              |
| 2:M:395:LYS:HE2   | 2:M:403:SER:HB2   | 1.92                     | 0.51              |
| 2:M:430:VAL:CG1   | 3:N:1075:HIS:HA   | 2.41                     | 0.51              |
| 2:M:524:VAL:HG13  | 2:M:528:GLU:OE1   | 2.10                     | 0.51              |
| 3:N:133:ILE:HG23  | 3:N:455:ARG:C     | 2.31                     | 0.51              |
| 3:N:148:GLU:HB3   | 3:N:151:GLN:HB3   | 1.93                     | 0.51              |
| 3:N:167:GLU:OE1   | 3:N:198:ARG:HB2   | 2.10                     | 0.51              |
| 3:N:407:VAL:CG2   | 3:N:408:GLU:H     | 2.05                     | 0.51              |
| 3:N:701:LEU:HD11  | 3:N:750:PRO:HG3   | 1.93                     | 0.51              |
| 3:N:758:GLU:CB    | 4:O:20:THR:HG21   | 2.41                     | 0.51              |
| 3:N:793:THR:HG21  | 3:N:906:GLN:HG2   | 1.93                     | 0.51              |
| 4:O:41:GLU:O      | 4:O:42:PRO:O      | 2.28                     | 0.51              |
| 2:C:148:PHE:HE2   | 2:C:160:ALA:HB1   | 1.75                     | 0.51              |
| 3:D:1205:TYR:HE1  | 3:D:1370:ILE:HD11 | 1.76                     | 0.51              |
| 3:D:1408:ILE:H    | 3:D:1408:ILE:HD12 | 1.76                     | 0.51              |
| 3:D:793:THR:HG21  | 3:D:906:GLN:HG2   | 1.93                     | 0.51              |
| 2:H:1095:LEU:HD11 | 2:H:1097:LEU:HD22 | 1.93                     | 0.51              |
| 3:D:207:PHE:CE1   | 2:H:283:ILE:HG13  | 2.42                     | 0.51              |
| 2:H:292:ARG:HD3   | 2:H:294:GLU:OE1   | 2.10                     | 0.51              |
| 2:H:598:GLU:HB2   | 2:H:615:TYR:OH    | 2.10                     | 0.51              |
| 2:H:86:LYS:O      | 2:H:813:VAL:HG23  | 2.10                     | 0.51              |
| 2:H:897:LEU:HD11  | 2:H:917:LEU:O     | 2.10                     | 0.51              |
| 3:I:10:ILE:HG22   | 3:I:10:ILE:O      | 2.11                     | 0.51              |
| 3:I:1108:ARG:N    | 3:I:1108:ARG:CD   | 2.74                     | 0.51              |
| 3:I:1098:LEU:HD21 | 3:I:1229:ILE:CG2  | 2.41                     | 0.51              |
| 3:I:1384:PRO:HG2  | 3:I:1388:ARG:NH2  | 2.26                     | 0.51              |
| 3:I:199:LEU:HD21  | 3:I:397:LYS:HZ1   | 1.76                     | 0.51              |
| 3:I:511:TRP:N     | 3:I:511:TRP:CE3   | 2.79                     | 0.51              |
| 3:I:826:PRO:HD2   | 3:I:829:VAL:CG2   | 2.40                     | 0.51              |
| 1:L:101:LEU:HD12  | 1:L:114:PHE:N     | 2.26                     | 0.51              |
| 2:M:317:VAL:HG11  | 2:M:320:HIS:NE2   | 2.25                     | 0.51              |
| 2:M:606:VAL:HG21  | 2:M:645:VAL:HG22  | 1.92                     | 0.51              |
| 3:N:1448:THR:O    | 3:N:1452:ILE:HD13 | 2.11                     | 0.51              |
| 3:N:50:PHE:HB3    | 3:N:522:PRO:HD2   | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:686:GLU:HA    | 3:N:689:ASP:OD2   | 2.10                     | 0.51              |
| 3:N:820:GLU:CB    | 3:N:836:VAL:HG21  | 2.40                     | 0.51              |
| 3:N:923:GLY:O     | 3:N:927:THR:OG1   | 2.28                     | 0.51              |
| 7:Y:74:ILE:HD12   | 7:Y:75:LEU:H      | 1.75                     | 0.51              |
| 2:C:108:ILE:CG2   | 2:C:109:LYS:N     | 2.72                     | 0.51              |
| 2:C:611:ILE:HD11  | 2:C:625:LEU:HD21  | 1.93                     | 0.51              |
| 2:C:579:VAL:CG1   | 2:C:887:GLU:HG3   | 2.35                     | 0.51              |
| 2:C:897:LEU:CD2   | 2:C:920:GLN:HG2   | 2.41                     | 0.51              |
| 3:D:104:PHE:O     | 3:D:112:ILE:HG22  | 2.10                     | 0.51              |
| 3:D:112:ILE:O     | 3:D:112:ILE:HD13  | 2.11                     | 0.51              |
| 3:D:1264:GLU:CD   | 3:D:1424:VAL:HG13 | 2.31                     | 0.51              |
| 3:D:1281:VAL:HG21 | 3:D:1313:VAL:HG22 | 1.93                     | 0.51              |
| 3:D:17:LYS:CG     | 3:D:21:TRP:HE1    | 2.20                     | 0.51              |
| 3:D:432:TYR:HB3   | 3:D:450:TYR:CB    | 2.40                     | 0.51              |
| 3:D:511:TRP:CE3   | 3:D:511:TRP:N     | 2.79                     | 0.51              |
| 3:D:785:ILE:CD1   | 3:D:939:PHE:CE2   | 2.94                     | 0.51              |
| 4:E:41:GLU:O      | 4:E:42:PRO:O      | 2.29                     | 0.51              |
| 1:F:216:GLU:OE2   | 1:F:219:ARG:NH2   | 2.44                     | 0.51              |
| 1:G:170:VAL:HG11  | 3:I:848:GLU:CD    | 2.31                     | 0.51              |
| 2:H:344:PHE:CD2   | 2:H:378:LEU:HD11  | 2.46                     | 0.51              |
| 2:H:701:THR:CG2   | 2:H:832:LYS:HG2   | 2.41                     | 0.51              |
| 3:I:28:LYS:CG     | 3:I:29:PRO:HD2    | 2.41                     | 0.51              |
| 3:I:547:LEU:HD11  | 3:I:578:VAL:HG23  | 1.93                     | 0.51              |
| 1:K:14:ARG:HH21   | 2:M:934:PHE:HZ    | 1.59                     | 0.51              |
| 1:L:48:ILE:CG2    | 1:L:173:PRO:HD2   | 2.41                     | 0.51              |
| 2:M:1044:GLY:HA3  | 4:O:17:TYR:HE1    | 1.75                     | 0.51              |
| 2:M:101:ILE:HB    | 2:M:108:ILE:CD1   | 2.40                     | 0.51              |
| 2:M:136:ILE:N     | 2:M:136:ILE:CD1   | 2.73                     | 0.51              |
| 2:M:249:LYS:O     | 2:M:250:ARG:C     | 2.49                     | 0.51              |
| 2:M:118:ILE:CG2   | 2:M:382:ILE:HD13  | 2.33                     | 0.51              |
| 2:M:881:ASN:O     | 2:M:884:GLN:HG3   | 2.11                     | 0.51              |
| 2:M:950:LEU:O     | 2:M:950:LEU:HD13  | 2.11                     | 0.51              |
| 3:N:142:LEU:HB3   | 3:N:144:GLY:N     | 2.22                     | 0.51              |
| 3:N:1442:ASN:O    | 3:N:1446:VAL:HG23 | 2.11                     | 0.51              |
| 3:N:145:VAL:HG22  | 3:N:146:PRO:HD2   | 1.93                     | 0.51              |
| 3:N:1496:GLU:HA   | 3:N:1499:ARG:HE   | 1.72                     | 0.51              |
| 3:N:432:TYR:CG    | 3:N:450:TYR:CD2   | 2.90                     | 0.51              |
| 3:N:924:MET:N     | 4:O:7:ASP:OD2     | 2.44                     | 0.51              |
| 3:N:956:ILE:HD13  | 3:N:1062:ARG:NH2  | 2.25                     | 0.51              |
| 3:D:991:GLN:CD    | 7:X:112:VAL:H     | 2.14                     | 0.51              |
| 7:X:85:LEU:HD21   | 7:X:121:ASP:HB2   | 1.93                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:Y:94:PRO:HD3    | 7:Y:148:GLU:O    | 2.10                     | 0.51              |
| 1:B:173:PRO:O     | 1:B:201:THR:CG2  | 2.59                     | 0.51              |
| 2:C:234:ALA:HA    | 2:C:237:ARG:HB2  | 1.93                     | 0.51              |
| 2:C:435:TYR:O     | 2:C:437:ARG:HD2  | 2.10                     | 0.51              |
| 2:C:524:VAL:CG1   | 2:C:525:SER:H    | 2.24                     | 0.51              |
| 2:C:950:LEU:O     | 2:C:950:LEU:HD13 | 2.11                     | 0.51              |
| 2:C:443:THR:HG21  | 3:D:1078:ARG:CD  | 2.41                     | 0.51              |
| 3:D:348:GLN:H     | 3:D:351:MET:HE2  | 1.75                     | 0.51              |
| 4:E:33:HIS:CG     | 4:E:89:MET:HG2   | 2.46                     | 0.51              |
| 4:E:47:LYS:N      | 4:E:54:LEU:HD13  | 2.26                     | 0.51              |
| 1:F:36:LEU:C      | 1:F:39:PRO:HD2   | 2.28                     | 0.51              |
| 1:F:9:PRO:HB2     | 1:G:224:TYR:HB3  | 1.93                     | 0.51              |
| 1:G:101:LEU:HD12  | 1:G:114:PHE:N    | 2.26                     | 0.51              |
| 2:H:197:LEU:HA    | 2:H:200:LEU:HD12 | 1.92                     | 0.51              |
| 2:H:25:SER:OG     | 2:H:335:THR:HB   | 2.10                     | 0.51              |
| 2:H:260:LEU:HA    | 2:H:291:ALA:HB2  | 1.93                     | 0.51              |
| 3:I:205:TYR:CD1   | 3:I:390:PRO:HB3  | 2.44                     | 0.51              |
| 3:I:611:GLN:HE22  | 6:S:9:U:C4'      | 2.00                     | 0.51              |
| 3:I:792:ILE:CD1   | 3:I:881:LEU:HD23 | 2.38                     | 0.51              |
| 1:K:184:THR:HG22  | 1:K:185:ARG:N    | 2.25                     | 0.51              |
| 1:L:70:GLY:O      | 1:L:132:LEU:HA   | 2.11                     | 0.51              |
| 2:M:363:SER:O     | 2:M:367:LEU:HG   | 2.10                     | 0.51              |
| 2:M:433:THR:HG21  | 2:M:488:ALA:HB1  | 1.93                     | 0.51              |
| 3:N:104:PHE:O     | 3:N:112:ILE:HG22 | 2.10                     | 0.51              |
| 3:N:479:GLU:O     | 3:N:483:HIS:ND1  | 2.42                     | 0.51              |
| 3:N:705:ALA:CB    | 3:N:706:PRO:CD   | 2.89                     | 0.51              |
| 1:A:85:LEU:HA     | 1:A:124:ASN:ND2  | 2.25                     | 0.51              |
| 1:A:26:GLU:HB2    | 1:A:27:PRO:HA    | 1.93                     | 0.51              |
| 1:B:132:LEU:HD23  | 1:B:136:GLY:O    | 2.11                     | 0.51              |
| 1:B:54:THR:C      | 1:B:167:VAL:HG23 | 2.32                     | 0.51              |
| 2:C:439:CYS:HB2   | 2:C:541:SER:HB2  | 1.92                     | 0.51              |
| 2:C:861:LEU:HD23  | 2:C:863:ASP:N    | 2.23                     | 0.51              |
| 3:D:1305:LEU:HD11 | 3:D:1326:THR:OG1 | 2.10                     | 0.51              |
| 3:D:356:PRO:HG2   | 3:D:359:ALA:HB2  | 1.93                     | 0.51              |
| 3:D:701:LEU:HD11  | 3:D:750:PRO:HG3  | 1.93                     | 0.51              |
| 1:F:68:ILE:O      | 1:F:71:VAL:HB    | 2.11                     | 0.51              |
| 1:G:109:VAL:HG23  | 1:G:132:LEU:HD13 | 1.91                     | 0.51              |
| 2:H:1096:ALA:HB1  | 3:I:12:LEU:CD2   | 2.41                     | 0.51              |
| 2:H:215:GLY:O     | 2:H:216:GLU:CB   | 2.59                     | 0.51              |
| 2:H:174:LEU:HD12  | 2:H:306:THR:CG2  | 2.41                     | 0.51              |
| 2:H:754:ILE:HG13  | 2:H:791:ARG:HH12 | 1.76                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:1434:TRP:CD1 | 3:I:1435:LEU:N    | 2.79                     | 0.51              |
| 3:I:451:ASP:OD1  | 3:I:452:ILE:N     | 2.43                     | 0.51              |
| 3:I:458:ALA:HB2  | 3:I:575:GLN:HE22  | 1.76                     | 0.51              |
| 3:I:793:THR:HG21 | 3:I:906:GLN:HG2   | 1.93                     | 0.51              |
| 4:J:54:LEU:CD2   | 4:J:58:PRO:HG2    | 2.41                     | 0.51              |
| 1:L:179:PHE:N    | 1:L:179:PHE:CD2   | 2.79                     | 0.51              |
| 2:M:437:ARG:CZ   | 2:M:488:ALA:HA    | 2.39                     | 0.51              |
| 2:M:848:VAL:HG12 | 2:M:849:VAL:N     | 2.26                     | 0.51              |
| 2:M:679:PHE:CE2  | 2:M:853:LEU:HD21  | 2.45                     | 0.51              |
| 2:M:861:LEU:HA   | 2:M:974:LEU:HD12  | 1.93                     | 0.51              |
| 3:N:1205:TYR:HE1 | 3:N:1370:ILE:HD11 | 1.76                     | 0.51              |
| 2:M:987:ILE:CD1  | 3:N:948:THR:HG23  | 2.41                     | 0.51              |
| 3:I:970:LYS:HZ3  | 7:Y:113:LEU:HA    | 1.75                     | 0.51              |
| 3:N:1235:GLN:HG2 | 7:Z:48:LEU:HD12   | 1.92                     | 0.51              |
| 1:A:150:TYR:CD1  | 2:C:696:LYS:HG2   | 2.46                     | 0.50              |
| 1:A:176:ARG:NH1  | 2:C:863:ASP:OD2   | 2.44                     | 0.50              |
| 1:A:33:GLY:O     | 1:A:195:LEU:HD13  | 2.11                     | 0.50              |
| 2:C:158:TYR:CD1  | 2:C:313:LEU:HD21  | 2.46                     | 0.50              |
| 2:C:17:PRO:HB2   | 2:C:20:GLU:HB3    | 1.92                     | 0.50              |
| 2:C:64:LEU:HD22  | 2:C:359:MET:HB2   | 1.93                     | 0.50              |
| 3:D:631:ILE:HG21 | 3:D:745:MET:HG3   | 1.93                     | 0.50              |
| 3:D:705:ALA:CB   | 3:D:706:PRO:CD    | 2.89                     | 0.50              |
| 3:D:795:VAL:CG2  | 3:D:879:ARG:HH12  | 2.24                     | 0.50              |
| 3:D:918:ALA:CB   | 3:D:927:THR:HG23  | 2.41                     | 0.50              |
| 2:H:158:TYR:N    | 2:H:158:TYR:CD1   | 2.78                     | 0.50              |
| 2:H:328:LEU:HD22 | 2:H:433:THR:O     | 2.10                     | 0.50              |
| 2:H:679:PHE:O    | 2:H:680:ASP:C     | 2.49                     | 0.50              |
| 3:I:1146:GLY:HA3 | 3:I:1207:TYR:HB2  | 1.93                     | 0.50              |
| 3:I:1434:TRP:NE1 | 3:I:1435:LEU:HD12 | 2.25                     | 0.50              |
| 3:I:701:LEU:HD11 | 3:I:750:PRO:HG3   | 1.93                     | 0.50              |
| 3:I:918:ALA:CB   | 3:I:927:THR:HG23  | 2.41                     | 0.50              |
| 1:K:128:HIS:HE1  | 1:K:131:THR:CG2   | 2.24                     | 0.50              |
| 1:L:45:LEU:HD11  | 1:L:177:VAL:HG22  | 1.93                     | 0.50              |
| 2:M:129:ILE:CD1  | 2:M:134:ARG:CB    | 2.88                     | 0.50              |
| 2:M:426:ASP:OD1  | 2:M:426:ASP:C     | 2.50                     | 0.50              |
| 3:N:511:TRP:N    | 3:N:511:TRP:CE3   | 2.79                     | 0.50              |
| 3:N:926:LYS:O    | 3:N:929:ARG:HB2   | 2.11                     | 0.50              |
| 6:U:12:G:N3      | 6:U:12:G:H2'      | 2.25                     | 0.50              |
| 7:Y:92:GLU:HA    | 7:Y:98:GLU:O      | 2.10                     | 0.50              |
| 7:Z:89:VAL:HG11  | 7:Z:151:VAL:HG13  | 1.91                     | 0.50              |
| 1:A:117:VAL:HB   | 1:A:120:VAL:HG13  | 1.92                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:187:ASN:O    | 2:C:188:LYS:HB3   | 2.10                     | 0.50              |
| 2:C:212:GLY:HA3  | 2:C:218:VAL:HG21  | 1.92                     | 0.50              |
| 2:C:41:ASN:O     | 2:C:46:ALA:HB2    | 2.11                     | 0.50              |
| 2:C:722:ILE:O    | 2:C:722:ILE:HG23  | 2.12                     | 0.50              |
| 2:C:754:ILE:HG13 | 2:C:791:ARG:HH12  | 1.76                     | 0.50              |
| 2:C:850:ALA:HA   | 3:D:632:VAL:HG11  | 1.93                     | 0.50              |
| 3:D:1258:ARG:O   | 3:D:1262:LEU:HB2  | 2.12                     | 0.50              |
| 3:D:1295:GLU:N   | 3:D:1295:GLU:OE2  | 2.44                     | 0.50              |
| 3:D:1356:TYR:HD2 | 3:D:1361:VAL:HG11 | 1.76                     | 0.50              |
| 3:D:1397:LYS:NZ  | 3:D:1432:LYS:HZ3  | 2.08                     | 0.50              |
| 3:D:1217:ILE:HB  | 3:D:1480:PHE:CE2  | 2.46                     | 0.50              |
| 3:D:347:VAL:CG2  | 3:D:368:VAL:HG11  | 2.41                     | 0.50              |
| 3:D:893:GLU:O    | 3:D:896:ALA:HB3   | 2.12                     | 0.50              |
| 3:D:975:GLU:O    | 3:D:979:GLU:HG3   | 2.11                     | 0.50              |
| 2:H:442:GLU:CG   | 2:H:454:SER:HB2   | 2.40                     | 0.50              |
| 2:H:861:LEU:HA   | 2:H:974:LEU:HD12  | 1.92                     | 0.50              |
| 2:H:897:LEU:CD2  | 2:H:920:GLN:HG2   | 2.40                     | 0.50              |
| 2:H:950:LEU:O    | 2:H:950:LEU:HD13  | 2.11                     | 0.50              |
| 2:H:577:PRO:HG3  | 2:H:993:PHE:CE1   | 2.45                     | 0.50              |
| 3:I:661:MET:HE2  | 3:I:673:ALA:HB1   | 1.92                     | 0.50              |
| 3:I:771:SER:HB2  | 3:I:778:LEU:CD1   | 2.37                     | 0.50              |
| 3:I:893:GLU:O    | 3:I:896:ALA:HB3   | 2.12                     | 0.50              |
| 3:I:50:PHE:O     | 3:I:89:ARG:HB2    | 2.11                     | 0.50              |
| 3:I:939:PHE:O    | 3:I:943:THR:HG23  | 2.11                     | 0.50              |
| 2:M:524:VAL:CG1  | 2:M:525:SER:H     | 2.24                     | 0.50              |
| 3:N:1189:ARG:HD2 | 3:N:1204:CYS:SG   | 2.52                     | 0.50              |
| 2:M:1046:ALA:HB1 | 3:N:1471:LEU:HD11 | 1.93                     | 0.50              |
| 3:N:81:THR:HB    | 3:N:85:VAL:HG21   | 1.93                     | 0.50              |
| 3:N:949:ILE:N    | 3:N:949:ILE:CD1   | 2.70                     | 0.50              |
| 3:N:975:GLU:O    | 3:N:979:GLU:HG3   | 2.12                     | 0.50              |
| 3:N:762:GLN:NE2  | 4:O:20:THR:CB     | 2.75                     | 0.50              |
| 3:D:783:ARG:NH1  | 7:X:41:ASP:CB     | 2.74                     | 0.50              |
| 2:C:428:ARG:O    | 3:D:1078:ARG:NH1  | 2.44                     | 0.50              |
| 2:C:29:ALA:O     | 2:C:43:GLY:HA3    | 2.11                     | 0.50              |
| 2:C:605:LYS:HB3  | 2:C:610:ARG:HH12  | 1.76                     | 0.50              |
| 2:C:657:ASP:CG   | 2:C:663:ASN:H     | 2.14                     | 0.50              |
| 2:C:93:PRO:HA    | 2:C:117:HIS:CD2   | 2.46                     | 0.50              |
| 3:D:119:SER:HB2  | 3:D:123:LEU:N     | 2.25                     | 0.50              |
| 3:D:190:GLU:HA   | 3:D:196:VAL:HG22  | 1.92                     | 0.50              |
| 3:D:187:LYS:HG3  | 3:D:198:ARG:C     | 2.32                     | 0.50              |
| 3:D:23:TYR:CE1   | 3:D:89:ARG:HG2    | 2.46                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:51:GLY:O      | 3:D:86:ARG:CZ     | 2.60                     | 0.50              |
| 2:H:1083:GLU:CD   | 2:H:1086:ARG:HD2  | 2.31                     | 0.50              |
| 2:H:272:ALA:HA    | 2:H:464:LEU:CD2   | 2.42                     | 0.50              |
| 2:H:571:LEU:HD21  | 2:H:699:PHE:O     | 2.11                     | 0.50              |
| 2:H:881:ASN:O     | 2:H:884:GLN:HG3   | 2.11                     | 0.50              |
| 3:I:10:ILE:CG2    | 3:I:1450:ALA:O    | 2.59                     | 0.50              |
| 3:I:127:LEU:HD21  | 3:I:461:ILE:HD11  | 1.93                     | 0.50              |
| 3:I:1468:LEU:HD13 | 3:I:1470:ARG:NE   | 2.19                     | 0.50              |
| 3:I:177:ALA:N     | 3:I:390:PRO:CD    | 2.73                     | 0.50              |
| 3:I:790:TYR:CG    | 3:I:1026:SER:OG   | 2.53                     | 0.50              |
| 1:K:99:LEU:HB3    | 1:K:114:PHE:CD2   | 2.45                     | 0.50              |
| 2:M:142:ARG:CD    | 2:M:325:ILE:HG23  | 2.41                     | 0.50              |
| 2:M:896:PHE:O     | 2:M:924:VAL:HG11  | 2.12                     | 0.50              |
| 3:N:112:ILE:HD13  | 3:N:112:ILE:O     | 2.11                     | 0.50              |
| 3:N:100:ALA:HB3   | 3:N:128:TYR:CE1   | 2.46                     | 0.50              |
| 1:L:185:ARG:CD    | 3:N:692:GLU:HG2   | 2.40                     | 0.50              |
| 3:N:792:ILE:CD1   | 3:N:881:LEU:HD23  | 2.38                     | 0.50              |
| 3:N:957:PRO:HG2   | 3:N:1007:VAL:CG2  | 2.40                     | 0.50              |
| 1:B:51:THR:HG21   | 1:B:87:VAL:O      | 2.11                     | 0.50              |
| 2:C:1012:PRO:HD2  | 2:C:1026:GLN:HB2  | 1.92                     | 0.50              |
| 2:C:188:LYS:HG3   | 2:C:188:LYS:O     | 2.10                     | 0.50              |
| 2:C:571:LEU:HD21  | 2:C:699:PHE:O     | 2.12                     | 0.50              |
| 2:C:549:PHE:CD2   | 2:C:886:LEU:HB3   | 2.47                     | 0.50              |
| 2:C:580:MET:HE2   | 2:C:902:ILE:HG12  | 1.94                     | 0.50              |
| 3:D:51:GLY:C      | 3:D:86:ARG:HD3    | 2.32                     | 0.50              |
| 3:D:52:PRO:O      | 3:D:86:ARG:CD     | 2.59                     | 0.50              |
| 3:D:1216:SER:HB3  | 4:E:15:SER:OG     | 2.11                     | 0.50              |
| 2:H:1008:ARG:HG2  | 2:H:1008:ARG:HH11 | 1.77                     | 0.50              |
| 2:H:1073:GLY:HA3  | 3:I:659:LYS:HG2   | 1.91                     | 0.50              |
| 3:I:926:LYS:O     | 3:I:929:ARG:HB2   | 2.11                     | 0.50              |
| 1:K:85:LEU:HA     | 1:K:124:ASN:ND2   | 2.26                     | 0.50              |
| 1:L:165:ILE:N     | 1:L:165:ILE:CD1   | 2.70                     | 0.50              |
| 2:M:399:ASN:O     | 2:M:402:SER:HB3   | 2.12                     | 0.50              |
| 2:M:554:ASP:CB    | 2:M:880:MET:HB2   | 2.41                     | 0.50              |
| 2:M:860:HIS:HA    | 2:M:866:PRO:HA    | 1.94                     | 0.50              |
| 2:M:6:PHE:HE2     | 2:M:917:LEU:HD11  | 1.77                     | 0.50              |
| 3:N:1468:LEU:CD2  | 3:N:1470:ARG:HD3  | 2.41                     | 0.50              |
| 3:N:179:VAL:HG11  | 3:N:185:VAL:CG2   | 2.41                     | 0.50              |
| 3:N:800:LYS:CD    | 3:N:804:LEU:HB3   | 2.41                     | 0.50              |
| 3:N:758:GLU:CA    | 4:O:20:THR:HG21   | 2.42                     | 0.50              |
| 7:X:99:ARG:HG3    | 7:X:99:ARG:NH1    | 2.27                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:99:LEU:HB3    | 1:A:114:PHE:CD2   | 2.46                     | 0.50              |
| 2:C:598:GLU:HB2   | 2:C:615:TYR:OH    | 2.12                     | 0.50              |
| 2:C:606:VAL:HG22  | 2:C:645:VAL:HG13  | 1.94                     | 0.50              |
| 2:C:857:ASP:HB2   | 2:C:978:ARG:CG    | 2.40                     | 0.50              |
| 2:C:911:GLU:OE2   | 3:D:1062:ARG:NH1  | 2.45                     | 0.50              |
| 3:D:1232:PRO:HB3  | 3:D:1361:VAL:HG21 | 1.93                     | 0.50              |
| 3:D:1448:THR:O    | 3:D:1451:ALA:HB3  | 2.11                     | 0.50              |
| 4:E:36:LYS:N      | 4:E:36:LYS:CE     | 2.74                     | 0.50              |
| 2:H:487:THR:HB    | 2:H:490:GLU:HG2   | 1.94                     | 0.50              |
| 2:H:535:SER:O     | 2:H:538:GLN:HG2   | 2.12                     | 0.50              |
| 2:H:923:GLU:O     | 2:H:927:GLY:HA3   | 2.11                     | 0.50              |
| 2:H:94:LEU:HD12   | 2:H:94:LEU:C      | 2.32                     | 0.50              |
| 2:H:9:ILE:O       | 2:H:9:ILE:CG1     | 2.60                     | 0.50              |
| 3:I:1150:ALA:O    | 3:I:1162:GLU:HG2  | 2.11                     | 0.50              |
| 3:I:1254:GLN:HA   | 3:I:1258:ARG:HB2  | 1.93                     | 0.50              |
| 3:I:38:LYS:O      | 3:I:39:PRO:C      | 2.50                     | 0.50              |
| 3:I:557:LEU:HD22  | 3:I:566:ILE:HG21  | 1.94                     | 0.50              |
| 2:H:1030:GLN:HE21 | 3:I:628:ARG:HD3   | 1.64                     | 0.50              |
| 3:I:631:ILE:HG21  | 3:I:745:MET:HG3   | 1.94                     | 0.50              |
| 3:I:699:VAL:HA    | 3:I:718:PRO:HD3   | 1.94                     | 0.50              |
| 1:K:101:LEU:HG    | 1:K:102:LYS:N     | 2.25                     | 0.50              |
| 2:M:63:GLY:HA3    | 2:M:103:LYS:HE3   | 1.93                     | 0.50              |
| 2:M:47:ALA:O      | 2:M:348:LEU:HD23  | 2.12                     | 0.50              |
| 2:M:572:ILE:HG23  | 2:M:703:ILE:CD1   | 2.41                     | 0.50              |
| 2:M:838:LYS:HD3   | 2:M:846:LYS:HZ3   | 1.76                     | 0.50              |
| 3:N:109:PRO:HB3   | 3:N:494:LYS:NZ    | 2.27                     | 0.50              |
| 3:N:1232:PRO:HB3  | 3:N:1361:VAL:HG21 | 1.93                     | 0.50              |
| 3:N:939:PHE:O     | 3:N:943:THR:HG23  | 2.12                     | 0.50              |
| 3:N:999:THR:CG2   | 3:N:1000:THR:N    | 2.75                     | 0.50              |
| 3:D:1052:THR:HG21 | 7:X:57:ARG:HH11   | 1.71                     | 0.50              |
| 2:C:194:VAL:HA    | 2:C:197:LEU:HD12  | 1.92                     | 0.50              |
| 2:C:6:PHE:CD1     | 2:C:909:ALA:HB2   | 2.47                     | 0.50              |
| 2:C:997:LEU:N     | 2:C:997:LEU:HD22  | 2.26                     | 0.50              |
| 3:D:400:VAL:CG2   | 3:D:443:VAL:HG21  | 2.42                     | 0.50              |
| 3:D:109:PRO:HB3   | 3:D:494:LYS:NZ    | 2.26                     | 0.50              |
| 3:D:699:VAL:HA    | 3:D:718:PRO:HD3   | 1.94                     | 0.50              |
| 3:D:770:LEU:HB2   | 3:D:1210:SER:O    | 2.11                     | 0.50              |
| 3:D:882:PHE:HE1   | 3:D:934:LEU:HD21  | 1.77                     | 0.50              |
| 4:E:36:LYS:HE2    | 4:E:36:LYS:N      | 2.26                     | 0.50              |
| 1:G:173:PRO:O     | 1:G:201:THR:CG2   | 2.59                     | 0.50              |
| 2:H:426:ASP:OD1   | 2:H:426:ASP:C     | 2.50                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:570:PRO:HD2   | 2:H:635:THR:CG2   | 2.42                     | 0.50              |
| 2:H:668:LEU:H     | 2:H:668:LEU:HD12  | 1.73                     | 0.50              |
| 3:I:112:ILE:O     | 3:I:112:ILE:HD13  | 2.11                     | 0.50              |
| 3:I:728:LEU:HD22  | 3:I:745:MET:SD    | 2.52                     | 0.50              |
| 3:I:957:PRO:HG2   | 3:I:1007:VAL:CG2  | 2.40                     | 0.50              |
| 1:K:50:GLY:HA3    | 1:K:173:PRO:HG3   | 1.93                     | 0.50              |
| 1:K:24:VAL:HG22   | 1:K:196:THR:HG22  | 1.94                     | 0.50              |
| 2:M:831:ARG:NH1   | 2:M:1002:GLU:HB2  | 2.27                     | 0.50              |
| 2:M:111:ASP:OD2   | 2:M:369:PRO:HB2   | 2.10                     | 0.50              |
| 2:M:263:ASP:OD2   | 2:M:263:ASP:N     | 2.43                     | 0.50              |
| 2:M:906:PHE:CZ    | 3:N:1067:VAL:HA   | 2.46                     | 0.50              |
| 3:N:127:LEU:O     | 3:N:457:GLY:HA2   | 2.12                     | 0.50              |
| 3:N:1381:VAL:O    | 3:N:1389:LEU:O    | 2.29                     | 0.50              |
| 3:N:1198:TYR:OH   | 3:N:1394:VAL:HG11 | 2.12                     | 0.50              |
| 3:N:1264:GLU:CD   | 3:N:1424:VAL:HG13 | 2.31                     | 0.50              |
| 3:N:1481:VAL:HG12 | 4:O:21:VAL:HG21   | 1.93                     | 0.50              |
| 3:N:893:GLU:O     | 3:N:896:ALA:HB3   | 2.12                     | 0.50              |
| 3:N:882:PHE:HE1   | 3:N:934:LEU:HD21  | 1.77                     | 0.50              |
| 3:I:1029:ARG:NH2  | 7:Y:41:ASP:OD2    | 2.39                     | 0.50              |
| 7:Z:83:ILE:CG1    | 7:Z:154:ILE:HD13  | 2.41                     | 0.50              |
| 1:A:89:PHE:HD1    | 1:A:120:VAL:CG2   | 2.25                     | 0.50              |
| 2:C:263:ASP:CB    | 2:C:264:PRO:HD3   | 2.42                     | 0.50              |
| 2:C:36:PRO:CB     | 2:C:70:GLU:HG2    | 2.42                     | 0.50              |
| 2:C:544:THR:O     | 2:C:547:ILE:HD12  | 2.12                     | 0.50              |
| 2:C:545:ASN:HA    | 2:C:905:ILE:HD11  | 1.93                     | 0.50              |
| 2:C:896:PHE:O     | 2:C:924:VAL:HG11  | 2.12                     | 0.50              |
| 2:C:99:GLN:HE21   | 2:C:101:ILE:HD11  | 1.77                     | 0.50              |
| 3:D:957:PRO:CG    | 3:D:1007:VAL:HG22 | 2.39                     | 0.50              |
| 3:D:1206:GLY:O    | 3:D:1215:VAL:HG23 | 2.12                     | 0.50              |
| 3:D:1491:THR:HA   | 3:D:1494:ALA:HB3  | 1.93                     | 0.50              |
| 3:D:173:PRO:HB3   | 2:H:279:GLU:OE2   | 2.12                     | 0.50              |
| 3:D:368:VAL:H     | 3:D:377:VAL:HB    | 1.76                     | 0.50              |
| 3:D:447:VAL:O     | 3:D:449:SER:N     | 2.44                     | 0.50              |
| 3:D:477:LEU:HD22  | 3:D:492:ALA:CB    | 2.40                     | 0.50              |
| 1:G:221:HIS:HA    | 1:G:224:TYR:HD2   | 1.77                     | 0.50              |
| 2:H:163:ILE:HG23  | 2:H:163:ILE:O     | 2.12                     | 0.50              |
| 2:H:249:LYS:O     | 2:H:250:ARG:C     | 2.50                     | 0.50              |
| 2:H:169:GLY:HA2   | 2:H:263:ASP:CB    | 2.42                     | 0.50              |
| 2:H:343:GLN:HA    | 2:H:346:VAL:CG2   | 2.42                     | 0.50              |
| 2:H:64:LEU:HD22   | 2:H:359:MET:HG3   | 1.92                     | 0.50              |
| 2:H:137:VAL:HG23  | 2:H:391:LEU:HD23  | 1.90                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:83:CYS:HB3    | 2:H:88:LEU:O      | 2.11                     | 0.50              |
| 2:H:848:VAL:HG12  | 2:H:849:VAL:N     | 2.26                     | 0.50              |
| 2:H:857:ASP:HB2   | 2:H:978:ARG:CG    | 2.40                     | 0.50              |
| 3:I:1277:ILE:N    | 3:I:1277:ILE:HD12 | 2.27                     | 0.50              |
| 3:I:1232:PRO:HB3  | 3:I:1361:VAL:HG21 | 1.93                     | 0.50              |
| 3:I:50:PHE:HA     | 3:I:89:ARG:CG     | 2.42                     | 0.50              |
| 3:I:550:ARG:HH11  | 3:I:573:MET:HB3   | 1.77                     | 0.50              |
| 2:M:361:MET:HG2   | 2:M:361:MET:O     | 2.11                     | 0.50              |
| 2:M:89:THR:HG21   | 2:M:383:ARG:HH22  | 1.77                     | 0.50              |
| 2:M:674:VAL:O     | 2:M:989:VAL:HA    | 2.12                     | 0.50              |
| 2:M:997:LEU:N     | 2:M:997:LEU:HD22  | 2.26                     | 0.50              |
| 3:N:957:PRO:CG    | 3:N:1007:VAL:HG22 | 2.39                     | 0.50              |
| 3:N:1087:ARG:HB2  | 3:N:1237:THR:OG1  | 2.12                     | 0.50              |
| 3:N:1277:ILE:N    | 3:N:1277:ILE:HD12 | 2.27                     | 0.50              |
| 3:N:1288:GLU:O    | 3:N:1307:LYS:CE   | 2.57                     | 0.50              |
| 3:N:1479:ASP:OD2  | 3:N:1482:ARG:NH2  | 2.44                     | 0.50              |
| 3:N:514:LEU:HD11  | 3:N:582:LEU:HD11  | 1.94                     | 0.50              |
| 3:N:631:ILE:HG21  | 3:N:745:MET:HG3   | 1.93                     | 0.50              |
| 3:N:699:VAL:HA    | 3:N:718:PRO:HD3   | 1.94                     | 0.50              |
| 3:N:771:SER:HB2   | 3:N:778:LEU:CD1   | 2.37                     | 0.50              |
| 1:A:50:GLY:HA3    | 1:A:173:PRO:HG3   | 1.93                     | 0.50              |
| 2:C:101:ILE:HD12  | 2:C:108:ILE:CD1   | 2.41                     | 0.50              |
| 2:C:272:ALA:O     | 2:C:464:LEU:HD22  | 2.12                     | 0.50              |
| 2:C:523:ILE:HD13  | 2:C:523:ILE:C     | 2.33                     | 0.50              |
| 2:C:679:PHE:O     | 2:C:680:ASP:C     | 2.49                     | 0.50              |
| 3:D:441:ARG:NH1   | 3:D:445:ARG:CZ    | 2.75                     | 0.50              |
| 3:D:86:ARG:HB3    | 3:D:523:ASP:OD2   | 2.11                     | 0.50              |
| 3:D:939:PHE:O     | 3:D:943:THR:HG23  | 2.11                     | 0.50              |
| 1:F:50:GLY:HA3    | 1:F:173:PRO:HG3   | 1.93                     | 0.50              |
| 2:H:182:VAL:O     | 2:H:193:LEU:HD11  | 2.08                     | 0.50              |
| 2:H:48:PHE:O      | 2:H:52:PHE:HB2    | 2.12                     | 0.50              |
| 2:H:797:GLY:O     | 2:H:829:GLN:NE2   | 2.45                     | 0.50              |
| 2:H:683:ASN:HB2   | 2:H:872:ASN:HB2   | 1.93                     | 0.50              |
| 3:I:1026:SER:O    | 3:I:1028:ALA:N    | 2.44                     | 0.50              |
| 3:I:1209:LEU:O    | 3:I:1210:SER:C    | 2.48                     | 0.50              |
| 3:I:502:PHE:CZ    | 3:I:1452:ILE:HG13 | 2.46                     | 0.50              |
| 3:I:806:PHE:C     | 3:I:808:THR:N     | 2.65                     | 0.50              |
| 2:M:1001:VAL:HG22 | 3:N:630:VAL:CG2   | 2.42                     | 0.50              |
| 2:M:380:ALA:O     | 2:M:384:GLU:HB2   | 2.12                     | 0.50              |
| 2:M:571:LEU:HD11  | 2:M:700:TYR:CA    | 2.40                     | 0.50              |
| 2:M:86:LYS:O      | 2:M:87:ASP:CB     | 2.52                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:923:GLU:O     | 2:M:927:GLY:HA3   | 2.11                     | 0.50              |
| 3:N:111:LYS:CE    | 3:N:1448:THR:HG22 | 2.42                     | 0.50              |
| 3:N:782:SER:H     | 3:N:785:ILE:HD13  | 1.77                     | 0.50              |
| 1:L:152:PRO:HG3   | 3:N:857:ILE:HG13  | 1.93                     | 0.50              |
| 3:N:987:GLU:OE1   | 7:Z:120:SER:CB    | 2.60                     | 0.50              |
| 7:Y:102:VAL:HG21  | 7:Y:125:MET:HE3   | 1.94                     | 0.50              |
| 1:B:110:LYS:HD3   | 1:B:126:ASP:HA    | 1.93                     | 0.50              |
| 1:B:153:ALA:HB2   | 1:B:168:ASP:N     | 2.27                     | 0.50              |
| 2:C:243:ARG:CB    | 2:C:244:PRO:HD3   | 2.42                     | 0.50              |
| 2:C:799:ILE:N     | 2:C:799:ILE:HD13  | 2.27                     | 0.50              |
| 2:C:879:ARG:CZ    | 7:X:42:ASP:CB     | 2.87                     | 0.50              |
| 2:C:885:ILE:HG13  | 3:D:949:ILE:HG21  | 1.94                     | 0.50              |
| 3:D:142:LEU:HD23  | 3:D:146:PRO:CA    | 2.41                     | 0.50              |
| 3:D:162:ARG:NE    | 3:D:452:ILE:HG21  | 2.26                     | 0.50              |
| 3:D:51:GLY:O      | 3:D:86:ARG:NE     | 2.45                     | 0.50              |
| 2:H:198:ARG:HD2   | 2:H:228:ALA:HA    | 1.93                     | 0.50              |
| 2:H:276:LYS:O     | 2:H:280:LYS:HB2   | 2.11                     | 0.50              |
| 2:H:36:PRO:HA     | 2:H:39:ARG:HB3    | 1.94                     | 0.50              |
| 2:H:799:ILE:N     | 2:H:799:ILE:HD13  | 2.27                     | 0.50              |
| 2:H:876:VAL:H     | 2:H:877:PRO:HD2   | 1.76                     | 0.50              |
| 2:H:98:LEU:CD1    | 2:H:98:LEU:N      | 2.60                     | 0.50              |
| 3:I:1024:ALA:HA   | 3:I:1029:ARG:O    | 2.12                     | 0.50              |
| 3:I:1093:TYR:CE2  | 3:I:1097:LYS:HE3  | 2.47                     | 0.50              |
| 3:I:1107:VAL:O    | 3:I:1107:VAL:HG12 | 2.12                     | 0.50              |
| 3:I:1256:LEU:O    | 3:I:1259:VAL:N    | 2.45                     | 0.50              |
| 3:I:1281:VAL:HG21 | 3:I:1313:VAL:HG21 | 1.94                     | 0.50              |
| 3:I:1472:ILE:HG22 | 3:I:1473:PRO:CD   | 2.40                     | 0.50              |
| 3:I:834:THR:HB    | 3:I:838:ARG:HD3   | 1.94                     | 0.50              |
| 1:K:88:ARG:HH12   | 1:K:90:LEU:HD11   | 1.76                     | 0.50              |
| 1:L:138:LEU:HD21  | 1:L:140:MET:SD    | 2.52                     | 0.50              |
| 1:L:73:GLU:HB2    | 1:L:78:ILE:CG1    | 2.42                     | 0.50              |
| 2:M:317:VAL:N     | 2:M:318:PRO:HD3   | 2.27                     | 0.50              |
| 2:M:570:PRO:HD2   | 2:M:635:THR:CG2   | 2.42                     | 0.50              |
| 2:M:878:SER:HA    | 3:N:1034:GLN:HE22 | 1.76                     | 0.50              |
| 3:N:1107:VAL:O    | 3:N:1218:GLY:N    | 2.43                     | 0.50              |
| 3:N:704:ARG:NH2   | 6:U:16:G:O2'      | 2.45                     | 0.50              |
| 7:Z:128:ALA:HB2   | 7:Z:140:LEU:HD21  | 1.93                     | 0.50              |
| 1:A:88:ARG:HH12   | 1:A:90:LEU:HD11   | 1.76                     | 0.49              |
| 2:C:1047:HIS:N    | 2:C:1047:HIS:CD2  | 2.80                     | 0.49              |
| 2:C:1047:HIS:H    | 2:C:1047:HIS:CD2  | 2.30                     | 0.49              |
| 2:C:188:LYS:NZ    | 2:C:188:LYS:HB2   | 2.25                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:426:ASP:OD1   | 2:C:426:ASP:C     | 2.50                     | 0.49              |
| 1:B:30:ARG:NH1    | 2:C:692:GLU:OE1   | 2.45                     | 0.49              |
| 2:C:966:LEU:HD11  | 2:C:986:PRO:HG2   | 1.94                     | 0.49              |
| 3:D:1098:LEU:HD21 | 3:D:1229:ILE:HG22 | 1.92                     | 0.49              |
| 3:D:13:ALA:CB     | 3:D:18:ILE:HD11   | 2.42                     | 0.49              |
| 3:D:390:PRO:HB2   | 3:D:393:ILE:HD11  | 1.93                     | 0.49              |
| 4:E:33:HIS:HB2    | 4:E:37:ASN:OD1    | 2.12                     | 0.49              |
| 2:H:215:GLY:O     | 2:H:216:GLU:HB3   | 2.12                     | 0.49              |
| 2:H:115:LEU:HA    | 2:H:375:SER:HB3   | 1.94                     | 0.49              |
| 2:H:860:HIS:HA    | 2:H:866:PRO:HA    | 1.94                     | 0.49              |
| 3:I:1408:ILE:HD12 | 3:I:1408:ILE:H    | 1.76                     | 0.49              |
| 3:I:401:TYR:HB3   | 3:I:427:VAL:HG13  | 1.93                     | 0.49              |
| 3:I:202:VAL:CG1   | 3:I:445:ARG:HH21  | 2.23                     | 0.49              |
| 3:I:447:VAL:O     | 3:I:449:SER:N     | 2.45                     | 0.49              |
| 4:J:31:LEU:HD12   | 4:J:32:ARG:H      | 1.76                     | 0.49              |
| 2:M:274:ARG:HD2   | 2:M:285:LEU:CD1   | 2.41                     | 0.49              |
| 2:M:383:ARG:CB    | 2:M:383:ARG:HH11  | 2.18                     | 0.49              |
| 2:M:720:GLU:HA    | 2:M:759:THR:O     | 2.11                     | 0.49              |
| 3:N:1264:GLU:OE2  | 3:N:1424:VAL:HG12 | 2.10                     | 0.49              |
| 3:N:162:ARG:HG2   | 3:N:162:ARG:HH11  | 1.77                     | 0.49              |
| 3:N:438:ASP:HB2   | 3:N:445:ARG:NH1   | 2.27                     | 0.49              |
| 3:N:481:MET:SD    | 3:N:496:LEU:HD23  | 2.52                     | 0.49              |
| 2:M:684:PHE:CB    | 3:N:633:VAL:HG21  | 2.41                     | 0.49              |
| 3:N:676:MET:O     | 3:N:680:GLN:N     | 2.44                     | 0.49              |
| 3:N:700:VAL:HG12  | 3:N:749:VAL:HG13  | 1.94                     | 0.49              |
| 3:N:705:ALA:HB3   | 3:N:706:PRO:HD3   | 1.94                     | 0.49              |
| 7:Y:128:ALA:CB    | 7:Y:140:LEU:HD11  | 2.41                     | 0.49              |
| 2:H:879:ARG:NE    | 7:Y:42:ASP:OD1    | 2.45                     | 0.49              |
| 1:B:73:GLU:HG3    | 1:B:130:ALA:HA    | 1.94                     | 0.49              |
| 1:B:212:ASN:O     | 1:B:215:VAL:CG2   | 2.54                     | 0.49              |
| 2:C:211:LEU:O     | 2:C:211:LEU:HD12  | 2.12                     | 0.49              |
| 2:C:267:TYR:N     | 2:C:267:TYR:CD2   | 2.80                     | 0.49              |
| 2:C:274:ARG:HG3   | 2:C:285:LEU:HB3   | 1.94                     | 0.49              |
| 2:C:338:GLU:C     | 2:C:341:THR:HG22  | 2.32                     | 0.49              |
| 2:C:570:PRO:HD2   | 2:C:635:THR:CG2   | 2.42                     | 0.49              |
| 2:C:579:VAL:HB    | 2:C:890:LEU:HD22  | 1.93                     | 0.49              |
| 3:D:1192:LEU:HB3  | 3:D:1345:GLU:OE2  | 2.13                     | 0.49              |
| 3:D:729:HIS:HB3   | 3:D:732:VAL:HG22  | 1.94                     | 0.49              |
| 2:C:886:LEU:CD1   | 3:D:951:ILE:HD12  | 2.43                     | 0.49              |
| 2:H:443:THR:HG21  | 3:I:1078:ARG:HD2  | 1.94                     | 0.49              |
| 2:H:662:GLU:O     | 2:H:662:GLU:OE1   | 2.30                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:756:VAL:HB    | 2:H:790:LEU:HB3   | 1.95                     | 0.49              |
| 2:H:896:PHE:O     | 2:H:924:VAL:HG11  | 2.12                     | 0.49              |
| 2:H:958:THR:CG2   | 2:H:961:GLU:HG3   | 2.35                     | 0.49              |
| 3:I:1192:LEU:HB3  | 3:I:1345:GLU:OE2  | 2.12                     | 0.49              |
| 3:I:606:ILE:HG13  | 3:I:606:ILE:O     | 2.12                     | 0.49              |
| 3:I:6:ARG:NH2     | 3:I:1482:ARG:NH2  | 2.59                     | 0.49              |
| 2:M:1038:TRP:O    | 2:M:1039:ALA:C    | 2.50                     | 0.49              |
| 2:M:1095:LEU:HD11 | 2:M:1097:LEU:HD22 | 1.93                     | 0.49              |
| 2:M:328:LEU:C     | 2:M:330:ASN:N     | 2.65                     | 0.49              |
| 2:M:492:ASP:OD2   | 2:M:518:LYS:HG3   | 2.12                     | 0.49              |
| 3:N:1047:LYS:HZ2  | 3:N:1053:PHE:HA   | 1.76                     | 0.49              |
| 3:N:1192:LEU:HB3  | 3:N:1345:GLU:OE2  | 2.12                     | 0.49              |
| 3:N:13:ALA:CB     | 3:N:18:ILE:HD11   | 2.42                     | 0.49              |
| 3:N:409:VAL:O     | 3:N:410:SER:OG    | 2.23                     | 0.49              |
| 3:N:804:LEU:CB    | 3:N:830:ALA:O     | 2.60                     | 0.49              |
| 3:N:834:THR:HB    | 3:N:838:ARG:HD3   | 1.94                     | 0.49              |
| 3:N:930:LEU:O     | 3:N:933:ALA:HB3   | 2.12                     | 0.49              |
| 4:O:73:LEU:H      | 4:O:73:LEU:HD12   | 1.77                     | 0.49              |
| 1:A:101:LEU:HG    | 1:A:102:LYS:N     | 2.25                     | 0.49              |
| 1:B:85:LEU:HA     | 1:B:124:ASN:HD22  | 1.77                     | 0.49              |
| 2:C:1054:THR:O    | 2:C:1056:LYS:N    | 2.46                     | 0.49              |
| 2:C:479:VAL:HG11  | 2:C:503:LEU:HD11  | 1.93                     | 0.49              |
| 2:C:535:SER:O     | 2:C:538:GLN:HG2   | 2.12                     | 0.49              |
| 2:C:6:PHE:CE1     | 2:C:909:ALA:HB2   | 2.47                     | 0.49              |
| 3:D:999:THR:CG2   | 3:D:1000:THR:N    | 2.75                     | 0.49              |
| 3:D:1026:SER:C    | 3:D:1028:ALA:H    | 2.15                     | 0.49              |
| 3:D:179:VAL:HG11  | 3:D:185:VAL:CG2   | 2.42                     | 0.49              |
| 3:D:685:ASP:O     | 3:D:689:ASP:OD1   | 2.28                     | 0.49              |
| 3:D:930:LEU:O     | 3:D:933:ALA:HB3   | 2.12                     | 0.49              |
| 1:G:179:PHE:CD2   | 1:G:179:PHE:N     | 2.79                     | 0.49              |
| 2:H:1074:GLU:CG   | 2:H:1075:ASP:H    | 2.05                     | 0.49              |
| 2:H:395:LYS:O     | 2:H:397:GLU:N     | 2.45                     | 0.49              |
| 2:H:524:VAL:CG1   | 2:H:525:SER:H     | 2.25                     | 0.49              |
| 2:H:565:GLN:NE2   | 2:H:842:ARG:CG    | 2.65                     | 0.49              |
| 2:H:650:ARG:HG2   | 2:H:653:ASP:OD2   | 2.13                     | 0.49              |
| 3:I:1384:PRO:HG2  | 3:I:1388:ARG:CZ   | 2.41                     | 0.49              |
| 3:I:1472:ILE:H    | 3:I:1472:ILE:CD1  | 2.15                     | 0.49              |
| 3:I:205:TYR:HB2   | 3:I:393:ILE:CG1   | 2.39                     | 0.49              |
| 3:I:514:LEU:HD12  | 3:I:578:VAL:HG11  | 1.92                     | 0.49              |
| 3:I:705:ALA:HB3   | 3:I:706:PRO:HD3   | 1.94                     | 0.49              |
| 3:I:765:SER:OG    | 3:I:766:ALA:N     | 2.46                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:87:ARG:O     | 3:I:88:TYR:HD2    | 1.87                     | 0.49              |
| 4:J:69:LEU:HD23  | 4:J:70:THR:CG2    | 2.41                     | 0.49              |
| 1:L:88:ARG:HB2   | 1:L:123:MET:SD    | 2.52                     | 0.49              |
| 2:M:662:GLU:O    | 2:M:662:GLU:OE1   | 2.30                     | 0.49              |
| 3:N:136:ASP:HB3  | 3:N:137:PRO:CD    | 2.41                     | 0.49              |
| 3:N:142:LEU:HD22 | 3:N:145:VAL:CA    | 2.41                     | 0.49              |
| 3:N:1440:PHE:O   | 3:N:1441:GLN:O    | 2.30                     | 0.49              |
| 3:N:441:ARG:HD2  | 3:N:445:ARG:HH22  | 1.75                     | 0.49              |
| 2:M:684:PHE:HB3  | 3:N:633:VAL:HG21  | 1.94                     | 0.49              |
| 3:N:646:LYS:HG3  | 3:N:647:ARG:N     | 2.27                     | 0.49              |
| 3:N:728:LEU:HD22 | 3:N:745:MET:SD    | 2.52                     | 0.49              |
| 3:N:810:GLU:C    | 3:N:812:ALA:N     | 2.64                     | 0.49              |
| 6:Q:13:G:H2'     | 6:Q:14:C:C6       | 2.47                     | 0.49              |
| 2:C:182:VAL:CG1  | 2:C:193:LEU:HB2   | 2.42                     | 0.49              |
| 2:C:218:VAL:C    | 2:C:220:GLY:N     | 2.64                     | 0.49              |
| 2:C:290:LEU:HD13 | 2:C:303:PHE:HE1   | 1.76                     | 0.49              |
| 2:C:317:VAL:C    | 2:C:319:GLY:N     | 2.62                     | 0.49              |
| 2:C:433:THR:CG2  | 2:C:488:ALA:HB1   | 2.42                     | 0.49              |
| 2:C:848:VAL:HG12 | 2:C:849:VAL:N     | 2.26                     | 0.49              |
| 2:C:860:HIS:HA   | 2:C:866:PRO:HA    | 1.94                     | 0.49              |
| 2:C:876:VAL:H    | 2:C:877:PRO:HD2   | 1.77                     | 0.49              |
| 3:D:111:LYS:HG2  | 3:D:1452:ILE:HD11 | 1.93                     | 0.49              |
| 3:D:116:LEU:CD2  | 3:D:118:LEU:CD1   | 2.90                     | 0.49              |
| 3:D:508:ARG:HB3  | 3:D:509:PRO:HD2   | 1.95                     | 0.49              |
| 3:D:52:PRO:O     | 3:D:86:ARG:HG3    | 2.12                     | 0.49              |
| 3:D:562:ALA:HB3  | 2:H:226:VAL:HG12  | 1.93                     | 0.49              |
| 3:D:700:VAL:HG12 | 3:D:749:VAL:HG13  | 1.95                     | 0.49              |
| 3:D:765:SER:OG   | 3:D:766:ALA:N     | 2.46                     | 0.49              |
| 3:D:834:THR:HB   | 3:D:838:ARG:HD3   | 1.95                     | 0.49              |
| 3:D:926:LYS:O    | 3:D:929:ARG:HB2   | 2.11                     | 0.49              |
| 4:E:48:MET:HG3   | 4:E:54:LEU:HG     | 1.94                     | 0.49              |
| 1:G:15:THR:O     | 1:G:15:THR:HG23   | 2.13                     | 0.49              |
| 1:G:70:GLY:O     | 1:G:132:LEU:HA    | 2.12                     | 0.49              |
| 2:H:294:GLU:CG   | 2:H:295:ASP:CG    | 2.80                     | 0.49              |
| 2:H:571:LEU:HD11 | 2:H:700:TYR:C     | 2.32                     | 0.49              |
| 2:H:728:HIS:O    | 2:H:729:LEU:HD22  | 2.12                     | 0.49              |
| 3:I:584:ASN:HD21 | 3:I:590:PRO:HD2   | 1.73                     | 0.49              |
| 4:J:3:GLU:OE1    | 4:J:4:PRO:HD3     | 2.13                     | 0.49              |
| 2:M:328:LEU:N    | 2:M:328:LEU:CD1   | 2.74                     | 0.49              |
| 3:N:436:GLU:OE1  | 3:N:447:VAL:HG13  | 2.12                     | 0.49              |
| 3:N:47:GLU:O     | 3:N:51:GLY:N      | 2.46                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:50:PHE:CB     | 3:N:522:PRO:CD    | 2.91                     | 0.49              |
| 3:N:664:LYS:O     | 3:N:666:ILE:N     | 2.46                     | 0.49              |
| 3:N:835:SER:O     | 3:N:837:GLY:N     | 2.46                     | 0.49              |
| 1:A:32:PHE:CZ     | 1:B:47:SER:HB2    | 2.48                     | 0.49              |
| 2:C:261:ILE:HD12  | 2:C:262:ALA:H     | 1.77                     | 0.49              |
| 2:C:292:ARG:HD2   | 2:C:299:LYS:CE    | 2.43                     | 0.49              |
| 2:C:359:MET:SD    | 2:C:359:MET:O     | 2.71                     | 0.49              |
| 2:C:806:LEU:HB2   | 2:C:822:VAL:HG22  | 1.95                     | 0.49              |
| 2:C:863:ASP:CG    | 2:C:865:THR:HG22  | 2.33                     | 0.49              |
| 2:C:89:THR:HG21   | 2:C:383:ARG:HH22  | 1.74                     | 0.49              |
| 3:D:1008:PHE:CE2  | 3:D:1035:ILE:HG21 | 2.47                     | 0.49              |
| 3:D:368:VAL:HB    | 3:D:377:VAL:HB    | 1.94                     | 0.49              |
| 3:D:412:GLY:HA2   | 3:D:434:ARG:HD3   | 1.93                     | 0.49              |
| 2:H:332:ARG:HH12  | 2:H:338:GLU:CD    | 2.15                     | 0.49              |
| 2:H:553:ASP:OD2   | 2:H:883:GLY:N     | 2.44                     | 0.49              |
| 2:H:6:PHE:CB      | 2:H:909:ALA:HA    | 2.41                     | 0.49              |
| 2:H:6:PHE:CZ      | 2:H:917:LEU:CD1   | 2.96                     | 0.49              |
| 2:H:966:LEU:HD11  | 2:H:986:PRO:HG2   | 1.94                     | 0.49              |
| 2:H:987:ILE:HG23  | 3:I:948:THR:CG2   | 2.23                     | 0.49              |
| 3:I:646:LYS:HG3   | 3:I:647:ARG:N     | 2.26                     | 0.49              |
| 1:G:185:ARG:NH1   | 3:I:692:GLU:HG2   | 2.12                     | 0.49              |
| 3:I:782:SER:H     | 3:I:785:ILE:HD13  | 1.77                     | 0.49              |
| 3:I:930:LEU:O     | 3:I:933:ALA:HB3   | 2.12                     | 0.49              |
| 4:J:47:LYS:N      | 4:J:54:LEU:HD13   | 2.27                     | 0.49              |
| 2:M:101:ILE:CG1   | 2:M:108:ILE:HD11  | 2.41                     | 0.49              |
| 2:M:317:VAL:C     | 2:M:319:GLY:N     | 2.65                     | 0.49              |
| 2:M:799:ILE:HD13  | 2:M:799:ILE:N     | 2.27                     | 0.49              |
| 3:N:1252:ILE:CG1  | 3:N:1253:THR:N    | 2.75                     | 0.49              |
| 3:N:126:VAL:O     | 3:N:130:SER:CB    | 2.60                     | 0.49              |
| 3:N:1280:VAL:O    | 3:N:1294:VAL:HA   | 2.13                     | 0.49              |
| 3:N:456:MET:CE    | 3:N:568:ARG:HH21  | 2.22                     | 0.49              |
| 5:R:20:DG:N2      | 6:S:11:C:H42      | 2.10                     | 0.49              |
| 1:A:22:GLU:OE2    | 1:A:198:ARG:CB    | 2.60                     | 0.49              |
| 2:C:203:ASP:OD1   | 2:C:205:GLU:HG2   | 2.13                     | 0.49              |
| 2:C:224:GLU:HG3   | 2:C:227:PHE:HB2   | 1.94                     | 0.49              |
| 2:C:338:GLU:O     | 2:C:341:THR:HG22  | 2.12                     | 0.49              |
| 2:C:650:ARG:HG2   | 2:C:653:ASP:OD2   | 2.13                     | 0.49              |
| 3:D:1137:ARG:HH11 | 3:D:1137:ARG:CB   | 2.21                     | 0.49              |
| 3:D:1189:ARG:HD2  | 3:D:1204:CYS:SG   | 2.52                     | 0.49              |
| 3:D:1381:VAL:O    | 3:D:1389:LEU:O    | 2.31                     | 0.49              |
| 3:D:160:GLU:HG2   | 3:D:165:LYS:CG    | 2.41                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:620:GLY:O    | 3:D:621:LYS:CG    | 2.54                     | 0.49              |
| 3:D:646:LYS:HG3  | 3:D:647:ARG:N     | 2.26                     | 0.49              |
| 3:D:1485:GLN:O   | 4:E:75:PHE:HA     | 2.13                     | 0.49              |
| 1:G:112:ARG:CD   | 1:G:125:PRO:CB    | 2.79                     | 0.49              |
| 2:H:691:SER:HB2  | 2:H:858:MET:SD    | 2.52                     | 0.49              |
| 2:H:882:LEU:HD12 | 3:I:1061:PHE:HB3  | 1.94                     | 0.49              |
| 2:H:549:PHE:CD2  | 2:H:886:LEU:HB3   | 2.47                     | 0.49              |
| 2:H:997:LEU:C    | 2:H:999:HIS:N     | 2.64                     | 0.49              |
| 3:I:1205:TYR:HE1 | 3:I:1370:ILE:HD11 | 1.76                     | 0.49              |
| 3:I:1264:GLU:OE2 | 3:I:1424:VAL:HG12 | 2.10                     | 0.49              |
| 3:I:481:MET:SD   | 3:I:496:LEU:HD23  | 2.53                     | 0.49              |
| 3:I:508:ARG:HB3  | 3:I:509:PRO:HD2   | 1.95                     | 0.49              |
| 3:I:584:ASN:CG   | 3:I:590:PRO:HD2   | 2.33                     | 0.49              |
| 1:K:89:PHE:HD1   | 1:K:120:VAL:CG2   | 2.25                     | 0.49              |
| 1:L:15:THR:O     | 1:L:15:THR:HG23   | 2.13                     | 0.49              |
| 2:M:1083:GLU:CD  | 2:M:1086:ARG:HD2  | 2.31                     | 0.49              |
| 2:M:1101:THR:C   | 2:M:1102:LEU:HD12 | 2.33                     | 0.49              |
| 2:M:523:ILE:HD13 | 2:M:523:ILE:C     | 2.32                     | 0.49              |
| 2:M:722:ILE:HD13 | 2:M:722:ILE:C     | 2.32                     | 0.49              |
| 2:M:94:LEU:HD12  | 2:M:95:TYR:N      | 2.28                     | 0.49              |
| 3:N:795:VAL:HG23 | 3:N:879:ARG:HH12  | 1.77                     | 0.49              |
| 2:H:879:ARG:CZ   | 7:Y:42:ASP:CG     | 2.81                     | 0.49              |
| 1:B:80:LEU:HG    | 3:D:844:ALA:HB2   | 1.95                     | 0.49              |
| 2:C:831:ARG:HH12 | 2:C:1002:GLU:HB2  | 1.77                     | 0.49              |
| 2:C:15:LEU:CD1   | 2:C:15:LEU:H      | 2.23                     | 0.49              |
| 2:C:682:TYR:CE1  | 2:C:851:LYS:HD3   | 2.47                     | 0.49              |
| 2:C:861:LEU:HD21 | 2:C:925:TYR:CE2   | 2.48                     | 0.49              |
| 3:D:1021:TYR:CE2 | 3:D:1025:GLN:CG   | 2.96                     | 0.49              |
| 3:D:404:GLU:N    | 3:D:423:ASP:OD2   | 2.42                     | 0.49              |
| 2:H:1036:GLU:O   | 2:H:1039:ALA:HB3  | 2.12                     | 0.49              |
| 2:H:226:VAL:HG13 | 2:H:227:PHE:N     | 2.28                     | 0.49              |
| 2:H:433:THR:HG21 | 2:H:488:ALA:HB1   | 1.95                     | 0.49              |
| 2:H:593:ALA:HB1  | 2:H:659:PRO:HD2   | 1.95                     | 0.49              |
| 2:H:685:GLU:OE2  | 3:I:783:ARG:HD2   | 2.12                     | 0.49              |
| 2:H:726:ILE:CG1  | 2:H:734:LEU:HD11  | 2.36                     | 0.49              |
| 2:H:861:LEU:HD21 | 2:H:925:TYR:CE2   | 2.48                     | 0.49              |
| 3:I:1147:ARG:HB3 | 3:I:1188:VAL:CG2  | 2.41                     | 0.49              |
| 3:I:143:ASN:HB3  | 3:I:161:LEU:HD13  | 1.94                     | 0.49              |
| 3:I:205:TYR:HD1  | 3:I:390:PRO:CB    | 2.25                     | 0.49              |
| 3:I:479:GLU:O    | 3:I:483:HIS:ND1   | 2.42                     | 0.49              |
| 3:I:546:ARG:HH11 | 3:I:546:ARG:HG2   | 1.78                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:684:PHE:CB   | 3:I:633:VAL:HG21  | 2.43                     | 0.49              |
| 3:I:975:GLU:O    | 3:I:979:GLU:HG3   | 2.12                     | 0.49              |
| 3:I:999:THR:CG2  | 3:I:1000:THR:N    | 2.75                     | 0.49              |
| 4:J:17:TYR:O     | 4:J:21:VAL:HG23   | 2.12                     | 0.49              |
| 1:L:73:GLU:HG3   | 1:L:130:ALA:HA    | 1.95                     | 0.49              |
| 1:L:42:ARG:CG    | 1:L:42:ARG:HH11   | 2.24                     | 0.49              |
| 2:M:31:GLN:HG2   | 2:M:34:VAL:CG2    | 2.43                     | 0.49              |
| 2:M:340:MET:C    | 2:M:340:MET:SD    | 2.91                     | 0.49              |
| 2:M:20:GLU:OE2   | 2:M:460:ARG:HB2   | 2.13                     | 0.49              |
| 2:M:966:LEU:HD11 | 2:M:986:PRO:HG2   | 1.94                     | 0.49              |
| 3:N:1297:GLU:OE1 | 3:N:1299:PHE:HE2  | 1.95                     | 0.49              |
| 3:N:165:LYS:NZ   | 3:N:199:LEU:HB3   | 2.27                     | 0.49              |
| 3:N:28:LYS:CG    | 3:N:29:PRO:HD2    | 2.41                     | 0.49              |
| 3:N:355:VAL:HG13 | 3:N:356:PRO:HD2   | 1.95                     | 0.49              |
| 3:N:508:ARG:HB3  | 3:N:509:PRO:HD2   | 1.94                     | 0.49              |
| 1:L:185:ARG:NH1  | 3:N:692:GLU:HG2   | 2.22                     | 0.49              |
| 3:N:896:ALA:O    | 3:N:900:ILE:HG23  | 2.12                     | 0.49              |
| 5:R:17:DG:H2''   | 5:R:18:DC:C5'     | 2.40                     | 0.49              |
| 7:X:30:THR:HG22  | 7:X:31:LYS:N      | 2.28                     | 0.49              |
| 7:Y:28:GLU:O     | 7:Y:32:ILE:HD13   | 2.13                     | 0.49              |
| 1:A:111:ALA:HB3  | 1:A:124:ASN:O     | 2.13                     | 0.49              |
| 1:B:132:LEU:HD11 | 1:B:138:LEU:HD13  | 1.94                     | 0.49              |
| 1:A:25:LEU:HD22  | 1:B:225:PHE:CE2   | 2.47                     | 0.49              |
| 2:C:182:VAL:CB   | 2:C:193:LEU:CB    | 2.91                     | 0.49              |
| 2:C:208:ALA:HB2  | 2:C:222:MET:CG    | 2.42                     | 0.49              |
| 2:C:36:PRO:HB2   | 2:C:70:GLU:HG2    | 1.93                     | 0.49              |
| 3:D:102:ILE:CD1  | 3:D:586:ARG:HG3   | 2.43                     | 0.49              |
| 3:D:105:VAL:HG21 | 3:D:128:TYR:CE2   | 2.48                     | 0.49              |
| 3:D:1444:THR:O   | 3:D:1448:THR:OG1  | 2.20                     | 0.49              |
| 3:D:481:MET:SD   | 3:D:496:LEU:HD23  | 2.52                     | 0.49              |
| 3:D:704:ARG:NH1  | 3:D:743:ASP:HB3   | 2.27                     | 0.49              |
| 3:D:835:SER:O    | 3:D:837:GLY:N     | 2.46                     | 0.49              |
| 3:D:896:ALA:O    | 3:D:900:ILE:HG23  | 2.12                     | 0.49              |
| 1:F:25:LEU:HD23  | 1:F:28:LEU:HD11   | 1.95                     | 0.49              |
| 1:G:76:VAL:CG1   | 3:I:872:ARG:NH1   | 2.76                     | 0.49              |
| 2:H:1075:ASP:HB2 | 4:J:31:LEU:CD1    | 2.43                     | 0.49              |
| 2:H:1101:THR:C   | 2:H:1102:LEU:HD12 | 2.33                     | 0.49              |
| 2:H:610:ARG:HH11 | 2:H:610:ARG:HG3   | 1.78                     | 0.49              |
| 2:H:806:LEU:HB2  | 2:H:822:VAL:HG22  | 1.95                     | 0.49              |
| 2:H:701:THR:CG2  | 2:H:832:LYS:HA    | 2.43                     | 0.49              |
| 2:H:690:ILE:HG23 | 2:H:852:ILE:HG23  | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1155:VAL:CG1  | 3:I:1177:ALA:CB   | 2.91                     | 0.49              |
| 3:I:1434:TRP:CZ3  | 3:I:1457:ASP:N    | 2.81                     | 0.49              |
| 3:I:521:PRO:HB2   | 3:I:524:LEU:HD13  | 1.94                     | 0.49              |
| 1:K:111:ALA:HB3   | 1:K:124:ASN:O     | 2.12                     | 0.49              |
| 2:M:1059:ASP:OD1  | 2:M:1061:GLU:HB3  | 2.13                     | 0.49              |
| 2:M:368:THR:CB    | 2:M:369:PRO:HD2   | 2.35                     | 0.49              |
| 2:M:432:ARG:NH2   | 3:N:1047:LYS:CD   | 2.46                     | 0.49              |
| 2:M:40:GLU:O      | 2:M:45:GLN:OE1    | 2.31                     | 0.49              |
| 2:M:52:PHE:CG     | 2:M:68:PHE:HB2    | 2.48                     | 0.49              |
| 2:M:612:VAL:HG22  | 2:M:622:GLU:HG3   | 1.94                     | 0.49              |
| 2:M:83:CYS:SG     | 2:M:90:TYR:HB2    | 2.53                     | 0.49              |
| 3:N:1117:TYR:HE1  | 3:N:1119:SER:HG   | 1.61                     | 0.49              |
| 3:N:1160:LEU:HD23 | 3:N:1164:ARG:NH1  | 2.27                     | 0.49              |
| 3:N:982:PHE:CE1   | 7:Z:100:LEU:HD21  | 2.48                     | 0.49              |
| 7:Y:111:ASN:ND2   | 7:Y:113:LEU:HD12  | 2.28                     | 0.49              |
| 3:N:991:GLN:OE1   | 7:Z:111:ASN:ND2   | 2.46                     | 0.49              |
| 1:A:12:THR:OG1    | 1:A:24:VAL:HB     | 2.12                     | 0.49              |
| 2:C:204:GLN:NE2   | 2:C:228:ALA:HB1   | 2.28                     | 0.49              |
| 2:C:662:GLU:O     | 2:C:662:GLU:OE1   | 2.30                     | 0.49              |
| 2:C:923:GLU:O     | 2:C:927:GLY:HA3   | 2.12                     | 0.49              |
| 3:D:350:HIS:CD2   | 3:D:371:ILE:HG12  | 2.48                     | 0.49              |
| 3:D:397:LYS:HE2   | 3:D:448:GLU:OE1   | 2.13                     | 0.49              |
| 3:D:813:LEU:CD1   | 3:D:814:ALA:N     | 2.72                     | 0.49              |
| 2:C:885:ILE:CG2   | 3:D:950:GLY:HA2   | 2.43                     | 0.49              |
| 1:G:87:VAL:CG2    | 1:G:144:VAL:HG11  | 2.42                     | 0.49              |
| 2:H:104:ASP:O     | 2:H:106:GLY:N     | 2.46                     | 0.49              |
| 2:H:127:PHE:O     | 2:H:133:ASP:HA    | 2.12                     | 0.49              |
| 2:H:447:ALA:O     | 2:H:448:ASN:CB    | 2.60                     | 0.49              |
| 2:H:602:GLU:CG    | 2:H:603:VAL:N     | 2.76                     | 0.49              |
| 2:H:861:LEU:HD23  | 2:H:863:ASP:N     | 2.24                     | 0.49              |
| 3:I:1063:GLU:CD   | 3:I:1064:GLY:H    | 2.16                     | 0.49              |
| 3:I:407:VAL:HA    | 3:I:422:ALA:CA    | 2.39                     | 0.49              |
| 3:I:593:ASN:ND2   | 3:I:594:PRO:HD2   | 2.28                     | 0.49              |
| 4:J:37:ASN:HA     | 4:J:93:TYR:CE2    | 2.48                     | 0.49              |
| 1:L:62:LEU:CD1    | 1:L:62:LEU:H      | 2.19                     | 0.49              |
| 2:M:1067:TYR:O    | 2:M:1071:ILE:HG12 | 2.13                     | 0.49              |
| 2:M:93:PRO:HB3    | 2:M:117:HIS:CE1   | 2.48                     | 0.49              |
| 2:M:281:LEU:HA    | 2:M:309:TYR:CE2   | 2.48                     | 0.49              |
| 2:M:217:LEU:CG    | 2:M:311:PHE:CD1   | 2.95                     | 0.49              |
| 2:M:342:ASP:O     | 2:M:345:ARG:HG2   | 2.12                     | 0.49              |
| 2:M:603:VAL:HG12  | 2:M:604:ALA:N     | 2.28                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:863:ASP:CG   | 2:M:865:THR:HG22  | 2.33                     | 0.49              |
| 2:M:861:LEU:HD21 | 2:M:925:TYR:CE2   | 2.47                     | 0.49              |
| 2:M:946:ARG:HD3  | 2:M:984:GLU:HB2   | 1.95                     | 0.49              |
| 2:M:997:LEU:C    | 2:M:999:HIS:N     | 2.64                     | 0.49              |
| 3:N:1089:ALA:C   | 3:N:1091:SER:N    | 2.65                     | 0.49              |
| 3:N:205:TYR:HD1  | 3:N:390:PRO:HG3   | 1.78                     | 0.49              |
| 3:N:133:ILE:CG2  | 3:N:455:ARG:O     | 2.61                     | 0.49              |
| 3:N:81:THR:HG21  | 3:N:85:VAL:CG1    | 2.41                     | 0.49              |
| 7:X:147:ARG:NH2  | 7:X:149:PHE:HZ    | 2.10                     | 0.49              |
| 7:Y:82:VAL:HG22  | 7:Y:133:ARG:HH21  | 1.76                     | 0.49              |
| 2:C:200:LEU:HD13 | 2:C:300:ASP:CG    | 2.33                     | 0.49              |
| 2:C:878:SER:HB3  | 3:D:1029:ARG:CZ   | 2.41                     | 0.49              |
| 3:D:1046:GLN:HA  | 3:D:1052:THR:HA   | 1.95                     | 0.49              |
| 2:C:911:GLU:OE2  | 3:D:1062:ARG:CZ   | 2.61                     | 0.49              |
| 3:D:102:ILE:HD11 | 3:D:106:LYS:HB2   | 1.95                     | 0.49              |
| 3:D:1264:GLU:HG2 | 3:D:1266:ARG:NH2  | 2.28                     | 0.49              |
| 3:D:36:THR:HB    | 3:D:38:LYS:HB2    | 1.95                     | 0.49              |
| 1:F:111:ALA:HB3  | 1:F:124:ASN:O     | 2.13                     | 0.49              |
| 1:G:112:ARG:HG3  | 1:G:125:PRO:CB    | 2.43                     | 0.49              |
| 2:H:380:ALA:O    | 2:H:384:GLU:HB2   | 2.12                     | 0.49              |
| 1:F:70:GLY:N     | 2:H:607:ASP:OD1   | 2.30                     | 0.49              |
| 2:H:662:GLU:OE1  | 2:H:663:ASN:HB2   | 2.13                     | 0.49              |
| 2:H:564:MET:HE2  | 2:H:846:LYS:CD    | 2.42                     | 0.49              |
| 3:I:1295:GLU:HB3 | 3:I:1300:SER:HB3  | 1.95                     | 0.49              |
| 3:I:1448:THR:O   | 3:I:1451:ALA:HB3  | 2.13                     | 0.49              |
| 3:I:615:ARG:CG   | 3:I:619:LEU:HD11  | 2.42                     | 0.49              |
| 3:I:660:LYS:CA   | 3:I:660:LYS:HZ1   | 2.25                     | 0.49              |
| 3:I:704:ARG:NH1  | 3:I:743:ASP:HB3   | 2.27                     | 0.49              |
| 1:G:80:LEU:HD23  | 3:I:867:ARG:CG    | 2.43                     | 0.49              |
| 1:K:117:VAL:CG1  | 1:K:120:VAL:CG1   | 2.91                     | 0.49              |
| 1:L:195:LEU:HD12 | 1:L:196:THR:N     | 2.28                     | 0.49              |
| 2:M:535:SER:O    | 2:M:538:GLN:HG2   | 2.12                     | 0.49              |
| 3:N:1046:GLN:HA  | 3:N:1052:THR:HA   | 1.95                     | 0.49              |
| 3:N:1063:GLU:CD  | 3:N:1064:GLY:H    | 2.15                     | 0.49              |
| 2:M:906:PHE:CE1  | 3:N:1067:VAL:HA   | 2.48                     | 0.49              |
| 3:N:141:ILE:C    | 3:N:141:ILE:HD13  | 2.32                     | 0.49              |
| 3:N:111:LYS:CD   | 3:N:1448:THR:HG22 | 2.43                     | 0.49              |
| 3:N:351:MET:O    | 3:N:352:ASN:OD1   | 2.31                     | 0.49              |
| 3:N:970:LYS:HE2  | 7:Z:113:LEU:CD2   | 2.39                     | 0.49              |
| 1:B:143:ARG:HD3  | 1:B:158:ILE:HG21  | 1.95                     | 0.48              |
| 2:C:11:GLU:CD    | 2:C:537:LYS:NZ    | 2.66                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:14:ARG:HH21   | 2:C:934:PHE:HZ    | 1.61                     | 0.48              |
| 3:D:1094:LEU:O    | 3:D:1098:LEU:HD13 | 2.13                     | 0.48              |
| 3:D:1312:LEU:HD12 | 3:D:1327:ARG:NH2  | 2.28                     | 0.48              |
| 3:D:431:VAL:HG12  | 3:D:432:TYR:N     | 2.27                     | 0.48              |
| 2:C:682:TYR:CD1   | 3:D:635:PRO:HG2   | 2.48                     | 0.48              |
| 3:D:705:ALA:HB3   | 3:D:706:PRO:HD3   | 1.94                     | 0.48              |
| 3:D:957:PRO:HG3   | 3:D:1007:VAL:HA   | 1.95                     | 0.48              |
| 4:E:41:GLU:N      | 4:E:42:PRO:CD     | 2.76                     | 0.48              |
| 2:H:1019:GLN:OE1  | 3:I:621:LYS:CB    | 2.61                     | 0.48              |
| 2:H:142:ARG:HD2   | 2:H:147:TYR:CE1   | 2.47                     | 0.48              |
| 2:H:278:GLU:HA    | 2:H:283:ILE:HA    | 1.94                     | 0.48              |
| 2:H:478:VAL:HA    | 2:H:506:ASN:O     | 2.13                     | 0.48              |
| 2:H:477:GLY:O     | 2:H:507:ARG:HA    | 2.13                     | 0.48              |
| 3:I:1356:TYR:HD2  | 3:I:1361:VAL:HG11 | 1.76                     | 0.48              |
| 3:I:89:ARG:O      | 3:I:521:PRO:CB    | 2.60                     | 0.48              |
| 4:J:40:LEU:C      | 4:J:40:LEU:HD12   | 2.34                     | 0.48              |
| 1:K:41:ARG:HG3    | 1:K:177:VAL:CG1   | 2.43                     | 0.48              |
| 2:M:258:TYR:OH    | 2:M:290:LEU:HD21  | 2.13                     | 0.48              |
| 2:M:650:ARG:HG2   | 2:M:653:ASP:OD2   | 2.13                     | 0.48              |
| 2:M:806:LEU:HB2   | 2:M:822:VAL:HG22  | 1.95                     | 0.48              |
| 2:M:6:PHE:CZ      | 2:M:901:TYR:HB3   | 2.46                     | 0.48              |
| 3:N:1114:THR:HG22 | 3:N:1195:GLN:HB3  | 1.93                     | 0.48              |
| 3:N:1256:LEU:O    | 3:N:1259:VAL:N    | 2.46                     | 0.48              |
| 3:N:100:ALA:CB    | 3:N:128:TYR:CZ    | 2.95                     | 0.48              |
| 3:N:1408:ILE:HD12 | 3:N:1408:ILE:H    | 1.76                     | 0.48              |
| 3:N:169:TYR:CE2   | 3:N:196:VAL:O     | 2.66                     | 0.48              |
| 3:N:205:TYR:C     | 3:N:205:TYR:CD2   | 2.86                     | 0.48              |
| 3:N:355:VAL:HG21  | 3:N:367:ILE:HG23  | 1.94                     | 0.48              |
| 3:N:432:TYR:CB    | 3:N:450:TYR:CD2   | 2.96                     | 0.48              |
| 3:N:525:ARG:HG2   | 3:N:525:ARG:O     | 2.12                     | 0.48              |
| 3:N:95:LEU:HA     | 3:N:551:ASN:OD1   | 2.13                     | 0.48              |
| 7:X:83:ILE:HD13   | 7:X:89:VAL:HG21   | 1.96                     | 0.48              |
| 7:Y:85:LEU:HD21   | 7:Y:121:ASP:CG    | 2.32                     | 0.48              |
| 2:C:185:LYS:HG2   | 2:C:190:LYS:HG3   | 1.87                     | 0.48              |
| 2:C:432:ARG:HH22  | 3:D:1047:LYS:CD   | 2.24                     | 0.48              |
| 2:C:501:THR:HG21  | 2:C:513:VAL:CG1   | 2.44                     | 0.48              |
| 2:C:52:PHE:CD2    | 2:C:68:PHE:HB2    | 2.48                     | 0.48              |
| 2:C:754:ILE:CD1   | 2:C:754:ILE:H     | 2.25                     | 0.48              |
| 3:D:1103:HIS:CD2  | 3:D:1463:LYS:HB2  | 2.48                     | 0.48              |
| 3:D:1106:VAL:HG12 | 3:D:1107:VAL:H    | 1.78                     | 0.48              |
| 3:D:415:VAL:HG12  | 3:D:416:ALA:N     | 2.28                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:1036:GLU:HG3 | 3:D:707:THR:CB    | 2.43                     | 0.48              |
| 3:D:796:ARG:HB2  | 3:D:828:LYS:HD3   | 1.95                     | 0.48              |
| 3:D:907:GLU:N    | 3:D:910:SER:OG    | 2.46                     | 0.48              |
| 1:F:69:PRO:O     | 1:F:71:VAL:HG23   | 2.13                     | 0.48              |
| 2:H:1085:PHE:CE2 | 3:I:1468:LEU:CG   | 2.91                     | 0.48              |
| 3:I:1437:ALA:HB3 | 3:I:1446:VAL:CG1  | 2.43                     | 0.48              |
| 3:I:982:PHE:HE1  | 7:Y:100:LEU:HD21  | 1.78                     | 0.48              |
| 1:K:8:ALA:O      | 1:K:9:PRO:C       | 2.52                     | 0.48              |
| 1:L:108:GLU:OE1  | 1:L:128:HIS:NE2   | 2.45                     | 0.48              |
| 2:M:163:ILE:O    | 2:M:163:ILE:HG23  | 2.14                     | 0.48              |
| 2:M:203:ASP:O    | 2:M:207:LEU:HB2   | 2.13                     | 0.48              |
| 2:M:265:ARG:HD3  | 2:M:267:TYR:CG    | 2.48                     | 0.48              |
| 2:M:437:ARG:HH22 | 2:M:488:ALA:HA    | 1.70                     | 0.48              |
| 3:N:1042:ARG:CB  | 3:N:1042:ARG:HH11 | 2.26                     | 0.48              |
| 2:M:432:ARG:HD3  | 3:N:1048:PRO:HG2  | 1.94                     | 0.48              |
| 3:N:1264:GLU:HG2 | 3:N:1266:ARG:NH2  | 2.28                     | 0.48              |
| 3:N:36:THR:HB    | 3:N:38:LYS:HB2    | 1.95                     | 0.48              |
| 3:N:729:HIS:HB3  | 3:N:732:VAL:HG22  | 1.94                     | 0.48              |
| 3:N:704:ARG:NH1  | 3:N:743:ASP:HB3   | 2.27                     | 0.48              |
| 3:N:841:TYR:HB2  | 3:N:864:VAL:HG11  | 1.96                     | 0.48              |
| 1:B:58:ILE:HG21  | 1:B:68:ILE:CD1    | 2.43                     | 0.48              |
| 2:C:1067:TYR:O   | 2:C:1071:ILE:HG12 | 2.13                     | 0.48              |
| 2:C:1101:THR:C   | 2:C:1102:LEU:HD12 | 2.33                     | 0.48              |
| 2:C:182:VAL:CG1  | 2:C:193:LEU:CB    | 2.90                     | 0.48              |
| 2:C:140:ILE:HG23 | 2:C:410:ILE:CG2   | 2.43                     | 0.48              |
| 3:D:1063:GLU:CD  | 3:D:1064:GLY:H    | 2.15                     | 0.48              |
| 3:D:33:ASN:HD21  | 3:D:35:ARG:CZ     | 2.26                     | 0.48              |
| 1:B:152:PRO:CG   | 3:D:857:ILE:HD11  | 2.42                     | 0.48              |
| 3:D:911:LEU:HD23 | 3:D:934:LEU:HD13  | 1.94                     | 0.48              |
| 4:E:47:LYS:C     | 4:E:54:LEU:HD12   | 2.32                     | 0.48              |
| 1:F:189:ARG:CG   | 1:F:189:ARG:NH1   | 2.72                     | 0.48              |
| 1:F:33:GLY:O     | 1:F:195:LEU:HD13  | 2.13                     | 0.48              |
| 1:F:35:THR:HG21  | 1:G:43:ILE:CD1    | 2.43                     | 0.48              |
| 1:G:195:LEU:HD12 | 1:G:196:THR:N     | 2.28                     | 0.48              |
| 2:H:1085:PHE:CD2 | 3:I:1468:LEU:HA   | 2.48                     | 0.48              |
| 2:H:211:LEU:HG   | 2:H:218:VAL:HG22  | 1.95                     | 0.48              |
| 2:H:50:GLU:HG3   | 2:H:266:ARG:NE    | 2.28                     | 0.48              |
| 2:H:544:THR:O    | 2:H:547:ILE:HD12  | 2.12                     | 0.48              |
| 3:I:1264:GLU:CD  | 3:I:1424:VAL:HG13 | 2.31                     | 0.48              |
| 3:I:182:GLY:N    | 3:I:441:ARG:HD3   | 2.28                     | 0.48              |
| 3:I:872:ARG:CZ   | 1:L:162:ILE:HG21  | 2.42                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:118:ILE:HD12  | 2:M:119:PRO:O     | 2.12                     | 0.48              |
| 2:M:154:ARG:NH1   | 2:M:178:PRO:HG3   | 2.28                     | 0.48              |
| 2:M:258:TYR:OH    | 2:M:290:LEU:CD2   | 2.62                     | 0.48              |
| 2:M:334:ARG:HG2   | 2:M:338:GLU:OE2   | 2.12                     | 0.48              |
| 2:M:544:THR:O     | 2:M:547:ILE:HD12  | 2.12                     | 0.48              |
| 2:M:54:ILE:O      | 2:M:54:ILE:CG2    | 2.60                     | 0.48              |
| 2:M:549:PHE:HB3   | 2:M:552:HIS:HD2   | 1.78                     | 0.48              |
| 2:M:86:LYS:O      | 2:M:813:VAL:HG23  | 2.14                     | 0.48              |
| 3:N:1111:ASP:CG   | 3:N:1203:LYS:HD2  | 2.33                     | 0.48              |
| 3:N:1384:PRO:CB   | 3:N:1388:ARG:HH12 | 2.26                     | 0.48              |
| 3:N:1397:LYS:NZ   | 3:N:1432:LYS:HZ3  | 2.12                     | 0.48              |
| 3:N:695:ILE:HD11  | 3:N:718:PRO:HB2   | 1.95                     | 0.48              |
| 4:O:41:GLU:HG2    | 4:O:42:PRO:N      | 2.27                     | 0.48              |
| 2:C:685:GLU:CD    | 7:X:41:ASP:OD1    | 2.51                     | 0.48              |
| 2:C:879:ARG:HH22  | 7:X:42:ASP:HB2    | 1.76                     | 0.48              |
| 3:D:1029:ARG:HH21 | 7:X:42:ASP:HB3    | 1.78                     | 0.48              |
| 7:Z:76:GLU:O      | 7:Z:76:GLU:OE2    | 2.32                     | 0.48              |
| 1:A:117:VAL:CG1   | 1:A:120:VAL:CG1   | 2.91                     | 0.48              |
| 1:B:122:ILE:CD1   | 1:B:122:ILE:N     | 2.70                     | 0.48              |
| 1:B:179:PHE:N     | 1:B:179:PHE:CD2   | 2.79                     | 0.48              |
| 1:B:195:LEU:HD12  | 1:B:196:THR:N     | 2.28                     | 0.48              |
| 2:C:165:LEU:CB    | 2:C:265:ARG:HH12  | 2.23                     | 0.48              |
| 2:C:208:ALA:HB2   | 2:C:222:MET:HG3   | 1.95                     | 0.48              |
| 2:C:265:ARG:HG2   | 2:C:267:TYR:H     | 1.78                     | 0.48              |
| 2:C:662:GLU:OE1   | 2:C:663:ASN:HB2   | 2.13                     | 0.48              |
| 2:C:756:VAL:HB    | 2:C:790:LEU:HB3   | 1.95                     | 0.48              |
| 3:D:1263:PHE:HB3  | 3:D:1424:VAL:HG11 | 1.96                     | 0.48              |
| 3:D:1434:TRP:CE2  | 3:D:1435:LEU:HD12 | 2.48                     | 0.48              |
| 2:C:1046:ALA:HB2  | 3:D:1476:THR:HB   | 1.94                     | 0.48              |
| 2:H:326:ASP:O     | 2:H:328:LEU:HD12  | 2.13                     | 0.48              |
| 2:H:379:GLU:O     | 2:H:383:ARG:HB3   | 2.14                     | 0.48              |
| 2:H:405:ARG:HD2   | 2:H:442:GLU:OE1   | 2.14                     | 0.48              |
| 2:H:591:SER:O     | 2:H:592:LEU:HB2   | 2.13                     | 0.48              |
| 2:H:863:ASP:CG    | 2:H:865:THR:HG22  | 2.33                     | 0.48              |
| 2:H:998:TYR:O     | 2:H:998:TYR:CG    | 2.66                     | 0.48              |
| 3:I:102:ILE:HD11  | 3:I:106:LYS:HB2   | 1.95                     | 0.48              |
| 3:I:1312:LEU:HD12 | 3:I:1327:ARG:NH2  | 2.28                     | 0.48              |
| 3:I:135:LEU:HD22  | 3:I:149:LYS:O     | 2.13                     | 0.48              |
| 3:I:617:ASN:HB3   | 3:I:1467:ILE:HA   | 1.95                     | 0.48              |
| 3:I:473:LEU:HA    | 3:I:476:GLU:HB2   | 1.96                     | 0.48              |
| 3:I:544:TYR:O     | 3:I:548:ILE:HG12  | 2.12                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:882:PHE:HE1   | 3:I:934:LEU:HD21  | 1.77                     | 0.48              |
| 3:I:896:ALA:O     | 3:I:900:ILE:HG23  | 2.12                     | 0.48              |
| 4:J:26:ARG:HE     | 4:J:30:LEU:HD11   | 1.78                     | 0.48              |
| 1:L:156:HIS:CE1   | 1:L:158:ILE:HG12  | 2.48                     | 0.48              |
| 2:M:1086:ARG:HH22 | 2:M:1111:ILE:HD11 | 1.78                     | 0.48              |
| 2:M:128:ILE:C     | 2:M:129:ILE:HD12  | 2.32                     | 0.48              |
| 2:M:794:PRO:HG2   | 2:M:1025:ALA:CA   | 2.40                     | 0.48              |
| 2:M:77:PRO:CD     | 2:M:91:GLN:O      | 2.61                     | 0.48              |
| 2:M:435:TYR:HA    | 3:N:1071:PHE:CE2  | 2.48                     | 0.48              |
| 3:N:1209:LEU:O    | 3:N:1210:SER:C    | 2.48                     | 0.48              |
| 3:N:1452:ILE:HD12 | 3:N:1452:ILE:N    | 2.29                     | 0.48              |
| 3:N:148:GLU:CG    | 3:N:151:GLN:HB3   | 2.41                     | 0.48              |
| 3:N:102:ILE:HG21  | 3:N:583:ASP:HB3   | 1.95                     | 0.48              |
| 3:N:804:LEU:HD23  | 3:N:804:LEU:H     | 1.78                     | 0.48              |
| 3:N:911:LEU:HD23  | 3:N:934:LEU:HD13  | 1.94                     | 0.48              |
| 4:O:41:GLU:N      | 4:O:42:PRO:CD     | 2.76                     | 0.48              |
| 1:B:221:HIS:HA    | 1:B:224:TYR:HD2   | 1.77                     | 0.48              |
| 2:C:1014:SER:HB2  | 2:C:1021:LEU:CD1  | 2.43                     | 0.48              |
| 2:C:104:ASP:O     | 2:C:106:GLY:N     | 2.46                     | 0.48              |
| 2:C:129:ILE:N     | 2:C:129:ILE:CD1   | 2.76                     | 0.48              |
| 2:C:185:LYS:HG2   | 2:C:190:LYS:CA    | 2.44                     | 0.48              |
| 2:C:26:TYR:CE2    | 2:C:127:PHE:CZ    | 3.02                     | 0.48              |
| 2:C:270:GLY:O     | 2:C:274:ARG:HB3   | 2.13                     | 0.48              |
| 2:C:322:VAL:O     | 2:C:322:VAL:HG23  | 2.13                     | 0.48              |
| 2:C:326:ASP:OD2   | 2:C:426:ASP:OD1   | 2.32                     | 0.48              |
| 2:C:546:LEU:C     | 2:C:581:THR:HG21  | 2.34                     | 0.48              |
| 2:C:640:ARG:NH1   | 2:C:640:ARG:HG2   | 2.29                     | 0.48              |
| 2:C:794:PRO:HD2   | 2:C:1024:LYS:O    | 2.13                     | 0.48              |
| 2:C:85:GLU:O      | 2:C:824:ARG:NH2   | 2.47                     | 0.48              |
| 2:C:998:TYR:O     | 2:C:998:TYR:CG    | 2.66                     | 0.48              |
| 3:D:124:GLU:CD    | 3:D:128:TYR:HE1   | 2.17                     | 0.48              |
| 3:D:1412:LYS:HE2  | 3:D:1414:PRO:HG3  | 1.96                     | 0.48              |
| 3:D:415:VAL:HG13  | 3:D:419:ASP:HB2   | 1.94                     | 0.48              |
| 3:D:728:LEU:HD22  | 3:D:745:MET:SD    | 2.52                     | 0.48              |
| 3:D:820:GLU:HG3   | 3:D:836:VAL:HG21  | 1.95                     | 0.48              |
| 2:H:508:ILE:HG22  | 2:H:509:ALA:H     | 1.78                     | 0.48              |
| 2:H:52:PHE:CE1    | 2:H:67:ASP:C      | 2.86                     | 0.48              |
| 2:H:549:PHE:HB3   | 2:H:552:HIS:HD2   | 1.78                     | 0.48              |
| 2:H:557:ARG:HG3   | 2:H:557:ARG:HH11  | 1.79                     | 0.48              |
| 2:H:583:LEU:O     | 2:H:587:VAL:HG23  | 2.14                     | 0.48              |
| 2:H:679:PHE:HB2   | 2:H:683:ASN:ND2   | 2.23                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:79:PRO:HG2    | 2:H:82:GLU:CG     | 2.43                     | 0.48              |
| 2:H:840:ALA:CB    | 2:H:846:LYS:HA    | 2.43                     | 0.48              |
| 2:H:689:VAL:HG11  | 2:H:853:LEU:HD22  | 1.95                     | 0.48              |
| 2:H:69:LEU:HG     | 2:H:97:ARG:O      | 2.14                     | 0.48              |
| 3:I:783:ARG:CZ    | 3:I:1029:ARG:NH2  | 2.76                     | 0.48              |
| 3:I:107:ASP:OD1   | 3:I:1444:THR:CG2  | 2.53                     | 0.48              |
| 3:I:1084:THR:HA   | 3:I:1087:ARG:HH11 | 1.78                     | 0.48              |
| 3:I:1089:ALA:C    | 3:I:1091:SER:N    | 2.66                     | 0.48              |
| 3:I:1440:PHE:O    | 3:I:1441:GLN:O    | 2.32                     | 0.48              |
| 3:I:202:VAL:HB    | 3:I:396:VAL:CG2   | 2.43                     | 0.48              |
| 3:I:621:LYS:HA    | 3:I:621:LYS:HD3   | 1.38                     | 0.48              |
| 1:L:221:HIS:HA    | 1:L:224:TYR:HD2   | 1.77                     | 0.48              |
| 1:L:77:GLU:HA     | 1:L:80:LEU:HD22   | 1.95                     | 0.48              |
| 1:L:78:ILE:O      | 1:L:82:LEU:HG     | 2.13                     | 0.48              |
| 2:M:708:TYR:CE2   | 2:M:793:PRO:HD2   | 2.49                     | 0.48              |
| 3:N:501:ALA:CB    | 3:N:1453:ALA:HB2  | 2.44                     | 0.48              |
| 3:N:103:TRP:NE1   | 3:N:604:THR:OG1   | 2.20                     | 0.48              |
| 3:N:638:LYS:HD3   | 3:N:932:ASP:CG    | 2.34                     | 0.48              |
| 3:N:849:ALA:O     | 3:N:853:VAL:HG23  | 2.14                     | 0.48              |
| 3:N:843:PHE:HB2   | 3:N:866:VAL:HG22  | 1.95                     | 0.48              |
| 4:O:43:GLU:O      | 4:O:44:GLU:HB2    | 2.14                     | 0.48              |
| 7:X:7:LEU:HD22    | 7:X:109:GLU:HB2   | 1.94                     | 0.48              |
| 1:B:73:GLU:CD     | 1:B:130:ALA:HA    | 2.33                     | 0.48              |
| 1:B:15:THR:O      | 1:B:15:THR:HG23   | 2.13                     | 0.48              |
| 2:C:1095:LEU:HD11 | 2:C:1097:LEU:HD22 | 1.93                     | 0.48              |
| 2:C:30:LEU:HB3    | 2:C:44:ILE:HG13   | 1.96                     | 0.48              |
| 2:C:327:HIS:CE1   | 2:C:488:ALA:HB1   | 2.49                     | 0.48              |
| 3:D:1209:LEU:HD12 | 3:D:1215:VAL:HA   | 1.94                     | 0.48              |
| 3:D:1257:PRO:O    | 3:D:1261:GLU:HB2  | 2.13                     | 0.48              |
| 3:D:1273:VAL:O    | 3:D:1325:LEU:HB2  | 2.13                     | 0.48              |
| 3:D:525:ARG:HG2   | 3:D:525:ARG:O     | 2.12                     | 0.48              |
| 3:D:687:VAL:HG13  | 3:D:688:TRP:N     | 2.28                     | 0.48              |
| 2:H:294:GLU:HG2   | 2:H:295:ASP:OD2   | 2.12                     | 0.48              |
| 2:H:338:GLU:C     | 2:H:341:THR:HG22  | 2.33                     | 0.48              |
| 2:H:724:ARG:HG2   | 2:H:724:ARG:O     | 2.14                     | 0.48              |
| 3:I:111:LYS:HG3   | 3:I:1452:ILE:HG12 | 1.95                     | 0.48              |
| 3:I:1161:GLU:CD   | 3:I:1164:ARG:HB2  | 2.34                     | 0.48              |
| 3:I:1264:GLU:HG2  | 3:I:1266:ARG:NH2  | 2.28                     | 0.48              |
| 3:I:1399:ASP:O    | 3:I:1403:LEU:HB2  | 2.14                     | 0.48              |
| 2:H:1046:ALA:HA   | 3:I:1472:ILE:HD13 | 1.95                     | 0.48              |
| 3:I:434:ARG:HB2   | 3:I:449:SER:OG    | 2.14                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:I:50:PHE:O      | 3:I:89:ARG:HG2   | 2.08                     | 0.48              |
| 3:I:546:ARG:HH12  | 3:I:550:ARG:HH21 | 1.60                     | 0.48              |
| 3:I:606:ILE:CD1   | 3:I:613:ARG:HE   | 2.26                     | 0.48              |
| 3:I:619:LEU:N     | 3:I:619:LEU:HD23 | 2.29                     | 0.48              |
| 3:I:820:GLU:HG3   | 3:I:836:VAL:HG21 | 1.95                     | 0.48              |
| 3:I:835:SER:O     | 3:I:837:GLY:N    | 2.46                     | 0.48              |
| 2:M:840:ALA:CB    | 2:M:846:LYS:HA   | 2.44                     | 0.48              |
| 3:N:1164:ARG:NH2  | 3:N:1170:ASP:OD1 | 2.47                     | 0.48              |
| 3:N:1273:VAL:O    | 3:N:1325:LEU:HB2 | 2.13                     | 0.48              |
| 3:N:171:LEU:C     | 3:N:171:LEU:HD23 | 2.34                     | 0.48              |
| 3:N:645:PRO:HG3   | 3:N:725:SER:O    | 2.14                     | 0.48              |
| 3:N:907:GLU:N     | 3:N:910:SER:OG   | 2.46                     | 0.48              |
| 3:N:704:ARG:NH2   | 6:U:16:G:C2'     | 2.76                     | 0.48              |
| 7:X:16:MET:SD     | 7:X:69:LEU:HD13  | 2.54                     | 0.48              |
| 1:B:80:LEU:HG     | 3:D:844:ALA:HA   | 1.96                     | 0.48              |
| 2:C:1072:LYS:O    | 3:D:659:LYS:HE2  | 2.13                     | 0.48              |
| 2:C:565:GLN:HE21  | 2:C:842:ARG:CG   | 2.07                     | 0.48              |
| 2:C:617:ASP:OD1   | 2:C:618:GLY:N    | 2.46                     | 0.48              |
| 3:D:583:ASP:HB2   | 3:D:604:THR:OG1  | 2.13                     | 0.48              |
| 1:F:42:ARG:NH1    | 1:G:34:VAL:CB    | 2.57                     | 0.48              |
| 1:G:115:LEU:HA    | 1:G:116:PRO:HD3  | 1.71                     | 0.48              |
| 1:G:212:ASN:O     | 1:G:215:VAL:CG2  | 2.54                     | 0.48              |
| 1:G:41:ARG:NH1    | 1:G:177:VAL:CG2  | 2.69                     | 0.48              |
| 1:G:86:VAL:HG12   | 1:G:124:ASN:HB2  | 1.96                     | 0.48              |
| 2:H:1013:TYR:HD1  | 2:H:1020:PRO:HA  | 1.79                     | 0.48              |
| 2:H:309:TYR:OH    | 2:H:319:GLY:O    | 2.30                     | 0.48              |
| 2:H:640:ARG:NH1   | 2:H:640:ARG:HG2  | 2.29                     | 0.48              |
| 3:I:1034:GLN:O    | 3:I:1037:GLN:N   | 2.46                     | 0.48              |
| 3:I:1273:VAL:O    | 3:I:1325:LEU:HB2 | 2.13                     | 0.48              |
| 3:I:501:ALA:HB1   | 3:I:1453:ALA:HB2 | 1.96                     | 0.48              |
| 3:I:729:HIS:HB3   | 3:I:732:VAL:HG22 | 1.94                     | 0.48              |
| 3:I:805:GLU:O     | 3:I:809:PRO:HD2  | 2.13                     | 0.48              |
| 3:I:922:LEU:N     | 3:I:922:LEU:CD2  | 2.75                     | 0.48              |
| 2:M:322:VAL:O     | 2:M:322:VAL:HG23 | 2.13                     | 0.48              |
| 1:K:150:TYR:OH    | 2:M:695:LEU:HD22 | 2.13                     | 0.48              |
| 3:N:102:ILE:HD11  | 3:N:106:LYS:HB2  | 1.95                     | 0.48              |
| 3:N:1312:LEU:HD12 | 3:N:1327:ARG:NH2 | 2.28                     | 0.48              |
| 3:N:1399:ASP:O    | 3:N:1403:LEU:HB2 | 2.14                     | 0.48              |
| 3:N:1434:TRP:CD1  | 3:N:1435:LEU:N   | 2.82                     | 0.48              |
| 3:N:813:LEU:CD1   | 3:N:814:ALA:N    | 2.72                     | 0.48              |
| 4:O:57:ASP:H      | 4:O:58:PRO:HD3   | 1.79                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:41:ARG:CG     | 1:B:177:VAL:HG21  | 2.27                     | 0.48              |
| 1:B:62:LEU:CD1    | 1:B:63:HIS:N      | 2.71                     | 0.48              |
| 2:C:133:ASP:OD2   | 2:C:133:ASP:N     | 2.45                     | 0.48              |
| 2:C:217:LEU:O     | 2:C:220:GLY:N     | 2.27                     | 0.48              |
| 2:C:886:LEU:HD11  | 3:D:951:ILE:HD12  | 1.95                     | 0.48              |
| 3:D:1401:GLU:OE1  | 3:D:1415:VAL:HG11 | 2.14                     | 0.48              |
| 3:D:1488:ASP:N    | 3:D:1488:ASP:OD1  | 2.46                     | 0.48              |
| 3:D:158:TYR:HD1   | 3:D:162:ARG:CB    | 2.20                     | 0.48              |
| 3:D:210:ARG:N     | 3:D:389:GLU:HB2   | 2.29                     | 0.48              |
| 3:D:563:PRO:HA    | 2:H:223:ASP:CB    | 2.34                     | 0.48              |
| 3:D:97:THR:HB     | 3:D:571:LYS:HE2   | 1.94                     | 0.48              |
| 1:F:128:HIS:HE1   | 1:F:131:THR:CG2   | 2.24                     | 0.48              |
| 1:F:89:PHE:HD1    | 1:F:120:VAL:CG2   | 2.25                     | 0.48              |
| 2:H:124:ASP:N     | 2:H:124:ASP:OD1   | 2.40                     | 0.48              |
| 2:H:200:LEU:HD13  | 2:H:300:ASP:OD2   | 2.14                     | 0.48              |
| 2:H:203:ASP:HB2   | 2:H:206:THR:HG22  | 1.96                     | 0.48              |
| 2:H:245:GLY:C     | 2:H:246:ASP:CG    | 2.71                     | 0.48              |
| 2:H:170:PRO:HG2   | 2:H:258:TYR:CD1   | 2.48                     | 0.48              |
| 2:H:332:ARG:HG3   | 2:H:465:GLY:CA    | 2.28                     | 0.48              |
| 2:H:523:ILE:HD13  | 2:H:523:ILE:C     | 2.32                     | 0.48              |
| 2:H:630:ARG:HD2   | 2:H:634:GLY:HA2   | 1.96                     | 0.48              |
| 2:H:754:ILE:CD1   | 2:H:754:ILE:H     | 2.25                     | 0.48              |
| 3:I:1042:ARG:HH11 | 3:I:1042:ARG:CB   | 2.26                     | 0.48              |
| 3:I:1195:GLN:HG3  | 3:I:1196:THR:N    | 2.29                     | 0.48              |
| 3:I:28:LYS:N      | 3:I:42:ASP:O      | 2.45                     | 0.48              |
| 3:I:645:PRO:HG3   | 3:I:725:SER:O     | 2.14                     | 0.48              |
| 3:I:661:MET:CE    | 3:I:673:ALA:HB1   | 2.44                     | 0.48              |
| 3:I:911:LEU:HD23  | 3:I:934:LEU:HD13  | 1.94                     | 0.48              |
| 1:L:41:ARG:NH1    | 1:L:177:VAL:CG2   | 2.74                     | 0.48              |
| 2:M:113:VAL:O     | 2:M:115:LEU:HD22  | 2.13                     | 0.48              |
| 2:M:302:VAL:C     | 2:M:305:PRO:HD2   | 2.33                     | 0.48              |
| 2:M:722:ILE:O     | 2:M:722:ILE:HG23  | 2.14                     | 0.48              |
| 2:M:831:ARG:HD2   | 2:M:1000:MET:CE   | 2.44                     | 0.48              |
| 2:M:1034:GLU:CD   | 3:N:1096:ARG:HH22 | 2.16                     | 0.48              |
| 3:N:1128:VAL:HG12 | 3:N:1129:THR:HG22 | 1.95                     | 0.48              |
| 3:N:1101:VAL:CG1  | 3:N:1424:VAL:HG23 | 2.40                     | 0.48              |
| 3:N:1434:TRP:NE1  | 3:N:1435:LEU:CD1  | 2.77                     | 0.48              |
| 3:N:701:LEU:HD13  | 3:N:748:HIS:HB2   | 1.96                     | 0.48              |
| 3:N:811:GLU:O     | 3:N:815:ALA:HB3   | 2.14                     | 0.48              |
| 5:R:20:DG:H22     | 6:S:11:C:H42      | 1.60                     | 0.48              |
| 2:C:1083:GLU:CD   | 2:C:1086:ARG:HD2  | 2.31                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:182:VAL:HG11  | 2:C:193:LEU:HD23  | 1.92                     | 0.48              |
| 2:C:267:TYR:CB    | 2:C:272:ALA:CB    | 2.79                     | 0.48              |
| 2:C:910:LYS:O     | 2:C:914:ILE:HG13  | 2.14                     | 0.48              |
| 3:D:1144:LEU:HD11 | 3:D:1186:VAL:HG21 | 1.96                     | 0.48              |
| 3:D:1176:LYS:O    | 3:D:1179:GLU:HB2  | 2.14                     | 0.48              |
| 2:C:1085:PHE:CD2  | 3:D:1468:LEU:HD23 | 2.48                     | 0.48              |
| 1:F:41:ARG:HG3    | 1:F:177:VAL:CG1   | 2.43                     | 0.48              |
| 1:G:110:LYS:HD3   | 1:G:126:ASP:HA    | 1.96                     | 0.48              |
| 1:F:13:VAL:N      | 1:G:229:GLN:O     | 2.36                     | 0.48              |
| 2:H:168:ARG:HG2   | 2:H:263:ASP:OD2   | 2.14                     | 0.48              |
| 2:H:26:TYR:CE2    | 2:H:30:LEU:HD21   | 2.49                     | 0.48              |
| 2:H:22:GLN:NE2    | 2:H:336:VAL:CG2   | 2.77                     | 0.48              |
| 2:H:701:THR:HG22  | 2:H:832:LYS:HA    | 1.96                     | 0.48              |
| 2:H:984:GLU:HG2   | 3:I:944:THR:O     | 2.13                     | 0.48              |
| 3:I:957:PRO:HG3   | 3:I:1007:VAL:HA   | 1.95                     | 0.48              |
| 3:I:199:LEU:HD23  | 3:I:200:ASP:N     | 2.29                     | 0.48              |
| 3:I:701:LEU:HD13  | 3:I:748:HIS:HB2   | 1.96                     | 0.48              |
| 3:I:700:VAL:HG12  | 3:I:749:VAL:HG13  | 1.95                     | 0.48              |
| 1:K:221:HIS:NE2   | 1:L:32:PHE:CE2    | 2.81                     | 0.48              |
| 2:M:230:ARG:NH1   | 2:M:230:ARG:HG2   | 2.28                     | 0.48              |
| 2:M:313:LEU:HD13  | 2:M:321:GLU:CG    | 2.42                     | 0.48              |
| 2:M:432:ARG:HD3   | 3:N:1048:PRO:CG   | 2.44                     | 0.48              |
| 2:M:487:THR:HG22  | 2:M:489:THR:OG1   | 2.13                     | 0.48              |
| 2:M:876:VAL:H     | 2:M:877:PRO:HD2   | 1.77                     | 0.48              |
| 2:M:96:ALA:O      | 2:M:98:LEU:CD1    | 2.61                     | 0.48              |
| 3:N:1176:LYS:O    | 3:N:1179:GLU:HB2  | 2.14                     | 0.48              |
| 3:N:123:LEU:O     | 3:N:126:VAL:HB    | 2.13                     | 0.48              |
| 3:N:1252:ILE:HD11 | 3:N:1329:ALA:HB2  | 1.95                     | 0.48              |
| 3:N:163:TYR:HA    | 3:N:163:TYR:HD2   | 1.60                     | 0.48              |
| 3:N:211:VAL:HG12  | 3:N:213:VAL:HG22  | 1.93                     | 0.48              |
| 3:N:799:LYS:HG2   | 3:N:799:LYS:O     | 2.10                     | 0.48              |
| 7:Y:6:LYS:HD3     | 7:Y:75:LEU:HD11   | 1.96                     | 0.48              |
| 7:Z:128:ALA:CB    | 7:Z:140:LEU:HD11  | 2.44                     | 0.48              |
| 2:C:1084:SER:CB   | 3:D:617:ASN:HD21  | 2.27                     | 0.48              |
| 2:C:1092:LEU:HD22 | 2:C:1099:VAL:HG23 | 1.96                     | 0.48              |
| 2:C:122:THR:CB    | 2:C:124:ASP:OD1   | 2.56                     | 0.48              |
| 2:C:153:ALA:O     | 2:C:155:PRO:HD3   | 2.14                     | 0.48              |
| 2:C:175:GLU:HG2   | 2:C:183:SER:OG    | 2.12                     | 0.48              |
| 2:C:51:THR:OG1    | 2:C:348:LEU:HB3   | 2.13                     | 0.48              |
| 2:C:401:LEU:HD13  | 2:C:587:VAL:HG11  | 1.95                     | 0.48              |
| 2:C:64:LEU:CD1    | 2:C:100:LEU:HD11  | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:708:TYR:CE2   | 2:C:793:PRO:HD2   | 2.49                     | 0.48              |
| 3:D:783:ARG:HA    | 3:D:1028:ALA:HA   | 1.96                     | 0.48              |
| 3:D:1372:VAL:O    | 3:D:1375:MET:HB2  | 2.14                     | 0.48              |
| 3:D:1264:GLU:OE2  | 3:D:1424:VAL:HG12 | 2.11                     | 0.48              |
| 3:D:1486:VAL:HG23 | 4:E:29:GLN:OE1    | 2.14                     | 0.48              |
| 3:D:28:LYS:HG3    | 3:D:29:PRO:HD2    | 1.93                     | 0.48              |
| 3:D:799:LYS:O     | 3:D:826:PRO:HD2   | 2.14                     | 0.48              |
| 1:G:170:VAL:O     | 1:G:170:VAL:HG23  | 2.14                     | 0.48              |
| 1:G:52:ALA:HB1    | 1:G:170:VAL:H     | 1.78                     | 0.48              |
| 1:G:57:TYR:CZ     | 1:G:59:GLU:HA     | 2.49                     | 0.48              |
| 2:H:218:VAL:HG12  | 2:H:222:MET:HG3   | 1.94                     | 0.48              |
| 2:H:304:LEU:O     | 2:H:308:ARG:N     | 2.46                     | 0.48              |
| 3:I:160:GLU:CG    | 3:I:165:LYS:HB2   | 2.42                     | 0.48              |
| 3:I:451:ASP:O     | 3:I:452:ILE:HG22  | 2.14                     | 0.48              |
| 3:I:639:LEU:HD22  | 3:I:766:ALA:HA    | 1.96                     | 0.48              |
| 1:L:115:LEU:HD12  | 1:L:115:LEU:C     | 2.34                     | 0.48              |
| 1:L:44:LEU:HA     | 1:L:48:ILE:CD1    | 2.40                     | 0.48              |
| 2:M:442:GLU:CG    | 2:M:454:SER:HB2   | 2.40                     | 0.48              |
| 2:M:449:ILE:CD1   | 3:N:1081:GLY:HA3  | 2.44                     | 0.48              |
| 2:M:516:ARG:HD2   | 3:N:1068:LEU:HD22 | 1.95                     | 0.48              |
| 2:M:697:ARG:CD    | 2:M:699:PHE:CD1   | 2.92                     | 0.48              |
| 2:M:754:ILE:CD1   | 2:M:754:ILE:H     | 2.25                     | 0.48              |
| 2:M:876:VAL:N     | 2:M:877:PRO:HD2   | 2.29                     | 0.48              |
| 3:N:957:PRO:HG3   | 3:N:1007:VAL:HA   | 1.95                     | 0.48              |
| 3:N:1140:ILE:HG22 | 3:N:1144:LEU:HD12 | 1.95                     | 0.48              |
| 2:M:1046:ALA:HB3  | 3:N:1476:THR:OG1  | 2.13                     | 0.48              |
| 3:N:153:LEU:C     | 3:N:153:LEU:CD1   | 2.82                     | 0.48              |
| 3:N:191:LEU:HD13  | 3:N:393:ILE:CG2   | 2.44                     | 0.48              |
| 3:N:199:LEU:HD23  | 3:N:200:ASP:H     | 1.79                     | 0.48              |
| 4:O:3:GLU:OE1     | 4:O:4:PRO:HD3     | 2.14                     | 0.48              |
| 1:A:21:GLY:HA3    | 1:A:207:PRO:CB    | 2.43                     | 0.47              |
| 2:C:1086:ARG:HD3  | 3:D:88:TYR:HE1    | 1.73                     | 0.47              |
| 2:C:278:GLU:HG3   | 2:C:279:GLU:N     | 2.28                     | 0.47              |
| 2:C:946:ARG:HD3   | 2:C:984:GLU:HB2   | 1.95                     | 0.47              |
| 2:C:992:MET:O     | 2:C:994:ILE:HD12  | 2.14                     | 0.47              |
| 2:C:878:SER:CB    | 3:D:1029:ARG:HD3  | 2.44                     | 0.47              |
| 3:D:1042:ARG:CB   | 3:D:1042:ARG:HH11 | 2.26                     | 0.47              |
| 3:D:1280:VAL:O    | 3:D:1294:VAL:HA   | 2.14                     | 0.47              |
| 3:D:135:LEU:HB2   | 3:D:151:GLN:O     | 2.14                     | 0.47              |
| 3:D:206:ARG:HB3   | 3:D:207:PHE:CE1   | 2.49                     | 0.47              |
| 3:D:638:LYS:HD3   | 3:D:932:ASP:CB    | 2.44                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:167:VAL:HG12  | 1:F:168:ASP:N     | 2.29                     | 0.47              |
| 1:F:169:ALA:HB1   | 1:F:171:PHE:CE2   | 2.49                     | 0.47              |
| 1:G:123:MET:C     | 1:G:125:PRO:HD3   | 2.34                     | 0.47              |
| 2:H:191:PHE:HB2   | 2:H:241:LEU:HD11  | 1.95                     | 0.47              |
| 2:H:358:ARG:HA    | 2:H:361:MET:HB3   | 1.96                     | 0.47              |
| 2:H:946:ARG:HD3   | 2:H:984:GLU:HB2   | 1.95                     | 0.47              |
| 3:I:1106:VAL:HG21 | 3:I:1474:ALA:HB2  | 1.96                     | 0.47              |
| 3:I:1176:LYS:O    | 3:I:1179:GLU:HB2  | 2.14                     | 0.47              |
| 3:I:1401:GLU:OE1  | 3:I:1415:VAL:HG11 | 2.14                     | 0.47              |
| 2:H:1085:PHE:CD2  | 3:I:1468:LEU:HD23 | 2.49                     | 0.47              |
| 3:I:1481:VAL:HG22 | 4:J:18:ARG:NH2    | 2.28                     | 0.47              |
| 3:I:462:GLN:O     | 3:I:466:LYS:HG3   | 2.14                     | 0.47              |
| 3:I:486:ARG:HA    | 3:I:489:ARG:CG    | 2.35                     | 0.47              |
| 1:K:26:GLU:HG3    | 1:K:185:ARG:HB2   | 1.96                     | 0.47              |
| 1:L:161:ARG:HG3   | 1:L:161:ARG:NH1   | 2.29                     | 0.47              |
| 1:L:58:ILE:CG2    | 1:L:61:VAL:HG23   | 2.44                     | 0.47              |
| 2:M:176:VAL:O     | 2:M:176:VAL:HG23  | 2.14                     | 0.47              |
| 2:M:333:ILE:CG1   | 2:M:410:ILE:HD11  | 2.44                     | 0.47              |
| 2:M:49:ARG:O      | 2:M:53:PRO:HD3    | 2.13                     | 0.47              |
| 2:M:546:LEU:C     | 2:M:581:THR:HG21  | 2.34                     | 0.47              |
| 2:M:679:PHE:O     | 2:M:680:ASP:C     | 2.49                     | 0.47              |
| 2:M:69:LEU:HD11   | 2:M:99:GLN:CD     | 2.34                     | 0.47              |
| 2:M:998:TYR:CG    | 2:M:998:TYR:O     | 2.66                     | 0.47              |
| 2:M:99:GLN:OE1    | 2:M:110:GLU:CG    | 2.59                     | 0.47              |
| 3:N:1147:ARG:O    | 3:N:1165:TYR:HA   | 2.13                     | 0.47              |
| 3:N:1401:GLU:OE1  | 3:N:1415:VAL:HG11 | 2.14                     | 0.47              |
| 3:N:367:ILE:HB    | 3:N:377:VAL:HG12  | 1.95                     | 0.47              |
| 3:N:438:ASP:HB2   | 3:N:445:ARG:HH12  | 1.79                     | 0.47              |
| 3:N:514:LEU:HD12  | 3:N:578:VAL:HG11  | 1.96                     | 0.47              |
| 2:M:850:ALA:CA    | 3:N:632:VAL:CG1   | 2.88                     | 0.47              |
| 3:N:97:THR:HB     | 3:N:571:LYS:HD2   | 1.96                     | 0.47              |
| 4:O:40:LEU:HD12   | 4:O:40:LEU:C      | 2.34                     | 0.47              |
| 7:X:6:LYS:HB3     | 7:X:75:LEU:CD1    | 2.44                     | 0.47              |
| 7:Z:22:GLU:HB3    | 7:Z:62:ILE:HD11   | 1.96                     | 0.47              |
| 1:A:91:ASN:HD22   | 1:A:93:SER:CB     | 2.27                     | 0.47              |
| 1:B:58:ILE:HG21   | 1:B:68:ILE:HD11   | 1.96                     | 0.47              |
| 2:C:236:ILE:HD12  | 2:C:236:ILE:N     | 2.29                     | 0.47              |
| 2:C:18:LEU:O      | 2:C:408:ARG:NH1   | 2.47                     | 0.47              |
| 2:C:546:LEU:HD13  | 2:C:565:GLN:OE1   | 2.14                     | 0.47              |
| 2:C:630:ARG:HD2   | 2:C:634:GLY:HA2   | 1.96                     | 0.47              |
| 3:D:102:ILE:HD13  | 3:D:106:LYS:HB2   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1299:PHE:N    | 3:D:1299:PHE:CD2  | 2.79                     | 0.47              |
| 3:D:180:LYS:HG2   | 3:D:183:GLU:HB2   | 1.97                     | 0.47              |
| 3:D:456:MET:O     | 3:D:459:GLU:HB3   | 2.14                     | 0.47              |
| 3:D:701:LEU:HD13  | 3:D:748:HIS:HB2   | 1.96                     | 0.47              |
| 3:D:843:PHE:HB2   | 3:D:866:VAL:HG22  | 1.95                     | 0.47              |
| 3:D:850:LEU:HA    | 3:D:853:VAL:HG23  | 1.96                     | 0.47              |
| 3:D:1216:SER:CB   | 4:E:16:LYS:H      | 2.28                     | 0.47              |
| 4:E:37:ASN:HD21   | 4:E:93:TYR:HB3    | 1.77                     | 0.47              |
| 1:F:117:VAL:CG1   | 1:F:120:VAL:CG1   | 2.91                     | 0.47              |
| 1:G:128:HIS:CE1   | 1:G:131:THR:HG23  | 2.50                     | 0.47              |
| 2:H:12:VAL:HG13   | 2:H:13:ILE:N      | 2.28                     | 0.47              |
| 3:I:1035:ILE:CA   | 3:I:1038:LEU:HD12 | 2.42                     | 0.47              |
| 3:I:1258:ARG:NH2  | 3:I:1262:LEU:CD1  | 2.77                     | 0.47              |
| 3:I:783:ARG:CD    | 7:Y:41:ASP:OD2    | 2.62                     | 0.47              |
| 3:I:811:GLU:O     | 3:I:815:ALA:HB3   | 2.14                     | 0.47              |
| 3:I:850:LEU:HA    | 3:I:853:VAL:HG23  | 1.96                     | 0.47              |
| 2:M:142:ARG:CD    | 2:M:325:ILE:CG2   | 2.91                     | 0.47              |
| 3:N:1026:SER:C    | 3:N:1028:ALA:H    | 2.18                     | 0.47              |
| 3:N:155:ASP:O     | 3:N:158:TYR:HB3   | 2.14                     | 0.47              |
| 3:N:465:LEU:HD21  | 3:N:509:PRO:CB    | 2.44                     | 0.47              |
| 2:M:1005:MET:HA   | 3:N:628:ARG:O     | 2.14                     | 0.47              |
| 3:N:925:GLU:OE2   | 4:O:3:GLU:O       | 2.32                     | 0.47              |
| 1:A:127:LEU:HD12  | 1:A:128:HIS:N     | 2.29                     | 0.47              |
| 1:A:169:ALA:HB1   | 1:A:171:PHE:CE2   | 2.49                     | 0.47              |
| 1:A:41:ARG:HG3    | 1:A:177:VAL:CG1   | 2.43                     | 0.47              |
| 1:A:79:ILE:HG13   | 1:A:80:LEU:N      | 2.29                     | 0.47              |
| 2:C:195:LEU:HD12  | 2:C:195:LEU:O     | 2.15                     | 0.47              |
| 2:C:198:ARG:NH1   | 2:C:204:GLN:HG2   | 2.29                     | 0.47              |
| 2:C:334:ARG:HB3   | 2:C:339:LEU:HD21  | 1.96                     | 0.47              |
| 2:C:455:LEU:HD12  | 2:C:455:LEU:C     | 2.35                     | 0.47              |
| 2:C:674:VAL:HG12  | 2:C:990:GLY:O     | 2.13                     | 0.47              |
| 2:C:571:LEU:HD11  | 2:C:700:TYR:C     | 2.33                     | 0.47              |
| 3:D:1089:ALA:C    | 3:D:1091:SER:N    | 2.66                     | 0.47              |
| 3:D:1366:LYS:HA   | 3:D:1369:GLU:OE1  | 2.15                     | 0.47              |
| 3:D:1442:ASN:HD22 | 3:D:1445:HIS:H    | 1.61                     | 0.47              |
| 3:D:361:VAL:HB    | 3:D:383:GLY:O     | 2.14                     | 0.47              |
| 3:D:546:ARG:HH11  | 3:D:546:ARG:CG    | 2.27                     | 0.47              |
| 3:D:660:LYS:HZ1   | 3:D:660:LYS:CA    | 2.27                     | 0.47              |
| 3:D:631:ILE:CD1   | 3:D:743:ASP:O     | 2.54                     | 0.47              |
| 3:D:849:ALA:O     | 3:D:853:VAL:HG23  | 2.14                     | 0.47              |
| 2:H:236:ILE:HD12  | 2:H:236:ILE:N     | 2.29                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:126:SER:CB    | 2:H:395:LYS:NZ    | 2.78                     | 0.47              |
| 2:H:469:THR:CG2   | 2:H:470:PRO:HD2   | 2.36                     | 0.47              |
| 2:H:402:SER:HA    | 2:H:566:THR:HG23  | 1.95                     | 0.47              |
| 2:H:676:ILE:HG21  | 2:H:988:VAL:CG1   | 2.36                     | 0.47              |
| 3:I:1098:LEU:HD21 | 3:I:1229:ILE:HG22 | 1.95                     | 0.47              |
| 3:I:133:ILE:O     | 3:I:152:LEU:HB3   | 2.14                     | 0.47              |
| 3:I:26:VAL:CG2    | 3:I:26:VAL:O      | 2.62                     | 0.47              |
| 3:I:810:GLU:C     | 3:I:812:ALA:H     | 2.15                     | 0.47              |
| 3:I:849:ALA:O     | 3:I:853:VAL:HG23  | 2.14                     | 0.47              |
| 1:K:167:VAL:HG12  | 1:K:168:ASP:N     | 2.28                     | 0.47              |
| 1:K:24:VAL:HG22   | 1:K:196:THR:CG2   | 2.43                     | 0.47              |
| 1:L:157:GLY:O     | 1:L:159:LYS:HD3   | 2.13                     | 0.47              |
| 1:L:95:GLN:HE21   | 1:L:95:GLN:HB2    | 1.57                     | 0.47              |
| 2:M:1081:VAL:HG12 | 2:M:1085:PHE:HB3  | 1.93                     | 0.47              |
| 2:M:136:ILE:CG2   | 2:M:336:VAL:HG13  | 2.43                     | 0.47              |
| 2:M:501:THR:CG2   | 2:M:513:VAL:HG13  | 2.44                     | 0.47              |
| 2:M:557:ARG:HH11  | 2:M:557:ARG:HG3   | 1.78                     | 0.47              |
| 1:K:67:THR:CG2    | 2:M:627:ARG:NH2   | 2.77                     | 0.47              |
| 2:M:653:ASP:OD1   | 2:M:654:LEU:HD23  | 2.14                     | 0.47              |
| 2:M:831:ARG:NH1   | 2:M:1000:MET:HG3  | 2.28                     | 0.47              |
| 2:M:831:ARG:NH1   | 2:M:1002:GLU:CB   | 2.76                     | 0.47              |
| 2:M:910:LYS:O     | 2:M:914:ILE:HG13  | 2.14                     | 0.47              |
| 2:M:992:MET:O     | 2:M:994:ILE:HD12  | 2.14                     | 0.47              |
| 3:N:115:LEU:O     | 3:N:115:LEU:HD23  | 2.14                     | 0.47              |
| 3:N:1137:ARG:NH2  | 3:N:1172:HIS:NE2  | 2.63                     | 0.47              |
| 3:N:1123:PHE:CE2  | 3:N:1184:GLN:HA   | 2.36                     | 0.47              |
| 3:N:1195:GLN:HG3  | 3:N:1196:THR:N    | 2.29                     | 0.47              |
| 3:N:1252:ILE:CD1  | 3:N:1329:ALA:HB2  | 2.44                     | 0.47              |
| 3:N:438:ASP:CB    | 3:N:445:ARG:HH12  | 2.28                     | 0.47              |
| 3:N:462:GLN:O     | 3:N:466:LYS:HG3   | 2.14                     | 0.47              |
| 2:M:1056:LYS:CB   | 3:N:623:VAL:HG13  | 2.45                     | 0.47              |
| 2:M:911:GLU:CD    | 3:N:951:ILE:CD1   | 2.74                     | 0.47              |
| 1:B:162:ILE:O     | 1:B:162:ILE:HD12  | 2.14                     | 0.47              |
| 1:B:179:PHE:N     | 1:B:179:PHE:HD2   | 2.12                     | 0.47              |
| 2:C:354:GLY:O     | 2:C:358:ARG:HD3   | 2.15                     | 0.47              |
| 2:C:557:ARG:HH11  | 2:C:557:ARG:HG3   | 1.79                     | 0.47              |
| 2:C:572:ILE:CD1   | 2:C:573:ARG:H     | 2.17                     | 0.47              |
| 2:C:691:SER:HB2   | 2:C:858:MET:SD    | 2.55                     | 0.47              |
| 3:D:1066:THR:HG22 | 3:D:1069:GLU:CB   | 2.38                     | 0.47              |
| 3:D:1089:ALA:C    | 3:D:1091:SER:H    | 2.18                     | 0.47              |
| 3:D:160:GLU:O     | 3:D:164:GLY:C     | 2.53                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:407:VAL:CG2   | 3:D:408:GLU:H     | 2.14                     | 0.47              |
| 3:D:433:GLY:HA3   | 3:D:447:VAL:O     | 2.14                     | 0.47              |
| 3:D:86:ARG:HB2    | 3:D:523:ASP:OD2   | 2.15                     | 0.47              |
| 3:D:553:ARG:HH12  | 3:D:573:MET:CE    | 2.27                     | 0.47              |
| 3:D:625:TYR:HB3   | 3:D:749:VAL:CG2   | 2.43                     | 0.47              |
| 3:D:645:PRO:HG3   | 3:D:725:SER:O     | 2.14                     | 0.47              |
| 1:F:46:SER:HB3    | 2:H:856:GLU:CG    | 2.44                     | 0.47              |
| 1:F:91:ASN:HD22   | 1:F:93:SER:CB     | 2.26                     | 0.47              |
| 1:G:51:THR:CG2    | 1:G:145:ASP:O     | 2.63                     | 0.47              |
| 2:H:12:VAL:CG1    | 2:H:534:VAL:HG13  | 2.44                     | 0.47              |
| 2:H:876:VAL:N     | 2:H:877:PRO:HD2   | 2.29                     | 0.47              |
| 3:I:1147:ARG:HD2  | 3:I:1188:VAL:HG21 | 1.95                     | 0.47              |
| 3:I:133:ILE:HG22  | 3:I:134:VAL:N     | 2.29                     | 0.47              |
| 3:I:1428:ALA:O    | 3:I:1431:THR:HG22 | 2.14                     | 0.47              |
| 3:I:593:ASN:CB    | 3:I:594:PRO:HD2   | 2.45                     | 0.47              |
| 3:I:810:GLU:C     | 3:I:812:ALA:N     | 2.67                     | 0.47              |
| 3:I:841:TYR:HB2   | 3:I:864:VAL:HG11  | 1.95                     | 0.47              |
| 1:K:127:LEU:HD12  | 1:K:128:HIS:N     | 2.29                     | 0.47              |
| 1:K:7:LYS:O       | 1:K:7:LYS:HD3     | 2.15                     | 0.47              |
| 1:L:52:ALA:HB1    | 1:L:170:VAL:H     | 1.79                     | 0.47              |
| 2:M:63:GLY:N      | 2:M:103:LYS:HG3   | 2.29                     | 0.47              |
| 2:M:704:HIS:O     | 2:M:828:ALA:HA    | 2.14                     | 0.47              |
| 3:N:1105:ILE:N    | 3:N:1105:ILE:CD1  | 2.77                     | 0.47              |
| 3:N:1274:ILE:HD12 | 3:N:1274:ILE:O    | 2.14                     | 0.47              |
| 3:N:1304:LYS:HE2  | 3:N:1304:LYS:HB3  | 1.64                     | 0.47              |
| 3:N:1372:VAL:O    | 3:N:1375:MET:HB2  | 2.14                     | 0.47              |
| 3:N:142:LEU:HA    | 3:N:145:VAL:O     | 2.14                     | 0.47              |
| 3:N:1462:LEU:HD23 | 3:N:1472:ILE:HG22 | 1.95                     | 0.47              |
| 3:N:169:TYR:HE1   | 3:N:198:ARG:HG3   | 1.79                     | 0.47              |
| 7:Y:66:GLU:O      | 7:Y:70:SER:HB3    | 2.15                     | 0.47              |
| 7:Z:58:ILE:HG22   | 7:Z:62:ILE:CD1    | 2.44                     | 0.47              |
| 1:A:167:VAL:HG12  | 1:A:168:ASP:N     | 2.29                     | 0.47              |
| 1:A:176:ARG:NH1   | 2:C:865:THR:HB    | 2.28                     | 0.47              |
| 1:B:65:PHE:CD1    | 3:D:813:LEU:HD22  | 2.49                     | 0.47              |
| 2:C:101:ILE:HD13  | 2:C:108:ILE:CG2   | 2.43                     | 0.47              |
| 2:C:549:PHE:HB3   | 2:C:552:HIS:HD2   | 1.79                     | 0.47              |
| 2:C:571:LEU:CD1   | 2:C:701:THR:H     | 2.27                     | 0.47              |
| 2:C:620:LEU:O     | 2:C:620:LEU:HD12  | 2.15                     | 0.47              |
| 3:D:682:ASP:HB3   | 3:D:684:LYS:H     | 1.80                     | 0.47              |
| 3:D:695:ILE:HD11  | 3:D:718:PRO:HB2   | 1.95                     | 0.47              |
| 3:D:639:LEU:HD22  | 3:D:766:ALA:HA    | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:811:GLU:O     | 3:D:815:ALA:HB3   | 2.14                     | 0.47              |
| 1:F:206:THR:HG23  | 1:F:208:LEU:H     | 1.79                     | 0.47              |
| 2:H:1012:PRO:HD2  | 2:H:1026:GLN:CB   | 2.44                     | 0.47              |
| 2:H:1067:TYR:O    | 2:H:1071:ILE:HG12 | 2.13                     | 0.47              |
| 2:H:115:LEU:N     | 2:H:115:LEU:HD23  | 2.30                     | 0.47              |
| 2:H:195:LEU:HD12  | 2:H:195:LEU:O     | 2.15                     | 0.47              |
| 2:H:332:ARG:CD    | 2:H:464:LEU:O     | 2.62                     | 0.47              |
| 2:H:498:GLN:HE21  | 2:H:498:GLN:CA    | 2.24                     | 0.47              |
| 2:H:714:ASP:OD1   | 2:H:719:PRO:HG3   | 2.15                     | 0.47              |
| 3:I:1046:GLN:HA   | 3:I:1052:THR:HA   | 1.95                     | 0.47              |
| 3:I:1462:LEU:HD22 | 3:I:1472:ILE:HG21 | 1.97                     | 0.47              |
| 3:I:167:GLU:HG2   | 3:I:169:TYR:CE1   | 2.50                     | 0.47              |
| 3:I:185:VAL:HG21  | 3:I:203:ALA:CB    | 2.44                     | 0.47              |
| 3:I:402:PRO:O     | 3:I:427:VAL:HG21  | 2.14                     | 0.47              |
| 3:I:457:GLY:C     | 3:I:459:GLU:N     | 2.66                     | 0.47              |
| 3:I:695:ILE:HD11  | 3:I:718:PRO:HB2   | 1.95                     | 0.47              |
| 3:I:984:THR:CG2   | 3:I:987:GLU:HG3   | 2.45                     | 0.47              |
| 2:M:204:GLN:NE2   | 2:M:228:ALA:CB    | 2.76                     | 0.47              |
| 2:M:290:LEU:HB2   | 2:M:302:VAL:HG11  | 1.88                     | 0.47              |
| 2:M:379:GLU:O     | 2:M:383:ARG:HB3   | 2.14                     | 0.47              |
| 2:M:474:VAL:CG2   | 2:M:479:VAL:HG12  | 2.45                     | 0.47              |
| 2:M:603:VAL:HA    | 2:M:613:VAL:HG12  | 1.95                     | 0.47              |
| 3:N:1011:PHE:HB3  | 3:N:1021:TYR:CD1  | 2.50                     | 0.47              |
| 3:N:1029:ARG:CG   | 3:N:1029:ARG:HH11 | 2.27                     | 0.47              |
| 3:N:26:VAL:CG2    | 3:N:26:VAL:O      | 2.62                     | 0.47              |
| 3:N:434:ARG:O     | 3:N:447:VAL:CG2   | 2.58                     | 0.47              |
| 3:N:415:VAL:HG23  | 3:N:435:VAL:HG23  | 1.95                     | 0.47              |
| 3:N:540:LEU:N     | 3:N:540:LEU:HD12  | 2.29                     | 0.47              |
| 3:N:54:LYS:HG3    | 3:N:55:ASP:H      | 1.80                     | 0.47              |
| 3:N:638:LYS:O     | 3:N:640:HIS:N     | 2.47                     | 0.47              |
| 3:N:639:LEU:HD22  | 3:N:766:ALA:HA    | 1.96                     | 0.47              |
| 3:N:781:PRO:HB2   | 3:N:786:ILE:CD1   | 2.44                     | 0.47              |
| 3:N:820:GLU:HG3   | 3:N:836:VAL:HG21  | 1.96                     | 0.47              |
| 3:N:984:THR:CG2   | 3:N:987:GLU:HG3   | 2.44                     | 0.47              |
| 7:X:103:GLN:NE2   | 7:X:105:VAL:CG1   | 2.77                     | 0.47              |
| 7:X:74:ILE:O      | 7:X:74:ILE:HG23   | 2.15                     | 0.47              |
| 7:Y:150:ARG:HB3   | 7:Y:150:ARG:HH11  | 1.79                     | 0.47              |
| 2:C:139:GLN:O     | 2:C:333:ILE:HA    | 2.15                     | 0.47              |
| 2:C:876:VAL:N     | 2:C:877:PRO:HD2   | 2.29                     | 0.47              |
| 3:D:148:GLU:N     | 3:D:148:GLU:OE2   | 2.48                     | 0.47              |
| 3:D:352:ASN:C     | 3:D:368:VAL:HG13  | 2.35                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:661:MET:CE    | 3:D:673:ALA:HB1  | 2.44                     | 0.47              |
| 3:D:799:LYS:HE2   | 3:D:824:ASN:O    | 2.14                     | 0.47              |
| 1:G:35:THR:O      | 1:G:39:PRO:HG2   | 2.14                     | 0.47              |
| 2:H:546:LEU:HD13  | 2:H:565:GLN:OE1  | 2.14                     | 0.47              |
| 2:H:546:LEU:C     | 2:H:581:THR:HG21 | 2.34                     | 0.47              |
| 2:H:610:ARG:NH1   | 2:H:610:ARG:HG3  | 2.29                     | 0.47              |
| 2:H:653:ASP:OD1   | 2:H:654:LEU:HD23 | 2.14                     | 0.47              |
| 2:H:910:LYS:O     | 2:H:914:ILE:HG13 | 2.14                     | 0.47              |
| 2:H:992:MET:O     | 2:H:994:ILE:HD12 | 2.14                     | 0.47              |
| 3:I:1106:VAL:CG1  | 3:I:1107:VAL:N   | 2.73                     | 0.47              |
| 3:I:1274:ILE:HD12 | 3:I:1274:ILE:O   | 2.14                     | 0.47              |
| 3:I:907:GLU:N     | 3:I:910:SER:OG   | 2.46                     | 0.47              |
| 1:K:169:ALA:HB1   | 1:K:171:PHE:CE2  | 2.49                     | 0.47              |
| 2:M:163:ILE:HD12  | 2:M:171:TRP:CZ3  | 2.50                     | 0.47              |
| 2:M:188:LYS:NZ    | 2:M:188:LYS:CA   | 2.78                     | 0.47              |
| 2:M:157:ARG:NE    | 2:M:314:THR:HG23 | 2.28                     | 0.47              |
| 2:M:140:ILE:CG2   | 2:M:410:ILE:HD13 | 2.44                     | 0.47              |
| 2:M:405:ARG:HD2   | 2:M:442:GLU:OE1  | 2.14                     | 0.47              |
| 2:M:332:ARG:HG3   | 2:M:465:GLY:HA3  | 1.96                     | 0.47              |
| 2:M:472:ARG:NH1   | 2:M:480:THR:O    | 2.47                     | 0.47              |
| 2:M:487:THR:HG22  | 2:M:489:THR:H    | 1.78                     | 0.47              |
| 2:M:630:ARG:HD2   | 2:M:634:GLY:HA2  | 1.96                     | 0.47              |
| 2:M:662:GLU:OE1   | 2:M:663:ASN:HB2  | 2.13                     | 0.47              |
| 2:M:694:LEU:HD11  | 2:M:868:ASP:HB3  | 1.96                     | 0.47              |
| 3:N:1041:LEU:HD12 | 3:N:1058:ARG:CA  | 2.44                     | 0.47              |
| 3:N:102:ILE:HD13  | 3:N:106:LYS:HB2  | 1.96                     | 0.47              |
| 3:N:1462:LEU:HD23 | 3:N:1472:ILE:CG2 | 2.45                     | 0.47              |
| 3:N:148:GLU:HB3   | 3:N:151:GLN:CB   | 2.45                     | 0.47              |
| 3:N:162:ARG:HA    | 3:N:162:ARG:HD3  | 1.71                     | 0.47              |
| 3:N:607:LEU:HD23  | 3:N:607:LEU:HA   | 1.65                     | 0.47              |
| 3:N:689:ASP:O     | 3:N:693:GLU:HB2  | 2.15                     | 0.47              |
| 1:B:32:PHE:O      | 1:B:36:LEU:HG    | 2.15                     | 0.47              |
| 2:C:251:ASP:O     | 2:C:253:ALA:N    | 2.48                     | 0.47              |
| 2:C:270:GLY:O     | 2:C:274:ARG:HD3  | 2.15                     | 0.47              |
| 2:C:302:VAL:O     | 2:C:306:THR:HG23 | 2.15                     | 0.47              |
| 2:C:319:GLY:O     | 2:C:321:GLU:CD   | 2.53                     | 0.47              |
| 2:C:367:LEU:O     | 2:C:367:LEU:HD12 | 2.14                     | 0.47              |
| 2:C:443:THR:HG21  | 3:D:1078:ARG:HD2 | 1.96                     | 0.47              |
| 3:D:1137:ARG:HH21 | 3:D:1172:HIS:CD2 | 2.31                     | 0.47              |
| 3:D:1274:ILE:HD12 | 3:D:1274:ILE:O   | 2.14                     | 0.47              |
| 3:D:393:ILE:N     | 3:D:393:ILE:CD1  | 2.75                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:484:PRO:HB3   | 3:D:488:ARG:CG    | 2.44                     | 0.47              |
| 3:D:95:LEU:CD2    | 3:D:574:LEU:HD21  | 2.44                     | 0.47              |
| 3:D:638:LYS:O     | 3:D:640:HIS:N     | 2.48                     | 0.47              |
| 2:H:1013:TYR:O    | 2:H:1015:LEU:HD12 | 2.14                     | 0.47              |
| 2:H:1092:LEU:HD22 | 2:H:1099:VAL:HG23 | 1.97                     | 0.47              |
| 2:H:338:GLU:HA    | 2:H:341:THR:HG22  | 1.96                     | 0.47              |
| 2:H:455:LEU:HD12  | 2:H:455:LEU:C     | 2.35                     | 0.47              |
| 2:H:487:THR:HB    | 2:H:490:GLU:CG    | 2.43                     | 0.47              |
| 2:H:606:VAL:HG21  | 2:H:645:VAL:HG22  | 1.97                     | 0.47              |
| 3:I:1120:VAL:HG23 | 3:I:1188:VAL:CG1  | 2.45                     | 0.47              |
| 3:I:1292:VAL:CG2  | 3:I:1311:LEU:HD13 | 2.45                     | 0.47              |
| 3:I:123:LEU:CD1   | 3:I:152:LEU:HD11  | 2.44                     | 0.47              |
| 3:I:814:ALA:O     | 3:I:818:ARG:HG3   | 2.15                     | 0.47              |
| 3:I:843:PHE:HB2   | 3:I:866:VAL:HG22  | 1.95                     | 0.47              |
| 4:J:25:LYS:C      | 4:J:28:GLN:HG3    | 2.35                     | 0.47              |
| 4:J:47:LYS:O      | 4:J:54:LEU:HD12   | 2.15                     | 0.47              |
| 1:K:91:ASN:HD22   | 1:K:93:SER:CB     | 2.27                     | 0.47              |
| 1:L:170:VAL:O     | 1:L:170:VAL:HG23  | 2.14                     | 0.47              |
| 2:M:199:VAL:HG12  | 2:M:298:PHE:CE1   | 2.49                     | 0.47              |
| 2:M:316:GLY:O     | 2:M:318:PRO:HD3   | 2.13                     | 0.47              |
| 2:M:640:ARG:HG2   | 2:M:640:ARG:NH1   | 2.29                     | 0.47              |
| 2:M:564:MET:SD    | 2:M:846:LYS:CE    | 3.03                     | 0.47              |
| 2:M:93:PRO:HA     | 2:M:117:HIS:ND1   | 2.30                     | 0.47              |
| 3:N:1035:ILE:CA   | 3:N:1038:LEU:HD12 | 2.41                     | 0.47              |
| 3:N:1145:TYR:O    | 3:N:1147:ARG:HG2  | 2.14                     | 0.47              |
| 3:N:1253:THR:O    | 3:N:1258:ARG:HB2  | 2.15                     | 0.47              |
| 3:N:191:LEU:O     | 3:N:192:ALA:CB    | 2.58                     | 0.47              |
| 3:N:441:ARG:HH11  | 3:N:445:ARG:NH2   | 2.12                     | 0.47              |
| 2:M:1051:GLU:OE1  | 3:N:750:PRO:HA    | 2.13                     | 0.47              |
| 4:O:59:ASN:HD21   | 4:O:61:VAL:HG23   | 1.80                     | 0.47              |
| 7:Y:88:VAL:HG23   | 7:Y:156:GLY:OXT   | 2.14                     | 0.47              |
| 1:B:100:LEU:HB2   | 1:B:115:LEU:HD21  | 1.97                     | 0.47              |
| 2:C:1010:THR:CG2  | 2:C:1011:GLY:N    | 2.77                     | 0.47              |
| 2:C:107:LEU:C     | 2:C:108:ILE:HG13  | 2.35                     | 0.47              |
| 3:D:1041:LEU:HD12 | 3:D:1058:ARG:CA   | 2.44                     | 0.47              |
| 3:D:10:ILE:O      | 3:D:1454:GLY:HA2  | 2.14                     | 0.47              |
| 3:D:1101:VAL:HG11 | 3:D:1424:VAL:CG2  | 2.42                     | 0.47              |
| 3:D:129:PHE:O     | 3:D:130:SER:CB    | 2.62                     | 0.47              |
| 3:D:1363:LEU:HD11 | 3:D:1368:ILE:HD11 | 1.97                     | 0.47              |
| 3:D:1459:LEU:HD11 | 3:D:1468:LEU:HD12 | 1.97                     | 0.47              |
| 3:D:145:VAL:CG2   | 3:D:146:PRO:CD    | 2.86                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:204:LEU:O     | 3:D:393:ILE:HA    | 2.15                     | 0.47              |
| 4:E:40:LEU:O      | 4:E:40:LEU:HD12   | 2.15                     | 0.47              |
| 2:H:195:LEU:HD13  | 2:H:234:ALA:HB1   | 1.92                     | 0.47              |
| 2:H:353:ARG:HG3   | 2:H:353:ARG:HH11  | 1.80                     | 0.47              |
| 2:H:444:PRO:CD    | 2:H:452:ILE:O     | 2.62                     | 0.47              |
| 2:H:604:ALA:HB3   | 2:H:612:VAL:O     | 2.14                     | 0.47              |
| 2:H:928:LYS:HZ3   | 2:H:932:GLU:HG3   | 1.79                     | 0.47              |
| 3:I:1282:ARG:HA   | 3:I:1315:ASP:HA   | 1.97                     | 0.47              |
| 3:I:1263:PHE:HB3  | 3:I:1424:VAL:HG11 | 1.96                     | 0.47              |
| 3:I:1459:LEU:HD13 | 3:I:1468:LEU:CD1  | 2.45                     | 0.47              |
| 3:I:456:MET:O     | 3:I:459:GLU:HB3   | 2.14                     | 0.47              |
| 3:I:949:ILE:HD12  | 3:I:949:ILE:N     | 2.29                     | 0.47              |
| 1:K:206:THR:CG2   | 1:K:209:GLU:HG3   | 2.45                     | 0.47              |
| 2:M:129:ILE:HG12  | 2:M:134:ARG:HD2   | 1.93                     | 0.47              |
| 2:M:402:SER:HA    | 2:M:566:THR:HG23  | 1.95                     | 0.47              |
| 2:M:588:VAL:HG11  | 2:M:661:SER:CB    | 2.45                     | 0.47              |
| 3:N:1031:ASN:O    | 3:N:1035:ILE:HG12 | 2.15                     | 0.47              |
| 3:N:1093:TYR:CE2  | 3:N:1097:LYS:HE3  | 2.49                     | 0.47              |
| 3:N:1282:ARG:HG2  | 3:N:1282:ARG:HH11 | 1.80                     | 0.47              |
| 3:N:1332:PRO:HB2  | 3:N:1421:LEU:HD21 | 1.96                     | 0.47              |
| 3:N:638:LYS:HD3   | 3:N:932:ASP:CB    | 2.44                     | 0.47              |
| 7:Y:89:VAL:HG22   | 7:Y:154:ILE:HG23  | 1.96                     | 0.47              |
| 1:B:165:ILE:HA    | 1:B:166:PRO:HD3   | 1.68                     | 0.47              |
| 2:C:13:ILE:O      | 2:C:13:ILE:HG13   | 2.14                     | 0.47              |
| 2:C:226:VAL:HG13  | 2:C:227:PHE:N     | 2.30                     | 0.47              |
| 2:C:402:SER:HA    | 2:C:566:THR:HG23  | 1.97                     | 0.47              |
| 3:D:1044:LEU:HD21 | 3:D:1056:PRO:HG3  | 1.97                     | 0.47              |
| 3:D:1399:ASP:O    | 3:D:1403:LEU:HB2  | 2.14                     | 0.47              |
| 3:D:1441:GLN:NE2  | 3:D:1442:ASN:H    | 2.12                     | 0.47              |
| 3:D:1481:VAL:HG12 | 3:D:1481:VAL:O    | 2.13                     | 0.47              |
| 3:D:457:GLY:C     | 3:D:459:GLU:N     | 2.66                     | 0.47              |
| 3:D:810:GLU:C     | 3:D:812:ALA:N     | 2.67                     | 0.47              |
| 4:E:83:ASP:O      | 4:E:86:GLN:HG2    | 2.15                     | 0.47              |
| 1:F:42:ARG:NH2    | 1:G:31:GLY:O      | 2.47                     | 0.47              |
| 1:G:79:ILE:HG13   | 1:G:80:LEU:N      | 2.30                     | 0.47              |
| 2:H:91:GLN:HB3    | 2:H:119:PRO:HA    | 1.97                     | 0.47              |
| 2:H:946:ARG:HH12  | 3:I:796:ARG:HH12  | 1.62                     | 0.47              |
| 3:I:956:ILE:HD11  | 3:I:1062:ARG:HG3  | 1.97                     | 0.47              |
| 3:I:1437:ALA:HB3  | 3:I:1446:VAL:HG13 | 1.96                     | 0.47              |
| 3:I:183:GLU:O     | 3:I:185:VAL:HG23  | 2.15                     | 0.47              |
| 3:I:689:ASP:O     | 3:I:693:GLU:HB2   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:6:ARG:HH21    | 3:I:1482:ARG:HH22 | 1.63                     | 0.47              |
| 1:K:222:LEU:HD21  | 1:L:218:LEU:HD23  | 1.97                     | 0.47              |
| 2:M:196:LEU:O     | 2:M:200:LEU:HG    | 2.15                     | 0.47              |
| 2:M:468:ARG:HG2   | 2:M:486:MET:C     | 2.34                     | 0.47              |
| 2:M:755:LEU:HG    | 2:M:792:VAL:HG22  | 1.96                     | 0.47              |
| 2:M:831:ARG:HH12  | 2:M:1002:GLU:HB3  | 1.80                     | 0.47              |
| 2:M:928:LYS:NZ    | 2:M:932:GLU:HG3   | 2.30                     | 0.47              |
| 3:N:1106:VAL:CG1  | 3:N:1107:VAL:H    | 2.22                     | 0.47              |
| 3:N:1297:GLU:CG   | 3:N:1298:GLY:N    | 2.69                     | 0.47              |
| 3:N:1263:PHE:HB3  | 3:N:1424:VAL:HG11 | 1.96                     | 0.47              |
| 3:N:672:ALA:O     | 3:N:675:ARG:HB2   | 2.15                     | 0.47              |
| 2:C:577:PRO:HG3   | 2:C:993:PHE:CD1   | 2.50                     | 0.47              |
| 2:C:701:THR:HA    | 2:C:831:ARG:O     | 2.15                     | 0.47              |
| 3:D:1120:VAL:HG23 | 3:D:1188:VAL:HG11 | 1.97                     | 0.47              |
| 3:D:1209:LEU:HD23 | 3:D:1210:SER:N    | 2.30                     | 0.47              |
| 3:D:1260:ILE:O    | 3:D:1264:GLU:HB2  | 2.14                     | 0.47              |
| 3:D:12:LEU:HA     | 3:D:12:LEU:HD23   | 1.61                     | 0.47              |
| 3:D:907:GLU:CG    | 3:D:908:LYS:N     | 2.78                     | 0.47              |
| 1:G:137:ARG:HB3   | 1:G:137:ARG:CZ    | 2.45                     | 0.47              |
| 1:G:179:PHE:HD2   | 1:G:179:PHE:N     | 2.12                     | 0.47              |
| 2:H:101:ILE:HG23  | 2:H:108:ILE:HG12  | 1.97                     | 0.47              |
| 2:H:344:PHE:O     | 2:H:348:LEU:HD13  | 2.15                     | 0.47              |
| 2:H:885:ILE:HG13  | 3:I:949:ILE:CG2   | 2.45                     | 0.47              |
| 2:H:886:LEU:HD12  | 2:H:886:LEU:HA    | 1.39                     | 0.47              |
| 2:H:966:LEU:HD21  | 2:H:986:PRO:HG2   | 1.97                     | 0.47              |
| 3:I:102:ILE:HD13  | 3:I:106:LYS:HB2   | 1.96                     | 0.47              |
| 3:I:1119:SER:HA   | 3:I:1186:VAL:O    | 2.15                     | 0.47              |
| 3:I:115:LEU:O     | 3:I:115:LEU:HD23  | 2.14                     | 0.47              |
| 3:I:481:MET:HE2   | 3:I:493:ARG:CB    | 2.45                     | 0.47              |
| 2:H:1091:GLU:CB   | 3:I:607:LEU:HD21  | 2.42                     | 0.47              |
| 3:I:800:LYS:HA    | 3:I:829:VAL:HG13  | 1.97                     | 0.47              |
| 1:K:64:GLU:O      | 1:K:75:VAL:HB     | 2.14                     | 0.47              |
| 2:M:266:ARG:NH1   | 2:M:288:ARG:HH21  | 2.11                     | 0.47              |
| 2:M:308:ARG:HG3   | 2:M:308:ARG:O     | 2.15                     | 0.47              |
| 2:M:109:LYS:HZ3   | 2:M:367:LEU:C     | 2.18                     | 0.47              |
| 2:M:515:ALA:O     | 2:M:516:ARG:HD3   | 2.15                     | 0.47              |
| 2:M:394:PHE:CD1   | 2:M:632:ASN:ND2   | 2.83                     | 0.47              |
| 3:N:102:ILE:HD13  | 3:N:102:ILE:C     | 2.35                     | 0.47              |
| 3:N:1290:LEU:CD1  | 3:N:1307:LYS:HA   | 2.45                     | 0.47              |
| 3:N:133:ILE:CG2   | 3:N:134:VAL:H     | 2.23                     | 0.47              |
| 3:N:814:ALA:O     | 3:N:818:ARG:HG3   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:X:89:VAL:HG12   | 7:X:90:GLU:N      | 2.30                     | 0.47              |
| 1:A:206:THR:HG23  | 1:A:208:LEU:H     | 1.80                     | 0.47              |
| 1:A:206:THR:CG2   | 1:A:209:GLU:HG3   | 2.45                     | 0.47              |
| 1:B:170:VAL:HG23  | 1:B:170:VAL:O     | 2.14                     | 0.47              |
| 1:B:48:ILE:HD12   | 1:B:48:ILE:H      | 1.79                     | 0.47              |
| 2:C:66:LEU:HD13   | 2:C:100:LEU:HB2   | 1.97                     | 0.47              |
| 2:C:209:ARG:O     | 2:C:213:ALA:HB2   | 2.14                     | 0.47              |
| 2:C:144:PRO:O     | 2:C:276:LYS:CE    | 2.63                     | 0.47              |
| 2:C:302:VAL:HG13  | 2:C:303:PHE:N     | 2.29                     | 0.47              |
| 2:C:397:GLU:HG2   | 2:C:403:SER:HB3   | 1.97                     | 0.47              |
| 2:C:835:VAL:O     | 2:C:849:VAL:O     | 2.33                     | 0.47              |
| 2:C:906:PHE:CZ    | 3:D:1067:VAL:HA   | 2.50                     | 0.47              |
| 3:D:1084:THR:HG22 | 3:D:1087:ARG:NH1  | 2.30                     | 0.47              |
| 3:D:1231:GLU:CB   | 3:D:1232:PRO:HD3  | 2.45                     | 0.47              |
| 3:D:1290:LEU:N    | 3:D:1290:LEU:HD12 | 2.30                     | 0.47              |
| 3:D:396:VAL:HG23  | 3:D:398:ALA:HB3   | 1.97                     | 0.47              |
| 3:D:481:MET:HE2   | 3:D:493:ARG:HB2   | 1.97                     | 0.47              |
| 3:D:783:ARG:HG2   | 3:D:784:ASP:N     | 2.27                     | 0.47              |
| 1:B:152:PRO:CG    | 3:D:857:ILE:CD1   | 2.91                     | 0.47              |
| 1:G:82:LEU:HD22   | 1:G:142:VAL:HG11  | 1.97                     | 0.47              |
| 1:G:185:ARG:HD3   | 3:I:692:GLU:CG    | 2.44                     | 0.47              |
| 2:H:1014:SER:C    | 2:H:1015:LEU:HD12 | 2.35                     | 0.47              |
| 3:D:173:PRO:HB3   | 2:H:279:GLU:CD    | 2.36                     | 0.47              |
| 2:H:285:LEU:HD21  | 2:H:287:GLY:O     | 2.15                     | 0.47              |
| 2:H:351:LEU:HD11  | 2:H:374:ASN:H     | 1.80                     | 0.47              |
| 3:I:1363:LEU:HD11 | 3:I:1368:ILE:HD11 | 1.97                     | 0.47              |
| 3:I:1441:GLN:CG   | 3:I:1442:ASN:N    | 2.77                     | 0.47              |
| 1:K:141:GLU:OE1   | 1:K:161:ARG:NH1   | 2.47                     | 0.47              |
| 1:K:184:THR:CG2   | 1:K:185:ARG:N     | 2.78                     | 0.47              |
| 1:L:190:THR:HG22  | 1:L:190:THR:O     | 2.15                     | 0.47              |
| 2:M:1095:LEU:CD1  | 2:M:1097:LEU:H    | 2.24                     | 0.47              |
| 2:M:13:ILE:HG13   | 2:M:13:ILE:O      | 2.15                     | 0.47              |
| 2:M:184:MET:HB2   | 2:M:193:LEU:HD21  | 1.97                     | 0.47              |
| 2:M:455:LEU:C     | 2:M:455:LEU:HD12  | 2.35                     | 0.47              |
| 2:M:545:ASN:HA    | 2:M:905:ILE:HD11  | 1.97                     | 0.47              |
| 2:M:835:VAL:O     | 2:M:849:VAL:O     | 2.33                     | 0.47              |
| 2:M:863:ASP:O     | 2:M:865:THR:N     | 2.48                     | 0.47              |
| 2:M:877:PRO:HG3   | 3:N:1023:MET:SD   | 2.55                     | 0.47              |
| 3:N:1120:VAL:HG23 | 3:N:1188:VAL:CG1  | 2.45                     | 0.47              |
| 3:N:1256:LEU:N    | 3:N:1257:PRO:CD   | 2.78                     | 0.47              |
| 3:N:1273:VAL:HG21 | 3:N:1305:LEU:HD21 | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:362:GLU:O     | 3:N:379:ALA:CB    | 2.62                     | 0.47              |
| 3:N:368:VAL:HB    | 3:N:377:VAL:CB    | 2.44                     | 0.47              |
| 3:N:796:ARG:HD3   | 3:N:1017:PHE:CE1  | 2.50                     | 0.47              |
| 3:N:850:LEU:HA    | 3:N:853:VAL:HG23  | 1.96                     | 0.47              |
| 3:N:907:GLU:CG    | 3:N:908:LYS:N     | 2.78                     | 0.47              |
| 4:O:35:PHE:CD2    | 4:O:56:ASP:O      | 2.68                     | 0.47              |
| 7:Y:73:VAL:HG12   | 7:Y:74:ILE:N      | 2.29                     | 0.47              |
| 1:B:48:ILE:CG2    | 1:B:173:PRO:HD2   | 2.45                     | 0.46              |
| 2:C:1015:LEU:N    | 2:C:1015:LEU:CD1  | 2.78                     | 0.46              |
| 2:C:1032:PHE:CZ   | 2:C:1040:LEU:HD22 | 2.50                     | 0.46              |
| 2:C:140:ILE:CG2   | 2:C:333:ILE:HG13  | 2.45                     | 0.46              |
| 2:C:723:THR:HG23  | 2:C:725:ASP:H     | 1.80                     | 0.46              |
| 3:D:1102:THR:HG1  | 3:D:1226:ALA:HB2  | 1.80                     | 0.46              |
| 3:D:127:LEU:HD13  | 3:D:461:ILE:HD11  | 1.97                     | 0.46              |
| 3:D:473:LEU:HA    | 3:D:476:GLU:HB2   | 1.96                     | 0.46              |
| 3:D:481:MET:HE2   | 3:D:493:ARG:CB    | 2.46                     | 0.46              |
| 3:D:546:ARG:HG2   | 3:D:546:ARG:NH1   | 2.30                     | 0.46              |
| 3:D:54:LYS:CG     | 3:D:55:ASP:N      | 2.78                     | 0.46              |
| 3:D:689:ASP:O     | 3:D:693:GLU:HB2   | 2.15                     | 0.46              |
| 3:D:755:ALA:O     | 3:D:758:GLU:HG2   | 2.15                     | 0.46              |
| 1:F:18:ARG:NH1    | 1:F:88:ARG:NE     | 2.63                     | 0.46              |
| 1:G:62:LEU:HD12   | 1:G:63:HIS:N      | 2.21                     | 0.46              |
| 2:H:440:PRO:HB2   | 3:I:1074:SER:OG   | 2.14                     | 0.46              |
| 2:H:515:ALA:O     | 2:H:516:ARG:HD3   | 2.15                     | 0.46              |
| 2:H:679:PHE:O     | 3:I:943:THR:HG22  | 2.15                     | 0.46              |
| 3:I:1029:ARG:NH2  | 7:Y:41:ASP:HB3    | 2.30                     | 0.46              |
| 3:I:1044:LEU:HD21 | 3:I:1056:PRO:HG3  | 1.97                     | 0.46              |
| 3:I:1260:ILE:O    | 3:I:1264:GLU:HB2  | 2.14                     | 0.46              |
| 3:I:1332:PRO:HB2  | 3:I:1421:LEU:HD21 | 1.97                     | 0.46              |
| 3:I:1366:LYS:HA   | 3:I:1369:GLU:OE1  | 2.15                     | 0.46              |
| 3:I:1412:LYS:HE2  | 3:I:1414:PRO:HG3  | 1.96                     | 0.46              |
| 3:I:202:VAL:O     | 3:I:395:VAL:CA    | 2.55                     | 0.46              |
| 3:I:950:GLY:O     | 3:I:953:ASP:HB2   | 2.16                     | 0.46              |
| 1:K:223:THR:C     | 1:K:225:PHE:H     | 2.19                     | 0.46              |
| 1:K:23:PHE:CD2    | 1:K:211:LEU:HD22  | 2.50                     | 0.46              |
| 1:L:179:PHE:N     | 1:L:179:PHE:HD2   | 2.12                     | 0.46              |
| 1:L:62:LEU:HD12   | 1:L:63:HIS:H      | 1.78                     | 0.46              |
| 2:M:1092:LEU:HD22 | 2:M:1099:VAL:HG23 | 1.97                     | 0.46              |
| 2:M:145:GLY:CA    | 2:M:276:LYS:HD3   | 2.44                     | 0.46              |
| 2:M:154:ARG:HH12  | 2:M:178:PRO:HD3   | 1.74                     | 0.46              |
| 3:N:1366:LYS:HA   | 3:N:1369:GLU:OE1  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:199:LEU:CG    | 3:N:200:ASP:H     | 2.29                     | 0.46              |
| 3:N:54:LYS:HG3    | 3:N:55:ASP:N      | 2.30                     | 0.46              |
| 3:N:800:LYS:CE    | 3:N:830:ALA:HB3   | 2.45                     | 0.46              |
| 1:A:128:HIS:HE1   | 1:A:131:THR:CG2   | 2.24                     | 0.46              |
| 2:C:1056:LYS:HD3  | 3:D:623:VAL:HG11  | 1.96                     | 0.46              |
| 2:C:1081:VAL:HG12 | 2:C:1085:PHE:HB3  | 1.93                     | 0.46              |
| 2:C:265:ARG:H     | 2:C:289:THR:CG2   | 2.20                     | 0.46              |
| 2:C:351:LEU:CD1   | 2:C:374:ASN:ND2   | 2.78                     | 0.46              |
| 2:C:361:MET:O     | 2:C:361:MET:HG2   | 2.15                     | 0.46              |
| 2:C:440:PRO:HB2   | 3:D:1074:SER:OG   | 2.15                     | 0.46              |
| 2:C:495:THR:HG21  | 2:C:517:ARG:HH21  | 1.80                     | 0.46              |
| 2:C:477:GLY:HA2   | 2:C:508:ILE:CD1   | 2.46                     | 0.46              |
| 2:C:515:ALA:O     | 2:C:516:ARG:HD3   | 2.15                     | 0.46              |
| 2:C:726:ILE:CG1   | 2:C:734:LEU:HD11  | 2.43                     | 0.46              |
| 3:D:1035:ILE:HA   | 3:D:1038:LEU:HD12 | 1.98                     | 0.46              |
| 3:D:1106:VAL:CB   | 3:D:1108:ARG:HE   | 2.09                     | 0.46              |
| 3:D:1165:TYR:CD1  | 3:D:1165:TYR:N    | 2.83                     | 0.46              |
| 3:D:1330:ILE:HG22 | 3:D:1331:ASP:N    | 2.30                     | 0.46              |
| 3:D:1332:PRO:HB2  | 3:D:1421:LEU:HD21 | 1.96                     | 0.46              |
| 3:D:1369:GLU:HA   | 3:D:1372:VAL:HG12 | 1.97                     | 0.46              |
| 3:D:1437:ALA:HB1  | 3:D:1446:VAL:HG22 | 1.96                     | 0.46              |
| 2:C:834:GLN:NE2   | 3:D:724:GLN:HG3   | 2.16                     | 0.46              |
| 3:D:810:GLU:C     | 3:D:812:ALA:H     | 2.16                     | 0.46              |
| 3:D:906:GLN:HB3   | 3:D:911:LEU:CD1   | 2.45                     | 0.46              |
| 1:G:190:THR:O     | 1:G:190:THR:HG22  | 2.15                     | 0.46              |
| 2:H:1084:SER:HA   | 2:H:1087:VAL:HG12 | 1.97                     | 0.46              |
| 2:H:1102:LEU:HA   | 2:H:1107:ASN:O    | 2.16                     | 0.46              |
| 2:H:332:ARG:CG    | 2:H:464:LEU:O     | 2.63                     | 0.46              |
| 2:H:399:ASN:ND2   | 2:H:568:ALA:HB3   | 2.30                     | 0.46              |
| 2:H:444:PRO:HD2   | 2:H:452:ILE:O     | 2.15                     | 0.46              |
| 2:H:483:VAL:HG12  | 2:H:484:VAL:N     | 2.30                     | 0.46              |
| 2:H:606:VAL:CG2   | 2:H:645:VAL:HG22  | 2.44                     | 0.46              |
| 2:H:4:LYS:NZ      | 2:H:917:LEU:HD21  | 2.31                     | 0.46              |
| 3:I:1119:SER:O    | 3:I:1121:PRO:HD3  | 2.15                     | 0.46              |
| 3:I:638:LYS:O     | 3:I:640:HIS:N     | 2.47                     | 0.46              |
| 3:I:800:LYS:HD3   | 3:I:830:ALA:O     | 2.15                     | 0.46              |
| 3:I:907:GLU:CG    | 3:I:908:LYS:N     | 2.78                     | 0.46              |
| 1:L:65:PHE:CD1    | 1:L:65:PHE:N      | 2.84                     | 0.46              |
| 2:M:207:LEU:HD22  | 2:M:221:LEU:HD11  | 1.97                     | 0.46              |
| 2:M:267:TYR:CD2   | 2:M:267:TYR:N     | 2.82                     | 0.46              |
| 2:M:304:LEU:HD11  | 2:M:308:ARG:CZ    | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:508:ILE:HG22  | 2:M:509:ALA:H     | 1.79                     | 0.46              |
| 3:N:1044:LEU:HD21 | 3:N:1056:PRO:HG3  | 1.97                     | 0.46              |
| 3:N:1120:VAL:O    | 3:N:1122:LEU:HD12 | 2.15                     | 0.46              |
| 3:N:1122:LEU:N    | 3:N:1122:LEU:CD1  | 2.75                     | 0.46              |
| 3:N:1305:LEU:HD12 | 3:N:1311:LEU:CD2  | 2.30                     | 0.46              |
| 3:N:402:PRO:N     | 3:N:443:VAL:HG23  | 2.29                     | 0.46              |
| 3:N:473:LEU:HA    | 3:N:476:GLU:HB2   | 1.96                     | 0.46              |
| 3:N:800:LYS:HE3   | 3:N:830:ALA:HB3   | 1.97                     | 0.46              |
| 4:O:25:LYS:O      | 4:O:28:GLN:HB2    | 2.15                     | 0.46              |
| 2:C:1038:TRP:O    | 2:C:1039:ALA:C    | 2.53                     | 0.46              |
| 2:C:390:GLN:NE2   | 6:Q:12:G:OP1      | 2.49                     | 0.46              |
| 2:C:479:VAL:CG2   | 2:C:506:ASN:HA    | 2.45                     | 0.46              |
| 2:C:588:VAL:HG11  | 2:C:661:SER:HB3   | 1.98                     | 0.46              |
| 2:C:840:ALA:CB    | 2:C:846:LYS:HA    | 2.43                     | 0.46              |
| 2:C:863:ASP:O     | 2:C:865:THR:N     | 2.48                     | 0.46              |
| 3:D:388:HIS:O     | 3:D:390:PRO:HD3   | 2.15                     | 0.46              |
| 3:D:408:GLU:CG    | 3:D:409:VAL:N     | 2.77                     | 0.46              |
| 3:D:465:LEU:CD1   | 3:D:510:GLU:HA    | 2.36                     | 0.46              |
| 4:E:31:LEU:HD12   | 4:E:32:ARG:N      | 2.30                     | 0.46              |
| 4:E:68:LEU:HD12   | 4:E:73:LEU:HD13   | 1.96                     | 0.46              |
| 2:H:437:ARG:HG2   | 2:H:467:ILE:HG22  | 1.96                     | 0.46              |
| 2:H:78:PHE:HB3    | 2:H:79:PRO:HD2    | 1.97                     | 0.46              |
| 2:H:578:VAL:HA    | 2:H:900:ARG:CG    | 2.45                     | 0.46              |
| 2:H:928:LYS:NZ    | 2:H:932:GLU:HG3   | 2.30                     | 0.46              |
| 3:I:1041:LEU:HD12 | 3:I:1058:ARG:CA   | 2.44                     | 0.46              |
| 3:I:1149:LEU:HG   | 3:I:1166:LEU:HD22 | 1.97                     | 0.46              |
| 2:M:108:ILE:HG22  | 2:M:109:LYS:N     | 2.30                     | 0.46              |
| 2:M:1112:PHE:O    | 2:M:1112:PHE:CG   | 2.67                     | 0.46              |
| 2:M:190:LYS:O     | 2:M:191:PHE:HB3   | 2.15                     | 0.46              |
| 2:M:252:LYS:HG2   | 2:M:252:LYS:H     | 1.42                     | 0.46              |
| 2:M:290:LEU:CB    | 2:M:302:VAL:CG1   | 2.80                     | 0.46              |
| 2:M:63:GLY:HA2    | 2:M:359:MET:HE1   | 1.96                     | 0.46              |
| 2:M:939:ARG:HA    | 2:M:939:ARG:NE    | 2.14                     | 0.46              |
| 3:N:1202:GLN:HB2  | 3:N:1217:ILE:HD11 | 1.97                     | 0.46              |
| 3:N:129:PHE:O     | 3:N:572:ARG:HG2   | 2.16                     | 0.46              |
| 3:N:1340:GLY:O    | 3:N:1344:VAL:HG23 | 2.15                     | 0.46              |
| 3:N:127:LEU:HD23  | 3:N:134:VAL:HG13  | 1.97                     | 0.46              |
| 3:N:1384:PRO:HG3  | 3:N:1389:LEU:CB   | 2.38                     | 0.46              |
| 3:N:143:ASN:CB    | 3:N:161:LEU:HD23  | 2.46                     | 0.46              |
| 3:N:401:TYR:C     | 3:N:443:VAL:HG23  | 2.35                     | 0.46              |
| 3:N:477:LEU:HD22  | 3:N:492:ALA:CB    | 2.40                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:687:VAL:O    | 3:N:690:ALA:HB3   | 2.16                     | 0.46              |
| 4:O:25:LYS:HE2   | 4:O:25:LYS:HB3    | 1.69                     | 0.46              |
| 4:O:29:GLN:OE1   | 4:O:89:MET:HE1    | 2.15                     | 0.46              |
| 1:A:34:VAL:HG13  | 1:B:42:ARG:HE     | 1.79                     | 0.46              |
| 2:C:170:PRO:CG   | 2:C:258:TYR:CD1   | 2.92                     | 0.46              |
| 2:C:80:GLN:O     | 2:C:83:CYS:N      | 2.49                     | 0.46              |
| 3:D:1061:PHE:CE1 | 3:D:1065:LEU:HD22 | 2.41                     | 0.46              |
| 3:D:1152:GLU:HG2 | 3:D:1160:LEU:O    | 2.14                     | 0.46              |
| 3:D:1195:GLN:HG3 | 3:D:1196:THR:N    | 2.29                     | 0.46              |
| 3:D:1221:VAL:O   | 3:D:1222:GLY:C    | 2.53                     | 0.46              |
| 3:D:126:VAL:HG12 | 3:D:132:TYR:CB    | 2.34                     | 0.46              |
| 3:D:1282:ARG:HA  | 3:D:1315:ASP:HA   | 1.96                     | 0.46              |
| 3:D:420:VAL:HG13 | 3:D:424:GLY:O     | 2.16                     | 0.46              |
| 1:F:18:ARG:O     | 1:F:201:THR:OG1   | 2.32                     | 0.46              |
| 1:G:188:GLN:CG   | 3:I:685:ASP:OD1   | 2.62                     | 0.46              |
| 2:H:335:THR:O    | 2:H:336:VAL:C     | 2.54                     | 0.46              |
| 2:H:415:PRO:HB2  | 2:H:418:LEU:CD1   | 2.46                     | 0.46              |
| 2:H:606:VAL:HG22 | 2:H:645:VAL:HG13  | 1.97                     | 0.46              |
| 2:H:6:PHE:HZ     | 2:H:917:LEU:CD1   | 2.27                     | 0.46              |
| 3:I:1372:VAL:O   | 3:I:1375:MET:HB2  | 2.14                     | 0.46              |
| 2:H:1093:GLN:OE1 | 3:I:21:TRP:CE3    | 2.68                     | 0.46              |
| 2:M:139:GLN:O    | 2:M:333:ILE:HA    | 2.14                     | 0.46              |
| 2:M:3:ILE:N      | 2:M:3:ILE:HD12    | 2.31                     | 0.46              |
| 2:M:415:PRO:HD2  | 2:M:418:LEU:HD13  | 1.98                     | 0.46              |
| 2:M:679:PHE:HB2  | 2:M:683:ASN:ND2   | 2.23                     | 0.46              |
| 2:M:795:GLY:O    | 2:M:796:GLU:HG2   | 2.16                     | 0.46              |
| 3:N:368:VAL:H    | 3:N:377:VAL:HB    | 1.80                     | 0.46              |
| 3:N:50:PHE:HD2   | 3:N:522:PRO:CD    | 1.74                     | 0.46              |
| 3:N:804:LEU:HB2  | 3:N:830:ALA:O     | 2.16                     | 0.46              |
| 3:N:880:ILE:CG2  | 3:N:881:LEU:N     | 2.78                     | 0.46              |
| 3:N:996:TRP:O    | 3:N:999:THR:HG22  | 2.16                     | 0.46              |
| 7:X:81:GLU:OE2   | 7:X:154:ILE:HD12  | 2.16                     | 0.46              |
| 7:Y:30:THR:HA    | 7:Y:55:LYS:HE2    | 1.98                     | 0.46              |
| 7:Y:91:LEU:HB3   | 7:Y:149:PHE:HB3   | 1.96                     | 0.46              |
| 1:A:156:HIS:CD2  | 1:A:158:ILE:CD1   | 2.99                     | 0.46              |
| 1:A:18:ARG:HH11  | 1:A:123:MET:CE    | 2.28                     | 0.46              |
| 1:B:44:LEU:HA    | 1:B:48:ILE:HD11   | 1.97                     | 0.46              |
| 1:B:85:LEU:HA    | 1:B:124:ASN:ND2   | 2.31                     | 0.46              |
| 2:C:1070:ILE:CG2 | 3:D:655:PRO:HB2   | 2.45                     | 0.46              |
| 2:C:1102:LEU:HA  | 2:C:1107:ASN:O    | 2.16                     | 0.46              |
| 2:C:333:ILE:HD12 | 2:C:333:ILE:N     | 2.31                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:334:ARG:CB   | 2:C:339:LEU:HD21  | 2.46                     | 0.46              |
| 2:C:361:MET:HE3  | 3:I:1317:ASP:HB2  | 1.97                     | 0.46              |
| 2:C:39:ARG:HB2   | 2:C:45:GLN:NE2    | 2.30                     | 0.46              |
| 2:C:64:LEU:HB2   | 2:C:359:MET:CE    | 2.46                     | 0.46              |
| 3:D:1425:THR:O   | 3:D:1428:ALA:HB3  | 2.16                     | 0.46              |
| 3:D:183:GLU:O    | 3:D:185:VAL:HG23  | 2.15                     | 0.46              |
| 3:D:792:ILE:CD1  | 3:D:881:LEU:HD23  | 2.38                     | 0.46              |
| 4:E:3:GLU:OE1    | 4:E:3:GLU:HA      | 2.15                     | 0.46              |
| 1:F:206:THR:CG2  | 1:F:209:GLU:HG3   | 2.45                     | 0.46              |
| 1:F:26:GLU:HB2   | 1:F:27:PRO:HA     | 1.98                     | 0.46              |
| 1:G:142:VAL:HG23 | 1:G:142:VAL:O     | 2.15                     | 0.46              |
| 1:G:159:LYS:H    | 1:G:159:LYS:HZ2   | 1.63                     | 0.46              |
| 2:H:1059:ASP:OD1 | 2:H:1062:GLY:N    | 2.45                     | 0.46              |
| 2:H:365:ASP:OD1  | 2:H:365:ASP:C     | 2.53                     | 0.46              |
| 2:H:508:ILE:HG22 | 2:H:509:ALA:N     | 2.31                     | 0.46              |
| 2:H:54:ILE:CG2   | 2:H:66:LEU:HB3    | 2.46                     | 0.46              |
| 2:H:626:ARG:HB3  | 2:H:629:TYR:CD1   | 2.51                     | 0.46              |
| 2:H:63:GLY:N     | 2:H:103:LYS:HG3   | 2.29                     | 0.46              |
| 2:H:953:VAL:O    | 2:H:955:PRO:HD3   | 2.15                     | 0.46              |
| 3:I:1202:GLN:HB2 | 3:I:1217:ILE:HD11 | 1.97                     | 0.46              |
| 3:I:1281:VAL:CG1 | 3:I:1282:ARG:N    | 2.78                     | 0.46              |
| 3:I:796:ARG:HD3  | 3:I:1017:PHE:HE1  | 1.79                     | 0.46              |
| 3:I:806:PHE:O    | 3:I:808:THR:N     | 2.48                     | 0.46              |
| 3:I:880:ILE:CG2  | 3:I:881:LEU:N     | 2.78                     | 0.46              |
| 3:I:881:LEU:HD12 | 3:I:885:ILE:HD11  | 1.98                     | 0.46              |
| 2:M:174:LEU:CD2  | 2:M:184:MET:HG3   | 2.45                     | 0.46              |
| 2:M:235:LEU:HD11 | 2:M:298:PHE:CE1   | 2.50                     | 0.46              |
| 2:M:571:LEU:CD1  | 2:M:701:THR:H     | 2.28                     | 0.46              |
| 2:M:798:GLY:C    | 2:M:799:ILE:HD13  | 2.36                     | 0.46              |
| 3:N:709:HIS:HA   | 3:N:1227:GLN:NE2  | 2.30                     | 0.46              |
| 3:N:1325:LEU:HA  | 3:N:1325:LEU:HD12 | 1.70                     | 0.46              |
| 3:N:1481:VAL:O   | 3:N:1481:VAL:HG12 | 2.16                     | 0.46              |
| 3:N:180:LYS:HZ1  | 3:N:386:HIS:CB    | 2.29                     | 0.46              |
| 3:N:791:TYR:CD2  | 3:N:945:SER:HB2   | 2.51                     | 0.46              |
| 3:N:996:TRP:CD1  | 3:N:1056:PRO:CG   | 2.98                     | 0.46              |
| 7:X:22:GLU:OE1   | 7:X:58:ILE:HD12   | 2.16                     | 0.46              |
| 1:B:7:LYS:HB3    | 1:B:7:LYS:HE3     | 1.70                     | 0.46              |
| 1:A:224:TYR:CD1  | 1:B:9:PRO:HD2     | 2.50                     | 0.46              |
| 2:C:95:TYR:CD2   | 2:C:114:PHE:CB    | 2.95                     | 0.46              |
| 2:C:184:MET:SD   | 2:C:191:PHE:HE1   | 2.39                     | 0.46              |
| 2:C:263:ASP:HB2  | 2:C:264:PRO:CD    | 2.46                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:269:LEU:CD2   | 2:C:269:LEU:C     | 2.84                     | 0.46              |
| 2:C:317:VAL:N     | 2:C:318:PRO:HD3   | 2.29                     | 0.46              |
| 2:C:516:ARG:CG    | 3:D:1068:LEU:HD13 | 2.46                     | 0.46              |
| 2:C:571:LEU:HD11  | 2:C:700:TYR:CA    | 2.44                     | 0.46              |
| 2:C:722:ILE:HG12  | 2:C:757:GLY:O     | 2.15                     | 0.46              |
| 2:C:798:GLY:C     | 2:C:799:ILE:HD13  | 2.36                     | 0.46              |
| 2:C:80:GLN:O      | 2:C:83:CYS:HB2    | 2.16                     | 0.46              |
| 2:C:877:PRO:HD3   | 3:D:949:ILE:HD11  | 1.98                     | 0.46              |
| 3:D:1094:LEU:HD21 | 3:D:1259:VAL:HG11 | 1.96                     | 0.46              |
| 3:D:1365:ASP:O    | 3:D:1366:LYS:C    | 2.53                     | 0.46              |
| 3:D:489:ARG:NH2   | 3:D:1389:LEU:HD21 | 2.30                     | 0.46              |
| 3:D:462:GLN:O     | 3:D:466:LYS:HG3   | 2.14                     | 0.46              |
| 3:D:682:ASP:O     | 3:D:683:ILE:CB    | 2.59                     | 0.46              |
| 2:C:1051:GLU:OE2  | 3:D:751:LEU:HB2   | 2.16                     | 0.46              |
| 3:D:925:GLU:HG2   | 3:D:926:LYS:N     | 2.31                     | 0.46              |
| 3:D:956:ILE:HD12  | 3:D:956:ILE:N     | 2.30                     | 0.46              |
| 1:F:127:LEU:HD12  | 1:F:128:HIS:N     | 2.29                     | 0.46              |
| 1:F:82:LEU:O      | 1:F:85:LEU:HB3    | 2.16                     | 0.46              |
| 2:H:794:PRO:CD    | 2:H:1025:ALA:HA   | 2.46                     | 0.46              |
| 2:H:269:LEU:HG    | 2:H:287:GLY:O     | 2.16                     | 0.46              |
| 3:I:1011:PHE:HB3  | 3:I:1021:TYR:CD1  | 2.50                     | 0.46              |
| 3:I:102:ILE:HD13  | 3:I:102:ILE:C     | 2.35                     | 0.46              |
| 3:I:1083:ASP:O    | 3:I:1087:ARG:HB3  | 2.16                     | 0.46              |
| 3:I:1330:ILE:HG22 | 3:I:1331:ASP:N    | 2.30                     | 0.46              |
| 2:H:874:LEU:HD21  | 3:I:787:LEU:HD22  | 1.97                     | 0.46              |
| 3:I:806:PHE:C     | 3:I:808:THR:H     | 2.17                     | 0.46              |
| 1:K:82:LEU:O      | 1:K:85:LEU:HB3    | 2.15                     | 0.46              |
| 2:M:1051:GLU:CD   | 3:N:751:LEU:H     | 2.19                     | 0.46              |
| 2:M:1084:SER:HA   | 2:M:1087:VAL:HG12 | 1.97                     | 0.46              |
| 2:M:182:VAL:HG12  | 2:M:193:LEU:HD13  | 1.97                     | 0.46              |
| 2:M:215:GLY:O     | 2:M:216:GLU:CB    | 2.63                     | 0.46              |
| 2:M:26:TYR:HA     | 2:M:29:ALA:CB     | 2.45                     | 0.46              |
| 2:M:626:ARG:HB3   | 2:M:629:TYR:CD1   | 2.51                     | 0.46              |
| 3:N:1231:GLU:CB   | 3:N:1232:PRO:HD3  | 2.45                     | 0.46              |
| 3:N:1261:GLU:O    | 3:N:1264:GLU:O    | 2.34                     | 0.46              |
| 3:N:1330:ILE:HG22 | 3:N:1331:ASP:N    | 2.30                     | 0.46              |
| 3:N:1347:TYR:HD2  | 3:N:1348:LEU:HD12 | 1.81                     | 0.46              |
| 3:N:765:SER:OG    | 3:N:766:ALA:N     | 2.46                     | 0.46              |
| 3:N:921:ARG:C     | 3:N:922:LEU:HD23  | 2.36                     | 0.46              |
| 2:M:984:GLU:HG3   | 3:N:944:THR:O     | 2.14                     | 0.46              |
| 3:D:970:LYS:HZ3   | 7:X:113:LEU:HD23  | 1.79                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:Z:139:SER:OG   | 7:Z:146:ARG:HG3   | 2.15                     | 0.46              |
| 1:A:82:LEU:O     | 1:A:85:LEU:HB3    | 2.15                     | 0.46              |
| 1:B:190:THR:O    | 1:B:190:THR:HG22  | 2.15                     | 0.46              |
| 1:B:76:VAL:HB    | 3:D:872:ARG:HH12  | 1.81                     | 0.46              |
| 1:B:94:LEU:HD13  | 1:B:120:VAL:HG22  | 1.97                     | 0.46              |
| 2:C:1084:SER:HA  | 2:C:1087:VAL:HG12 | 1.96                     | 0.46              |
| 2:C:449:ILE:CD1  | 3:D:1081:GLY:HA3  | 2.45                     | 0.46              |
| 2:C:953:VAL:O    | 2:C:955:PRO:HD3   | 2.16                     | 0.46              |
| 3:D:1011:PHE:HB3 | 3:D:1021:TYR:CD1  | 2.50                     | 0.46              |
| 3:D:1132:LEU:H   | 3:D:1132:LEU:HD12 | 1.81                     | 0.46              |
| 3:D:154:THR:HG21 | 3:D:157:GLU:OE2   | 2.16                     | 0.46              |
| 3:D:832:ARG:NE   | 3:D:832:ARG:HA    | 2.31                     | 0.46              |
| 3:D:835:SER:N    | 3:D:838:ARG:CD    | 2.79                     | 0.46              |
| 3:D:956:ILE:HD11 | 3:D:1062:ARG:CB   | 2.46                     | 0.46              |
| 1:F:180:GLN:HB3  | 1:F:180:GLN:HE21  | 1.55                     | 0.46              |
| 1:F:223:THR:C    | 1:F:225:PHE:H     | 2.19                     | 0.46              |
| 1:G:154:GLU:OE2  | 3:I:840:LYS:HE2   | 2.16                     | 0.46              |
| 2:H:176:VAL:HG12 | 2:H:182:VAL:HG22  | 1.97                     | 0.46              |
| 3:D:391:ALA:HB3  | 2:H:283:ILE:HG21  | 1.98                     | 0.46              |
| 2:H:281:LEU:HD12 | 2:H:306:THR:HA    | 1.97                     | 0.46              |
| 2:H:325:ILE:N    | 2:H:325:ILE:HD12  | 2.31                     | 0.46              |
| 2:H:336:VAL:O    | 2:H:339:LEU:HB2   | 2.15                     | 0.46              |
| 2:H:500:ASN:H    | 2:H:500:ASN:ND2   | 2.14                     | 0.46              |
| 2:H:6:PHE:CD1    | 2:H:909:ALA:HB2   | 2.50                     | 0.46              |
| 2:H:722:ILE:HD13 | 2:H:722:ILE:C     | 2.36                     | 0.46              |
| 2:H:798:GLY:C    | 2:H:799:ILE:HD13  | 2.36                     | 0.46              |
| 2:H:835:VAL:O    | 2:H:849:VAL:O     | 2.34                     | 0.46              |
| 2:H:84:ARG:HG2   | 2:H:131:GLY:O     | 2.15                     | 0.46              |
| 2:H:80:GLN:HA    | 2:H:90:TYR:CD2    | 2.51                     | 0.46              |
| 3:I:123:LEU:HD21 | 3:I:151:GLN:HE22  | 1.76                     | 0.46              |
| 3:I:1340:GLY:O   | 3:I:1344:VAL:HG23 | 2.15                     | 0.46              |
| 3:I:182:GLY:CA   | 3:I:441:ARG:HD3   | 2.45                     | 0.46              |
| 3:I:415:VAL:O    | 3:I:432:TYR:HA    | 2.16                     | 0.46              |
| 3:I:481:MET:HE2  | 3:I:493:ARG:HB2   | 1.97                     | 0.46              |
| 3:I:50:PHE:CE2   | 3:I:522:PRO:CD    | 2.98                     | 0.46              |
| 3:I:639:LEU:CD1  | 3:I:640:HIS:N     | 2.79                     | 0.46              |
| 2:H:1044:GLY:HA3 | 4:J:17:TYR:HE1    | 1.81                     | 0.46              |
| 4:J:32:ARG:HB2   | 4:J:32:ARG:NH1    | 2.30                     | 0.46              |
| 4:J:41:GLU:N     | 4:J:42:PRO:CD     | 2.79                     | 0.46              |
| 1:K:102:LYS:HB3  | 1:K:139:ASN:ND2   | 2.31                     | 0.46              |
| 1:K:21:GLY:HA3   | 1:K:207:PRO:CB    | 2.46                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:100:LEU:O    | 2:M:108:ILE:CG2   | 2.56                     | 0.46              |
| 2:M:165:LEU:HA   | 2:M:166:PRO:O     | 2.15                     | 0.46              |
| 2:M:294:GLU:HG2  | 2:M:295:ASP:N     | 2.31                     | 0.46              |
| 2:M:424:GLY:O    | 2:M:425:PHE:C     | 2.53                     | 0.46              |
| 2:M:328:LEU:HB2  | 2:M:488:ALA:CB    | 2.46                     | 0.46              |
| 2:M:966:LEU:HD21 | 2:M:986:PRO:HG2   | 1.97                     | 0.46              |
| 3:N:1108:ARG:HA  | 3:N:1217:ILE:HG23 | 1.98                     | 0.46              |
| 3:N:1165:TYR:CE2 | 3:N:1214:PRO:HB3  | 2.51                     | 0.46              |
| 3:N:481:MET:O    | 3:N:489:ARG:HB2   | 2.16                     | 0.46              |
| 3:N:755:ALA:O    | 3:N:758:GLU:HG2   | 2.15                     | 0.46              |
| 3:N:827:ILE:N    | 3:N:827:ILE:HD12  | 2.27                     | 0.46              |
| 3:N:906:GLN:HB3  | 3:N:911:LEU:CD1   | 2.45                     | 0.46              |
| 3:N:997:THR:CG2  | 7:Z:61:ARG:NH1    | 2.79                     | 0.46              |
| 4:O:37:ASN:ND2   | 4:O:93:TYR:CD2    | 2.83                     | 0.46              |
| 7:X:128:ALA:O    | 7:X:138:LEU:CD1   | 2.63                     | 0.46              |
| 1:A:102:LYS:HB3  | 1:A:139:ASN:ND2   | 2.31                     | 0.46              |
| 1:A:223:THR:C    | 1:A:225:PHE:H     | 2.19                     | 0.46              |
| 1:B:34:VAL:CG2   | 1:B:181:VAL:HG21  | 2.45                     | 0.46              |
| 2:C:443:THR:HA   | 2:C:444:PRO:HD3   | 1.74                     | 0.46              |
| 2:C:625:LEU:O    | 2:C:627:ARG:N     | 2.49                     | 0.46              |
| 2:C:626:ARG:HB3  | 2:C:629:TYR:CD1   | 2.50                     | 0.46              |
| 2:C:64:LEU:HB2   | 2:C:359:MET:HE2   | 1.98                     | 0.46              |
| 2:C:706:GLU:HB3  | 2:C:708:TYR:CE1   | 2.50                     | 0.46              |
| 2:C:863:ASP:OD2  | 2:C:863:ASP:C     | 2.54                     | 0.46              |
| 2:C:957:LYS:O    | 2:C:962:GLN:NE2   | 2.25                     | 0.46              |
| 3:D:1395:LEU:C   | 3:D:1395:LEU:HD23 | 2.35                     | 0.46              |
| 3:D:1459:LEU:CD1 | 3:D:1468:LEU:HD12 | 2.45                     | 0.46              |
| 3:D:184:GLU:OE1  | 3:D:201:GLY:O     | 2.34                     | 0.46              |
| 3:D:661:MET:HE2  | 3:D:673:ALA:HB1   | 1.96                     | 0.46              |
| 3:D:720:LEU:H    | 3:D:720:LEU:HD12  | 1.81                     | 0.46              |
| 3:D:921:ARG:C    | 3:D:922:LEU:HD23  | 2.36                     | 0.46              |
| 1:F:102:LYS:HB3  | 1:F:139:ASN:ND2   | 2.31                     | 0.46              |
| 2:H:611:ILE:HG13 | 2:H:625:LEU:HD21  | 1.98                     | 0.46              |
| 2:H:728:HIS:O    | 2:H:729:LEU:CB    | 2.63                     | 0.46              |
| 3:I:1103:HIS:CD2 | 3:I:1463:LYS:HB2  | 2.51                     | 0.46              |
| 3:I:1258:ARG:O   | 3:I:1262:LEU:HB2  | 2.15                     | 0.46              |
| 3:I:1369:GLU:HA  | 3:I:1372:VAL:HG12 | 1.97                     | 0.46              |
| 3:I:483:HIS:CB   | 3:I:484:PRO:HD3   | 2.40                     | 0.46              |
| 3:I:832:ARG:HA   | 3:I:832:ARG:NE    | 2.31                     | 0.46              |
| 3:I:907:GLU:CD   | 3:I:909:ASN:HD22  | 2.19                     | 0.46              |
| 2:M:1102:LEU:HA  | 2:M:1107:ASN:O    | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:235:LEU:CD1   | 2:M:298:PHE:CE1   | 2.98                     | 0.46              |
| 2:M:274:ARG:CD    | 2:M:285:LEU:HD13  | 2.45                     | 0.46              |
| 2:M:281:LEU:HD11  | 2:M:306:THR:HG22  | 1.98                     | 0.46              |
| 2:M:333:ILE:HD11  | 2:M:467:ILE:HG13  | 1.98                     | 0.46              |
| 2:M:39:ARG:HH12   | 2:M:70:GLU:HA     | 1.80                     | 0.46              |
| 2:M:557:ARG:HG2   | 2:M:881:ASN:HD22  | 1.76                     | 0.46              |
| 2:M:749:VAL:HB    | 2:M:792:VAL:HG21  | 1.97                     | 0.46              |
| 2:M:859:PRO:HB2   | 2:M:867:VAL:CG2   | 2.46                     | 0.46              |
| 2:M:953:VAL:O     | 2:M:955:PRO:HD3   | 2.15                     | 0.46              |
| 3:N:1042:ARG:HH11 | 3:N:1042:ARG:HB2  | 1.81                     | 0.46              |
| 3:N:12:LEU:HD23   | 3:N:12:LEU:HA     | 1.62                     | 0.46              |
| 3:N:166:GLN:CD    | 3:N:394:LEU:HD12  | 2.36                     | 0.46              |
| 3:N:956:ILE:N     | 3:N:956:ILE:HD12  | 2.31                     | 0.46              |
| 3:N:758:GLU:HA    | 4:O:20:THR:HG21   | 1.97                     | 0.46              |
| 7:Y:105:VAL:O     | 7:Y:121:ASP:N     | 2.49                     | 0.46              |
| 1:B:156:HIS:CD2   | 1:B:156:HIS:H     | 2.34                     | 0.46              |
| 2:C:95:TYR:CD2    | 2:C:114:PHE:HB3   | 2.45                     | 0.46              |
| 2:C:140:ILE:HG22  | 2:C:333:ILE:HD11  | 1.97                     | 0.46              |
| 2:C:333:ILE:HG12  | 2:C:410:ILE:HD13  | 1.98                     | 0.46              |
| 2:C:140:ILE:HD11  | 2:C:412:ALA:CB    | 2.46                     | 0.46              |
| 2:C:653:ASP:OD1   | 2:C:654:LEU:HD23  | 2.14                     | 0.46              |
| 2:C:588:VAL:HG11  | 2:C:661:SER:CB    | 2.45                     | 0.46              |
| 2:C:928:LYS:NZ    | 2:C:932:GLU:HG3   | 2.30                     | 0.46              |
| 3:D:115:LEU:O     | 3:D:115:LEU:HD23  | 2.14                     | 0.46              |
| 3:D:1202:GLN:HB2  | 3:D:1217:ILE:HD11 | 1.97                     | 0.46              |
| 3:D:1286:THR:O    | 3:D:1287:GLU:CB   | 2.64                     | 0.46              |
| 3:D:171:LEU:HD12  | 3:D:393:ILE:HD13  | 1.98                     | 0.46              |
| 3:D:799:LYS:HD3   | 3:D:826:PRO:CG    | 2.46                     | 0.46              |
| 3:D:984:THR:CG2   | 3:D:987:GLU:HG3   | 2.44                     | 0.46              |
| 2:H:1065:ALA:CB   | 2:H:1077:PRO:HG2  | 2.36                     | 0.46              |
| 2:H:273:GLY:HA2   | 2:H:276:LYS:HD2   | 1.97                     | 0.46              |
| 2:H:368:THR:HB    | 2:H:369:PRO:HD2   | 1.97                     | 0.46              |
| 2:H:572:ILE:HG23  | 2:H:703:ILE:CD1   | 2.39                     | 0.46              |
| 2:H:6:PHE:HZ      | 2:H:917:LEU:HD11  | 1.81                     | 0.46              |
| 3:I:1021:TYR:CE2  | 3:I:1025:GLN:HG2  | 2.51                     | 0.46              |
| 3:I:996:TRP:CG    | 3:I:1056:PRO:HG2  | 2.51                     | 0.46              |
| 3:I:1148:VAL:HG13 | 3:I:1163:GLY:O    | 2.15                     | 0.46              |
| 3:I:1155:VAL:CG1  | 3:I:1177:ALA:HB1  | 2.46                     | 0.46              |
| 3:I:408:GLU:CG    | 3:I:409:VAL:N     | 2.58                     | 0.46              |
| 3:I:520:LEU:HD12  | 3:I:521:PRO:CD    | 2.44                     | 0.46              |
| 3:I:551:ASN:O     | 3:I:555:LYS:HG3   | 2.16                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:I:562:ALA:HB1   | 3:I:567:ILE:HD11 | 1.98                     | 0.46              |
| 3:I:458:ALA:HB2   | 3:I:575:GLN:NE2  | 2.30                     | 0.46              |
| 4:J:61:VAL:HG23   | 4:J:62:THR:N     | 2.31                     | 0.46              |
| 1:L:7:LYS:HB3     | 1:L:7:LYS:HE3    | 1.70                     | 0.46              |
| 2:M:176:VAL:CG1   | 2:M:182:VAL:HG13 | 2.42                     | 0.46              |
| 2:M:338:GLU:HA    | 2:M:341:THR:HG22 | 1.97                     | 0.46              |
| 2:M:546:LEU:HD13  | 2:M:565:GLN:OE1  | 2.14                     | 0.46              |
| 2:M:625:LEU:O     | 2:M:627:ARG:N    | 2.49                     | 0.46              |
| 2:M:863:ASP:C     | 2:M:863:ASP:OD2  | 2.54                     | 0.46              |
| 3:N:1087:ARG:HG2  | 3:N:1234:THR:O   | 2.16                     | 0.46              |
| 3:N:1412:LYS:HE2  | 3:N:1414:PRO:HG3 | 1.96                     | 0.46              |
| 3:N:1468:LEU:HD22 | 3:N:1470:ARG:HD3 | 1.98                     | 0.46              |
| 3:N:180:LYS:HZ2   | 3:N:387:LEU:N    | 2.14                     | 0.46              |
| 3:N:465:LEU:HD22  | 3:N:510:GLU:CA   | 2.46                     | 0.46              |
| 3:N:50:PHE:HB3    | 3:N:522:PRO:CD   | 2.46                     | 0.46              |
| 3:N:29:PRO:HD3    | 3:N:548:ILE:HG22 | 1.98                     | 0.46              |
| 1:B:56:VAL:CG1    | 1:B:57:TYR:N     | 2.78                     | 0.46              |
| 2:C:187:ASN:O     | 2:C:188:LYS:CB   | 2.64                     | 0.46              |
| 2:C:258:TYR:CE1   | 2:C:264:PRO:HG3  | 2.51                     | 0.46              |
| 2:C:333:ILE:CG1   | 2:C:410:ILE:HD13 | 2.46                     | 0.46              |
| 2:C:859:PRO:HB2   | 2:C:867:VAL:CG2  | 2.46                     | 0.46              |
| 3:D:116:LEU:CD2   | 3:D:118:LEU:CG   | 2.72                     | 0.46              |
| 3:D:1397:LYS:NZ   | 3:D:1432:LYS:NZ  | 2.63                     | 0.46              |
| 3:D:179:VAL:HG13  | 3:D:183:GLU:CG   | 2.46                     | 0.46              |
| 3:D:170:PRO:HA    | 3:D:392:SER:HB3  | 1.98                     | 0.46              |
| 3:D:465:LEU:HD21  | 3:D:509:PRO:CB   | 2.44                     | 0.46              |
| 4:E:61:VAL:CG2    | 4:E:62:THR:N     | 2.79                     | 0.46              |
| 1:G:51:THR:HG22   | 1:G:145:ASP:O    | 2.16                     | 0.46              |
| 2:H:1046:ALA:CB   | 3:I:1476:THR:HB  | 2.46                     | 0.46              |
| 2:H:1078:GLU:HA   | 2:H:1079:PRO:HD3 | 1.79                     | 0.46              |
| 2:H:144:PRO:O     | 2:H:276:LYS:HD3  | 2.16                     | 0.46              |
| 2:H:184:MET:SD    | 2:H:191:PHE:CE1  | 3.09                     | 0.46              |
| 2:H:251:ASP:O     | 2:H:252:LYS:C    | 2.54                     | 0.46              |
| 2:H:332:ARG:NE    | 2:H:464:LEU:CD1  | 2.78                     | 0.46              |
| 3:I:100:ALA:CB    | 3:I:128:TYR:OH   | 2.64                     | 0.46              |
| 3:I:123:LEU:CD1   | 3:I:152:LEU:HD21 | 2.44                     | 0.46              |
| 3:I:141:ILE:HG13  | 3:I:448:GLU:CD   | 2.37                     | 0.46              |
| 3:I:47:GLU:O      | 3:I:51:GLY:CA    | 2.64                     | 0.46              |
| 3:I:564:GLU:C     | 3:I:566:ILE:H    | 2.18                     | 0.46              |
| 3:I:593:ASN:O     | 3:I:594:PRO:C    | 2.54                     | 0.46              |
| 3:I:90:MET:HG2    | 3:I:521:PRO:HG3  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:3:GLU:OE1     | 4:J:4:PRO:CD      | 2.64                     | 0.46              |
| 1:K:156:HIS:CD2   | 1:K:158:ILE:CD1   | 2.99                     | 0.46              |
| 1:K:165:ILE:HG12  | 1:K:165:ILE:O     | 2.16                     | 0.46              |
| 1:K:206:THR:HG23  | 1:K:208:LEU:H     | 1.79                     | 0.46              |
| 2:M:31:GLN:NE2    | 2:M:34:VAL:HG22   | 2.31                     | 0.46              |
| 2:M:374:ASN:O     | 2:M:374:ASN:ND2   | 2.49                     | 0.46              |
| 2:M:791:ARG:HG2   | 2:M:791:ARG:HH11  | 1.81                     | 0.46              |
| 3:N:1007:VAL:CG1  | 3:N:1039:CYS:HB2  | 2.37                     | 0.46              |
| 2:M:906:PHE:CD1   | 3:N:1067:VAL:HG13 | 2.51                     | 0.46              |
| 3:N:178:LEU:CD1   | 3:N:179:VAL:HG23  | 2.44                     | 0.46              |
| 3:N:180:LYS:NZ    | 3:N:387:LEU:N     | 2.64                     | 0.46              |
| 3:N:631:ILE:CD1   | 3:N:743:ASP:O     | 2.53                     | 0.46              |
| 3:N:835:SER:C     | 3:N:837:GLY:N     | 2.69                     | 0.46              |
| 3:N:925:GLU:HG2   | 3:N:926:LYS:N     | 2.31                     | 0.46              |
| 7:X:109:GLU:HG3   | 7:X:118:LYS:HD3   | 1.96                     | 0.46              |
| 7:Z:115:THR:CB    | 7:Z:116:PRO:CD    | 2.94                     | 0.46              |
| 1:B:152:PRO:HA    | 1:B:168:ASP:OD1   | 2.16                     | 0.45              |
| 1:B:57:TYR:CE1    | 1:B:163:ASN:OD1   | 2.68                     | 0.45              |
| 1:B:227:ASN:HD22  | 1:B:227:ASN:N     | 2.14                     | 0.45              |
| 2:C:336:VAL:O     | 2:C:339:LEU:HB2   | 2.16                     | 0.45              |
| 2:C:139:GLN:NE2   | 2:C:415:PRO:CD    | 2.76                     | 0.45              |
| 1:A:83:LYS:NZ     | 2:C:698:ASP:OD2   | 2.49                     | 0.45              |
| 2:C:671:ASN:OD1   | 2:C:993:PHE:HD2   | 1.99                     | 0.45              |
| 3:D:953:ASP:OD1   | 3:D:1019:PRO:HG2  | 2.17                     | 0.45              |
| 2:C:1098:ASP:O    | 3:D:10:ILE:HA     | 2.16                     | 0.45              |
| 3:D:129:PHE:O     | 3:D:130:SER:OG    | 2.30                     | 0.45              |
| 3:D:1340:GLY:O    | 3:D:1344:VAL:HG23 | 2.15                     | 0.45              |
| 3:D:1472:ILE:HD13 | 3:D:1474:ALA:O    | 2.15                     | 0.45              |
| 3:D:388:HIS:C     | 3:D:390:PRO:HD3   | 2.36                     | 0.45              |
| 3:D:589:ALA:HA    | 3:D:590:PRO:HD3   | 1.74                     | 0.45              |
| 3:D:814:ALA:O     | 3:D:818:ARG:HG3   | 2.15                     | 0.45              |
| 3:D:996:TRP:O     | 3:D:999:THR:HG22  | 2.16                     | 0.45              |
| 1:F:156:HIS:CD2   | 1:F:158:ILE:CD1   | 2.99                     | 0.45              |
| 2:H:854:PRO:HB2   | 2:H:856:GLU:CD    | 2.36                     | 0.45              |
| 3:I:1221:VAL:O    | 3:I:1222:GLY:C    | 2.53                     | 0.45              |
| 3:I:1231:GLU:CB   | 3:I:1232:PRO:HD3  | 2.45                     | 0.45              |
| 3:I:608:SER:HB3   | 3:I:1443:THR:OG1  | 2.16                     | 0.45              |
| 3:I:204:LEU:HB3   | 3:I:394:LEU:CG    | 2.26                     | 0.45              |
| 3:I:481:MET:O     | 3:I:489:ARG:HB2   | 2.17                     | 0.45              |
| 3:I:525:ARG:HG3   | 3:I:540:LEU:HD13  | 1.98                     | 0.45              |
| 3:I:667:ALA:HA    | 3:I:668:PRO:HD3   | 1.72                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:791:TYR:CD1   | 3:I:1022:VAL:HG11 | 2.51                     | 0.45              |
| 3:I:813:LEU:CD1   | 3:I:814:ALA:N     | 2.73                     | 0.45              |
| 3:I:921:ARG:C     | 3:I:922:LEU:HD23  | 2.36                     | 0.45              |
| 1:L:149:GLY:O     | 1:L:171:PHE:HB2   | 2.17                     | 0.45              |
| 1:L:80:LEU:HD12   | 1:L:83:LYS:HE3    | 1.98                     | 0.45              |
| 3:N:1363:LEU:HD11 | 3:N:1368:ILE:HD11 | 1.96                     | 0.45              |
| 3:N:511:TRP:C     | 3:N:513:ILE:H     | 2.20                     | 0.45              |
| 4:O:70:THR:OG1    | 4:O:72:ARG:CG     | 2.64                     | 0.45              |
| 7:Y:84:GLY:O      | 7:Y:87:SER:OG     | 2.28                     | 0.45              |
| 7:Z:89:VAL:CG1    | 7:Z:90:GLU:N      | 2.78                     | 0.45              |
| 1:A:19:GLU:N      | 1:A:19:GLU:CD     | 2.68                     | 0.45              |
| 1:B:73:GLU:HG3    | 1:B:130:ALA:CB    | 2.46                     | 0.45              |
| 2:C:95:TYR:HB3    | 2:C:114:PHE:HA    | 1.97                     | 0.45              |
| 2:C:207:LEU:CD2   | 2:C:221:LEU:CD2   | 2.90                     | 0.45              |
| 2:C:267:TYR:O     | 2:C:267:TYR:HD2   | 2.00                     | 0.45              |
| 2:C:325:ILE:N     | 2:C:325:ILE:CD1   | 2.66                     | 0.45              |
| 2:C:367:LEU:HD13  | 2:C:372:LEU:HD11  | 1.98                     | 0.45              |
| 2:C:854:PRO:HB2   | 2:C:856:GLU:CD    | 2.36                     | 0.45              |
| 3:D:102:ILE:HD13  | 3:D:102:ILE:C     | 2.35                     | 0.45              |
| 3:D:1109:GLU:CD   | 3:D:1201:CYS:HB2  | 2.37                     | 0.45              |
| 3:D:1223:ILE:HD11 | 3:D:1462:LEU:CD1  | 2.46                     | 0.45              |
| 3:D:169:TYR:HE2   | 3:D:197:SER:HA    | 1.77                     | 0.45              |
| 3:D:348:GLN:HB2   | 3:D:351:MET:CE    | 2.46                     | 0.45              |
| 3:D:44:LEU:O      | 3:D:50:PHE:HE1    | 1.95                     | 0.45              |
| 3:D:457:GLY:O     | 3:D:458:ALA:C     | 2.54                     | 0.45              |
| 3:D:617:ASN:HB2   | 3:D:1467:ILE:HG23 | 1.98                     | 0.45              |
| 3:D:787:LEU:HD12  | 3:D:787:LEU:C     | 2.36                     | 0.45              |
| 3:D:841:TYR:HB2   | 3:D:864:VAL:HG11  | 1.96                     | 0.45              |
| 3:D:994:GLN:OE1   | 3:D:994:GLN:HA    | 2.16                     | 0.45              |
| 1:F:21:GLY:HA3    | 1:F:207:PRO:CB    | 2.46                     | 0.45              |
| 1:G:143:ARG:HD3   | 1:G:158:ILE:HG21  | 1.98                     | 0.45              |
| 1:G:38:ASN:O      | 1:G:41:ARG:HB3    | 2.15                     | 0.45              |
| 2:H:170:PRO:HB2   | 2:H:172:ILE:HD11  | 1.97                     | 0.45              |
| 2:H:189:ARG:HA    | 2:H:189:ARG:HD3   | 1.69                     | 0.45              |
| 2:H:221:LEU:HD12  | 2:H:222:MET:N     | 2.31                     | 0.45              |
| 2:H:863:ASP:OD2   | 2:H:863:ASP:C     | 2.54                     | 0.45              |
| 3:I:111:LYS:HE3   | 3:I:1449:GLU:HA   | 1.98                     | 0.45              |
| 3:I:141:ILE:CD1   | 3:I:448:GLU:OE2   | 2.64                     | 0.45              |
| 3:I:166:GLN:HE21  | 3:I:396:VAL:HG12  | 1.78                     | 0.45              |
| 3:I:204:LEU:HD11  | 3:I:441:ARG:NH2   | 2.23                     | 0.45              |
| 3:I:433:GLY:CA    | 3:I:447:VAL:O     | 2.65                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:I:786:ILE:O     | 3:I:787:LEU:C    | 2.55                     | 0.45              |
| 2:M:162:ILE:CG2   | 2:M:172:ILE:HD13 | 2.46                     | 0.45              |
| 2:M:361:MET:HE3   | 2:M:361:MET:O    | 2.15                     | 0.45              |
| 2:M:36:PRO:C      | 2:M:39:ARG:HB2   | 2.37                     | 0.45              |
| 2:M:857:ASP:HB2   | 2:M:978:ARG:CG   | 2.40                     | 0.45              |
| 2:M:946:ARG:CB    | 2:M:946:ARG:HH11 | 2.25                     | 0.45              |
| 3:N:1258:ARG:NH2  | 3:N:1351:GLU:HG2 | 2.29                     | 0.45              |
| 3:N:1365:ASP:O    | 3:N:1366:LYS:C   | 2.54                     | 0.45              |
| 3:N:189:GLN:HB3   | 3:N:189:GLN:HE21 | 1.60                     | 0.45              |
| 3:N:481:MET:HE2   | 3:N:493:ARG:HB2  | 1.97                     | 0.45              |
| 3:N:660:LYS:NZ    | 3:N:660:LYS:CA   | 2.79                     | 0.45              |
| 3:N:720:LEU:H     | 3:N:720:LEU:HD12 | 1.81                     | 0.45              |
| 3:N:907:GLU:CD    | 3:N:909:ASN:HD22 | 2.19                     | 0.45              |
| 3:N:99:ALA:O      | 3:N:514:LEU:N    | 2.48                     | 0.45              |
| 7:X:32:ILE:HG22   | 7:X:33:LEU:N     | 2.31                     | 0.45              |
| 7:Y:89:VAL:HG12   | 7:Y:91:LEU:HD23  | 1.97                     | 0.45              |
| 1:A:9:PRO:CB      | 1:A:25:LEU:HD11  | 2.46                     | 0.45              |
| 2:C:137:VAL:O     | 2:C:391:LEU:HD21 | 2.16                     | 0.45              |
| 2:C:175:GLU:N     | 2:C:183:SER:O    | 2.39                     | 0.45              |
| 2:C:285:LEU:HG    | 2:C:286:SER:N    | 2.30                     | 0.45              |
| 2:C:363:SER:OG    | 2:C:366:SER:CB   | 2.64                     | 0.45              |
| 2:C:66:LEU:HD22   | 2:C:372:LEU:HD22 | 1.97                     | 0.45              |
| 2:C:710:ILE:HB    | 2:C:790:LEU:HB2  | 1.98                     | 0.45              |
| 2:C:946:ARG:HH11  | 2:C:946:ARG:CB   | 2.25                     | 0.45              |
| 3:D:1262:LEU:HD12 | 3:D:1262:LEU:HA  | 1.84                     | 0.45              |
| 2:H:272:ALA:O     | 2:H:276:LYS:NZ   | 2.33                     | 0.45              |
| 2:H:9:ILE:HD13    | 2:H:536:PRO:CD   | 2.47                     | 0.45              |
| 2:H:124:ASP:CG    | 2:H:592:LEU:HD12 | 2.36                     | 0.45              |
| 2:H:554:ASP:HB2   | 2:H:880:MET:HB2  | 1.97                     | 0.45              |
| 3:I:762:GLN:NE2   | 4:J:20:THR:CG2   | 2.54                     | 0.45              |
| 3:I:994:GLN:OE1   | 3:I:994:GLN:HA   | 2.17                     | 0.45              |
| 4:J:32:ARG:HB2    | 4:J:32:ARG:HH11  | 1.82                     | 0.45              |
| 1:L:211:LEU:O     | 1:L:214:ALA:HB3  | 2.17                     | 0.45              |
| 2:M:1096:ALA:HB1  | 3:N:12:LEU:CD2   | 2.46                     | 0.45              |
| 2:M:144:PRO:O     | 2:M:276:LYS:CE   | 2.65                     | 0.45              |
| 2:M:267:TYR:CE1   | 2:M:273:GLY:HA3  | 2.52                     | 0.45              |
| 2:M:756:VAL:HB    | 2:M:790:LEU:HB3  | 1.98                     | 0.45              |
| 2:M:882:LEU:HD12  | 3:N:1061:PHE:HB3 | 1.98                     | 0.45              |
| 2:M:897:LEU:HD21  | 2:M:921:ALA:N    | 2.32                     | 0.45              |
| 3:N:1145:TYR:CG   | 3:N:1146:GLY:N   | 2.85                     | 0.45              |
| 3:N:116:LEU:O     | 3:N:117:ASP:HB3  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:1221:VAL:O   | 3:N:1222:GLY:C    | 2.53                     | 0.45              |
| 2:M:1086:ARG:CD  | 3:N:88:TYR:CE2    | 2.96                     | 0.45              |
| 4:O:57:ASP:N     | 4:O:58:PRO:HD3    | 2.30                     | 0.45              |
| 7:Y:128:ALA:HB2  | 7:Y:140:LEU:HD21  | 1.97                     | 0.45              |
| 1:B:56:VAL:HG21  | 1:B:82:LEU:HD13   | 1.97                     | 0.45              |
| 2:C:334:ARG:O    | 2:C:339:LEU:HD11  | 2.16                     | 0.45              |
| 2:C:22:GLN:HE21  | 2:C:336:VAL:CG2   | 2.29                     | 0.45              |
| 2:C:64:LEU:HD13  | 2:C:359:MET:HG2   | 1.97                     | 0.45              |
| 2:C:462:ASP:HB3  | 2:C:468:ARG:HD2   | 1.99                     | 0.45              |
| 2:C:12:VAL:CB    | 2:C:472:ARG:HH11  | 2.30                     | 0.45              |
| 2:C:540:PHE:HZ   | 3:D:1070:TYR:HD1  | 1.64                     | 0.45              |
| 2:C:674:VAL:HB   | 2:C:869:VAL:HG13  | 1.98                     | 0.45              |
| 2:C:966:LEU:HD21 | 2:C:986:PRO:HG2   | 1.97                     | 0.45              |
| 3:D:1138:ALA:O   | 3:D:1141:GLU:HB2  | 2.17                     | 0.45              |
| 3:D:1113:GLY:N   | 3:D:1195:GLN:OE1  | 2.50                     | 0.45              |
| 3:D:1208:ASP:O   | 3:D:1215:VAL:HG22 | 2.16                     | 0.45              |
| 3:D:171:LEU:HB2  | 3:D:392:SER:HA    | 1.98                     | 0.45              |
| 3:D:759:ALA:O    | 3:D:763:MET:HB3   | 2.17                     | 0.45              |
| 1:F:72:LYS:HE2   | 2:H:641:PRO:O     | 2.16                     | 0.45              |
| 2:H:1019:GLN:OE1 | 3:I:621:LYS:HD3   | 2.13                     | 0.45              |
| 2:H:1068:GLU:O   | 2:H:1071:ILE:HB   | 2.17                     | 0.45              |
| 2:H:17:PRO:HD2   | 2:H:20:GLU:OE2    | 2.17                     | 0.45              |
| 2:H:281:LEU:CD1  | 2:H:306:THR:HA    | 2.46                     | 0.45              |
| 2:H:332:ARG:NE   | 2:H:464:LEU:HG    | 2.32                     | 0.45              |
| 2:H:863:ASP:O    | 2:H:865:THR:N     | 2.48                     | 0.45              |
| 3:I:1045:MET:O   | 3:I:1053:PHE:HB2  | 2.17                     | 0.45              |
| 3:I:956:ILE:N    | 3:I:956:ILE:HD12  | 2.30                     | 0.45              |
| 4:J:53:GLY:C     | 4:J:55:PHE:H      | 2.20                     | 0.45              |
| 1:K:65:PHE:HE1   | 2:M:799:ILE:HG13  | 1.81                     | 0.45              |
| 1:L:227:ASN:HD22 | 1:L:227:ASN:N     | 2.14                     | 0.45              |
| 2:M:1047:HIS:O   | 2:M:1051:GLU:HB2  | 2.17                     | 0.45              |
| 2:M:1068:GLU:O   | 2:M:1071:ILE:HB   | 2.17                     | 0.45              |
| 2:M:48:PHE:HA    | 2:M:348:LEU:HD21  | 1.98                     | 0.45              |
| 2:M:571:LEU:CD1  | 2:M:701:THR:N     | 2.78                     | 0.45              |
| 2:M:585:GLU:CD   | 2:M:585:GLU:C     | 2.75                     | 0.45              |
| 2:M:854:PRO:HB2  | 2:M:856:GLU:CD    | 2.36                     | 0.45              |
| 2:M:1095:LEU:HA  | 3:N:101:HIS:HE2   | 1.82                     | 0.45              |
| 3:N:1031:ASN:CG  | 3:N:1032:PRO:HD2  | 2.37                     | 0.45              |
| 3:N:1092:GLY:O   | 3:N:1095:THR:OG1  | 2.24                     | 0.45              |
| 3:N:1109:GLU:CG  | 3:N:1202:GLN:H    | 2.26                     | 0.45              |
| 3:N:1209:LEU:CD2 | 3:N:1211:MET:H    | 2.24                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1348:LEU:HD23 | 3:N:1372:VAL:HG23 | 1.99                     | 0.45              |
| 3:N:1428:ALA:O    | 3:N:1431:THR:HG22 | 2.17                     | 0.45              |
| 3:N:1477:GLY:O    | 3:N:1478:SER:C    | 2.54                     | 0.45              |
| 3:N:162:ARG:C     | 3:N:452:ILE:HG21  | 2.37                     | 0.45              |
| 3:N:179:VAL:HG13  | 3:N:183:GLU:CD    | 2.36                     | 0.45              |
| 3:N:400:VAL:O     | 3:N:400:VAL:HG13  | 2.16                     | 0.45              |
| 3:N:787:LEU:HD12  | 3:N:787:LEU:C     | 2.36                     | 0.45              |
| 3:N:832:ARG:HA    | 3:N:832:ARG:NE    | 2.31                     | 0.45              |
| 7:Y:18:GLN:NE2    | 7:Y:65:LEU:HD21   | 2.32                     | 0.45              |
| 1:A:10:VAL:O      | 1:A:12:THR:HG23   | 2.16                     | 0.45              |
| 1:A:42:ARG:HH11   | 1:B:34:VAL:HG12   | 1.80                     | 0.45              |
| 1:B:52:ALA:HB2    | 1:B:170:VAL:O     | 2.16                     | 0.45              |
| 2:C:1008:ARG:HH12 | 2:C:1011:GLY:N    | 2.15                     | 0.45              |
| 2:C:1046:ALA:HB3  | 2:C:1047:HIS:HD2  | 1.80                     | 0.45              |
| 2:C:204:GLN:NE2   | 2:C:228:ALA:CB    | 2.79                     | 0.45              |
| 2:C:642:ARG:CD    | 2:C:642:ARG:O     | 2.56                     | 0.45              |
| 2:C:548:PRO:HG2   | 2:C:842:ARG:NH2   | 2.32                     | 0.45              |
| 3:D:1139:ASP:O    | 3:D:1142:ALA:HB3  | 2.16                     | 0.45              |
| 3:D:1426:LYS:HA   | 3:D:1429:LEU:HB2  | 1.99                     | 0.45              |
| 3:D:1428:ALA:O    | 3:D:1429:LEU:C    | 2.55                     | 0.45              |
| 3:D:348:GLN:HB2   | 3:D:351:MET:HE1   | 1.99                     | 0.45              |
| 3:D:907:GLU:CD    | 3:D:909:ASN:HD22  | 2.19                     | 0.45              |
| 2:H:307:LEU:HD11  | 2:H:311:PHE:CE2   | 2.52                     | 0.45              |
| 2:H:90:TYR:O      | 2:H:90:TYR:HD1    | 2.00                     | 0.45              |
| 2:H:577:PRO:HG3   | 2:H:993:PHE:CZ    | 2.51                     | 0.45              |
| 3:I:1089:ALA:C    | 3:I:1091:SER:H    | 2.19                     | 0.45              |
| 3:I:116:LEU:O     | 3:I:117:ASP:HB3   | 2.16                     | 0.45              |
| 3:I:1273:VAL:HG21 | 3:I:1305:LEU:HD21 | 1.97                     | 0.45              |
| 3:I:1434:TRP:CG   | 3:I:1435:LEU:N    | 2.84                     | 0.45              |
| 3:I:191:LEU:HD21  | 3:I:203:ALA:CB    | 2.47                     | 0.45              |
| 3:I:465:LEU:HD22  | 3:I:510:GLU:CA    | 2.46                     | 0.45              |
| 3:I:660:LYS:NZ    | 3:I:660:LYS:CA    | 2.79                     | 0.45              |
| 3:I:759:ALA:O     | 3:I:763:MET:HB3   | 2.17                     | 0.45              |
| 1:K:61:VAL:HG13   | 1:K:66:SER:HB3    | 1.99                     | 0.45              |
| 2:M:200:LEU:HB3   | 2:M:300:ASP:OD1   | 2.15                     | 0.45              |
| 2:M:282:GLY:C     | 2:M:283:ILE:CG1   | 2.85                     | 0.45              |
| 2:M:39:ARG:NH1    | 2:M:70:GLU:HA     | 2.31                     | 0.45              |
| 2:M:54:ILE:O      | 2:M:65:VAL:HA     | 2.17                     | 0.45              |
| 2:M:681:GLY:C     | 3:N:635:PRO:CG    | 2.82                     | 0.45              |
| 3:N:1045:MET:HG3  | 3:N:1073:SER:OG   | 2.17                     | 0.45              |
| 3:N:1089:ALA:C    | 3:N:1091:SER:H    | 2.18                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:1256:LEU:O   | 3:N:1260:ILE:N    | 2.46                     | 0.45              |
| 3:N:1397:LYS:NZ  | 3:N:1432:LYS:NZ   | 2.65                     | 0.45              |
| 3:N:149:LYS:CE   | 3:N:149:LYS:H     | 2.30                     | 0.45              |
| 3:N:157:GLU:O    | 3:N:161:LEU:N     | 2.50                     | 0.45              |
| 2:M:1093:GLN:CB  | 3:N:21:TRP:CZ3    | 2.72                     | 0.45              |
| 3:N:407:VAL:HG21 | 3:N:437:VAL:HG11  | 1.98                     | 0.45              |
| 3:N:158:TYR:HE1  | 3:N:452:ILE:HD11  | 1.81                     | 0.45              |
| 3:N:464:LEU:HD23 | 3:N:464:LEU:HA    | 1.73                     | 0.45              |
| 3:N:642:CYS:O    | 3:N:642:CYS:SG    | 2.74                     | 0.45              |
| 3:N:827:ILE:H    | 3:N:827:ILE:CD1   | 2.28                     | 0.45              |
| 7:X:123:SER:O    | 7:X:127:LYS:N     | 2.47                     | 0.45              |
| 7:X:21:ARG:O     | 7:X:25:ARG:HG3    | 2.16                     | 0.45              |
| 1:A:174:VAL:HG13 | 1:A:200:TRP:O     | 2.17                     | 0.45              |
| 1:B:149:GLY:O    | 1:B:171:PHE:HB2   | 2.17                     | 0.45              |
| 2:C:224:GLU:HB3  | 2:C:228:ALA:CA    | 2.42                     | 0.45              |
| 2:C:81:ASP:HA    | 2:C:84:ARG:NH1    | 2.31                     | 0.45              |
| 3:D:13:ALA:HB1   | 3:D:18:ILE:CD1    | 2.46                     | 0.45              |
| 3:D:162:ARG:HD2  | 3:D:162:ARG:HA    | 1.45                     | 0.45              |
| 3:D:402:PRO:HA   | 3:D:443:VAL:HG23  | 1.98                     | 0.45              |
| 3:D:96:ALA:CB    | 3:D:554:LEU:HD23  | 2.37                     | 0.45              |
| 3:D:771:SER:HB2  | 3:D:778:LEU:CD1   | 2.37                     | 0.45              |
| 3:D:972:LEU:C    | 3:D:976:GLN:HE21  | 2.20                     | 0.45              |
| 4:E:33:HIS:CD2   | 4:E:89:MET:HG2    | 2.51                     | 0.45              |
| 2:H:9:ILE:HG12   | 2:H:907:ASP:CG    | 2.36                     | 0.45              |
| 3:I:1347:TYR:HD2 | 3:I:1348:LEU:HD12 | 1.81                     | 0.45              |
| 3:I:127:LEU:HD22 | 3:I:134:VAL:CG1   | 2.45                     | 0.45              |
| 3:I:1365:ASP:O   | 3:I:1366:LYS:C    | 2.54                     | 0.45              |
| 3:I:465:LEU:HD21 | 3:I:509:PRO:CB    | 2.44                     | 0.45              |
| 3:I:546:ARG:HG2  | 3:I:546:ARG:NH1   | 2.32                     | 0.45              |
| 3:I:557:LEU:CD2  | 3:I:566:ILE:HG21  | 2.47                     | 0.45              |
| 3:I:755:ALA:O    | 3:I:758:GLU:HG2   | 2.15                     | 0.45              |
| 1:L:142:VAL:HG23 | 1:L:142:VAL:O     | 2.17                     | 0.45              |
| 1:L:65:PHE:CE1   | 3:N:813:LEU:HD22  | 2.52                     | 0.45              |
| 2:M:290:LEU:HB3  | 2:M:302:VAL:CG1   | 2.22                     | 0.45              |
| 2:M:399:ASN:OD1  | 2:M:402:SER:CB    | 2.60                     | 0.45              |
| 3:N:1257:PRO:CA  | 3:N:1260:ILE:CD1  | 2.87                     | 0.45              |
| 3:N:1369:GLU:HA  | 3:N:1372:VAL:HG12 | 1.96                     | 0.45              |
| 3:N:148:GLU:CG   | 3:N:151:GLN:CB    | 2.94                     | 0.45              |
| 3:N:1491:THR:HA  | 3:N:1494:ALA:HB3  | 1.99                     | 0.45              |
| 3:N:355:VAL:CG1  | 3:N:356:PRO:HD2   | 2.47                     | 0.45              |
| 3:N:486:ARG:HA   | 3:N:489:ARG:CG    | 2.35                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:720:LEU:N     | 3:N:720:LEU:HD12  | 2.32                     | 0.45              |
| 4:O:45:ARG:HH21   | 4:O:63:TRP:HH2    | 1.64                     | 0.45              |
| 3:D:970:LYS:CE    | 7:X:113:LEU:HD23  | 2.46                     | 0.45              |
| 7:Y:111:ASN:HD21  | 7:Y:113:LEU:HD12  | 1.82                     | 0.45              |
| 7:Z:105:VAL:O     | 7:Z:121:ASP:N     | 2.49                     | 0.45              |
| 7:Z:89:VAL:HG13   | 7:Z:151:VAL:HG13  | 1.99                     | 0.45              |
| 1:B:29:GLU:HB2    | 1:B:32:PHE:CD1    | 2.51                     | 0.45              |
| 1:B:76:VAL:HB     | 3:D:872:ARG:NH1   | 2.32                     | 0.45              |
| 2:C:273:GLY:HA2   | 2:C:276:LYS:CD    | 2.47                     | 0.45              |
| 1:A:70:GLY:N      | 2:C:607:ASP:OD1   | 2.46                     | 0.45              |
| 2:C:625:LEU:O     | 2:C:626:ARG:C     | 2.56                     | 0.45              |
| 2:C:699:PHE:HB3   | 2:C:700:TYR:HD1   | 1.81                     | 0.45              |
| 2:C:950:LEU:CD1   | 2:C:950:LEU:O     | 2.65                     | 0.45              |
| 2:C:516:ARG:HD2   | 3:D:1068:LEU:HD22 | 1.99                     | 0.45              |
| 3:D:1118:ILE:HG13 | 3:D:1192:LEU:HD12 | 1.99                     | 0.45              |
| 3:D:115:LEU:HD12  | 3:D:502:PHE:CE1   | 2.51                     | 0.45              |
| 3:D:1107:VAL:HG13 | 3:D:1200:VAL:O    | 2.17                     | 0.45              |
| 3:D:1434:TRP:HZ3  | 3:D:1457:ASP:N    | 2.14                     | 0.45              |
| 3:D:179:VAL:HG13  | 3:D:183:GLU:CB    | 2.44                     | 0.45              |
| 3:D:210:ARG:CZ    | 3:D:389:GLU:OE2   | 2.65                     | 0.45              |
| 3:D:451:ASP:C     | 3:D:452:ILE:HG23  | 2.37                     | 0.45              |
| 3:D:465:LEU:HD22  | 3:D:510:GLU:CA    | 2.46                     | 0.45              |
| 3:D:835:SER:N     | 3:D:838:ARG:HD3   | 2.32                     | 0.45              |
| 3:D:875:THR:CG2   | 3:D:879:ARG:CB    | 2.95                     | 0.45              |
| 1:F:124:ASN:HD21  | 1:F:127:LEU:CD2   | 2.26                     | 0.45              |
| 1:F:26:GLU:HB3    | 1:F:194:LYS:HG3   | 1.98                     | 0.45              |
| 2:H:110:GLU:O     | 2:H:111:ASP:CG    | 2.55                     | 0.45              |
| 2:H:146:VAL:HG22  | 2:H:162:ILE:HG12  | 1.99                     | 0.45              |
| 2:H:403:SER:O     | 2:H:407:LYS:HG3   | 2.17                     | 0.45              |
| 2:H:631:SER:CB    | 2:H:637:LEU:HD11  | 2.47                     | 0.45              |
| 2:H:595:LEU:HG    | 2:H:655:LEU:HD12  | 1.98                     | 0.45              |
| 2:H:691:SER:O     | 2:H:692:GLU:C     | 2.55                     | 0.45              |
| 2:H:897:LEU:HD21  | 2:H:921:ALA:N     | 2.32                     | 0.45              |
| 2:H:987:ILE:HD12  | 3:I:948:THR:CG2   | 2.46                     | 0.45              |
| 3:I:1045:MET:HG3  | 3:I:1073:SER:OG   | 2.17                     | 0.45              |
| 3:I:1258:ARG:CZ   | 3:I:1262:LEU:HD13 | 2.47                     | 0.45              |
| 3:I:687:VAL:O     | 3:I:690:ALA:HB3   | 2.16                     | 0.45              |
| 3:I:835:SER:N     | 3:I:838:ARG:HD3   | 2.32                     | 0.45              |
| 3:I:875:THR:CG2   | 3:I:879:ARG:CB    | 2.94                     | 0.45              |
| 3:I:87:ARG:HD3    | 3:I:87:ARG:HA     | 1.61                     | 0.45              |
| 1:K:11:PHE:HB2    | 1:K:25:LEU:CD1    | 2.46                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:26:GLU:HB3    | 1:K:194:LYS:HG3   | 1.99                     | 0.45              |
| 2:M:1019:GLN:HG3  | 3:N:621:LYS:HD2   | 1.99                     | 0.45              |
| 2:M:12:VAL:HG21   | 2:M:472:ARG:NH1   | 2.32                     | 0.45              |
| 2:M:154:ARG:HH12  | 2:M:177:GLU:HA    | 1.82                     | 0.45              |
| 2:M:100:LEU:CD2   | 2:M:372:LEU:HD21  | 2.47                     | 0.45              |
| 2:M:697:ARG:HD2   | 2:M:699:PHE:CE1   | 2.50                     | 0.45              |
| 2:M:69:LEU:HB2    | 2:M:97:ARG:O      | 2.16                     | 0.45              |
| 2:M:730:SER:O     | 2:M:734:LEU:HD22  | 2.16                     | 0.45              |
| 2:M:969:GLN:HB3   | 2:M:969:GLN:HE21  | 1.47                     | 0.45              |
| 3:N:1147:ARG:HB3  | 3:N:1188:VAL:CG2  | 2.43                     | 0.45              |
| 3:N:1275:SER:HB2  | 3:N:1294:VAL:HG21 | 1.97                     | 0.45              |
| 3:N:141:ILE:HG23  | 3:N:162:ARG:NH1   | 2.32                     | 0.45              |
| 3:N:50:PHE:CB     | 3:N:522:PRO:CG    | 2.87                     | 0.45              |
| 3:N:835:SER:N     | 3:N:838:ARG:CD    | 2.79                     | 0.45              |
| 3:N:994:GLN:HA    | 3:N:994:GLN:OE1   | 2.16                     | 0.45              |
| 7:Y:31:LYS:HB3    | 7:Y:31:LYS:HE2    | 1.72                     | 0.45              |
| 7:Z:5:VAL:CG2     | 7:Z:71:ARG:NH1    | 2.80                     | 0.45              |
| 7:Z:76:GLU:O      | 7:Z:76:GLU:CD     | 2.55                     | 0.45              |
| 1:A:61:VAL:HG13   | 1:A:66:SER:HB3    | 1.99                     | 0.45              |
| 1:B:56:VAL:HG13   | 1:B:142:VAL:HG12  | 1.98                     | 0.45              |
| 2:C:148:PHE:CE2   | 2:C:160:ALA:HB1   | 2.52                     | 0.45              |
| 2:C:191:PHE:CD2   | 2:C:195:LEU:HD23  | 2.47                     | 0.45              |
| 2:C:267:TYR:OH    | 2:C:289:THR:CG2   | 2.64                     | 0.45              |
| 2:C:449:ILE:C     | 2:C:451:LEU:H     | 2.20                     | 0.45              |
| 2:C:631:SER:CB    | 2:C:637:LEU:HD11  | 2.47                     | 0.45              |
| 2:C:931:GLY:C     | 2:C:933:GLY:N     | 2.70                     | 0.45              |
| 2:C:878:SER:HB3   | 3:D:1029:ARG:HD3  | 1.99                     | 0.45              |
| 3:D:1486:VAL:HG12 | 4:E:22:VAL:HG12   | 1.97                     | 0.45              |
| 3:D:618:LEU:HD21  | 3:D:1463:LYS:CE   | 2.45                     | 0.45              |
| 3:D:639:LEU:CD1   | 3:D:640:HIS:N     | 2.79                     | 0.45              |
| 3:D:720:LEU:N     | 3:D:720:LEU:HD12  | 2.32                     | 0.45              |
| 3:D:783:ARG:CZ    | 7:X:41:ASP:CB     | 2.95                     | 0.45              |
| 1:G:95:GLN:HA     | 1:G:146:ARG:HD2   | 1.97                     | 0.45              |
| 1:G:45:LEU:HD11   | 1:G:177:VAL:HG22  | 1.99                     | 0.45              |
| 2:H:269:LEU:C     | 2:H:269:LEU:HD23  | 2.38                     | 0.45              |
| 2:H:342:ASP:HA    | 2:H:345:ARG:CD    | 2.42                     | 0.45              |
| 2:H:859:PRO:HB2   | 2:H:867:VAL:CG2   | 2.46                     | 0.45              |
| 2:H:873:PRO:HB3   | 3:I:949:ILE:HD12  | 1.98                     | 0.45              |
| 3:I:135:LEU:HD22  | 3:I:149:LYS:C     | 2.36                     | 0.45              |
| 3:I:947:ILE:C     | 3:I:947:ILE:HD12  | 2.36                     | 0.45              |
| 3:I:972:LEU:C     | 3:I:976:GLN:HE21  | 2.20                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:83:LYS:HE2    | 1:L:167:VAL:CG1   | 2.47                     | 0.45              |
| 2:M:1056:LYS:HD3  | 3:N:623:VAL:HG11  | 1.97                     | 0.45              |
| 2:M:443:THR:HA    | 2:M:444:PRO:HD3   | 1.74                     | 0.45              |
| 2:M:487:THR:CG2   | 2:M:489:THR:OG1   | 2.65                     | 0.45              |
| 2:M:544:THR:C     | 2:M:546:LEU:H     | 2.20                     | 0.45              |
| 2:M:592:LEU:HD23  | 2:M:592:LEU:N     | 2.32                     | 0.45              |
| 1:K:178:ALA:HB2   | 2:M:864:GLY:H     | 1.81                     | 0.45              |
| 3:N:1045:MET:O    | 3:N:1053:PHE:HB2  | 2.17                     | 0.45              |
| 3:N:1288:GLU:C    | 3:N:1307:LYS:HG2  | 2.36                     | 0.45              |
| 3:N:639:LEU:CD1   | 3:N:640:HIS:N     | 2.79                     | 0.45              |
| 4:O:68:LEU:HA     | 4:O:73:LEU:CD1    | 2.47                     | 0.45              |
| 7:X:22:GLU:OE2    | 7:X:25:ARG:NH1    | 2.47                     | 0.45              |
| 1:A:18:ARG:O      | 1:A:201:THR:OG1   | 2.35                     | 0.45              |
| 2:C:151:ASP:CG    | 2:C:152:PRO:CD    | 2.84                     | 0.45              |
| 2:C:26:TYR:HD1    | 2:C:26:TYR:HA     | 1.66                     | 0.45              |
| 2:C:26:TYR:CE1    | 2:C:340:MET:HE2   | 2.45                     | 0.45              |
| 2:C:496:ILE:O     | 2:C:515:ALA:HB1   | 2.17                     | 0.45              |
| 3:D:1042:ARG:HH11 | 3:D:1042:ARG:HB2  | 1.81                     | 0.45              |
| 3:D:1045:MET:O    | 3:D:1053:PHE:HB2  | 2.17                     | 0.45              |
| 3:D:116:LEU:O     | 3:D:116:LEU:HD23  | 2.17                     | 0.45              |
| 3:D:28:LYS:HG3    | 3:D:29:PRO:CD     | 2.47                     | 0.45              |
| 3:D:204:LEU:HD13  | 3:D:441:ARG:HH12  | 1.81                     | 0.45              |
| 3:D:650:LEU:CD1   | 3:D:688:TRP:HZ3   | 2.26                     | 0.45              |
| 3:D:841:TYR:O     | 3:D:864:VAL:HG12  | 2.17                     | 0.45              |
| 3:D:880:ILE:CG2   | 3:D:881:LEU:N     | 2.79                     | 0.45              |
| 1:F:165:ILE:HG12  | 1:F:165:ILE:O     | 2.16                     | 0.45              |
| 1:G:211:LEU:O     | 1:G:214:ALA:HB3   | 2.17                     | 0.45              |
| 2:H:1007:ALA:O    | 2:H:1027:PHE:CE2  | 2.70                     | 0.45              |
| 2:H:1016:ILE:HG13 | 2:H:1017:THR:N    | 2.32                     | 0.45              |
| 2:H:137:VAL:HG23  | 2:H:391:LEU:HD21  | 1.98                     | 0.45              |
| 2:H:304:LEU:H     | 2:H:304:LEU:CD2   | 2.25                     | 0.45              |
| 2:H:11:GLU:CD     | 2:H:537:LYS:HZ2   | 2.19                     | 0.45              |
| 2:H:544:THR:C     | 2:H:546:LEU:H     | 2.20                     | 0.45              |
| 2:H:577:PRO:C     | 2:H:579:VAL:N     | 2.71                     | 0.45              |
| 2:H:754:ILE:CD1   | 2:H:754:ILE:N     | 2.71                     | 0.45              |
| 3:I:1084:THR:HA   | 3:I:1087:ARG:CD   | 2.47                     | 0.45              |
| 3:I:1144:LEU:HA   | 3:I:1147:ARG:HG3  | 1.99                     | 0.45              |
| 3:I:1155:VAL:HG12 | 3:I:1177:ALA:HB1  | 1.99                     | 0.45              |
| 3:I:1256:LEU:C    | 3:I:1260:ILE:HG13 | 2.35                     | 0.45              |
| 3:I:1261:GLU:O    | 3:I:1264:GLU:O    | 2.34                     | 0.45              |
| 3:I:1491:THR:HA   | 3:I:1494:ALA:HB3  | 1.97                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:I:557:LEU:HD22  | 3:I:566:ILE:CG2  | 2.47                     | 0.45              |
| 3:I:720:LEU:H     | 3:I:720:LEU:HD12 | 1.81                     | 0.45              |
| 3:I:720:LEU:N     | 3:I:720:LEU:HD12 | 2.32                     | 0.45              |
| 3:I:925:GLU:HG2   | 3:I:926:LYS:N    | 2.31                     | 0.45              |
| 1:K:174:VAL:HG13  | 1:K:200:TRP:O    | 2.17                     | 0.45              |
| 2:M:39:ARG:HD2    | 2:M:45:GLN:CG    | 2.47                     | 0.45              |
| 2:M:557:ARG:HD3   | 2:M:879:ARG:HB3  | 1.99                     | 0.45              |
| 1:K:65:PHE:HE1    | 2:M:799:ILE:CG1  | 2.30                     | 0.45              |
| 3:N:963:TYR:HD2   | 3:N:1002:LYS:HD3 | 1.81                     | 0.45              |
| 1:B:165:ILE:CD1   | 1:B:165:ILE:N    | 2.76                     | 0.45              |
| 1:B:81:ASN:O      | 1:B:84:GLU:HB3   | 2.17                     | 0.45              |
| 2:C:1097:LEU:CD1  | 3:D:1451:ALA:HA  | 2.47                     | 0.45              |
| 2:C:267:TYR:CG    | 2:C:272:ALA:HB1  | 2.52                     | 0.45              |
| 2:C:265:ARG:N     | 2:C:289:THR:HG21 | 2.19                     | 0.45              |
| 2:C:317:VAL:C     | 2:C:319:GLY:H    | 2.20                     | 0.45              |
| 2:C:426:ASP:O     | 2:C:426:ASP:OD1  | 2.35                     | 0.45              |
| 2:C:544:THR:C     | 2:C:546:LEU:H    | 2.20                     | 0.45              |
| 3:D:1381:VAL:HB   | 3:D:1389:LEU:HA  | 1.99                     | 0.45              |
| 3:D:153:LEU:HD12  | 3:D:153:LEU:O    | 2.17                     | 0.45              |
| 3:D:212:ARG:HB3   | 3:D:386:HIS:HB2  | 1.99                     | 0.45              |
| 4:E:60:ALA:O      | 4:E:63:TRP:HB2   | 2.17                     | 0.45              |
| 1:F:18:ARG:HH12   | 1:F:88:ARG:NE    | 2.15                     | 0.45              |
| 1:G:227:ASN:HD22  | 1:G:227:ASN:N    | 2.14                     | 0.45              |
| 2:H:1088:LEU:HD21 | 3:I:614:PHE:CZ   | 2.51                     | 0.45              |
| 2:H:178:PRO:C     | 2:H:180:GLY:N    | 2.70                     | 0.45              |
| 2:H:191:PHE:HB2   | 2:H:241:LEU:CD1  | 2.47                     | 0.45              |
| 2:H:391:LEU:C     | 2:H:391:LEU:HD23 | 2.37                     | 0.45              |
| 2:H:496:ILE:H     | 2:H:496:ILE:CD1  | 2.29                     | 0.45              |
| 2:H:576:ALA:CB    | 2:H:900:ARG:NH1  | 2.60                     | 0.45              |
| 2:H:950:LEU:O     | 2:H:950:LEU:CD1  | 2.65                     | 0.45              |
| 2:H:915:LYS:HE2   | 2:H:968:LEU:O    | 2.17                     | 0.45              |
| 2:H:96:ALA:O      | 2:H:98:LEU:HD11  | 2.17                     | 0.45              |
| 3:I:1114:THR:O    | 3:I:1114:THR:CG2 | 2.64                     | 0.45              |
| 3:I:157:GLU:O     | 3:I:161:LEU:N    | 2.40                     | 0.45              |
| 3:I:189:GLN:HG2   | 3:I:190:GLU:N    | 2.32                     | 0.45              |
| 3:I:452:ILE:C     | 3:I:452:ILE:HD13 | 2.37                     | 0.45              |
| 3:I:572:ARG:O     | 3:I:573:MET:C    | 2.56                     | 0.45              |
| 3:I:827:ILE:H     | 3:I:827:ILE:CD1  | 2.28                     | 0.45              |
| 3:I:835:SER:N     | 3:I:838:ARG:CD   | 2.79                     | 0.45              |
| 1:L:57:TYR:C      | 1:L:58:ILE:HD12  | 2.37                     | 0.45              |
| 2:M:154:ARG:HH12  | 2:M:178:PRO:N    | 2.15                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:449:ILE:C     | 2:M:451:LEU:H     | 2.19                     | 0.45              |
| 2:M:54:ILE:HG22   | 2:M:66:LEU:H      | 1.82                     | 0.45              |
| 2:M:54:ILE:O      | 2:M:54:ILE:HG22   | 2.15                     | 0.45              |
| 2:M:588:VAL:HG12  | 2:M:661:SER:HB3   | 1.98                     | 0.45              |
| 2:M:600:ASP:OD1   | 2:M:649:VAL:O     | 2.35                     | 0.45              |
| 2:M:679:PHE:C     | 3:N:943:THR:CG2   | 2.85                     | 0.45              |
| 2:M:671:ASN:OD1   | 2:M:993:PHE:HD2   | 2.00                     | 0.45              |
| 3:N:348:GLN:H     | 3:N:351:MET:CE    | 2.29                     | 0.45              |
| 3:N:415:VAL:O     | 3:N:432:TYR:HA    | 2.16                     | 0.45              |
| 3:N:875:THR:CG2   | 3:N:879:ARG:CB    | 2.95                     | 0.45              |
| 4:O:24:ALA:O      | 4:O:25:LYS:C      | 2.55                     | 0.45              |
| 7:X:78:GLY:O      | 7:X:156:GLY:HA2   | 2.16                     | 0.45              |
| 7:X:89:VAL:HG13   | 7:X:151:VAL:HG13  | 1.98                     | 0.45              |
| 7:Z:75:LEU:O      | 7:Z:77:GLU:HG3    | 2.17                     | 0.45              |
| 1:A:186:LEU:CD2   | 1:A:187:GLY:N     | 2.77                     | 0.44              |
| 2:C:1052:MET:SD   | 2:C:1056:LYS:CD   | 3.06                     | 0.44              |
| 2:C:1068:GLU:O    | 2:C:1071:ILE:HB   | 2.17                     | 0.44              |
| 2:C:187:ASN:O     | 2:C:187:ASN:OD1   | 2.36                     | 0.44              |
| 2:C:148:PHE:HE1   | 2:C:309:TYR:HB3   | 1.76                     | 0.44              |
| 2:C:442:GLU:CD    | 2:C:543:ASN:HD22  | 2.20                     | 0.44              |
| 2:C:83:CYS:HA     | 2:C:88:LEU:HB3    | 1.99                     | 0.44              |
| 3:D:957:PRO:HG2   | 3:D:1007:VAL:CA   | 2.47                     | 0.44              |
| 3:D:1144:LEU:HD22 | 3:D:1166:LEU:CD1  | 2.47                     | 0.44              |
| 3:D:1287:GLU:C    | 3:D:1289:LYS:H    | 2.19                     | 0.44              |
| 3:D:511:TRP:C     | 3:D:513:ILE:H     | 2.20                     | 0.44              |
| 3:D:54:LYS:CG     | 3:D:55:ASP:H      | 2.29                     | 0.44              |
| 3:D:643:GLY:N     | 3:D:727:GLN:O     | 2.50                     | 0.44              |
| 1:G:66:SER:OG     | 1:G:75:VAL:HG21   | 2.17                     | 0.44              |
| 2:H:11:GLU:HG2    | 2:H:537:LYS:NZ    | 2.33                     | 0.44              |
| 2:H:129:ILE:HD11  | 2:H:386:PHE:CD2   | 2.49                     | 0.44              |
| 2:H:185:LYS:CG    | 2:H:190:LYS:HA    | 2.46                     | 0.44              |
| 2:H:426:ASP:OD1   | 2:H:426:ASP:O     | 2.35                     | 0.44              |
| 2:H:430:VAL:HG13  | 3:I:1075:HIS:ND1  | 2.31                     | 0.44              |
| 2:H:642:ARG:CD    | 2:H:642:ARG:O     | 2.56                     | 0.44              |
| 2:H:674:VAL:HG23  | 2:H:869:VAL:O     | 2.16                     | 0.44              |
| 3:I:1020:LEU:HD12 | 3:I:1020:LEU:HA   | 1.80                     | 0.44              |
| 3:I:1029:ARG:HH21 | 7:Y:41:ASP:CG     | 2.21                     | 0.44              |
| 2:H:878:SER:C     | 3:I:1034:GLN:HE22 | 2.19                     | 0.44              |
| 3:I:1043:GLY:O    | 3:I:1057:VAL:N    | 2.42                     | 0.44              |
| 3:I:116:LEU:O     | 3:I:116:LEU:HD23  | 2.17                     | 0.44              |
| 3:I:127:LEU:CD1   | 3:I:127:LEU:O     | 2.59                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1462:LEU:N    | 3:I:1462:LEU:HD23 | 2.32                     | 0.44              |
| 3:I:162:ARG:HB3   | 3:I:452:ILE:HG21  | 1.99                     | 0.44              |
| 3:I:514:LEU:HD11  | 3:I:582:LEU:HD11  | 1.99                     | 0.44              |
| 3:I:642:CYS:SG    | 3:I:642:CYS:O     | 2.74                     | 0.44              |
| 4:J:23:VAL:HG13   | 4:J:65:MET:HG3    | 1.98                     | 0.44              |
| 1:K:230:ALA:HB2   | 1:L:13:VAL:O      | 2.17                     | 0.44              |
| 1:K:30:ARG:HA     | 1:K:193:ASP:OD1   | 2.16                     | 0.44              |
| 1:K:88:ARG:NH1    | 1:K:90:LEU:HD11   | 2.32                     | 0.44              |
| 2:M:197:LEU:HA    | 2:M:200:LEU:CD1   | 2.20                     | 0.44              |
| 2:M:336:VAL:O     | 2:M:339:LEU:HB2   | 2.16                     | 0.44              |
| 2:M:374:ASN:N     | 2:M:374:ASN:ND2   | 2.64                     | 0.44              |
| 2:M:413:LEU:O     | 2:M:413:LEU:HD12  | 2.17                     | 0.44              |
| 2:M:725:ASP:O     | 2:M:727:PRO:HD3   | 2.17                     | 0.44              |
| 2:M:915:LYS:HE2   | 2:M:968:LEU:O     | 2.17                     | 0.44              |
| 2:M:878:SER:HA    | 3:N:1034:GLN:NE2  | 2.31                     | 0.44              |
| 3:N:1487:VAL:CG1  | 3:N:1488:ASP:H    | 2.29                     | 0.44              |
| 3:N:160:GLU:HA    | 3:N:165:LYS:HB2   | 1.99                     | 0.44              |
| 3:N:179:VAL:HG13  | 3:N:183:GLU:CB    | 2.47                     | 0.44              |
| 3:N:483:HIS:CB    | 3:N:484:PRO:HD3   | 2.40                     | 0.44              |
| 3:N:621:LYS:HA    | 3:N:621:LYS:HD3   | 1.43                     | 0.44              |
| 3:N:795:VAL:HG12  | 3:N:796:ARG:N     | 2.32                     | 0.44              |
| 5:T:18:DC:H2'     | 5:T:19:DC:H6      | 1.82                     | 0.44              |
| 7:X:14:ARG:HB3    | 7:X:14:ARG:HH11   | 1.81                     | 0.44              |
| 7:X:93:ASP:OD2    | 7:X:96:SER:OG     | 2.35                     | 0.44              |
| 7:Y:78:GLY:O      | 7:Y:156:GLY:HA2   | 2.17                     | 0.44              |
| 1:A:141:GLU:OE1   | 1:A:161:ARG:NH1   | 2.47                     | 0.44              |
| 1:A:222:LEU:HD21  | 1:B:218:LEU:HD23  | 1.99                     | 0.44              |
| 1:A:83:LYS:HD3    | 1:A:167:VAL:HG12  | 1.99                     | 0.44              |
| 2:C:1087:VAL:O    | 2:C:1091:GLU:HG3  | 2.18                     | 0.44              |
| 2:C:473:ARG:CA    | 2:C:531:PHE:CE1   | 2.99                     | 0.44              |
| 2:C:690:ILE:HG23  | 2:C:852:ILE:HG23  | 1.99                     | 0.44              |
| 1:A:14:ARG:NH2    | 2:C:934:PHE:HZ    | 2.15                     | 0.44              |
| 3:D:1109:GLU:HG2  | 3:D:1201:CYS:HB2  | 1.99                     | 0.44              |
| 3:D:1348:LEU:HD23 | 3:D:1372:VAL:HG23 | 1.99                     | 0.44              |
| 3:D:207:PHE:CE1   | 2:H:283:ILE:CB    | 2.97                     | 0.44              |
| 3:D:451:ASP:O     | 3:D:452:ILE:CG2   | 2.65                     | 0.44              |
| 3:D:925:GLU:CD    | 4:E:6:ILE:HG22    | 2.37                     | 0.44              |
| 4:E:67:GLU:HB3    | 4:E:73:LEU:HD11   | 1.99                     | 0.44              |
| 2:H:229:MET:CB    | 2:H:230:ARG:HH12  | 2.30                     | 0.44              |
| 2:H:284:ARG:HG2   | 2:H:285:LEU:N     | 2.33                     | 0.44              |
| 2:H:625:LEU:O     | 2:H:627:ARG:N     | 2.49                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:865:THR:HA    | 2:H:866:PRO:HD3   | 1.74                     | 0.44              |
| 3:I:1325:LEU:HD12 | 3:I:1325:LEU:HA   | 1.70                     | 0.44              |
| 3:I:202:VAL:HG11  | 3:I:445:ARG:CZ    | 2.48                     | 0.44              |
| 2:H:1088:LEU:HD11 | 3:I:614:PHE:CE1   | 2.52                     | 0.44              |
| 3:I:642:CYS:HB3   | 3:I:716:PHE:HB3   | 1.99                     | 0.44              |
| 3:I:701:LEU:H     | 3:I:701:LEU:HD12  | 1.82                     | 0.44              |
| 3:I:761:ILE:HG21  | 4:J:20:THR:HG23   | 2.00                     | 0.44              |
| 3:I:787:LEU:HD12  | 3:I:787:LEU:C     | 2.36                     | 0.44              |
| 3:I:827:ILE:HD12  | 3:I:827:ILE:N     | 2.27                     | 0.44              |
| 3:I:804:LEU:CB    | 3:I:830:ALA:O     | 2.65                     | 0.44              |
| 3:I:50:PHE:C      | 3:I:89:ARG:CG     | 2.84                     | 0.44              |
| 3:I:996:TRP:O     | 3:I:999:THR:HG22  | 2.16                     | 0.44              |
| 1:K:124:ASN:HD21  | 1:K:127:LEU:CD2   | 2.26                     | 0.44              |
| 1:L:56:VAL:CG2    | 1:L:142:VAL:HG12  | 2.45                     | 0.44              |
| 1:L:73:GLU:HB2    | 1:L:78:ILE:HD11   | 2.00                     | 0.44              |
| 2:M:63:GLY:CA     | 2:M:103:LYS:CG    | 2.94                     | 0.44              |
| 2:M:1085:PHE:CD1  | 2:M:1085:PHE:C    | 2.91                     | 0.44              |
| 2:M:577:PRO:C     | 2:M:579:VAL:N     | 2.71                     | 0.44              |
| 2:M:625:LEU:O     | 2:M:626:ARG:C     | 2.55                     | 0.44              |
| 2:M:931:GLY:C     | 2:M:933:GLY:N     | 2.70                     | 0.44              |
| 3:N:189:GLN:HE21  | 3:N:190:GLU:N     | 2.14                     | 0.44              |
| 3:N:759:ALA:O     | 3:N:763:MET:HB3   | 2.17                     | 0.44              |
| 5:R:18:DC:H2'     | 5:R:19:DC:C5      | 2.52                     | 0.44              |
| 1:B:80:LEU:HA     | 1:B:83:LYS:HE3    | 1.98                     | 0.44              |
| 2:C:1095:LEU:HD12 | 2:C:1097:LEU:N    | 2.24                     | 0.44              |
| 2:C:114:PHE:O     | 2:C:375:SER:OG    | 2.30                     | 0.44              |
| 2:C:223:ASP:OD1   | 2:C:224:GLU:N     | 2.50                     | 0.44              |
| 2:C:516:ARG:NE    | 3:D:1068:LEU:HD22 | 2.32                     | 0.44              |
| 2:C:584:GLU:H     | 2:C:584:GLU:CD    | 2.21                     | 0.44              |
| 2:C:706:GLU:HB3   | 2:C:708:TYR:HE1   | 1.81                     | 0.44              |
| 3:D:1347:TYR:HD2  | 3:D:1348:LEU:HD12 | 1.81                     | 0.44              |
| 3:D:159:ARG:HH22  | 2:H:218:VAL:CG2   | 2.31                     | 0.44              |
| 3:D:426:LYS:CE    | 3:D:427:VAL:HG23  | 2.46                     | 0.44              |
| 1:F:58:ILE:HB     | 1:F:61:VAL:HB     | 1.99                     | 0.44              |
| 2:H:30:LEU:HB3    | 2:H:44:ILE:CG1    | 2.46                     | 0.44              |
| 2:H:134:ARG:NH1   | 2:H:386:PHE:O     | 2.50                     | 0.44              |
| 2:H:518:LYS:HE2   | 2:H:518:LYS:HB2   | 1.73                     | 0.44              |
| 3:I:1232:PRO:HB2  | 3:I:1356:TYR:HE2  | 1.82                     | 0.44              |
| 3:I:1256:LEU:CD2  | 3:I:1260:ILE:HD11 | 2.48                     | 0.44              |
| 3:I:145:VAL:HG22  | 3:I:146:PRO:CD    | 2.44                     | 0.44              |
| 3:I:806:PHE:HE1   | 3:I:813:LEU:HB3   | 1.80                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:957:PRO:HG2  | 3:I:1007:VAL:CA  | 2.47                     | 0.44              |
| 1:K:79:ILE:CG1   | 1:K:80:LEU:N     | 2.75                     | 0.44              |
| 1:G:73:GLU:HA    | 1:L:162:ILE:CD1  | 2.48                     | 0.44              |
| 2:M:101:ILE:CB   | 2:M:108:ILE:HG12 | 2.46                     | 0.44              |
| 2:M:124:ASP:N    | 2:M:124:ASP:OD1  | 2.40                     | 0.44              |
| 2:M:274:ARG:HG2  | 2:M:274:ARG:NH1  | 2.31                     | 0.44              |
| 2:M:474:VAL:HG23 | 2:M:478:VAL:O    | 2.17                     | 0.44              |
| 2:M:557:ARG:HH21 | 2:M:879:ARG:NE   | 2.12                     | 0.44              |
| 3:N:1025:GLN:NE2 | 3:N:1025:GLN:CA  | 2.79                     | 0.44              |
| 3:N:105:VAL:HG21 | 3:N:128:TYR:HE1  | 1.83                     | 0.44              |
| 3:N:1304:LYS:O   | 3:N:1306:PRO:HD3 | 2.18                     | 0.44              |
| 3:N:137:PRO:HD3  | 3:N:453:ASP:CB   | 2.35                     | 0.44              |
| 3:N:17:LYS:CD    | 3:N:21:TRP:HE1   | 2.30                     | 0.44              |
| 3:N:341:GLU:HA   | 3:N:342:PRO:HD2  | 1.83                     | 0.44              |
| 3:N:701:LEU:HD12 | 3:N:701:LEU:H    | 1.82                     | 0.44              |
| 3:N:806:PHE:C    | 3:N:808:THR:N    | 2.70                     | 0.44              |
| 3:N:835:SER:N    | 3:N:838:ARG:HD3  | 2.32                     | 0.44              |
| 7:X:5:VAL:O      | 7:X:72:ALA:HA    | 2.18                     | 0.44              |
| 3:I:1359:GLN:NE2 | 7:Y:52:LYS:HD3   | 2.23                     | 0.44              |
| 3:N:970:LYS:NZ   | 7:Z:113:LEU:CA   | 2.77                     | 0.44              |
| 2:C:1085:PHE:CD1 | 2:C:1085:PHE:C   | 2.91                     | 0.44              |
| 2:C:92:ALA:N     | 2:C:118:ILE:O    | 2.40                     | 0.44              |
| 1:A:133:GLU:OE2  | 2:C:605:LYS:HB3  | 2.18                     | 0.44              |
| 2:C:82:GLU:OE1   | 2:C:86:LYS:HE3   | 2.17                     | 0.44              |
| 2:C:897:LEU:HD21 | 2:C:921:ALA:N    | 2.32                     | 0.44              |
| 3:D:23:TYR:O     | 3:D:49:ILE:CG2   | 2.63                     | 0.44              |
| 1:G:80:LEU:O     | 1:G:83:LYS:HG3   | 2.17                     | 0.44              |
| 2:H:1085:PHE:CD1 | 2:H:1085:PHE:C   | 2.91                     | 0.44              |
| 2:H:265:ARG:HG2  | 2:H:267:TYR:CB   | 2.47                     | 0.44              |
| 2:H:294:GLU:HG2  | 2:H:295:ASP:N    | 2.31                     | 0.44              |
| 2:H:399:ASN:O    | 2:H:402:SER:HB3  | 2.18                     | 0.44              |
| 2:H:720:GLU:HA   | 2:H:759:THR:O    | 2.17                     | 0.44              |
| 2:H:6:PHE:HB2    | 2:H:909:ALA:CA   | 2.46                     | 0.44              |
| 3:I:1047:LYS:HZ1 | 3:I:1053:PHE:HA  | 1.80                     | 0.44              |
| 1:K:73:GLU:OE1   | 1:K:129:ILE:O    | 2.35                     | 0.44              |
| 1:K:73:GLU:HB2   | 1:K:78:ILE:HD11  | 1.99                     | 0.44              |
| 2:M:1087:VAL:O   | 2:M:1091:GLU:HG3 | 2.18                     | 0.44              |
| 2:M:254:VAL:CA   | 2:M:257:VAL:HG23 | 2.47                     | 0.44              |
| 2:M:48:PHE:HA    | 2:M:348:LEU:CD2  | 2.48                     | 0.44              |
| 2:M:631:SER:CB   | 2:M:637:LEU:HD11 | 2.47                     | 0.44              |
| 2:M:950:LEU:O    | 2:M:950:LEU:CD1  | 2.65                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1066:THR:HG22 | 3:N:1069:GLU:CB   | 2.38                     | 0.44              |
| 3:N:112:ILE:CD1   | 3:N:112:ILE:C     | 2.78                     | 0.44              |
| 3:N:1434:TRP:CD1  | 3:N:1434:TRP:C    | 2.90                     | 0.44              |
| 3:N:204:LEU:HD12  | 3:N:205:TYR:N     | 2.31                     | 0.44              |
| 3:N:415:VAL:CG2   | 3:N:435:VAL:CG2   | 2.95                     | 0.44              |
| 3:N:454:ALA:C     | 3:N:455:ARG:HG2   | 2.37                     | 0.44              |
| 3:N:972:LEU:C     | 3:N:976:GLN:HE21  | 2.20                     | 0.44              |
| 7:X:102:VAL:HG13  | 7:X:119:ILE:HG12  | 1.99                     | 0.44              |
| 7:X:128:ALA:O     | 7:X:138:LEU:HD13  | 2.17                     | 0.44              |
| 7:Y:115:THR:CB    | 7:Y:116:PRO:CD    | 2.91                     | 0.44              |
| 1:A:124:ASN:HD21  | 1:A:127:LEU:CD2   | 2.26                     | 0.44              |
| 1:A:165:ILE:O     | 1:A:165:ILE:HG12  | 2.16                     | 0.44              |
| 1:B:206:THR:HG23  | 1:B:207:PRO:N     | 2.32                     | 0.44              |
| 2:C:1040:LEU:O    | 2:C:1041:GLU:C    | 2.55                     | 0.44              |
| 2:C:185:LYS:HD2   | 2:C:190:LYS:CE    | 2.47                     | 0.44              |
| 2:C:264:PRO:CB    | 2:C:289:THR:HG21  | 2.48                     | 0.44              |
| 2:C:395:LYS:O     | 2:C:397:GLU:N     | 2.50                     | 0.44              |
| 2:C:431:HIS:CD2   | 2:C:433:THR:OG1   | 2.70                     | 0.44              |
| 2:C:481:ASP:N     | 2:C:481:ASP:OD1   | 2.50                     | 0.44              |
| 2:C:536:PRO:HB3   | 2:C:906:PHE:HD1   | 1.83                     | 0.44              |
| 2:C:931:GLY:O     | 2:C:933:GLY:N     | 2.51                     | 0.44              |
| 3:D:1310:ARG:HD3  | 3:D:1310:ARG:HA   | 1.77                     | 0.44              |
| 3:D:1441:GLN:HB3  | 3:D:1441:GLN:HE21 | 1.58                     | 0.44              |
| 3:D:9:ARG:CD      | 3:D:1456:LYS:HE2  | 2.41                     | 0.44              |
| 3:D:166:GLN:HE21  | 3:D:396:VAL:CG1   | 2.29                     | 0.44              |
| 3:D:642:CYS:SG    | 3:D:642:CYS:O     | 2.74                     | 0.44              |
| 4:E:35:PHE:C      | 4:E:36:LYS:CE     | 2.84                     | 0.44              |
| 1:F:88:ARG:NH1    | 1:F:90:LEU:HD11   | 2.32                     | 0.44              |
| 1:G:41:ARG:NH1    | 1:G:177:VAL:O     | 2.51                     | 0.44              |
| 1:G:86:VAL:O      | 1:G:86:VAL:HG13   | 2.18                     | 0.44              |
| 2:H:1008:ARG:NH2  | 2:H:1011:GLY:N    | 2.65                     | 0.44              |
| 2:H:1051:GLU:CG   | 2:H:1055:LEU:HD12 | 2.48                     | 0.44              |
| 2:H:1085:PHE:HD2  | 3:I:1468:LEU:HA   | 1.82                     | 0.44              |
| 2:H:136:ILE:CB    | 2:H:336:VAL:HG13  | 2.47                     | 0.44              |
| 2:H:431:HIS:CD2   | 2:H:433:THR:OG1   | 2.71                     | 0.44              |
| 2:H:464:LEU:HB3   | 2:H:466:PHE:HE2   | 1.81                     | 0.44              |
| 2:H:442:GLU:CD    | 2:H:543:ASN:HD22  | 2.21                     | 0.44              |
| 2:H:548:PRO:HG2   | 2:H:842:ARG:NH2   | 2.33                     | 0.44              |
| 2:H:52:PHE:CZ     | 2:H:98:LEU:HB3    | 2.51                     | 0.44              |
| 3:I:1033:GLN:OE1  | 3:I:1036:ARG:NH1  | 2.50                     | 0.44              |
| 3:I:1304:LYS:O    | 3:I:1306:PRO:HD3  | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1491:THR:HG22 | 3:I:1491:THR:O    | 2.16                     | 0.44              |
| 3:I:615:ARG:HG3   | 3:I:619:LEU:HD11  | 2.00                     | 0.44              |
| 1:K:78:ILE:HD12   | 1:K:130:ALA:HB2   | 2.00                     | 0.44              |
| 2:M:204:GLN:OE1   | 2:M:204:GLN:N     | 2.50                     | 0.44              |
| 2:M:267:TYR:CB    | 2:M:272:ALA:CB    | 2.81                     | 0.44              |
| 2:M:235:LEU:CD1   | 2:M:298:PHE:HZ    | 2.19                     | 0.44              |
| 2:M:691:SER:O     | 2:M:692:GLU:C     | 2.55                     | 0.44              |
| 3:N:116:LEU:HD23  | 3:N:116:LEU:O     | 2.18                     | 0.44              |
| 3:N:1232:PRO:HB2  | 3:N:1356:TYR:HE2  | 1.81                     | 0.44              |
| 3:N:141:ILE:CD1   | 3:N:448:GLU:OE2   | 2.66                     | 0.44              |
| 2:M:1046:ALA:CA   | 3:N:1472:ILE:HD11 | 2.41                     | 0.44              |
| 3:N:170:PRO:O     | 3:N:195:VAL:HG21  | 2.18                     | 0.44              |
| 3:N:23:TYR:CE1    | 3:N:89:ARG:HG2    | 2.53                     | 0.44              |
| 3:N:643:GLY:N     | 3:N:727:GLN:O     | 2.50                     | 0.44              |
| 7:X:9:LYS:HB3     | 7:X:9:LYS:HE2     | 1.79                     | 0.44              |
| 7:Y:127:LYS:O     | 7:Y:127:LYS:HD3   | 2.16                     | 0.44              |
| 7:Z:92:GLU:HA     | 7:Z:98:GLU:O      | 2.18                     | 0.44              |
| 1:B:211:LEU:O     | 1:B:214:ALA:HB3   | 2.17                     | 0.44              |
| 2:C:1071:ILE:HG23 | 3:D:670:VAL:HG11  | 2.00                     | 0.44              |
| 2:C:182:VAL:HB    | 2:C:193:LEU:CB    | 2.48                     | 0.44              |
| 2:C:217:LEU:O     | 2:C:218:VAL:C     | 2.56                     | 0.44              |
| 2:C:335:THR:O     | 2:C:336:VAL:C     | 2.56                     | 0.44              |
| 2:C:358:ARG:HH12  | 2:C:374:ASN:ND2   | 2.16                     | 0.44              |
| 2:C:376:ARG:HB3   | 2:C:377:PRO:HD3   | 1.99                     | 0.44              |
| 2:C:480:THR:HG22  | 2:C:481:ASP:H     | 1.83                     | 0.44              |
| 2:C:640:ARG:HH11  | 2:C:640:ARG:HG2   | 1.83                     | 0.44              |
| 2:C:754:ILE:CG1   | 2:C:791:ARG:HH12  | 2.31                     | 0.44              |
| 2:C:554:ASP:HB2   | 2:C:880:MET:HB2   | 2.00                     | 0.44              |
| 2:C:915:LYS:HE2   | 2:C:968:LEU:O     | 2.17                     | 0.44              |
| 2:C:957:LYS:CD    | 2:C:961:GLU:CB    | 2.95                     | 0.44              |
| 3:D:1055:VAL:HA   | 3:D:1056:PRO:HD3  | 1.84                     | 0.44              |
| 3:D:26:VAL:CG2    | 3:D:26:VAL:O      | 2.62                     | 0.44              |
| 3:D:631:ILE:HG21  | 3:D:745:MET:CG    | 2.48                     | 0.44              |
| 3:D:660:LYS:NZ    | 3:D:660:LYS:CA    | 2.79                     | 0.44              |
| 3:D:727:GLN:HB3   | 3:D:727:GLN:HE21  | 1.65                     | 0.44              |
| 1:F:101:LEU:HD12  | 1:F:113:ASP:O     | 2.18                     | 0.44              |
| 1:F:168:ASP:OD1   | 2:H:832:LYS:NZ    | 2.51                     | 0.44              |
| 1:G:94:LEU:CD1    | 1:G:119:ASP:HB2   | 2.44                     | 0.44              |
| 1:G:26:GLU:CB     | 1:G:27:PRO:HA     | 2.47                     | 0.44              |
| 2:H:1102:LEU:HD23 | 2:H:1106:ASP:HB3  | 2.00                     | 0.44              |
| 2:H:367:LEU:HA    | 2:H:371:LYS:HE3   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:503:LEU:HD23  | 2:H:507:ARG:C     | 2.38                     | 0.44              |
| 3:I:1042:ARG:HH11 | 3:I:1042:ARG:HB2  | 1.82                     | 0.44              |
| 3:I:1205:TYR:OH   | 3:I:1367:HIS:CE1  | 2.71                     | 0.44              |
| 3:I:457:GLY:O     | 3:I:458:ALA:C     | 2.54                     | 0.44              |
| 1:K:83:LYS:HD3    | 1:K:167:VAL:HG12  | 1.99                     | 0.44              |
| 2:M:1038:TRP:CE2  | 3:N:1099:VAL:HG11 | 2.53                     | 0.44              |
| 2:M:1037:VAL:HG13 | 2:M:1049:LEU:HD11 | 2.00                     | 0.44              |
| 2:M:169:GLY:HA2   | 2:M:170:PRO:HD3   | 1.85                     | 0.44              |
| 2:M:266:ARG:HD3   | 2:M:266:ARG:O     | 2.17                     | 0.44              |
| 2:M:394:PHE:CE2   | 5:T:20:DG:H4'     | 2.53                     | 0.44              |
| 2:M:431:HIS:CD2   | 2:M:433:THR:OG1   | 2.71                     | 0.44              |
| 2:M:591:SER:O     | 2:M:592:LEU:HB2   | 2.17                     | 0.44              |
| 2:M:642:ARG:O     | 2:M:642:ARG:CD    | 2.55                     | 0.44              |
| 3:N:368:VAL:HB    | 3:N:377:VAL:HG21  | 2.00                     | 0.44              |
| 3:N:408:GLU:HG2   | 3:N:420:VAL:O     | 2.18                     | 0.44              |
| 3:N:42:ASP:H      | 3:N:46:ASP:HB2    | 1.83                     | 0.44              |
| 3:N:511:TRP:C     | 3:N:513:ILE:N     | 2.71                     | 0.44              |
| 3:N:645:PRO:CD    | 3:N:726:ILE:HG12  | 2.45                     | 0.44              |
| 3:N:729:HIS:HE2   | 3:N:935:LYS:HD3   | 1.81                     | 0.44              |
| 3:N:1209:LEU:CD2  | 4:O:16:LYS:HE3    | 2.42                     | 0.44              |
| 5:T:18:DC:C2      | 6:U:13:G:N2       | 2.82                     | 0.44              |
| 1:A:58:ILE:HB     | 1:A:61:VAL:HB     | 2.00                     | 0.44              |
| 1:A:88:ARG:NH1    | 1:A:90:LEU:HD11   | 2.32                     | 0.44              |
| 2:C:148:PHE:CE2   | 2:C:160:ALA:CB    | 3.01                     | 0.44              |
| 2:C:22:GLN:HE21   | 2:C:336:VAL:HG22  | 1.83                     | 0.44              |
| 2:C:3:ILE:N       | 2:C:3:ILE:CD1     | 2.80                     | 0.44              |
| 2:C:673:LEU:CB    | 2:C:868:ASP:OD1   | 2.65                     | 0.44              |
| 2:C:673:LEU:HB3   | 2:C:868:ASP:OD1   | 2.18                     | 0.44              |
| 2:C:922:PHE:HZ    | 2:C:963:LEU:HB3   | 1.83                     | 0.44              |
| 3:D:1045:MET:HG3  | 3:D:1073:SER:OG   | 2.17                     | 0.44              |
| 3:D:1325:LEU:HD12 | 3:D:1325:LEU:HA   | 1.70                     | 0.44              |
| 3:D:1422:MET:HE2  | 3:D:1427:SER:HA   | 2.00                     | 0.44              |
| 3:D:205:TYR:HD1   | 3:D:390:PRO:CB    | 2.30                     | 0.44              |
| 3:D:412:GLY:HA2   | 3:D:434:ARG:NE    | 2.32                     | 0.44              |
| 3:D:432:TYR:HB3   | 3:D:450:TYR:CG    | 2.52                     | 0.44              |
| 3:D:521:PRO:HA    | 3:D:522:PRO:HD3   | 1.88                     | 0.44              |
| 3:D:644:LEU:HA    | 3:D:645:PRO:HD3   | 1.84                     | 0.44              |
| 2:H:141:HIS:HD1   | 2:H:144:PRO:HD3   | 1.83                     | 0.44              |
| 2:H:167:LYS:HG2   | 2:H:167:LYS:O     | 2.17                     | 0.44              |
| 2:H:311:PHE:N     | 2:H:311:PHE:CD2   | 2.86                     | 0.44              |
| 2:H:72:ARG:CZ     | 2:H:95:TYR:CE1    | 3.01                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:861:LEU:CD2   | 2:H:862:PRO:HD2   | 2.48                     | 0.44              |
| 2:H:931:GLY:C     | 2:H:933:GLY:N     | 2.70                     | 0.44              |
| 3:I:1066:THR:HG22 | 3:I:1069:GLU:CB   | 2.38                     | 0.44              |
| 3:I:1348:LEU:HD23 | 3:I:1372:VAL:HG23 | 1.99                     | 0.44              |
| 3:I:631:ILE:HG21  | 3:I:745:MET:CG    | 2.48                     | 0.44              |
| 3:I:781:PRO:HB2   | 3:I:786:ILE:CD1   | 2.43                     | 0.44              |
| 3:I:794:GLN:CG    | 3:I:1017:PHE:CE2  | 3.01                     | 0.44              |
| 3:I:963:TYR:HD2   | 3:I:1002:LYS:HD3  | 1.81                     | 0.44              |
| 4:J:54:LEU:CA     | 4:J:58:PRO:HG2    | 2.47                     | 0.44              |
| 1:K:73:GLU:OE1    | 1:K:78:ILE:HD13   | 2.18                     | 0.44              |
| 1:L:42:ARG:CG     | 1:L:42:ARG:NH1    | 2.80                     | 0.44              |
| 2:M:278:GLU:HA    | 2:M:283:ILE:HA    | 1.99                     | 0.44              |
| 2:M:363:SER:HB2   | 2:M:366:SER:CB    | 2.47                     | 0.44              |
| 2:M:575:GLN:C     | 2:M:667:ALA:HB1   | 2.38                     | 0.44              |
| 2:M:722:ILE:O     | 2:M:722:ILE:CD1   | 2.64                     | 0.44              |
| 3:N:1168:MET:HE3  | 3:N:1168:MET:HA   | 1.99                     | 0.44              |
| 3:N:1205:TYR:OH   | 3:N:1367:HIS:CE1  | 2.71                     | 0.44              |
| 3:N:1384:PRO:CB   | 3:N:1388:ARG:NH1  | 2.81                     | 0.44              |
| 3:N:148:GLU:CB    | 3:N:151:GLN:HB3   | 2.48                     | 0.44              |
| 3:N:183:GLU:O     | 3:N:185:VAL:HG23  | 2.18                     | 0.44              |
| 3:N:461:ILE:HD13  | 3:N:461:ILE:N     | 2.33                     | 0.44              |
| 3:N:502:PHE:CZ    | 3:N:509:PRO:HB3   | 2.53                     | 0.44              |
| 3:N:881:LEU:HD12  | 3:N:885:ILE:HD11  | 1.98                     | 0.44              |
| 7:Z:120:SER:HB2   | 7:Z:123:SER:OG    | 2.17                     | 0.44              |
| 1:B:34:VAL:HG11   | 2:C:978:ARG:HB3   | 2.00                     | 0.44              |
| 1:B:95:GLN:HB2    | 1:B:95:GLN:HE21   | 1.57                     | 0.44              |
| 2:C:328:LEU:CD1   | 2:C:328:LEU:N     | 2.80                     | 0.44              |
| 2:C:358:ARG:HH12  | 2:C:374:ASN:CG    | 2.21                     | 0.44              |
| 2:C:73:LEU:HD12   | 2:C:74:GLY:N      | 2.32                     | 0.44              |
| 3:D:1253:THR:HG21 | 3:D:1269:LYS:HG3  | 2.00                     | 0.44              |
| 3:D:1277:ILE:HD12 | 3:D:1277:ILE:N    | 2.33                     | 0.44              |
| 3:D:129:PHE:HZ    | 3:D:587:ARG:HD2   | 1.82                     | 0.44              |
| 3:D:766:ALA:HB1   | 4:E:2:ALA:HB2     | 2.00                     | 0.44              |
| 3:D:801:GLY:O     | 3:D:802:ALA:CB    | 2.65                     | 0.44              |
| 1:G:51:THR:HG22   | 1:G:144:VAL:HG12  | 2.00                     | 0.44              |
| 1:G:206:THR:HG23  | 1:G:207:PRO:N     | 2.32                     | 0.44              |
| 1:G:80:LEU:HG     | 3:I:844:ALA:HB2   | 1.98                     | 0.44              |
| 2:H:1008:ARG:NH2  | 2:H:1011:GLY:O    | 2.51                     | 0.44              |
| 2:H:265:ARG:CB    | 2:H:267:TYR:CZ    | 2.93                     | 0.44              |
| 2:H:322:VAL:O     | 2:H:322:VAL:CG2   | 2.62                     | 0.44              |
| 2:H:341:THR:CG2   | 2:H:342:ASP:N     | 2.80                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:H:126:SER:CB    | 2:H:395:LYS:HZ1  | 2.31                     | 0.44              |
| 2:H:413:LEU:HD12  | 2:H:413:LEU:O    | 2.17                     | 0.44              |
| 2:H:42:VAL:O      | 2:H:43:GLY:C     | 2.56                     | 0.44              |
| 2:H:332:ARG:CD    | 2:H:464:LEU:HG   | 2.47                     | 0.44              |
| 2:H:695:LEU:HD21  | 2:H:832:LYS:HB3  | 1.99                     | 0.44              |
| 2:H:897:LEU:HD22  | 2:H:920:GLN:CG   | 2.48                     | 0.44              |
| 1:F:38:ASN:HB2    | 2:H:980:GLY:HA3  | 1.99                     | 0.44              |
| 3:I:17:LYS:CD     | 3:I:21:TRP:HE1   | 2.30                     | 0.44              |
| 2:M:1003:ASP:O    | 2:M:1004:LYS:HD3 | 2.17                     | 0.44              |
| 2:M:1082:PRO:O    | 2:M:1085:PHE:N   | 2.48                     | 0.44              |
| 2:M:224:GLU:OE1   | 2:M:227:PHE:HD1  | 2.01                     | 0.44              |
| 2:M:410:ILE:HG22  | 2:M:410:ILE:O    | 2.18                     | 0.44              |
| 2:M:584:GLU:H     | 2:M:584:GLU:CD   | 2.21                     | 0.44              |
| 2:M:687:ALA:HB1   | 2:M:850:ALA:HB2  | 1.99                     | 0.44              |
| 2:M:939:ARG:CD    | 2:M:982:PRO:HD3  | 2.47                     | 0.44              |
| 3:N:1155:VAL:O    | 3:N:1182:GLU:OE2 | 2.36                     | 0.44              |
| 3:N:9:ARG:NH1     | 3:N:11:ALA:HB2   | 2.33                     | 0.44              |
| 3:N:1384:PRO:HB3  | 3:N:1388:ARG:NH1 | 2.32                     | 0.44              |
| 3:N:982:PHE:HA    | 7:Z:125:MET:HB3  | 2.00                     | 0.44              |
| 1:B:51:THR:HG22   | 1:B:89:PHE:CE2   | 2.52                     | 0.44              |
| 2:C:129:ILE:CG2   | 2:C:130:ASN:N    | 2.62                     | 0.44              |
| 2:C:473:ARG:HA    | 2:C:531:PHE:CE1  | 2.52                     | 0.44              |
| 2:C:700:TYR:N     | 2:C:700:TYR:CD1  | 2.86                     | 0.44              |
| 3:D:1120:VAL:HA   | 3:D:1121:PRO:HD3 | 1.76                     | 0.44              |
| 3:D:141:ILE:HG13  | 3:D:448:GLU:OE2  | 2.17                     | 0.44              |
| 3:D:159:ARG:HH22  | 2:H:218:VAL:HB   | 1.82                     | 0.44              |
| 3:D:511:TRP:C     | 3:D:513:ILE:N    | 2.71                     | 0.44              |
| 3:D:701:LEU:H     | 3:D:701:LEU:HD12 | 1.82                     | 0.44              |
| 3:D:827:ILE:HD12  | 3:D:827:ILE:N    | 2.27                     | 0.44              |
| 3:D:881:LEU:HD12  | 3:D:885:ILE:HD11 | 1.98                     | 0.44              |
| 3:D:881:LEU:O     | 3:D:885:ILE:HG12 | 2.18                     | 0.44              |
| 3:D:991:GLN:NE2   | 7:X:112:VAL:CG2  | 2.81                     | 0.44              |
| 1:F:189:ARG:HG2   | 1:F:189:ARG:NH1  | 2.33                     | 0.44              |
| 2:H:1095:LEU:HD12 | 2:H:1097:LEU:N   | 2.24                     | 0.44              |
| 2:H:151:ASP:OD1   | 2:H:152:PRO:HD2  | 2.18                     | 0.44              |
| 2:H:16:PRO:HB3    | 2:H:17:PRO:CD    | 2.48                     | 0.44              |
| 2:H:18:LEU:CD1    | 2:H:586:ARG:HH12 | 2.29                     | 0.44              |
| 2:H:194:VAL:HA    | 2:H:197:LEU:HD12 | 1.99                     | 0.44              |
| 2:H:273:GLY:HA2   | 2:H:276:LYS:NZ   | 2.33                     | 0.44              |
| 2:H:332:ARG:HE    | 2:H:464:LEU:HG   | 1.83                     | 0.44              |
| 2:H:25:SER:CB     | 2:H:335:THR:HB   | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:946:ARG:HH11  | 2:H:946:ARG:CB    | 2.25                     | 0.44              |
| 3:I:1304:LYS:HB3  | 3:I:1304:LYS:HE2  | 1.64                     | 0.44              |
| 3:I:1472:ILE:N    | 3:I:1472:ILE:HD12 | 2.25                     | 0.44              |
| 3:I:407:VAL:HA    | 3:I:422:ALA:CB    | 2.47                     | 0.44              |
| 3:I:461:ILE:N     | 3:I:461:ILE:HD13  | 2.33                     | 0.44              |
| 4:J:47:LYS:HA     | 4:J:54:LEU:CB     | 2.45                     | 0.44              |
| 1:K:58:ILE:HB     | 1:K:61:VAL:HB     | 2.00                     | 0.44              |
| 1:L:26:GLU:CB     | 1:L:27:PRO:HA     | 2.47                     | 0.44              |
| 2:M:174:LEU:HD22  | 2:M:193:LEU:CD2   | 2.37                     | 0.44              |
| 2:M:403:SER:O     | 2:M:407:LYS:HG3   | 2.17                     | 0.44              |
| 2:M:442:GLU:CD    | 2:M:543:ASN:HD22  | 2.21                     | 0.44              |
| 2:M:688:ILE:HG12  | 2:M:871:LEU:HD23  | 2.00                     | 0.44              |
| 2:M:758:ARG:NH2   | 2:M:788:THR:HG22  | 2.33                     | 0.44              |
| 2:M:705:ILE:HG12  | 2:M:828:ALA:HB2   | 2.00                     | 0.44              |
| 2:M:931:GLY:O     | 2:M:933:GLY:N     | 2.51                     | 0.44              |
| 3:N:1139:ASP:O    | 3:N:1142:ALA:HB3  | 2.17                     | 0.44              |
| 3:N:1235:GLN:HG2  | 7:Z:48:LEU:HD11   | 1.99                     | 0.44              |
| 3:N:1262:LEU:HD12 | 3:N:1262:LEU:HA   | 1.84                     | 0.44              |
| 3:N:1297:GLU:HG2  | 3:N:1298:GLY:H    | 1.75                     | 0.44              |
| 3:N:1294:VAL:O    | 3:N:1300:SER:HA   | 2.18                     | 0.44              |
| 3:N:1468:LEU:CD2  | 3:N:1470:ARG:HB2  | 2.32                     | 0.44              |
| 3:N:161:LEU:HA    | 3:N:397:LYS:NZ    | 2.30                     | 0.44              |
| 3:N:176:ASP:CB    | 3:N:389:GLU:HG2   | 2.47                     | 0.44              |
| 3:N:351:MET:HA    | 3:N:370:ALA:HB2   | 2.00                     | 0.44              |
| 3:N:802:ALA:O     | 3:N:803:GLY:C     | 2.55                     | 0.44              |
| 1:A:101:LEU:HD12  | 1:A:113:ASP:O     | 2.18                     | 0.43              |
| 1:A:8:ALA:O       | 1:A:9:PRO:C       | 2.56                     | 0.43              |
| 1:B:73:GLU:CG     | 1:B:130:ALA:HA    | 2.48                     | 0.43              |
| 2:C:1013:TYR:HD1  | 2:C:1020:PRO:HA   | 1.83                     | 0.43              |
| 2:C:173:ASP:O     | 2:C:184:MET:HA    | 2.18                     | 0.43              |
| 2:C:226:VAL:HG13  | 2:C:227:PHE:H     | 1.83                     | 0.43              |
| 2:C:939:ARG:CD    | 2:C:982:PRO:HD3   | 2.47                     | 0.43              |
| 2:C:447:ALA:HA    | 3:D:1085:ALA:HB1  | 1.98                     | 0.43              |
| 2:C:1084:SER:HB2  | 3:D:617:ASN:HD21  | 1.83                     | 0.43              |
| 2:C:1043:TYR:CE1  | 3:D:710:ARG:O     | 2.71                     | 0.43              |
| 3:D:800:LYS:CD    | 3:D:804:LEU:HD13  | 2.48                     | 0.43              |
| 1:G:45:LEU:HD11   | 1:G:177:VAL:CG2   | 2.48                     | 0.43              |
| 1:G:56:VAL:O      | 1:G:165:ILE:HD13  | 2.18                     | 0.43              |
| 2:H:1087:VAL:O    | 2:H:1091:GLU:HG3  | 2.18                     | 0.43              |
| 2:H:1095:LEU:CD1  | 2:H:1097:LEU:H    | 2.24                     | 0.43              |
| 2:H:238:LEU:O     | 2:H:241:LEU:CB    | 2.66                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:64:LEU:HD22   | 2:H:359:MET:CG    | 2.48                     | 0.43              |
| 2:H:410:ILE:O     | 2:H:410:ILE:HG22  | 2.18                     | 0.43              |
| 2:H:42:VAL:CG2    | 2:H:43:GLY:N      | 2.69                     | 0.43              |
| 3:I:1293:PHE:CD2  | 3:I:1300:SER:HB2  | 2.53                     | 0.43              |
| 3:I:41:ARG:HD2    | 3:I:41:ARG:C      | 2.38                     | 0.43              |
| 3:I:99:ALA:O      | 3:I:514:LEU:CA    | 2.66                     | 0.43              |
| 3:I:583:ASP:OD2   | 3:I:604:THR:HG21  | 2.17                     | 0.43              |
| 2:H:684:PHE:HB3   | 3:I:633:VAL:HG21  | 2.00                     | 0.43              |
| 3:I:757:ALA:O     | 3:I:761:ILE:HG12  | 2.18                     | 0.43              |
| 4:J:43:GLU:O      | 4:J:44:GLU:HB2    | 2.17                     | 0.43              |
| 3:I:925:GLU:CD    | 4:J:6:ILE:HG22    | 2.38                     | 0.43              |
| 1:L:77:GLU:O      | 1:L:80:LEU:HB2    | 2.17                     | 0.43              |
| 2:M:1038:TRP:CA   | 2:M:1041:GLU:HG3  | 2.46                     | 0.43              |
| 2:M:1041:GLU:OE1  | 3:N:1462:LEU:HB3  | 2.18                     | 0.43              |
| 2:M:317:VAL:C     | 2:M:319:GLY:H     | 2.19                     | 0.43              |
| 3:N:13:ALA:HB1    | 3:N:18:ILE:CD1    | 2.47                     | 0.43              |
| 3:N:141:ILE:CD1   | 3:N:142:LEU:N     | 2.64                     | 0.43              |
| 3:N:179:VAL:HG13  | 3:N:183:GLU:OE2   | 2.18                     | 0.43              |
| 3:N:631:ILE:HG21  | 3:N:745:MET:CG    | 2.48                     | 0.43              |
| 4:O:54:LEU:HA     | 4:O:58:PRO:CG     | 2.47                     | 0.43              |
| 7:Y:94:PRO:HB2    | 7:Y:95:LEU:H      | 1.57                     | 0.43              |
| 2:C:1035:MET:HA   | 2:C:1038:TRP:CZ3  | 2.53                     | 0.43              |
| 2:C:136:ILE:HG23  | 2:C:391:LEU:HD22  | 1.98                     | 0.43              |
| 2:C:141:HIS:O     | 2:C:331:ARG:HA    | 2.18                     | 0.43              |
| 2:C:449:ILE:O     | 2:C:451:LEU:N     | 2.51                     | 0.43              |
| 2:C:479:VAL:N     | 2:C:506:ASN:O     | 2.48                     | 0.43              |
| 2:C:691:SER:O     | 2:C:692:GLU:C     | 2.55                     | 0.43              |
| 2:C:673:LEU:CD2   | 2:C:867:VAL:HG12  | 2.46                     | 0.43              |
| 2:C:897:LEU:HD22  | 2:C:920:GLN:CG    | 2.48                     | 0.43              |
| 3:D:1090:ASP:O    | 3:D:1093:TYR:HB2  | 2.18                     | 0.43              |
| 3:D:1102:THR:C    | 3:D:1105:ILE:HD13 | 2.38                     | 0.43              |
| 3:D:1147:ARG:O    | 3:D:1166:LEU:HD23 | 2.18                     | 0.43              |
| 3:D:1123:PHE:HZ   | 3:D:1178:ALA:HB1  | 1.80                     | 0.43              |
| 3:D:1468:LEU:HD22 | 3:D:1470:ARG:HD3  | 1.99                     | 0.43              |
| 3:D:54:LYS:HG3    | 3:D:55:ASP:N      | 2.34                     | 0.43              |
| 3:D:97:THR:HB     | 3:D:571:LYS:CE    | 2.48                     | 0.43              |
| 2:H:354:GLY:O     | 2:H:358:ARG:HD3   | 2.18                     | 0.43              |
| 2:H:494:TYR:CE2   | 2:H:531:PHE:HE2   | 2.34                     | 0.43              |
| 2:H:681:GLY:C     | 3:I:635:PRO:CG    | 2.85                     | 0.43              |
| 2:H:950:LEU:CD1   | 2:H:952:LEU:HD21  | 2.46                     | 0.43              |
| 3:I:1107:VAL:O    | 3:I:1218:GLY:N    | 2.47                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1158:VAL:HG12 | 3:I:1159:ARG:N    | 2.33                     | 0.43              |
| 3:I:1425:THR:HG23 | 3:I:1429:LEU:HD13 | 2.01                     | 0.43              |
| 3:I:436:GLU:OE1   | 3:I:445:ARG:HG3   | 2.17                     | 0.43              |
| 2:H:1056:LYS:CB   | 3:I:623:VAL:HG13  | 2.48                     | 0.43              |
| 3:I:645:PRO:CD    | 3:I:726:ILE:HG12  | 2.45                     | 0.43              |
| 3:I:841:TYR:O     | 3:I:864:VAL:HG12  | 2.17                     | 0.43              |
| 4:J:19:LEU:HD12   | 4:J:23:VAL:HG23   | 1.99                     | 0.43              |
| 2:M:1102:LEU:HD23 | 2:M:1106:ASP:HB3  | 2.00                     | 0.43              |
| 2:M:199:VAL:CG1   | 2:M:298:PHE:CE1   | 3.01                     | 0.43              |
| 2:M:254:VAL:HA    | 2:M:257:VAL:HG23  | 2.00                     | 0.43              |
| 2:M:258:TYR:CG    | 2:M:258:TYR:O     | 2.71                     | 0.43              |
| 2:M:426:ASP:OD1   | 2:M:426:ASP:O     | 2.35                     | 0.43              |
| 2:M:572:ILE:CD1   | 2:M:573:ARG:H     | 2.17                     | 0.43              |
| 2:M:612:VAL:HG13  | 2:M:621:VAL:O     | 2.18                     | 0.43              |
| 2:M:922:PHE:HZ    | 2:M:963:LEU:HB3   | 1.83                     | 0.43              |
| 2:M:577:PRO:HG3   | 2:M:993:PHE:CZ    | 2.53                     | 0.43              |
| 3:N:100:ALA:HB2   | 3:N:128:TYR:CZ    | 2.53                     | 0.43              |
| 3:N:1090:ASP:OD2  | 3:N:1256:LEU:CD2  | 2.66                     | 0.43              |
| 3:N:398:ALA:CB    | 3:N:447:VAL:HA    | 2.46                     | 0.43              |
| 3:N:471:GLU:H     | 3:N:471:GLU:HG2   | 1.54                     | 0.43              |
| 3:N:970:LYS:HG2   | 3:N:995:LEU:CD1   | 2.48                     | 0.43              |
| 7:X:115:THR:CB    | 7:X:116:PRO:CD    | 2.94                     | 0.43              |
| 7:Z:85:LEU:HD22   | 7:Z:105:VAL:HA    | 2.00                     | 0.43              |
| 7:Z:21:ARG:N      | 7:Z:21:ARG:CD     | 2.81                     | 0.43              |
| 1:A:83:LYS:HZ2    | 1:A:168:ASP:HB2   | 1.83                     | 0.43              |
| 2:C:1102:LEU:HD23 | 2:C:1106:ASP:HB3  | 2.00                     | 0.43              |
| 2:C:1105:LYS:O    | 2:C:1107:ASN:N    | 2.51                     | 0.43              |
| 2:C:148:PHE:HD2   | 2:C:160:ALA:HA    | 1.82                     | 0.43              |
| 2:C:189:ARG:HD2   | 2:C:190:LYS:H     | 1.83                     | 0.43              |
| 2:C:207:LEU:HD21  | 2:C:221:LEU:HD22  | 1.99                     | 0.43              |
| 2:C:31:GLN:O      | 2:C:31:GLN:NE2    | 2.47                     | 0.43              |
| 2:C:438:ILE:HD11  | 2:C:467:ILE:HD12  | 2.00                     | 0.43              |
| 2:C:52:PHE:O      | 2:C:53:PRO:C      | 2.57                     | 0.43              |
| 2:C:575:GLN:C     | 2:C:667:ALA:HB1   | 2.38                     | 0.43              |
| 2:C:710:ILE:HD11  | 2:C:758:ARG:NE    | 2.31                     | 0.43              |
| 3:D:1205:TYR:OH   | 3:D:1367:HIS:CE1  | 2.70                     | 0.43              |
| 3:D:1437:ALA:C    | 3:D:1439:SER:N    | 2.71                     | 0.43              |
| 3:D:1452:ILE:HG22 | 3:D:1453:ALA:N    | 2.32                     | 0.43              |
| 3:D:593:ASN:HB3   | 3:D:594:PRO:HD2   | 2.01                     | 0.43              |
| 3:D:683:ILE:CD1   | 3:D:687:VAL:HG21  | 2.36                     | 0.43              |
| 2:H:185:LYS:HG2   | 2:H:190:LYS:CA    | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:258:TYR:CE2   | 2:H:290:LEU:CD1   | 2.97                     | 0.43              |
| 2:H:625:LEU:O     | 2:H:626:ARG:C     | 2.56                     | 0.43              |
| 2:H:565:GLN:HG2   | 2:H:995:MET:CE    | 2.48                     | 0.43              |
| 3:I:1258:ARG:HG3  | 3:I:1262:LEU:HD22 | 2.00                     | 0.43              |
| 3:I:1438:ALA:N    | 3:I:1446:VAL:HG11 | 2.33                     | 0.43              |
| 3:I:1441:GLN:CG   | 3:I:1442:ASN:H    | 2.31                     | 0.43              |
| 3:I:160:GLU:CG    | 3:I:165:LYS:HG3   | 2.32                     | 0.43              |
| 3:I:470:LEU:CB    | 3:I:503:LEU:HD21  | 2.44                     | 0.43              |
| 3:I:502:PHE:CZ    | 3:I:509:PRO:HB3   | 2.53                     | 0.43              |
| 3:I:511:TRP:C     | 3:I:513:ILE:N     | 2.71                     | 0.43              |
| 3:I:696:HIS:NE2   | 4:J:54:LEU:CD1    | 2.81                     | 0.43              |
| 3:I:881:LEU:O     | 3:I:885:ILE:HG12  | 2.18                     | 0.43              |
| 3:I:970:LYS:HG2   | 3:I:995:LEU:CD1   | 2.48                     | 0.43              |
| 3:I:970:LYS:O     | 3:I:974:ILE:HG13  | 2.19                     | 0.43              |
| 2:M:274:ARG:NE    | 2:M:285:LEU:HD22  | 2.33                     | 0.43              |
| 2:M:468:ARG:HB3   | 2:M:485:TYR:HB3   | 2.00                     | 0.43              |
| 2:M:52:PHE:O      | 2:M:53:PRO:C      | 2.56                     | 0.43              |
| 3:N:1213:ARG:HH12 | 4:O:10:PHE:C      | 2.22                     | 0.43              |
| 3:N:1434:TRP:CZ3  | 3:N:1455:LYS:O    | 2.71                     | 0.43              |
| 3:N:162:ARG:HG2   | 3:N:162:ARG:NH1   | 2.34                     | 0.43              |
| 3:N:55:ASP:O      | 3:N:56:TYR:CB     | 2.66                     | 0.43              |
| 3:N:914:LEU:HD23  | 3:N:914:LEU:O     | 2.19                     | 0.43              |
| 2:M:873:PRO:HB3   | 3:N:949:ILE:CD1   | 2.48                     | 0.43              |
| 7:X:98:GLU:OE1    | 7:X:98:GLU:HA     | 2.18                     | 0.43              |
| 2:C:217:LEU:C     | 2:C:219:GLN:N     | 2.70                     | 0.43              |
| 2:C:232:GLU:CD    | 2:C:250:ARG:HH12  | 2.22                     | 0.43              |
| 2:C:352:ALA:HA    | 2:C:355:VAL:HG12  | 1.99                     | 0.43              |
| 2:C:462:ASP:CG    | 2:C:463:GLU:N     | 2.70                     | 0.43              |
| 2:C:11:GLU:CG     | 2:C:537:LYS:HZ1   | 2.30                     | 0.43              |
| 2:C:553:ASP:OD2   | 2:C:883:GLY:N     | 2.47                     | 0.43              |
| 2:C:577:PRO:C     | 2:C:579:VAL:N     | 2.71                     | 0.43              |
| 2:C:654:LEU:HD13  | 2:C:663:ASN:O     | 2.18                     | 0.43              |
| 2:C:861:LEU:CD2   | 2:C:862:PRO:HD2   | 2.48                     | 0.43              |
| 3:D:1156:LEU:HD11 | 3:D:1177:ALA:HA   | 1.99                     | 0.43              |
| 3:D:1389:LEU:H    | 3:D:1389:LEU:HD23 | 1.83                     | 0.43              |
| 2:C:1085:PHE:HD2  | 3:D:1468:LEU:HA   | 1.84                     | 0.43              |
| 3:D:41:ARG:H      | 3:D:41:ARG:HG3    | 1.49                     | 0.43              |
| 3:D:438:ASP:HB3   | 3:D:441:ARG:NH2   | 2.33                     | 0.43              |
| 3:D:129:PHE:HZ    | 3:D:587:ARG:CD    | 2.30                     | 0.43              |
| 3:D:639:LEU:HD11  | 3:D:928:ALA:HB1   | 1.99                     | 0.43              |
| 3:D:786:ILE:O     | 3:D:787:LEU:C     | 2.55                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:176:ARG:NH1   | 2:H:863:ASP:OD2   | 2.52                     | 0.43              |
| 1:F:61:VAL:HG13   | 1:F:66:SER:HB3    | 1.99                     | 0.43              |
| 2:H:1054:THR:O    | 2:H:1056:LYS:N    | 2.51                     | 0.43              |
| 2:H:22:GLN:OE1    | 2:H:336:VAL:HG21  | 2.18                     | 0.43              |
| 2:H:939:ARG:CD    | 2:H:982:PRO:HD3   | 2.48                     | 0.43              |
| 3:I:1095:THR:O    | 3:I:1099:VAL:CG2  | 2.62                     | 0.43              |
| 3:I:1101:VAL:HG11 | 3:I:1424:VAL:O    | 2.19                     | 0.43              |
| 3:I:1479:ASP:OD2  | 3:I:1482:ARG:NH2  | 2.52                     | 0.43              |
| 3:I:766:ALA:CB    | 4:J:2:ALA:HB2     | 2.47                     | 0.43              |
| 3:I:835:SER:C     | 3:I:837:GLY:N     | 2.69                     | 0.43              |
| 3:I:50:PHE:CA     | 3:I:89:ARG:CB     | 2.97                     | 0.43              |
| 2:H:885:ILE:HG13  | 3:I:949:ILE:HG22  | 2.01                     | 0.43              |
| 4:J:80:VAL:HG13   | 4:J:81:PRO:HD2    | 1.99                     | 0.43              |
| 2:M:11:GLU:HG2    | 2:M:537:LYS:HZ1   | 1.84                     | 0.43              |
| 2:M:449:ILE:O     | 2:M:451:LEU:N     | 2.51                     | 0.43              |
| 2:M:474:VAL:HB    | 2:M:479:VAL:HG12  | 2.01                     | 0.43              |
| 2:M:886:LEU:HA    | 2:M:886:LEU:HD12  | 1.38                     | 0.43              |
| 2:M:958:THR:CG2   | 2:M:961:GLU:HG3   | 2.35                     | 0.43              |
| 3:N:1194:CYS:SG   | 3:N:1204:CYS:SG   | 3.16                     | 0.43              |
| 3:N:1288:GLU:HG2  | 3:N:1307:LYS:CE   | 2.43                     | 0.43              |
| 3:N:141:ILE:HD13  | 3:N:142:LEU:C     | 2.38                     | 0.43              |
| 3:N:1425:THR:HG23 | 3:N:1429:LEU:HD13 | 2.01                     | 0.43              |
| 3:N:786:ILE:O     | 3:N:787:LEU:C     | 2.55                     | 0.43              |
| 3:N:841:TYR:O     | 3:N:864:VAL:HG12  | 2.17                     | 0.43              |
| 1:A:20:TYR:O      | 1:A:207:PRO:HG2   | 2.18                     | 0.43              |
| 2:C:206:THR:HG23  | 2:C:207:LEU:N     | 2.34                     | 0.43              |
| 2:C:22:GLN:HG2    | 2:C:336:VAL:CG2   | 2.47                     | 0.43              |
| 2:C:266:ARG:HA    | 2:C:288:ARG:HD3   | 2.00                     | 0.43              |
| 2:C:52:PHE:HB3    | 2:C:53:PRO:CD     | 2.48                     | 0.43              |
| 2:C:654:LEU:CD1   | 2:C:663:ASN:O     | 2.67                     | 0.43              |
| 2:C:950:LEU:CD1   | 2:C:952:LEU:HD21  | 2.46                     | 0.43              |
| 3:D:1029:ARG:NH2  | 7:X:42:ASP:HB3    | 2.32                     | 0.43              |
| 3:D:100:ALA:HB3   | 3:D:128:TYR:HE2   | 1.83                     | 0.43              |
| 3:D:17:LYS:CD     | 3:D:21:TRP:HE1    | 2.30                     | 0.43              |
| 3:D:353:VAL:HG23  | 3:D:353:VAL:O     | 2.18                     | 0.43              |
| 3:D:461:ILE:HD13  | 3:D:461:ILE:N     | 2.33                     | 0.43              |
| 3:D:87:ARG:CB     | 3:D:523:ASP:CB    | 2.50                     | 0.43              |
| 3:D:829:VAL:O     | 3:D:831:GLY:N     | 2.52                     | 0.43              |
| 2:C:885:ILE:CG1   | 3:D:949:ILE:HG22  | 2.45                     | 0.43              |
| 4:E:84:ARG:O      | 4:E:88:GLU:HG2    | 2.19                     | 0.43              |
| 1:F:174:VAL:HG13  | 1:F:200:TRP:O     | 2.17                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:206:THR:OG1   | 1:F:207:PRO:HD2   | 2.19                     | 0.43              |
| 2:H:1038:TRP:HD1  | 2:H:1041:GLU:OE2  | 2.01                     | 0.43              |
| 2:H:1052:MET:CG   | 3:I:623:VAL:HG21  | 2.48                     | 0.43              |
| 2:H:182:VAL:CA    | 2:H:193:LEU:HD11  | 2.49                     | 0.43              |
| 2:H:445:GLU:HG3   | 2:H:560:MET:HE3   | 2.01                     | 0.43              |
| 2:H:473:ARG:HA    | 2:H:531:PHE:CD1   | 2.54                     | 0.43              |
| 2:H:583:LEU:HD12  | 2:H:583:LEU:N     | 2.34                     | 0.43              |
| 2:H:654:LEU:HD13  | 2:H:663:ASN:O     | 2.18                     | 0.43              |
| 2:H:575:GLN:C     | 2:H:667:ALA:HB1   | 2.38                     | 0.43              |
| 2:H:684:PHE:CG    | 2:H:685:GLU:N     | 2.86                     | 0.43              |
| 2:H:691:SER:C     | 2:H:693:GLU:N     | 2.72                     | 0.43              |
| 2:H:754:ILE:CG1   | 2:H:791:ARG:HH12  | 2.31                     | 0.43              |
| 2:H:536:PRO:HB3   | 2:H:906:PHE:HD1   | 1.82                     | 0.43              |
| 2:H:943:VAL:HG23  | 2:H:985:GLY:N     | 2.18                     | 0.43              |
| 2:H:922:PHE:HZ    | 2:H:963:LEU:HB3   | 1.83                     | 0.43              |
| 3:I:1117:TYR:CZ   | 3:I:1151:ARG:HD2  | 2.53                     | 0.43              |
| 3:I:1136:LYS:HB2  | 3:I:1139:ASP:OD2  | 2.19                     | 0.43              |
| 3:I:1455:LYS:HD3  | 3:I:1455:LYS:HA   | 1.70                     | 0.43              |
| 3:I:438:ASP:OD1   | 3:I:441:ARG:NH2   | 2.51                     | 0.43              |
| 1:K:206:THR:OG1   | 1:K:207:PRO:HD2   | 2.19                     | 0.43              |
| 1:L:206:THR:HG23  | 1:L:207:PRO:N     | 2.32                     | 0.43              |
| 2:M:1071:ILE:HG23 | 3:N:670:VAL:HG11  | 2.01                     | 0.43              |
| 2:M:182:VAL:CG1   | 2:M:193:LEU:HD13  | 2.49                     | 0.43              |
| 2:M:431:HIS:CD2   | 2:M:433:THR:H     | 2.37                     | 0.43              |
| 2:M:473:ARG:HA    | 2:M:531:PHE:CD1   | 2.53                     | 0.43              |
| 2:M:874:LEU:CD1   | 3:N:784:ASP:OD2   | 2.67                     | 0.43              |
| 2:M:943:VAL:HG23  | 2:M:985:GLY:N     | 2.18                     | 0.43              |
| 3:N:1458:GLU:HA   | 3:N:1458:GLU:OE2  | 2.19                     | 0.43              |
| 2:M:946:ARG:HH12  | 3:N:796:ARG:HH22  | 1.66                     | 0.43              |
| 3:N:87:ARG:HA     | 3:N:523:ASP:HB2   | 2.01                     | 0.43              |
| 3:N:970:LYS:O     | 3:N:974:ILE:HG13  | 2.19                     | 0.43              |
| 1:A:206:THR:OG1   | 1:A:207:PRO:HD2   | 2.18                     | 0.43              |
| 2:C:293:PHE:HA    | 2:C:298:PHE:CD2   | 2.53                     | 0.43              |
| 2:C:710:ILE:HG21  | 2:C:756:VAL:HG11  | 2.01                     | 0.43              |
| 2:C:899:GLN:HG3   | 2:C:901:TYR:CZ    | 2.54                     | 0.43              |
| 3:D:101:HIS:O     | 3:D:105:VAL:HG23  | 2.18                     | 0.43              |
| 3:D:1198:TYR:OH   | 3:D:1394:VAL:HG21 | 2.18                     | 0.43              |
| 3:D:1087:ARG:HG2  | 3:D:1234:THR:O    | 2.18                     | 0.43              |
| 3:D:1346:ARG:HD2  | 3:D:1346:ARG:HA   | 1.84                     | 0.43              |
| 2:C:1097:LEU:CD1  | 3:D:1451:ALA:CA   | 2.92                     | 0.43              |
| 3:D:38:LYS:HA     | 3:D:39:PRO:HD3    | 1.89                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:682:ASP:C    | 3:D:684:LYS:H     | 2.20                     | 0.43              |
| 3:D:806:PHE:C    | 3:D:808:THR:N     | 2.71                     | 0.43              |
| 1:F:141:GLU:OE1  | 1:F:161:ARG:NH1   | 2.47                     | 0.43              |
| 1:F:83:LYS:HD3   | 1:F:167:VAL:HG12  | 1.99                     | 0.43              |
| 1:G:149:GLY:O    | 1:G:171:PHE:HB2   | 2.18                     | 0.43              |
| 2:H:205:GLU:HG3  | 2:H:205:GLU:H     | 1.57                     | 0.43              |
| 2:H:285:LEU:HG   | 2:H:286:SER:N     | 2.33                     | 0.43              |
| 2:H:290:LEU:CB   | 2:H:302:VAL:CG1   | 2.92                     | 0.43              |
| 2:H:313:LEU:CB   | 2:H:320:HIS:ND1   | 2.80                     | 0.43              |
| 2:H:431:HIS:CD2  | 2:H:433:THR:H     | 2.37                     | 0.43              |
| 2:H:512:ARG:CG   | 2:H:523:ILE:CD1   | 2.96                     | 0.43              |
| 2:H:602:GLU:O    | 2:H:613:VAL:HB    | 2.18                     | 0.43              |
| 2:H:703:ILE:CD1  | 2:H:703:ILE:N     | 2.82                     | 0.43              |
| 2:H:939:ARG:NE   | 2:H:939:ARG:HA    | 2.14                     | 0.43              |
| 3:I:1209:LEU:CD2 | 3:I:1211:MET:H    | 2.25                     | 0.43              |
| 3:I:1287:GLU:C   | 3:I:1289:LYS:H    | 2.22                     | 0.43              |
| 3:I:130:SER:OG   | 3:I:132:TYR:HD1   | 2.02                     | 0.43              |
| 3:I:1353:GLN:HB3 | 3:I:1357:ARG:NE   | 2.34                     | 0.43              |
| 3:I:1434:TRP:C   | 3:I:1434:TRP:CD1  | 2.91                     | 0.43              |
| 3:I:133:ILE:O    | 3:I:152:LEU:CB    | 2.67                     | 0.43              |
| 3:I:465:LEU:HD11 | 3:I:512:MET:HB2   | 2.00                     | 0.43              |
| 3:I:676:MET:CE   | 3:I:684:LYS:HE3   | 2.49                     | 0.43              |
| 3:I:914:LEU:HD23 | 3:I:914:LEU:O     | 2.19                     | 0.43              |
| 1:K:18:ARG:O     | 1:K:201:THR:OG1   | 2.36                     | 0.43              |
| 1:K:206:THR:HG23 | 1:K:208:LEU:N     | 2.34                     | 0.43              |
| 2:M:100:LEU:HD12 | 2:M:100:LEU:C     | 2.39                     | 0.43              |
| 2:M:100:LEU:HD23 | 2:M:372:LEU:HD21  | 2.00                     | 0.43              |
| 2:M:395:LYS:CE   | 2:M:403:SER:HB2   | 2.49                     | 0.43              |
| 2:M:48:PHE:HD1   | 2:M:48:PHE:HA     | 1.73                     | 0.43              |
| 2:M:545:ASN:OD1  | 2:M:905:ILE:CG1   | 2.66                     | 0.43              |
| 2:M:553:ASP:OD1  | 2:M:843:HIS:ND1   | 2.50                     | 0.43              |
| 2:M:684:PHE:CG   | 2:M:685:GLU:N     | 2.86                     | 0.43              |
| 2:M:36:PRO:HB3   | 2:M:70:GLU:HG3    | 2.01                     | 0.43              |
| 3:N:1020:LEU:HA  | 3:N:1020:LEU:HD12 | 1.81                     | 0.43              |
| 3:N:820:GLU:HG2  | 3:N:825:ALA:O     | 2.19                     | 0.43              |
| 3:N:829:VAL:H    | 3:N:835:SER:HB2   | 1.84                     | 0.43              |
| 3:N:957:PRO:HG2  | 3:N:1007:VAL:CA   | 2.47                     | 0.43              |
| 5:R:17:DG:H2'    | 5:R:18:DC:H6      | 1.82                     | 0.43              |
| 7:X:33:LEU:HD11  | 7:X:52:LYS:CG     | 2.44                     | 0.43              |
| 7:Y:123:SER:O    | 7:Y:127:LYS:N     | 2.48                     | 0.43              |
| 7:Z:82:VAL:HG22  | 7:Z:133:ARG:HH21  | 1.83                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:124:ASN:ND2   | 1:A:127:LEU:CD2   | 2.82                     | 0.43              |
| 1:B:198:ARG:O     | 1:B:199:ILE:HD13  | 2.19                     | 0.43              |
| 1:B:226:SER:O     | 1:B:228:PRO:HD3   | 2.18                     | 0.43              |
| 2:C:205:GLU:HG3   | 2:C:206:THR:H     | 1.83                     | 0.43              |
| 2:C:428:ARG:HG2   | 2:C:451:LEU:HG    | 2.01                     | 0.43              |
| 2:C:554:ASP:HB2   | 3:D:1061:PHE:HE2  | 1.82                     | 0.43              |
| 2:C:588:VAL:HG13  | 2:C:666:LEU:HB2   | 2.01                     | 0.43              |
| 2:C:630:ARG:HD3   | 2:C:705:ILE:HB    | 2.00                     | 0.43              |
| 3:D:1152:GLU:CG   | 3:D:1161:GLU:HA   | 2.49                     | 0.43              |
| 3:D:1366:LYS:O    | 3:D:1370:ILE:HG13 | 2.19                     | 0.43              |
| 3:D:1377:LYS:CG   | 3:D:1377:LYS:O    | 2.67                     | 0.43              |
| 3:D:1217:ILE:HB   | 3:D:1480:PHE:CD2  | 2.53                     | 0.43              |
| 3:D:159:ARG:HH22  | 2:H:218:VAL:HG21  | 1.83                     | 0.43              |
| 3:D:42:ASP:H      | 3:D:46:ASP:HB2    | 1.83                     | 0.43              |
| 3:D:695:ILE:O     | 3:D:696:HIS:C     | 2.57                     | 0.43              |
| 3:D:757:ALA:O     | 3:D:761:ILE:HG12  | 2.18                     | 0.43              |
| 3:D:820:GLU:HG2   | 3:D:825:ALA:O     | 2.19                     | 0.43              |
| 3:D:87:ARG:HB3    | 3:D:523:ASP:HB3   | 1.81                     | 0.43              |
| 1:F:68:ILE:HA     | 1:F:69:PRO:HD3    | 1.86                     | 0.43              |
| 1:G:81:ASN:O      | 1:G:84:GLU:HB3    | 2.19                     | 0.43              |
| 2:H:1040:LEU:O    | 2:H:1041:GLU:C    | 2.56                     | 0.43              |
| 2:H:101:ILE:HD12  | 2:H:108:ILE:HD13  | 1.99                     | 0.43              |
| 2:H:1105:LYS:O    | 2:H:1107:ASN:N    | 2.51                     | 0.43              |
| 2:H:223:ASP:OD1   | 2:H:224:GLU:N     | 2.50                     | 0.43              |
| 2:H:899:GLN:HG3   | 2:H:901:TYR:CZ    | 2.54                     | 0.43              |
| 2:H:931:GLY:O     | 2:H:933:GLY:N     | 2.51                     | 0.43              |
| 2:H:957:LYS:CD    | 2:H:961:GLU:CB    | 2.95                     | 0.43              |
| 3:I:101:HIS:O     | 3:I:105:VAL:HG23  | 2.18                     | 0.43              |
| 3:I:1120:VAL:HG23 | 3:I:1188:VAL:HG11 | 2.00                     | 0.43              |
| 3:I:1293:PHE:HE2  | 3:I:1300:SER:HG   | 1.63                     | 0.43              |
| 3:I:204:LEU:CD1   | 3:I:441:ARG:NH2   | 2.77                     | 0.43              |
| 3:I:564:GLU:O     | 3:I:566:ILE:N     | 2.52                     | 0.43              |
| 3:I:829:VAL:O     | 3:I:831:GLY:N     | 2.52                     | 0.43              |
| 1:G:80:LEU:HD23   | 3:I:867:ARG:HE    | 1.84                     | 0.43              |
| 1:L:56:VAL:CG1    | 1:L:57:TYR:N      | 2.81                     | 0.43              |
| 2:M:223:ASP:OD1   | 2:M:224:GLU:N     | 2.49                     | 0.43              |
| 2:M:363:SER:HB2   | 2:M:366:SER:HB2   | 2.01                     | 0.43              |
| 2:M:431:HIS:CG    | 2:M:432:ARG:N     | 2.87                     | 0.43              |
| 2:M:862:PRO:CG    | 2:M:925:TYR:OH    | 2.67                     | 0.43              |
| 3:N:1384:PRO:HB3  | 3:N:1387:SER:O    | 2.19                     | 0.43              |
| 3:N:1437:ALA:HB3  | 3:N:1446:VAL:CG1  | 2.49                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1447:LEU:HD12 | 3:N:1447:LEU:N    | 2.34                     | 0.43              |
| 3:N:153:LEU:O     | 3:N:153:LEU:HD12  | 2.18                     | 0.43              |
| 3:N:93:ILE:HG21   | 3:N:548:ILE:HD13  | 2.01                     | 0.43              |
| 7:Z:123:SER:O     | 7:Z:127:LYS:N     | 2.49                     | 0.43              |
| 1:B:197:LEU:HD21  | 1:B:199:ILE:CG1   | 2.49                     | 0.43              |
| 1:B:198:ARG:H     | 1:B:198:ARG:HG2   | 1.61                     | 0.43              |
| 1:B:30:ARG:NH1    | 2:C:692:GLU:OE2   | 2.52                     | 0.43              |
| 2:C:42:VAL:O      | 2:C:43:GLY:C      | 2.57                     | 0.43              |
| 3:D:127:LEU:C     | 3:D:127:LEU:HD12  | 2.39                     | 0.43              |
| 3:D:127:LEU:HD12  | 3:D:128:TYR:N     | 2.34                     | 0.43              |
| 3:D:1293:PHE:O    | 3:D:1295:GLU:OE2  | 2.35                     | 0.43              |
| 3:D:1273:VAL:CG2  | 3:D:1305:LEU:HD21 | 2.47                     | 0.43              |
| 3:D:162:ARG:O     | 3:D:450:TYR:O     | 2.37                     | 0.43              |
| 3:D:53:ILE:HG13   | 3:D:53:ILE:O      | 2.18                     | 0.43              |
| 3:D:850:LEU:HA    | 3:D:853:VAL:CG2   | 2.49                     | 0.43              |
| 2:H:182:VAL:O     | 2:H:192:PRO:HA    | 2.19                     | 0.43              |
| 2:H:229:MET:HB3   | 2:H:230:ARG:HH12  | 1.84                     | 0.43              |
| 2:H:325:ILE:H     | 2:H:325:ILE:CD1   | 2.32                     | 0.43              |
| 2:H:135:VAL:CG1   | 2:H:407:LYS:HA    | 2.41                     | 0.43              |
| 2:H:584:GLU:CD    | 2:H:584:GLU:H     | 2.21                     | 0.43              |
| 2:H:603:VAL:HA    | 2:H:613:VAL:CG1   | 2.19                     | 0.43              |
| 3:I:1047:LYS:HZ2  | 3:I:1053:PHE:HA   | 1.82                     | 0.43              |
| 3:I:1117:TYR:CD2  | 3:I:1117:TYR:N    | 2.84                     | 0.43              |
| 3:I:156:GLU:O     | 3:I:160:GLU:HB2   | 2.18                     | 0.43              |
| 3:I:517:VAL:HG21  | 3:I:547:LEU:HD21  | 2.00                     | 0.43              |
| 3:I:703:ASN:HD22  | 3:I:704:ARG:H     | 1.67                     | 0.43              |
| 3:I:800:LYS:HD3   | 3:I:830:ALA:HB3   | 2.00                     | 0.43              |
| 1:K:62:LEU:N      | 1:K:62:LEU:CD1    | 2.76                     | 0.43              |
| 2:M:224:GLU:HB2   | 2:M:228:ALA:HB2   | 2.01                     | 0.43              |
| 2:M:344:PHE:CE2   | 2:M:378:LEU:HD21  | 2.53                     | 0.43              |
| 2:M:654:LEU:CD1   | 2:M:663:ASN:O     | 2.67                     | 0.43              |
| 2:M:679:PHE:O     | 3:N:943:THR:HG22  | 2.18                     | 0.43              |
| 2:M:861:LEU:CD2   | 2:M:862:PRO:HD2   | 2.48                     | 0.43              |
| 2:M:928:LYS:HZ3   | 2:M:932:GLU:HG3   | 1.82                     | 0.43              |
| 3:N:1061:PHE:CE1  | 3:N:1065:LEU:HD22 | 2.41                     | 0.43              |
| 2:M:1034:GLU:CD   | 3:N:1096:ARG:NH2  | 2.72                     | 0.43              |
| 3:N:1281:VAL:CG1  | 3:N:1282:ARG:N    | 2.81                     | 0.43              |
| 3:N:1437:ALA:HB3  | 3:N:1446:VAL:HG13 | 2.01                     | 0.43              |
| 3:N:511:TRP:O     | 3:N:513:ILE:N     | 2.52                     | 0.43              |
| 3:N:26:VAL:HG23   | 3:N:548:ILE:HD11  | 1.99                     | 0.43              |
| 3:N:757:ALA:O     | 3:N:761:ILE:HG12  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:Z:31:LYS:O      | 7:Z:35:GLU:HG2    | 2.19                     | 0.43              |
| 1:A:35:THR:CG2    | 1:B:43:ILE:HD11   | 2.35                     | 0.43              |
| 2:C:1044:GLY:HA2  | 3:D:1475:GLY:CA   | 2.48                     | 0.43              |
| 2:C:1095:LEU:CD1  | 2:C:1097:LEU:H    | 2.24                     | 0.43              |
| 2:C:211:LEU:HD21  | 2:C:311:PHE:CE1   | 2.54                     | 0.43              |
| 2:C:393:GLN:HE21  | 2:C:393:GLN:HB2   | 1.62                     | 0.43              |
| 2:C:674:VAL:HG23  | 2:C:869:VAL:O     | 2.17                     | 0.43              |
| 3:D:1020:LEU:HA   | 3:D:1020:LEU:HD12 | 1.81                     | 0.43              |
| 3:D:1254:GLN:HB2  | 3:D:1255:GLY:H    | 1.64                     | 0.43              |
| 2:H:229:MET:HB2   | 2:H:230:ARG:NH1   | 2.34                     | 0.43              |
| 2:H:328:LEU:N     | 2:H:328:LEU:HD12  | 2.33                     | 0.43              |
| 2:H:336:VAL:HA    | 2:H:339:LEU:HD12  | 2.01                     | 0.43              |
| 2:H:443:THR:HA    | 2:H:444:PRO:HD3   | 1.68                     | 0.43              |
| 2:H:551:GLU:O     | 3:I:1065:LEU:HB3  | 2.19                     | 0.43              |
| 2:H:654:LEU:CD1   | 2:H:663:ASN:O     | 2.67                     | 0.43              |
| 3:I:1488:ASP:N    | 3:I:1488:ASP:OD1  | 2.51                     | 0.43              |
| 3:I:204:LEU:CB    | 3:I:394:LEU:O     | 2.66                     | 0.43              |
| 3:I:511:TRP:C     | 3:I:513:ILE:H     | 2.20                     | 0.43              |
| 3:I:29:PRO:HG3    | 3:I:549:ASN:ND2   | 2.34                     | 0.43              |
| 3:I:99:ALA:HA     | 3:I:575:GLN:HE22  | 1.84                     | 0.43              |
| 1:K:189:ARG:HA    | 1:K:189:ARG:HD2   | 1.84                     | 0.43              |
| 1:K:35:THR:O      | 1:K:35:THR:HG22   | 2.18                     | 0.43              |
| 1:L:226:SER:O     | 1:L:228:PRO:HD3   | 2.18                     | 0.43              |
| 2:M:1008:ARG:HG2  | 2:M:1008:ARG:HH11 | 1.84                     | 0.43              |
| 2:M:1105:LYS:O    | 2:M:1107:ASN:N    | 2.51                     | 0.43              |
| 2:M:471:TYR:O     | 2:M:483:VAL:HG13  | 2.19                     | 0.43              |
| 2:M:603:VAL:HG11  | 2:M:606:VAL:HG13  | 2.01                     | 0.43              |
| 2:M:703:ILE:HD12  | 2:M:703:ILE:N     | 2.33                     | 0.43              |
| 3:N:1209:LEU:HD21 | 4:O:16:LYS:HZ2    | 1.74                     | 0.43              |
| 3:N:1366:LYS:O    | 3:N:1370:ILE:HG13 | 2.19                     | 0.43              |
| 3:N:177:ALA:HA    | 3:N:192:ALA:HA    | 2.01                     | 0.43              |
| 3:N:682:ASP:OD2   | 3:N:682:ASP:O     | 2.36                     | 0.43              |
| 3:N:851:LEU:H     | 3:N:851:LEU:HG    | 1.47                     | 0.43              |
| 1:L:74:ASP:CG     | 3:N:872:ARG:NH2   | 2.72                     | 0.43              |
| 3:N:766:ALA:CB    | 4:O:2:ALA:HB2     | 2.48                     | 0.43              |
| 7:X:75:LEU:HB3    | 7:X:77:GLU:OE2    | 2.18                     | 0.43              |
| 1:A:92:PRO:C      | 1:A:94:LEU:N      | 2.73                     | 0.43              |
| 2:C:1048:THR:HG21 | 3:D:763:MET:HE3   | 2.00                     | 0.43              |
| 2:C:251:ASP:O     | 2:C:252:LYS:C     | 2.56                     | 0.43              |
| 2:C:293:PHE:HA    | 2:C:298:PHE:HD2   | 1.83                     | 0.43              |
| 2:C:351:LEU:HD13  | 2:C:374:ASN:ND2   | 2.34                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:717:LEU:HB3   | 2:C:761:PHE:CD2   | 2.54                     | 0.43              |
| 2:C:71:TYR:O      | 2:C:71:TYR:CG     | 2.71                     | 0.43              |
| 2:C:939:ARG:NE    | 2:C:939:ARG:CA    | 2.79                     | 0.43              |
| 2:C:972:VAL:HG23  | 2:C:973:VAL:N     | 2.33                     | 0.43              |
| 3:D:1108:ARG:HH11 | 3:D:1108:ARG:HG3  | 1.83                     | 0.43              |
| 3:D:9:ARG:NH1     | 3:D:11:ALA:HB2    | 2.33                     | 0.43              |
| 3:D:1424:VAL:HG13 | 3:D:1425:THR:H    | 1.83                     | 0.43              |
| 3:D:1437:ALA:HB3  | 3:D:1446:VAL:HG11 | 2.00                     | 0.43              |
| 3:D:502:PHE:CZ    | 3:D:509:PRO:HB3   | 2.53                     | 0.43              |
| 3:D:52:PRO:O      | 3:D:86:ARG:CG     | 2.66                     | 0.43              |
| 3:D:54:LYS:HE3    | 3:D:55:ASP:OD1    | 2.18                     | 0.43              |
| 3:D:687:VAL:CG1   | 3:D:688:TRP:N     | 2.82                     | 0.43              |
| 2:C:988:VAL:CG1   | 3:D:948:THR:OG1   | 2.63                     | 0.43              |
| 3:D:970:LYS:HG2   | 3:D:995:LEU:CD1   | 2.48                     | 0.43              |
| 4:E:14:ASP:OD1    | 4:E:18:ARG:NH2    | 2.51                     | 0.43              |
| 1:F:206:THR:HG23  | 1:F:208:LEU:N     | 2.34                     | 0.43              |
| 1:F:18:ARG:HH12   | 1:F:88:ARG:CZ     | 2.32                     | 0.43              |
| 1:G:152:PRO:HG2   | 3:I:857:ILE:CD1   | 2.48                     | 0.43              |
| 1:G:153:ALA:HB2   | 1:G:168:ASP:N     | 2.33                     | 0.43              |
| 2:H:1051:GLU:HG2  | 2:H:1055:LEU:HD12 | 2.01                     | 0.43              |
| 2:H:333:ILE:N     | 2:H:333:ILE:CD1   | 2.80                     | 0.43              |
| 2:H:431:HIS:CG    | 2:H:432:ARG:N     | 2.87                     | 0.43              |
| 2:H:580:MET:O     | 2:H:903:SER:N     | 2.51                     | 0.43              |
| 3:I:1299:PHE:N    | 3:I:1299:PHE:CD2  | 2.87                     | 0.43              |
| 3:I:50:PHE:CA     | 3:I:89:ARG:HG2    | 2.48                     | 0.43              |
| 3:I:511:TRP:O     | 3:I:513:ILE:N     | 2.52                     | 0.43              |
| 3:I:649:ALA:O     | 3:I:650:LEU:C     | 2.57                     | 0.43              |
| 3:I:835:SER:O     | 3:I:836:VAL:C     | 2.58                     | 0.43              |
| 3:I:850:LEU:HA    | 3:I:853:VAL:CG2   | 2.49                     | 0.43              |
| 3:I:906:GLN:HB3   | 3:I:911:LEU:CD1   | 2.45                     | 0.43              |
| 1:L:161:ARG:HH11  | 1:L:161:ARG:HG3   | 1.84                     | 0.43              |
| 1:L:198:ARG:O     | 1:L:199:ILE:HD13  | 2.18                     | 0.43              |
| 2:M:1050:GLN:CA   | 2:M:1050:GLN:HE21 | 2.32                     | 0.43              |
| 2:M:99:GLN:CA     | 2:M:109:LYS:O     | 2.66                     | 0.43              |
| 2:M:15:LEU:O      | 2:M:586:ARG:NH2   | 2.52                     | 0.43              |
| 2:M:185:LYS:HG2   | 2:M:190:LYS:CG    | 2.48                     | 0.43              |
| 2:M:274:ARG:HG2   | 2:M:274:ARG:HH11  | 1.83                     | 0.43              |
| 2:M:333:ILE:CG2   | 2:M:410:ILE:HD11  | 2.49                     | 0.43              |
| 2:M:343:GLN:NE2   | 2:M:343:GLN:HA    | 2.32                     | 0.43              |
| 2:M:487:THR:O     | 2:M:488:ALA:C     | 2.57                     | 0.43              |
| 2:M:518:LYS:HB2   | 2:M:518:LYS:HE2   | 1.73                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:99:GLN:HB3    | 2:M:110:GLU:HA    | 2.01                     | 0.43              |
| 3:N:1311:LEU:H    | 3:N:1311:LEU:HD23 | 1.83                     | 0.43              |
| 3:N:1437:ALA:C    | 3:N:1439:SER:N    | 2.71                     | 0.43              |
| 3:N:158:TYR:CE1   | 3:N:452:ILE:HD11  | 2.54                     | 0.43              |
| 3:N:465:LEU:HD11  | 3:N:512:MET:HB2   | 2.00                     | 0.43              |
| 3:N:881:LEU:O     | 3:N:885:ILE:HG12  | 2.18                     | 0.43              |
| 2:C:352:ALA:HA    | 2:C:355:VAL:CG1   | 2.49                     | 0.42              |
| 2:C:385:PHE:HD1   | 2:C:389:SER:HB2   | 1.84                     | 0.42              |
| 2:C:437:ARG:CZ    | 2:C:488:ALA:HA    | 2.50                     | 0.42              |
| 2:C:886:LEU:HA    | 2:C:886:LEU:HD12  | 1.39                     | 0.42              |
| 3:D:1353:GLN:HB3  | 3:D:1357:ARG:NE   | 2.34                     | 0.42              |
| 3:D:160:GLU:HB3   | 3:D:161:LEU:HD12  | 2.01                     | 0.42              |
| 3:D:469:ASP:O     | 3:D:470:LEU:C     | 2.57                     | 0.42              |
| 3:D:584:ASN:HD21  | 3:D:590:PRO:HG2   | 1.83                     | 0.42              |
| 3:D:649:ALA:O     | 3:D:650:LEU:C     | 2.57                     | 0.42              |
| 3:D:829:VAL:H     | 3:D:835:SER:HB2   | 1.84                     | 0.42              |
| 3:D:835:SER:O     | 3:D:836:VAL:C     | 2.58                     | 0.42              |
| 3:D:914:LEU:O     | 3:D:914:LEU:HD23  | 2.19                     | 0.42              |
| 1:F:186:LEU:CD2   | 1:F:187:GLY:N     | 2.77                     | 0.42              |
| 1:G:111:ALA:HB3   | 1:G:124:ASN:O     | 2.19                     | 0.42              |
| 1:G:197:LEU:HD21  | 1:G:199:ILE:CG1   | 2.49                     | 0.42              |
| 2:H:154:ARG:HH12  | 2:H:178:PRO:HD2   | 1.83                     | 0.42              |
| 2:H:251:ASP:O     | 2:H:253:ALA:N     | 2.51                     | 0.42              |
| 2:H:724:ARG:HG3   | 2:H:737:LEU:HD22  | 2.01                     | 0.42              |
| 2:H:84:ARG:HG3    | 2:H:84:ARG:HH11   | 1.84                     | 0.42              |
| 2:H:862:PRO:CG    | 2:H:925:TYR:OH    | 2.67                     | 0.42              |
| 3:I:1436:SER:O    | 3:I:1439:SER:HB2  | 2.19                     | 0.42              |
| 2:H:1097:LEU:CD2  | 3:I:1447:LEU:HB3  | 2.46                     | 0.42              |
| 3:I:1486:VAL:HG11 | 4:J:22:VAL:HG13   | 2.00                     | 0.42              |
| 3:I:153:LEU:HD12  | 3:I:153:LEU:O     | 2.19                     | 0.42              |
| 3:I:84:ILE:O      | 3:I:84:ILE:HG12   | 2.12                     | 0.42              |
| 3:I:873:LEU:HA    | 3:I:873:LEU:HD23  | 1.82                     | 0.42              |
| 3:I:89:ARG:O      | 3:I:521:PRO:HB3   | 2.18                     | 0.42              |
| 4:J:53:GLY:C      | 4:J:55:PHE:N      | 2.72                     | 0.42              |
| 1:K:218:LEU:HD23  | 1:L:222:LEU:CD2   | 2.48                     | 0.42              |
| 2:M:178:PRO:C     | 2:M:180:GLY:N     | 2.72                     | 0.42              |
| 2:M:364:GLU:O     | 2:M:367:LEU:CG    | 2.60                     | 0.42              |
| 2:M:512:ARG:HG2   | 2:M:523:ILE:CD1   | 2.49                     | 0.42              |
| 2:M:644:VAL:HG22  | 2:M:647:GLN:OE1   | 2.19                     | 0.42              |
| 2:M:679:PHE:C     | 3:N:943:THR:HG22  | 2.40                     | 0.42              |
| 2:M:571:LEU:HD21  | 2:M:700:TYR:HA    | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:837:ASP:O    | 2:M:848:VAL:HG13 | 2.19                     | 0.42              |
| 2:M:88:LEU:HD22  | 2:M:814:GLU:CG   | 2.39                     | 0.42              |
| 2:M:899:GLN:HG3  | 2:M:901:TYR:CZ   | 2.54                     | 0.42              |
| 3:N:101:HIS:O    | 3:N:105:VAL:HG23 | 2.18                     | 0.42              |
| 3:N:1346:ARG:HD2 | 3:N:1346:ARG:HA  | 1.84                     | 0.42              |
| 3:N:835:SER:O    | 3:N:836:VAL:C    | 2.58                     | 0.42              |
| 3:N:926:LYS:NZ   | 3:N:929:ARG:HH12 | 2.17                     | 0.42              |
| 2:H:879:ARG:NE   | 7:Y:42:ASP:CG    | 2.72                     | 0.42              |
| 7:Z:102:VAL:HG13 | 7:Z:103:GLN:N    | 2.34                     | 0.42              |
| 1:A:189:ARG:HG2  | 1:A:189:ARG:NH1  | 2.33                     | 0.42              |
| 1:B:111:ALA:HB3  | 1:B:124:ASN:O    | 2.19                     | 0.42              |
| 1:B:170:VAL:HG11 | 3:D:848:GLU:OE2  | 2.19                     | 0.42              |
| 1:B:25:LEU:HD23  | 1:B:25:LEU:O     | 2.19                     | 0.42              |
| 2:C:212:GLY:HA3  | 2:C:218:VAL:CG2  | 2.49                     | 0.42              |
| 2:C:146:VAL:HG11 | 2:C:281:LEU:HD11 | 2.01                     | 0.42              |
| 2:C:289:THR:C    | 2:C:291:ALA:N    | 2.72                     | 0.42              |
| 2:C:295:ASP:C    | 2:C:297:GLU:H    | 2.21                     | 0.42              |
| 2:C:25:SER:O     | 2:C:29:ALA:HB2   | 2.19                     | 0.42              |
| 2:C:512:ARG:HG2  | 2:C:523:ILE:CD1  | 2.50                     | 0.42              |
| 2:C:405:ARG:CZ   | 2:C:566:THR:HG21 | 2.49                     | 0.42              |
| 2:C:583:LEU:N    | 2:C:583:LEU:HD12 | 2.34                     | 0.42              |
| 2:C:644:VAL:HG22 | 2:C:647:GLN:OE1  | 2.19                     | 0.42              |
| 2:C:691:SER:C    | 2:C:693:GLU:N    | 2.72                     | 0.42              |
| 2:C:754:ILE:N    | 2:C:754:ILE:CD1  | 2.71                     | 0.42              |
| 3:D:1232:PRO:HB2 | 3:D:1356:TYR:HE2 | 1.82                     | 0.42              |
| 3:D:1258:ARG:HG3 | 3:D:1258:ARG:NH1 | 2.34                     | 0.42              |
| 3:D:1375:MET:C   | 3:D:1376:MET:HG3 | 2.40                     | 0.42              |
| 3:D:10:ILE:HD12  | 3:D:1434:TRP:CE2 | 2.55                     | 0.42              |
| 3:D:185:VAL:CG1  | 3:D:186:VAL:N    | 2.82                     | 0.42              |
| 3:D:511:TRP:O    | 3:D:513:ILE:N    | 2.52                     | 0.42              |
| 4:E:25:LYS:O     | 4:E:28:GLN:HB2   | 2.19                     | 0.42              |
| 1:F:107:LYS:HG2  | 1:F:108:GLU:N    | 2.34                     | 0.42              |
| 1:G:122:ILE:H    | 1:G:122:ILE:HD12 | 1.82                     | 0.42              |
| 1:G:128:HIS:HE1  | 1:G:131:THR:HG23 | 1.83                     | 0.42              |
| 1:G:133:GLU:CG   | 1:G:134:GLU:H    | 2.25                     | 0.42              |
| 2:H:239:PHE:HZ   | 2:H:252:LYS:O    | 2.01                     | 0.42              |
| 2:H:272:ALA:O    | 2:H:464:LEU:CD2  | 2.67                     | 0.42              |
| 2:H:358:ARG:HH22 | 2:H:374:ASN:CB   | 2.32                     | 0.42              |
| 2:H:39:ARG:HB2   | 2:H:45:GLN:HE22  | 1.78                     | 0.42              |
| 2:H:512:ARG:HG2  | 2:H:523:ILE:CD1  | 2.49                     | 0.42              |
| 2:H:96:ALA:O     | 2:H:98:LEU:CD1   | 2.68                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:783:ARG:HA   | 3:I:1028:ALA:HA   | 2.00                     | 0.42              |
| 3:I:1105:ILE:N   | 3:I:1105:ILE:CD1  | 2.81                     | 0.42              |
| 3:I:1256:LEU:HG  | 3:I:1260:ILE:CD1  | 2.41                     | 0.42              |
| 3:I:1481:VAL:O   | 3:I:1483:PHE:N    | 2.51                     | 0.42              |
| 3:I:1487:VAL:CG1 | 3:I:1488:ASP:N    | 2.82                     | 0.42              |
| 3:I:705:ALA:HB3  | 3:I:706:PRO:CD    | 2.49                     | 0.42              |
| 3:I:829:VAL:H    | 3:I:835:SER:HB2   | 1.84                     | 0.42              |
| 2:H:1086:ARG:NH2 | 3:I:88:TYR:CZ     | 2.87                     | 0.42              |
| 3:I:926:LYS:NZ   | 3:I:929:ARG:HH12  | 2.17                     | 0.42              |
| 4:J:43:GLU:O     | 4:J:44:GLU:CB     | 2.67                     | 0.42              |
| 4:J:86:GLN:O     | 4:J:90:GLU:HG3    | 2.18                     | 0.42              |
| 1:K:107:LYS:HG2  | 1:K:108:GLU:N     | 2.34                     | 0.42              |
| 1:K:101:LEU:HD12 | 1:K:113:ASP:O     | 2.18                     | 0.42              |
| 1:K:109:VAL:HG21 | 1:K:138:LEU:HD23  | 2.01                     | 0.42              |
| 1:K:21:GLY:O     | 1:K:23:PHE:CE2    | 2.72                     | 0.42              |
| 1:L:197:LEU:HD21 | 1:L:199:ILE:CG1   | 2.49                     | 0.42              |
| 2:M:162:ILE:O    | 2:M:164:PRO:HD3   | 2.18                     | 0.42              |
| 2:M:487:THR:HB   | 2:M:490:GLU:HG3   | 2.00                     | 0.42              |
| 2:M:640:ARG:HG2  | 2:M:640:ARG:HH11  | 1.83                     | 0.42              |
| 2:M:555:ALA:HA   | 3:N:1070:TYR:OH   | 2.20                     | 0.42              |
| 3:N:384:VAL:HG12 | 3:N:385:VAL:N     | 2.34                     | 0.42              |
| 3:N:469:ASP:O    | 3:N:470:LEU:C     | 2.57                     | 0.42              |
| 3:N:695:ILE:O    | 3:N:696:HIS:C     | 2.58                     | 0.42              |
| 3:N:829:VAL:O    | 3:N:831:GLY:N     | 2.52                     | 0.42              |
| 3:N:850:LEU:HA   | 3:N:853:VAL:CG2   | 2.49                     | 0.42              |
| 7:Z:102:VAL:HG11 | 7:Z:125:MET:HE2   | 1.98                     | 0.42              |
| 1:A:117:VAL:HB   | 1:A:120:VAL:CG1   | 2.49                     | 0.42              |
| 1:A:109:VAL:HG21 | 1:A:138:LEU:HD23  | 2.01                     | 0.42              |
| 1:A:206:THR:HG23 | 1:A:208:LEU:N     | 2.34                     | 0.42              |
| 2:C:1032:PHE:HZ  | 2:C:1040:LEU:HD13 | 1.84                     | 0.42              |
| 2:C:1074:GLU:CG  | 2:C:1075:ASP:H    | 2.05                     | 0.42              |
| 2:C:12:VAL:HB    | 2:C:472:ARG:HH11  | 1.84                     | 0.42              |
| 2:C:431:HIS:CD2  | 2:C:433:THR:H     | 2.37                     | 0.42              |
| 2:C:836:GLY:O    | 2:C:848:VAL:HG13  | 2.19                     | 0.42              |
| 3:D:1094:LEU:HG  | 3:D:1098:LEU:HD11 | 2.01                     | 0.42              |
| 3:D:1312:LEU:HA  | 3:D:1312:LEU:HD23 | 1.87                     | 0.42              |
| 3:D:1437:ALA:HB3 | 3:D:1446:VAL:HG13 | 2.01                     | 0.42              |
| 3:D:546:ARG:NH1  | 3:D:546:ARG:CG    | 2.82                     | 0.42              |
| 3:D:621:LYS:HD3  | 3:D:621:LYS:HA    | 1.79                     | 0.42              |
| 3:D:703:ASN:HD22 | 3:D:704:ARG:H     | 1.67                     | 0.42              |
| 3:D:87:ARG:O     | 3:D:524:LEU:CD1   | 2.68                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:62:THR:O      | 4:E:66:LYS:HB2    | 2.19                     | 0.42              |
| 1:G:97:VAL:HG11   | 1:G:120:VAL:HG21  | 2.01                     | 0.42              |
| 2:H:1082:PRO:O    | 2:H:1085:PHE:N    | 2.48                     | 0.42              |
| 2:H:1109:VAL:HG11 | 3:I:5:VAL:HG13    | 2.02                     | 0.42              |
| 2:H:273:GLY:HA2   | 2:H:276:LYS:CD    | 2.49                     | 0.42              |
| 2:H:42:VAL:O      | 2:H:43:GLY:O      | 2.37                     | 0.42              |
| 2:H:572:ILE:CD1   | 2:H:573:ARG:H     | 2.17                     | 0.42              |
| 2:H:693:GLU:HG2   | 2:H:697:ARG:HH21  | 1.84                     | 0.42              |
| 3:I:1258:ARG:HE   | 3:I:1262:LEU:HD22 | 1.84                     | 0.42              |
| 3:I:1401:GLU:OE2  | 3:I:1402:ALA:N    | 2.52                     | 0.42              |
| 3:I:554:LEU:HD22  | 3:I:574:LEU:HD22  | 2.01                     | 0.42              |
| 3:I:787:LEU:HD21  | 3:I:947:ILE:HD13  | 2.00                     | 0.42              |
| 1:K:144:VAL:HG12  | 1:K:145:ASP:N     | 2.35                     | 0.42              |
| 2:M:121:MET:HE3   | 2:M:125:GLY:O     | 2.19                     | 0.42              |
| 2:M:242:LEU:HD11  | 2:M:254:VAL:CG1   | 2.35                     | 0.42              |
| 2:M:367:LEU:H     | 2:M:367:LEU:HG    | 1.68                     | 0.42              |
| 2:M:39:ARG:HD2    | 2:M:71:TYR:HE2    | 1.85                     | 0.42              |
| 2:M:512:ARG:CG    | 2:M:523:ILE:CD1   | 2.96                     | 0.42              |
| 2:M:654:LEU:HD13  | 2:M:663:ASN:O     | 2.19                     | 0.42              |
| 1:K:83:LYS:NZ     | 2:M:698:ASP:OD2   | 2.51                     | 0.42              |
| 1:K:198:ARG:NH2   | 2:M:934:PHE:CD1   | 2.87                     | 0.42              |
| 3:N:1084:THR:CB   | 3:N:1087:ARG:NH1  | 2.82                     | 0.42              |
| 3:N:1129:THR:HG23 | 3:N:1130:ARG:N    | 2.34                     | 0.42              |
| 3:N:1135:ARG:O    | 3:N:1140:ILE:HD11 | 2.19                     | 0.42              |
| 3:N:1310:ARG:HD3  | 3:N:1310:ARG:HA   | 1.88                     | 0.42              |
| 3:N:133:ILE:CG2   | 3:N:134:VAL:N     | 2.82                     | 0.42              |
| 3:N:1353:GLN:HB3  | 3:N:1357:ARG:NE   | 2.34                     | 0.42              |
| 3:N:1372:VAL:HG13 | 3:N:1373:ARG:N    | 2.34                     | 0.42              |
| 3:N:1442:ASN:HD22 | 3:N:1445:HIS:HB2  | 1.84                     | 0.42              |
| 3:N:1491:THR:HA   | 3:N:1494:ALA:CB   | 2.50                     | 0.42              |
| 3:N:178:LEU:CD1   | 3:N:191:LEU:HA    | 2.48                     | 0.42              |
| 3:N:379:ALA:C     | 3:N:380:GLU:HG3   | 2.39                     | 0.42              |
| 3:N:137:PRO:HG3   | 3:N:453:ASP:HB2   | 1.99                     | 0.42              |
| 3:N:649:ALA:O     | 3:N:650:LEU:C     | 2.57                     | 0.42              |
| 3:N:860:LEU:HD22  | 3:N:878:GLY:CA    | 2.49                     | 0.42              |
| 4:O:68:LEU:HA     | 4:O:73:LEU:HD13   | 2.01                     | 0.42              |
| 1:B:106:PRO:CG    | 1:B:134:GLU:OE2   | 2.68                     | 0.42              |
| 2:C:205:GLU:O     | 2:C:209:ARG:HD2   | 2.19                     | 0.42              |
| 2:C:195:LEU:CG    | 2:C:238:LEU:HG    | 2.44                     | 0.42              |
| 2:C:395:LYS:HE3   | 2:C:407:LYS:HE3   | 2.01                     | 0.42              |
| 2:C:431:HIS:CG    | 2:C:432:ARG:N     | 2.87                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:585:GLU:O     | 2:C:588:VAL:CG2   | 2.67                     | 0.42              |
| 3:D:963:TYR:CE2   | 3:D:1002:LYS:HD3  | 2.55                     | 0.42              |
| 3:D:1292:VAL:HG22 | 3:D:1311:LEU:HD13 | 2.00                     | 0.42              |
| 3:D:1305:LEU:HD12 | 3:D:1309:ALA:CB   | 2.49                     | 0.42              |
| 3:D:127:LEU:HD22  | 3:D:134:VAL:CG1   | 2.48                     | 0.42              |
| 3:D:471:GLU:H     | 3:D:471:GLU:HG2   | 1.54                     | 0.42              |
| 3:D:97:THR:CB     | 3:D:571:LYS:HE2   | 2.49                     | 0.42              |
| 1:B:185:ARG:HD3   | 3:D:692:GLU:CG    | 2.49                     | 0.42              |
| 3:D:820:GLU:HG3   | 3:D:836:VAL:CG2   | 2.49                     | 0.42              |
| 3:D:925:GLU:OE1   | 4:E:6:ILE:HG22    | 2.20                     | 0.42              |
| 4:E:35:PHE:C      | 4:E:36:LYS:NZ     | 2.72                     | 0.42              |
| 1:F:109:VAL:HG21  | 1:F:138:LEU:HD23  | 2.01                     | 0.42              |
| 1:G:25:LEU:O      | 1:G:25:LEU:HD23   | 2.19                     | 0.42              |
| 2:H:124:ASP:HA    | 2:H:592:LEU:HG    | 2.01                     | 0.42              |
| 2:H:260:LEU:HD23  | 2:H:261:ILE:HA    | 2.01                     | 0.42              |
| 2:H:294:GLU:HG3   | 2:H:295:ASP:OD2   | 2.19                     | 0.42              |
| 2:H:345:ARG:HA    | 2:H:348:LEU:HB2   | 2.01                     | 0.42              |
| 2:H:360:LEU:H     | 2:H:360:LEU:CD2   | 2.30                     | 0.42              |
| 2:H:48:PHE:CE2    | 2:H:71:TYR:HB3    | 2.54                     | 0.42              |
| 2:H:573:ARG:CB    | 2:H:670:GLN:NE2   | 2.83                     | 0.42              |
| 3:I:1258:ARG:HH21 | 3:I:1351:GLU:HG2  | 1.83                     | 0.42              |
| 3:I:1278:ASP:HA   | 3:I:1319:VAL:O    | 2.20                     | 0.42              |
| 3:I:1254:GLN:HG3  | 3:I:1355:VAL:HG13 | 2.01                     | 0.42              |
| 3:I:1363:LEU:H    | 3:I:1363:LEU:HD23 | 1.84                     | 0.42              |
| 3:I:1377:LYS:CG   | 3:I:1377:LYS:O    | 2.67                     | 0.42              |
| 3:I:1434:TRP:HZ3  | 3:I:1457:ASP:N    | 2.17                     | 0.42              |
| 3:I:546:ARG:NH1   | 3:I:550:ARG:NH2   | 2.65                     | 0.42              |
| 3:I:643:GLY:N     | 3:I:727:GLN:O     | 2.50                     | 0.42              |
| 4:J:60:ALA:O      | 4:J:63:TRP:HB2    | 2.20                     | 0.42              |
| 2:M:184:MET:O     | 2:M:191:PHE:CD1   | 2.72                     | 0.42              |
| 2:M:588:VAL:HG11  | 2:M:661:SER:HB2   | 2.01                     | 0.42              |
| 2:M:65:VAL:O      | 2:M:101:ILE:N     | 2.53                     | 0.42              |
| 2:M:836:GLY:O     | 2:M:848:VAL:HG13  | 2.19                     | 0.42              |
| 3:N:963:TYR:CE2   | 3:N:1002:LYS:HD3  | 2.55                     | 0.42              |
| 3:N:1384:PRO:HB3  | 3:N:1388:ARG:HH12 | 1.85                     | 0.42              |
| 3:N:199:LEU:CD2   | 3:N:200:ASP:H     | 2.33                     | 0.42              |
| 3:N:199:LEU:HG    | 3:N:200:ASP:H     | 1.84                     | 0.42              |
| 3:N:470:LEU:CB    | 3:N:503:LEU:HD21  | 2.44                     | 0.42              |
| 3:N:93:ILE:HG22   | 3:N:551:ASN:HD22  | 1.84                     | 0.42              |
| 3:N:572:ARG:O     | 3:N:573:MET:C     | 2.55                     | 0.42              |
| 3:N:667:ALA:HA    | 3:N:668:PRO:HD3   | 1.83                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:801:GLY:O     | 3:N:802:ALA:HB2   | 2.19                     | 0.42              |
| 3:N:820:GLU:HG3   | 3:N:836:VAL:CG2   | 2.49                     | 0.42              |
| 2:M:1090:LYS:CD   | 3:N:90:MET:SD     | 3.08                     | 0.42              |
| 4:O:47:LYS:HA     | 4:O:54:LEU:CB     | 2.45                     | 0.42              |
| 4:O:45:ARG:NH2    | 4:O:55:PHE:O      | 2.52                     | 0.42              |
| 4:O:93:TYR:HA     | 4:O:94:PRO:HD3    | 1.83                     | 0.42              |
| 1:B:124:ASN:N     | 1:B:125:PRO:CD    | 2.81                     | 0.42              |
| 2:C:91:GLN:HB2    | 2:C:117:HIS:HB3   | 2.01                     | 0.42              |
| 2:C:254:VAL:HA    | 2:C:257:VAL:HG23  | 2.01                     | 0.42              |
| 2:C:396:ASP:OD1   | 2:C:402:SER:OG    | 2.38                     | 0.42              |
| 2:C:512:ARG:CG    | 2:C:523:ILE:CD1   | 2.96                     | 0.42              |
| 2:C:557:ARG:HH21  | 2:C:879:ARG:HE    | 1.67                     | 0.42              |
| 2:C:605:LYS:CB    | 2:C:610:ARG:HH12  | 2.33                     | 0.42              |
| 2:C:64:LEU:HD22   | 2:C:359:MET:CB    | 2.50                     | 0.42              |
| 3:D:127:LEU:C     | 3:D:127:LEU:CD1   | 2.88                     | 0.42              |
| 3:D:139:GLY:HA3   | 3:D:147:VAL:HG21  | 2.00                     | 0.42              |
| 3:D:99:ALA:CB     | 3:D:575:GLN:OE1   | 2.61                     | 0.42              |
| 3:D:705:ALA:HB3   | 3:D:706:PRO:CD    | 2.49                     | 0.42              |
| 3:D:704:ARG:CG    | 3:D:736:PHE:HB3   | 2.50                     | 0.42              |
| 3:D:887:ALA:HB1   | 3:D:893:GLU:HG3   | 2.02                     | 0.42              |
| 1:F:124:ASN:ND2   | 1:F:127:LEU:CD2   | 2.82                     | 0.42              |
| 1:G:198:ARG:O     | 1:G:199:ILE:HD13  | 2.19                     | 0.42              |
| 1:G:7:LYS:HB3     | 1:G:7:LYS:HE3     | 1.70                     | 0.42              |
| 2:H:1038:TRP:O    | 2:H:1039:ALA:C    | 2.57                     | 0.42              |
| 2:H:12:VAL:HG22   | 2:H:13:ILE:HG23   | 2.01                     | 0.42              |
| 2:H:140:ILE:CG2   | 2:H:410:ILE:HD13  | 2.49                     | 0.42              |
| 2:H:338:GLU:CA    | 2:H:341:THR:HG22  | 2.50                     | 0.42              |
| 2:H:836:GLY:O     | 2:H:848:VAL:HG13  | 2.19                     | 0.42              |
| 3:I:1123:PHE:HD1  | 3:I:1133:ARG:O    | 2.03                     | 0.42              |
| 3:I:1305:LEU:HD23 | 3:I:1305:LEU:N    | 2.35                     | 0.42              |
| 3:I:1327:ARG:HG3  | 3:I:1328:GLY:N    | 2.35                     | 0.42              |
| 3:I:1366:LYS:O    | 3:I:1370:ILE:HG13 | 2.19                     | 0.42              |
| 3:I:1422:MET:HE1  | 3:I:1427:SER:HA   | 2.01                     | 0.42              |
| 2:H:1070:ILE:CG2  | 3:I:655:PRO:HB2   | 2.49                     | 0.42              |
| 4:J:24:ALA:O      | 4:J:25:LYS:C      | 2.58                     | 0.42              |
| 1:K:223:THR:O     | 1:K:225:PHE:N     | 2.52                     | 0.42              |
| 1:K:26:GLU:OE2    | 1:K:194:LYS:HE3   | 2.19                     | 0.42              |
| 2:M:1083:GLU:O    | 2:M:1087:VAL:HB   | 2.19                     | 0.42              |
| 2:M:154:ARG:CZ    | 2:M:178:PRO:HG3   | 2.49                     | 0.42              |
| 2:M:449:ILE:HD13  | 3:N:1082:ALA:N    | 2.34                     | 0.42              |
| 2:M:487:THR:O     | 2:M:490:GLU:N     | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:585:GLU:CD    | 2:M:585:GLU:O     | 2.57                     | 0.42              |
| 2:M:835:VAL:HA    | 2:M:849:VAL:HG12  | 2.02                     | 0.42              |
| 3:N:1260:ILE:O    | 3:N:1264:GLU:HB2  | 2.19                     | 0.42              |
| 3:N:1327:ARG:HG3  | 3:N:1328:GLY:N    | 2.35                     | 0.42              |
| 3:N:1401:GLU:OE2  | 3:N:1402:ALA:N    | 2.52                     | 0.42              |
| 2:M:1046:ALA:HB3  | 3:N:1476:THR:CB   | 2.49                     | 0.42              |
| 3:N:390:PRO:HB2   | 3:N:393:ILE:HD11  | 2.01                     | 0.42              |
| 3:N:657:LEU:O     | 3:N:661:MET:HG2   | 2.19                     | 0.42              |
| 3:D:982:PHE:CD1   | 7:X:125:MET:CE    | 3.03                     | 0.42              |
| 7:X:26:LEU:HD13   | 7:X:58:ILE:HG21   | 2.00                     | 0.42              |
| 7:Z:132:HIS:CD2   | 7:Z:138:LEU:HD22  | 2.53                     | 0.42              |
| 7:Z:77:GLU:OE1    | 7:Z:77:GLU:O      | 2.37                     | 0.42              |
| 2:C:831:ARG:NH1   | 2:C:1002:GLU:HB2  | 2.34                     | 0.42              |
| 2:C:31:GLN:O      | 2:C:71:TYR:OH     | 2.28                     | 0.42              |
| 2:C:516:ARG:CZ    | 3:D:1068:LEU:HD22 | 2.50                     | 0.42              |
| 2:C:588:VAL:HG12  | 2:C:661:SER:HB3   | 2.01                     | 0.42              |
| 2:C:9:ILE:CD1     | 2:C:907:ASP:CB    | 2.97                     | 0.42              |
| 3:D:135:LEU:HD23  | 3:D:135:LEU:HA    | 1.91                     | 0.42              |
| 3:D:1431:THR:O    | 3:D:1431:THR:HG23 | 2.20                     | 0.42              |
| 3:D:158:TYR:HD1   | 3:D:162:ARG:HB2   | 1.82                     | 0.42              |
| 3:D:187:LYS:H     | 3:D:200:ASP:CG    | 2.23                     | 0.42              |
| 3:D:213:VAL:HG12  | 3:D:384:VAL:O     | 2.19                     | 0.42              |
| 3:D:401:TYR:CD1   | 3:D:401:TYR:N     | 2.88                     | 0.42              |
| 3:D:464:LEU:HD23  | 3:D:464:LEU:HA    | 1.73                     | 0.42              |
| 2:C:1019:GLN:HG3  | 3:D:621:LYS:HD2   | 2.02                     | 0.42              |
| 2:C:1070:ILE:HG23 | 3:D:656:PHE:CD1   | 2.54                     | 0.42              |
| 3:D:657:LEU:O     | 3:D:661:MET:HG2   | 2.19                     | 0.42              |
| 4:E:36:LYS:HZ3    | 4:E:36:LYS:N      | 2.17                     | 0.42              |
| 1:F:18:ARG:NH1    | 1:F:123:MET:CE    | 2.82                     | 0.42              |
| 1:G:122:ILE:CD1   | 1:G:122:ILE:N     | 2.77                     | 0.42              |
| 2:H:1083:GLU:O    | 2:H:1087:VAL:HB   | 2.19                     | 0.42              |
| 2:H:196:LEU:HD22  | 2:H:303:PHE:CD1   | 2.54                     | 0.42              |
| 2:H:260:LEU:CD2   | 2:H:260:LEU:C     | 2.81                     | 0.42              |
| 2:H:328:LEU:HD13  | 2:H:433:THR:CB    | 2.23                     | 0.42              |
| 2:H:437:ARG:CZ    | 2:H:488:ALA:HA    | 2.48                     | 0.42              |
| 2:H:640:ARG:HH11  | 2:H:640:ARG:HG2   | 1.83                     | 0.42              |
| 2:H:720:GLU:OE1   | 2:H:758:ARG:NH1   | 2.52                     | 0.42              |
| 2:H:76:PRO:O      | 2:H:77:PRO:C      | 2.57                     | 0.42              |
| 3:I:111:LYS:HD3   | 3:I:1448:THR:HG21 | 2.02                     | 0.42              |
| 3:I:1356:TYR:N    | 3:I:1356:TYR:CD1  | 2.88                     | 0.42              |
| 3:I:618:LEU:CD2   | 3:I:619:LEU:HD23  | 2.47                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:695:ILE:O     | 3:I:696:HIS:C     | 2.57                     | 0.42              |
| 3:I:887:ALA:HB1   | 3:I:893:GLU:HG3   | 2.01                     | 0.42              |
| 2:H:1086:ARG:NH2  | 3:I:88:TYR:OH     | 2.53                     | 0.42              |
| 1:L:143:ARG:NH1   | 1:L:158:ILE:HG23  | 2.34                     | 0.42              |
| 1:L:76:VAL:O      | 1:L:80:LEU:HD13   | 2.19                     | 0.42              |
| 2:M:418:LEU:CD1   | 2:M:418:LEU:N     | 2.79                     | 0.42              |
| 2:M:897:LEU:HD22  | 2:M:920:GLN:CG    | 2.49                     | 0.42              |
| 3:N:1305:LEU:O    | 3:N:1306:PRO:O    | 2.38                     | 0.42              |
| 3:N:1281:VAL:HG11 | 3:N:1313:VAL:HG13 | 2.02                     | 0.42              |
| 3:N:134:VAL:HG21  | 3:N:460:ALA:HB1   | 2.02                     | 0.42              |
| 3:N:434:ARG:HB2   | 3:N:449:SER:OG    | 2.19                     | 0.42              |
| 4:O:59:ASN:HD21   | 4:O:61:VAL:HG22   | 1.84                     | 0.42              |
| 7:X:11:GLY:HA3    | 7:X:109:GLU:OE1   | 2.19                     | 0.42              |
| 7:Y:7:LEU:N       | 7:Y:7:LEU:HD23    | 2.35                     | 0.42              |
| 1:A:107:LYS:HG2   | 1:A:108:GLU:N     | 2.34                     | 0.42              |
| 1:A:170:VAL:O     | 1:A:170:VAL:CG2   | 2.63                     | 0.42              |
| 2:C:243:ARG:N     | 2:C:244:PRO:CD    | 2.83                     | 0.42              |
| 2:C:30:LEU:O      | 2:C:30:LEU:CD1    | 2.60                     | 0.42              |
| 2:C:405:ARG:HG3   | 2:C:442:GLU:OE1   | 2.19                     | 0.42              |
| 2:C:328:LEU:HD21  | 2:C:434:HIS:HA    | 2.01                     | 0.42              |
| 2:C:693:GLU:CG    | 2:C:697:ARG:HH21  | 2.33                     | 0.42              |
| 3:D:1292:VAL:HG11 | 3:D:1325:LEU:HG   | 2.01                     | 0.42              |
| 3:D:348:GLN:H     | 3:D:351:MET:CE    | 2.32                     | 0.42              |
| 3:D:677:LEU:CD2   | 3:D:683:ILE:HD11  | 2.28                     | 0.42              |
| 3:D:827:ILE:H     | 3:D:827:ILE:CD1   | 2.28                     | 0.42              |
| 3:D:899:LEU:HD13  | 3:D:914:LEU:CD2   | 2.50                     | 0.42              |
| 3:D:922:LEU:CD2   | 3:D:922:LEU:N     | 2.75                     | 0.42              |
| 3:D:978:TYR:C     | 3:D:980:MET:H     | 2.23                     | 0.42              |
| 1:F:39:PRO:HG3    | 1:G:39:PRO:CG     | 2.50                     | 0.42              |
| 2:H:230:ARG:NH1   | 2:H:230:ARG:HG2   | 2.34                     | 0.42              |
| 2:H:313:LEU:CA    | 2:H:320:HIS:CE1   | 3.01                     | 0.42              |
| 2:H:415:PRO:HD2   | 2:H:418:LEU:HD13  | 2.00                     | 0.42              |
| 2:H:469:THR:CG2   | 2:H:470:PRO:N     | 2.83                     | 0.42              |
| 2:H:603:VAL:HG12  | 2:H:604:ALA:N     | 2.34                     | 0.42              |
| 3:I:963:TYR:CE2   | 3:I:1002:LYS:HD3  | 2.55                     | 0.42              |
| 3:I:1123:PHE:HE2  | 3:I:1184:GLN:HG3  | 1.81                     | 0.42              |
| 3:I:123:LEU:CG    | 3:I:152:LEU:HD21  | 2.49                     | 0.42              |
| 2:C:371:LYS:HD3   | 3:I:1317:ASP:OD2  | 2.20                     | 0.42              |
| 3:I:657:LEU:O     | 3:I:661:MET:HG2   | 2.19                     | 0.42              |
| 3:I:631:ILE:CD1   | 3:I:743:ASP:O     | 2.53                     | 0.42              |
| 3:I:820:GLU:HG2   | 3:I:825:ALA:O     | 2.18                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:117:VAL:HB    | 1:K:120:VAL:CG1   | 2.50                     | 0.42              |
| 1:K:78:ILE:CD1    | 1:K:130:ALA:HB2   | 2.49                     | 0.42              |
| 1:L:212:ASN:O     | 1:L:215:VAL:CG2   | 2.54                     | 0.42              |
| 2:M:1103:ASP:HB3  | 2:M:1105:LYS:NZ   | 2.35                     | 0.42              |
| 2:M:274:ARG:CG    | 2:M:285:LEU:HD13  | 2.50                     | 0.42              |
| 2:M:274:ARG:O     | 2:M:277:ALA:HB3   | 2.19                     | 0.42              |
| 2:M:428:ARG:HG2   | 2:M:451:LEU:HG    | 2.01                     | 0.42              |
| 3:N:949:ILE:HD11  | 3:N:1023:MET:CE   | 2.49                     | 0.42              |
| 3:N:1120:VAL:HG23 | 3:N:1188:VAL:HG11 | 2.00                     | 0.42              |
| 3:N:1258:ARG:O    | 3:N:1262:LEU:HB2  | 2.19                     | 0.42              |
| 3:N:1363:LEU:HD23 | 3:N:1363:LEU:H    | 1.84                     | 0.42              |
| 3:N:169:TYR:CG    | 3:N:197:SER:HA    | 2.54                     | 0.42              |
| 3:N:397:LYS:HZ3   | 3:N:448:GLU:CD    | 2.22                     | 0.42              |
| 3:N:481:MET:HE1   | 3:N:496:LEU:HD23  | 2.00                     | 0.42              |
| 4:O:31:LEU:HD12   | 4:O:31:LEU:H      | 1.84                     | 0.42              |
| 7:X:92:GLU:HA     | 7:X:98:GLU:O      | 2.19                     | 0.42              |
| 3:I:1128:VAL:HG22 | 7:Y:23:ARG:NH2    | 2.35                     | 0.42              |
| 1:A:32:PHE:HZ     | 1:B:47:SER:CB     | 2.33                     | 0.42              |
| 2:C:170:PRO:CD    | 2:C:263:ASP:CB    | 2.90                     | 0.42              |
| 2:C:260:LEU:HA    | 2:C:291:ALA:HB2   | 2.00                     | 0.42              |
| 2:C:31:GLN:HE21   | 2:C:71:TYR:HH     | 1.62                     | 0.42              |
| 2:C:328:LEU:HD13  | 2:C:328:LEU:H     | 1.85                     | 0.42              |
| 2:C:50:GLU:OE2    | 2:C:345:ARG:HB2   | 2.20                     | 0.42              |
| 2:C:518:LYS:HE2   | 2:C:518:LYS:HB2   | 1.73                     | 0.42              |
| 2:C:836:GLY:HA3   | 2:C:1001:VAL:CG2  | 2.49                     | 0.42              |
| 3:D:956:ILE:CD1   | 3:D:1062:ARG:HG3  | 2.49                     | 0.42              |
| 2:C:521:PRO:HG3   | 3:D:1068:LEU:CD2  | 2.49                     | 0.42              |
| 3:D:1477:GLY:O    | 3:D:1478:SER:C    | 2.57                     | 0.42              |
| 3:D:465:LEU:HD11  | 3:D:512:MET:HB2   | 2.01                     | 0.42              |
| 3:D:956:ILE:HD11  | 3:D:1062:ARG:HB3  | 2.01                     | 0.42              |
| 2:C:1099:VAL:HA   | 3:D:9:ARG:O       | 2.18                     | 0.42              |
| 3:D:207:PHE:CD1   | 2:H:283:ILE:HB    | 2.52                     | 0.42              |
| 2:H:368:THR:CB    | 2:H:369:PRO:CD    | 2.98                     | 0.42              |
| 2:H:39:ARG:HD3    | 2:H:45:GLN:OE1    | 2.20                     | 0.42              |
| 2:H:557:ARG:HH21  | 2:H:879:ARG:HE    | 1.67                     | 0.42              |
| 2:H:722:ILE:CD1   | 2:H:741:GLY:HA3   | 2.50                     | 0.42              |
| 2:H:80:GLN:O      | 2:H:83:CYS:N      | 2.52                     | 0.42              |
| 3:I:617:ASN:HB2   | 3:I:1467:ILE:HG23 | 2.02                     | 0.42              |
| 3:I:703:ASN:ND2   | 3:I:704:ARG:H     | 2.18                     | 0.42              |
| 3:I:802:ALA:O     | 3:I:803:GLY:C     | 2.58                     | 0.42              |
| 3:I:1481:VAL:HG12 | 4:J:21:VAL:HG21   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:57:ASP:N      | 4:J:58:PRO:HD3    | 2.34                     | 0.42              |
| 2:M:236:ILE:H     | 2:M:236:ILE:HD13  | 1.80                     | 0.42              |
| 2:M:83:CYS:HB3    | 2:M:128:ILE:HG21  | 2.02                     | 0.42              |
| 2:M:72:ARG:CZ     | 2:M:95:TYR:OH     | 2.67                     | 0.42              |
| 3:N:1132:LEU:N    | 3:N:1132:LEU:HD12 | 2.34                     | 0.42              |
| 3:N:1377:LYS:O    | 3:N:1377:LYS:CG   | 2.67                     | 0.42              |
| 3:N:1437:ALA:O    | 3:N:1439:SER:N    | 2.53                     | 0.42              |
| 3:N:189:GLN:NE2   | 3:N:190:GLU:N     | 2.57                     | 0.42              |
| 3:N:639:LEU:HD12  | 3:N:640:HIS:H     | 1.85                     | 0.42              |
| 3:N:705:ALA:HB3   | 3:N:706:PRO:CD    | 2.49                     | 0.42              |
| 4:O:33:HIS:HE1    | 4:O:90:GLU:OE2    | 2.02                     | 0.42              |
| 2:H:838:LYS:NZ    | 6:S:15:G:O2'      | 2.53                     | 0.42              |
| 1:B:159:LYS:H     | 1:B:159:LYS:HZ2   | 1.67                     | 0.42              |
| 1:B:24:VAL:HG13   | 1:B:196:THR:HG22  | 2.02                     | 0.42              |
| 2:C:1083:GLU:O    | 2:C:1087:VAL:HB   | 2.19                     | 0.42              |
| 2:C:184:MET:HE2   | 2:C:186:VAL:CG1   | 2.49                     | 0.42              |
| 2:C:20:GLU:HG3    | 2:C:21:ILE:N      | 2.35                     | 0.42              |
| 2:C:569:VAL:HA    | 2:C:570:PRO:HD3   | 1.93                     | 0.42              |
| 2:C:684:PHE:CG    | 2:C:685:GLU:N     | 2.86                     | 0.42              |
| 2:C:752:GLY:H     | 2:C:792:VAL:HB    | 1.85                     | 0.42              |
| 3:D:1149:LEU:CD2  | 3:D:1187:PRO:O    | 2.68                     | 0.42              |
| 3:D:1442:ASN:ND2  | 3:D:1445:HIS:H    | 2.17                     | 0.42              |
| 3:D:412:GLY:HA2   | 3:D:434:ARG:CD    | 2.49                     | 0.42              |
| 1:B:185:ARG:HD3   | 3:D:692:GLU:HG2   | 2.01                     | 0.42              |
| 3:D:785:ILE:CD1   | 3:D:785:ILE:N     | 2.51                     | 0.42              |
| 1:F:111:ALA:HA    | 1:F:129:ILE:HD11  | 2.02                     | 0.42              |
| 1:G:82:LEU:HD11   | 1:G:140:MET:HE1   | 2.01                     | 0.42              |
| 1:G:172:SER:HA    | 1:G:173:PRO:HD3   | 1.92                     | 0.42              |
| 2:H:1055:LEU:O    | 2:H:1063:ARG:HB2  | 2.20                     | 0.42              |
| 2:H:147:TYR:CE2   | 2:H:330:ASN:HB3   | 2.55                     | 0.42              |
| 2:H:209:ARG:O     | 2:H:213:ALA:HB2   | 2.19                     | 0.42              |
| 2:H:198:ARG:NH1   | 2:H:228:ALA:O     | 2.52                     | 0.42              |
| 3:I:1031:ASN:HB3  | 3:I:1034:GLN:HG3  | 2.02                     | 0.42              |
| 3:I:1311:LEU:HD23 | 3:I:1311:LEU:H    | 1.83                     | 0.42              |
| 3:I:1477:GLY:O    | 3:I:1478:SER:C    | 2.58                     | 0.42              |
| 3:I:29:PRO:HG3    | 3:I:549:ASN:HD21  | 1.85                     | 0.42              |
| 3:I:469:ASP:O     | 3:I:470:LEU:C     | 2.57                     | 0.42              |
| 3:I:511:TRP:N     | 3:I:511:TRP:CD2   | 2.88                     | 0.42              |
| 3:I:93:ILE:HG13   | 3:I:519:VAL:CG2   | 2.50                     | 0.42              |
| 3:I:625:TYR:HB3   | 3:I:749:VAL:CG2   | 2.47                     | 0.42              |
| 1:K:30:ARG:HH11   | 1:K:30:ARG:HG2    | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:92:PRO:C      | 1:K:94:LEU:N      | 2.73                     | 0.42              |
| 2:M:128:ILE:HG12  | 2:M:133:ASP:OD1   | 2.19                     | 0.42              |
| 2:M:205:GLU:HA    | 2:M:209:ARG:NH1   | 2.34                     | 0.42              |
| 2:M:353:ARG:HH11  | 2:M:353:ARG:HG3   | 1.85                     | 0.42              |
| 2:M:545:ASN:O     | 2:M:905:ILE:HD11  | 2.20                     | 0.42              |
| 2:M:568:ALA:HB2   | 2:M:995:MET:SD    | 2.60                     | 0.42              |
| 3:N:1146:GLY:CA   | 3:N:1207:TYR:HB2  | 2.50                     | 0.42              |
| 3:N:1437:ALA:HB1  | 3:N:1446:VAL:HG22 | 2.01                     | 0.42              |
| 3:N:143:ASN:HB2   | 3:N:161:LEU:HD23  | 2.01                     | 0.42              |
| 3:N:375:GLU:HG2   | 3:N:375:GLU:O     | 2.18                     | 0.42              |
| 3:N:180:LYS:HZ1   | 3:N:386:HIS:HB3   | 1.85                     | 0.42              |
| 3:N:520:LEU:HD11  | 3:N:524:LEU:CD2   | 2.49                     | 0.42              |
| 3:N:727:GLN:HE21  | 3:N:727:GLN:HB3   | 1.65                     | 0.42              |
| 3:N:804:LEU:HB3   | 3:N:830:ALA:O     | 2.20                     | 0.42              |
| 3:N:86:ARG:HG2    | 3:N:87:ARG:N      | 2.35                     | 0.42              |
| 3:N:885:ILE:HD12  | 3:N:937:TYR:CZ    | 2.55                     | 0.42              |
| 7:Z:84:GLY:HA2    | 7:Z:130:LEU:CD1   | 2.48                     | 0.42              |
| 2:C:54:ILE:HD12   | 2:C:355:VAL:HG13  | 2.01                     | 0.42              |
| 2:C:568:ALA:HB1   | 2:C:668:LEU:HB3   | 2.02                     | 0.42              |
| 2:C:691:SER:O     | 2:C:693:GLU:N     | 2.53                     | 0.42              |
| 2:C:835:VAL:HA    | 2:C:849:VAL:HG12  | 2.01                     | 0.42              |
| 2:C:918:LEU:HD23  | 2:C:968:LEU:HA    | 2.02                     | 0.42              |
| 2:C:862:PRO:CG    | 2:C:925:TYR:OH    | 2.67                     | 0.42              |
| 2:C:927:GLY:HA2   | 2:C:930:LYS:HD3   | 2.02                     | 0.42              |
| 3:D:1025:GLN:HA   | 3:D:1025:GLN:NE2  | 2.35                     | 0.42              |
| 2:C:1019:GLN:OE1  | 3:D:621:LYS:HB3   | 2.20                     | 0.42              |
| 3:D:645:PRO:CD    | 3:D:726:ILE:HG12  | 2.45                     | 0.42              |
| 3:D:814:ALA:HB1   | 3:D:818:ARG:NE    | 2.34                     | 0.42              |
| 1:F:144:VAL:HG12  | 1:F:145:ASP:N     | 2.35                     | 0.42              |
| 1:F:185:ARG:NH2   | 1:F:194:LYS:NZ    | 2.68                     | 0.42              |
| 2:H:159:ILE:C     | 2:H:159:ILE:HD12  | 2.39                     | 0.42              |
| 2:H:218:VAL:HA    | 2:H:221:LEU:CD2   | 2.50                     | 0.42              |
| 2:H:258:TYR:OH    | 2:H:290:LEU:HD21  | 2.20                     | 0.42              |
| 2:H:343:GLN:HE21  | 2:H:343:GLN:CA    | 2.33                     | 0.42              |
| 2:H:498:GLN:NE2   | 2:H:498:GLN:CA    | 2.73                     | 0.42              |
| 2:H:54:ILE:HG21   | 2:H:66:LEU:HB3    | 2.02                     | 0.42              |
| 2:H:644:VAL:HG22  | 2:H:647:GLN:OE1   | 2.19                     | 0.42              |
| 2:H:837:ASP:O     | 2:H:848:VAL:HG13  | 2.19                     | 0.42              |
| 3:I:1155:VAL:HG11 | 3:I:1177:ALA:CB   | 2.50                     | 0.42              |
| 3:I:845:ASN:O     | 3:I:848:GLU:HB2   | 2.20                     | 0.42              |
| 3:I:885:ILE:HD12  | 3:I:937:TYR:CZ    | 2.55                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:67:THR:CB    | 1:L:159:LYS:HG3   | 2.50                     | 0.42              |
| 2:M:1074:GLU:CG  | 2:M:1075:ASP:N    | 2.71                     | 0.42              |
| 2:M:175:GLU:HG2  | 2:M:177:GLU:CD    | 2.40                     | 0.42              |
| 2:M:304:LEU:O    | 2:M:308:ARG:N     | 2.47                     | 0.42              |
| 2:M:368:THR:HG22 | 2:M:369:PRO:CD    | 2.48                     | 0.42              |
| 2:M:401:LEU:CD1  | 2:M:587:VAL:HG11  | 2.43                     | 0.42              |
| 2:M:568:ALA:HB1  | 2:M:668:LEU:HB3   | 2.02                     | 0.42              |
| 2:M:974:LEU:HA   | 2:M:974:LEU:HD12  | 1.88                     | 0.42              |
| 3:N:1305:LEU:N   | 3:N:1305:LEU:HD23 | 2.35                     | 0.42              |
| 3:N:1314:LYS:HG3 | 3:N:1314:LYS:HZ3  | 1.03                     | 0.42              |
| 3:N:1356:TYR:N   | 3:N:1356:TYR:CD1  | 2.88                     | 0.42              |
| 3:N:116:LEU:CD1  | 3:N:461:ILE:HG23  | 2.50                     | 0.42              |
| 2:M:1094:ALA:CB  | 3:N:603:LEU:CD1   | 2.97                     | 0.42              |
| 3:N:704:ARG:CG   | 3:N:736:PHE:HB3   | 2.50                     | 0.42              |
| 3:N:922:LEU:N    | 3:N:922:LEU:CD2   | 2.75                     | 0.42              |
| 3:N:975:GLU:HA   | 3:N:975:GLU:OE1   | 2.20                     | 0.42              |
| 4:O:3:GLU:HA     | 4:O:3:GLU:OE1     | 2.19                     | 0.42              |
| 7:Y:21:ARG:O     | 7:Y:25:ARG:HG3    | 2.19                     | 0.42              |
| 1:A:223:THR:O    | 1:A:225:PHE:N     | 2.52                     | 0.41              |
| 1:B:151:VAL:HB   | 1:B:169:ALA:HB3   | 2.02                     | 0.41              |
| 2:C:831:ARG:NH1  | 2:C:1000:MET:HG3  | 2.35                     | 0.41              |
| 2:C:1103:ASP:HB3 | 2:C:1105:LYS:NZ   | 2.35                     | 0.41              |
| 2:C:277:ALA:O    | 2:C:278:GLU:C     | 2.58                     | 0.41              |
| 2:C:348:LEU:HD12 | 2:C:348:LEU:HA    | 1.83                     | 0.41              |
| 2:C:539:VAL:HG12 | 2:C:539:VAL:O     | 2.19                     | 0.41              |
| 2:C:670:GLN:HB2  | 2:C:700:TYR:CE1   | 2.55                     | 0.41              |
| 2:C:728:HIS:O    | 2:C:729:LEU:CD2   | 2.68                     | 0.41              |
| 2:C:754:ILE:CD1  | 2:C:791:ARG:HH12  | 2.33                     | 0.41              |
| 2:C:837:ASP:O    | 2:C:848:VAL:HG13  | 2.19                     | 0.41              |
| 3:D:1130:ARG:C   | 3:D:1131:SER:OG   | 2.58                     | 0.41              |
| 3:D:1287:GLU:CA  | 3:D:1287:GLU:OE1  | 2.66                     | 0.41              |
| 3:D:1363:LEU:H   | 3:D:1363:LEU:HD23 | 1.84                     | 0.41              |
| 3:D:1401:GLU:OE2 | 3:D:1402:ALA:N    | 2.52                     | 0.41              |
| 3:D:451:ASP:O    | 3:D:452:ILE:HG23  | 2.20                     | 0.41              |
| 3:D:806:PHE:CE1  | 3:D:813:LEU:CB    | 2.88                     | 0.41              |
| 3:D:885:ILE:HD12 | 3:D:937:TYR:CZ    | 2.55                     | 0.41              |
| 3:D:970:LYS:HA   | 3:D:973:GLN:HE21  | 1.86                     | 0.41              |
| 3:D:970:LYS:O    | 3:D:974:ILE:HG13  | 2.19                     | 0.41              |
| 3:D:975:GLU:OE1  | 3:D:975:GLU:HA    | 2.20                     | 0.41              |
| 3:D:1487:VAL:CG2 | 4:E:79:LEU:HD23   | 2.50                     | 0.41              |
| 1:G:165:ILE:HA   | 1:G:166:PRO:HD3   | 1.82                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:140:ILE:HG22 | 2:H:333:ILE:HG13  | 2.02                     | 0.41              |
| 2:H:141:HIS:CD2  | 2:H:334:ARG:HD2   | 2.55                     | 0.41              |
| 2:H:557:ARG:HG3  | 2:H:557:ARG:NH1   | 2.35                     | 0.41              |
| 2:H:701:THR:HA   | 2:H:831:ARG:O     | 2.20                     | 0.41              |
| 2:H:742:VAL:CG1  | 2:H:743:VAL:N     | 2.83                     | 0.41              |
| 2:H:918:LEU:HD23 | 2:H:968:LEU:HA    | 2.01                     | 0.41              |
| 2:H:972:VAL:HG23 | 2:H:973:VAL:N     | 2.33                     | 0.41              |
| 3:I:129:PHE:CD2  | 3:I:575:GLN:HG2   | 2.55                     | 0.41              |
| 3:I:12:LEU:HD23  | 3:I:12:LEU:HA     | 1.81                     | 0.41              |
| 3:I:1305:LEU:O   | 3:I:1306:PRO:O    | 2.38                     | 0.41              |
| 3:I:131:LYS:O    | 3:I:132:TYR:C     | 2.57                     | 0.41              |
| 3:I:844:ALA:O    | 3:I:867:ARG:HB3   | 2.20                     | 0.41              |
| 4:J:26:ARG:NH2   | 4:J:67:GLU:OE1    | 2.53                     | 0.41              |
| 4:J:26:ARG:HD3   | 4:J:73:LEU:HD21   | 2.01                     | 0.41              |
| 1:K:124:ASN:ND2  | 1:K:127:LEU:CD2   | 2.82                     | 0.41              |
| 1:K:39:PRO:HG3   | 1:L:39:PRO:HG3    | 2.00                     | 0.41              |
| 2:M:101:ILE:HG23 | 2:M:101:ILE:O     | 2.19                     | 0.41              |
| 2:M:1049:LEU:O   | 2:M:1053:LEU:HG   | 2.19                     | 0.41              |
| 2:M:258:TYR:CZ   | 2:M:290:LEU:HD21  | 2.55                     | 0.41              |
| 2:M:452:ILE:HD12 | 2:M:452:ILE:N     | 2.35                     | 0.41              |
| 2:M:539:VAL:O    | 2:M:539:VAL:HG12  | 2.19                     | 0.41              |
| 2:M:688:ILE:HG23 | 2:M:869:VAL:HG23  | 2.02                     | 0.41              |
| 2:M:708:TYR:N    | 2:M:708:TYR:CD1   | 2.88                     | 0.41              |
| 2:M:911:GLU:OE1  | 3:N:951:ILE:HG12  | 2.17                     | 0.41              |
| 2:M:972:VAL:HG23 | 2:M:973:VAL:N     | 2.34                     | 0.41              |
| 3:N:1106:VAL:CG1 | 3:N:1107:VAL:N    | 2.79                     | 0.41              |
| 3:N:1161:GLU:N   | 3:N:1161:GLU:OE2  | 2.53                     | 0.41              |
| 3:N:1403:LEU:O   | 3:N:1407:LEU:HD13 | 2.20                     | 0.41              |
| 3:N:615:ARG:HG3  | 3:N:619:LEU:CD1   | 2.50                     | 0.41              |
| 3:N:686:GLU:H    | 3:N:686:GLU:HG3   | 1.56                     | 0.41              |
| 3:N:703:ASN:HD22 | 3:N:704:ARG:H     | 1.67                     | 0.41              |
| 3:N:879:ARG:HH11 | 3:N:879:ARG:CG    | 2.33                     | 0.41              |
| 4:O:53:GLY:C     | 4:O:55:PHE:N      | 2.73                     | 0.41              |
| 2:H:879:ARG:CZ   | 7:Y:42:ASP:OD1    | 2.68                     | 0.41              |
| 1:A:26:GLU:HB3   | 1:A:194:LYS:HG3   | 2.01                     | 0.41              |
| 1:B:101:LEU:HD12 | 1:B:114:PHE:CA    | 2.50                     | 0.41              |
| 2:C:1090:LYS:CE  | 3:D:90:MET:SD     | 3.07                     | 0.41              |
| 2:C:1081:VAL:HB  | 2:C:1111:ILE:HG22 | 1.99                     | 0.41              |
| 2:C:151:ASP:OD2  | 2:C:152:PRO:HD2   | 2.19                     | 0.41              |
| 2:C:452:ILE:N    | 2:C:452:ILE:HD12  | 2.36                     | 0.41              |
| 2:C:557:ARG:NH1  | 2:C:557:ARG:HG3   | 2.34                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:706:GLU:CG    | 2:C:708:TYR:CE1   | 3.03                     | 0.41              |
| 2:C:75:GLU:OE1    | 2:C:75:GLU:HA     | 2.20                     | 0.41              |
| 3:D:1014:ASN:C    | 3:D:1016:PRO:HD3  | 2.40                     | 0.41              |
| 3:D:108:VAL:CB    | 3:D:109:PRO:CD    | 2.95                     | 0.41              |
| 3:D:1146:GLY:C    | 3:D:1207:TYR:HB2  | 2.41                     | 0.41              |
| 3:D:1256:LEU:HB3  | 3:D:1257:PRO:CD   | 2.46                     | 0.41              |
| 3:D:185:VAL:O     | 3:D:200:ASP:HA    | 2.20                     | 0.41              |
| 3:D:660:LYS:HA    | 3:D:660:LYS:CE    | 2.50                     | 0.41              |
| 3:D:926:LYS:NZ    | 3:D:929:ARG:HH12  | 2.18                     | 0.41              |
| 2:C:987:ILE:CD1   | 3:D:948:THR:HG23  | 2.49                     | 0.41              |
| 1:F:223:THR:O     | 1:F:225:PHE:N     | 2.52                     | 0.41              |
| 1:G:228:PRO:O     | 1:G:229:GLN:HG3   | 2.20                     | 0.41              |
| 2:H:1046:ALA:HA   | 3:I:1472:ILE:CD1  | 2.51                     | 0.41              |
| 2:H:1084:SER:HB3  | 3:I:617:ASN:CG    | 2.33                     | 0.41              |
| 2:H:1103:ASP:HB3  | 2:H:1105:LYS:NZ   | 2.35                     | 0.41              |
| 2:H:340:MET:C     | 2:H:340:MET:SD    | 2.98                     | 0.41              |
| 2:H:395:LYS:HG2   | 2:H:397:GLU:CG    | 2.51                     | 0.41              |
| 2:H:470:PRO:HB2   | 2:H:534:VAL:HG21  | 2.02                     | 0.41              |
| 2:H:676:ILE:HG23  | 3:I:948:THR:HB    | 2.02                     | 0.41              |
| 2:H:754:ILE:CD1   | 2:H:791:ARG:HH12  | 2.33                     | 0.41              |
| 2:H:851:LYS:HG2   | 2:H:853:LEU:CD1   | 2.50                     | 0.41              |
| 3:I:955:VAL:O     | 3:I:1039:CYS:HB3  | 2.20                     | 0.41              |
| 3:I:1258:ARG:HE   | 3:I:1262:LEU:CD2  | 2.33                     | 0.41              |
| 3:I:1372:VAL:HG13 | 3:I:1373:ARG:N    | 2.34                     | 0.41              |
| 3:I:1481:VAL:C    | 3:I:1483:PHE:N    | 2.73                     | 0.41              |
| 3:I:704:ARG:CG    | 3:I:736:PHE:HB3   | 2.50                     | 0.41              |
| 2:M:1050:GLN:HA   | 2:M:1050:GLN:HE21 | 1.85                     | 0.41              |
| 2:M:1074:GLU:CG   | 2:M:1075:ASP:H    | 2.05                     | 0.41              |
| 2:M:1095:LEU:HB2  | 3:N:101:HIS:HE1   | 1.81                     | 0.41              |
| 2:M:231:PRO:HB2   | 2:M:232:GLU:H     | 1.52                     | 0.41              |
| 2:M:320:HIS:CD2   | 2:M:320:HIS:H     | 2.38                     | 0.41              |
| 2:M:470:PRO:HB2   | 2:M:534:VAL:HG21  | 2.01                     | 0.41              |
| 2:M:573:ARG:CB    | 2:M:670:GLN:NE2   | 2.83                     | 0.41              |
| 2:M:691:SER:O     | 2:M:693:GLU:N     | 2.53                     | 0.41              |
| 2:M:83:CYS:HB3    | 2:M:88:LEU:O      | 2.19                     | 0.41              |
| 3:N:1278:ASP:HB3  | 3:N:1321:ALA:N    | 2.35                     | 0.41              |
| 3:N:131:LYS:HG2   | 3:N:456:MET:SD    | 2.61                     | 0.41              |
| 3:N:514:LEU:HD12  | 3:N:578:VAL:CG1   | 2.50                     | 0.41              |
| 3:N:87:ARG:CB     | 3:N:524:LEU:HD12  | 2.50                     | 0.41              |
| 3:N:925:GLU:O     | 3:N:928:ALA:HB3   | 2.20                     | 0.41              |
| 4:O:22:VAL:H      | 4:O:22:VAL:HG23   | 1.60                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:X:124:PRO:O    | 7:X:140:LEU:HD11  | 2.19                     | 0.41              |
| 1:A:39:PRO:CG    | 1:B:39:PRO:HG2    | 2.43                     | 0.41              |
| 1:B:56:VAL:O     | 1:B:164:ALA:HB1   | 2.19                     | 0.41              |
| 2:C:184:MET:SD   | 2:C:191:PHE:CE1   | 3.13                     | 0.41              |
| 2:C:22:GLN:HB3   | 2:C:121:MET:HE2   | 2.01                     | 0.41              |
| 2:C:252:LYS:O    | 2:C:255:ALA:HB3   | 2.20                     | 0.41              |
| 2:C:265:ARG:HB3  | 2:C:267:TYR:CD1   | 2.55                     | 0.41              |
| 2:C:276:LYS:HA   | 2:C:280:LYS:CD    | 2.39                     | 0.41              |
| 2:C:276:LYS:CA   | 2:C:280:LYS:HD2   | 2.40                     | 0.41              |
| 2:C:42:VAL:HB    | 2:C:43:GLY:H      | 1.60                     | 0.41              |
| 2:C:470:PRO:HB2  | 2:C:534:VAL:HG21  | 2.02                     | 0.41              |
| 2:C:612:VAL:HG22 | 2:C:622:GLU:HG3   | 2.02                     | 0.41              |
| 2:C:80:GLN:C     | 2:C:84:ARG:NH1    | 2.73                     | 0.41              |
| 3:D:919:PHE:HZ   | 3:D:1211:MET:HA   | 1.85                     | 0.41              |
| 3:D:1330:ILE:CD1 | 3:D:1347:TYR:OH   | 2.63                     | 0.41              |
| 3:D:1434:TRP:O   | 3:D:1435:LEU:C    | 2.59                     | 0.41              |
| 3:D:351:MET:HG3  | 3:D:370:ALA:HB2   | 2.02                     | 0.41              |
| 3:D:11:ALA:HB1   | 3:D:507:ASN:HD22  | 1.84                     | 0.41              |
| 3:D:632:VAL:CG2  | 3:D:725:SER:CB    | 2.99                     | 0.41              |
| 3:D:879:ARG:CG   | 3:D:879:ARG:HH11  | 2.33                     | 0.41              |
| 3:D:925:GLU:O    | 3:D:928:ALA:HB3   | 2.21                     | 0.41              |
| 2:H:1076:VAL:HA  | 2:H:1077:PRO:HD3  | 1.98                     | 0.41              |
| 2:H:229:MET:CB   | 2:H:230:ARG:NH1   | 2.83                     | 0.41              |
| 2:H:266:ARG:HD3  | 2:H:288:ARG:NE    | 2.34                     | 0.41              |
| 2:H:292:ARG:CB   | 2:H:299:LYS:HE2   | 2.50                     | 0.41              |
| 2:H:500:ASN:H    | 2:H:500:ASN:HD22  | 1.60                     | 0.41              |
| 2:H:539:VAL:O    | 2:H:539:VAL:HG12  | 2.19                     | 0.41              |
| 3:I:1084:THR:HA  | 3:I:1087:ARG:HD3  | 2.02                     | 0.41              |
| 3:I:1288:GLU:HA  | 3:I:1307:LYS:HD3  | 2.03                     | 0.41              |
| 3:I:660:LYS:HA   | 3:I:660:LYS:CE    | 2.50                     | 0.41              |
| 3:I:650:LEU:CD1  | 3:I:688:TRP:HZ3   | 2.26                     | 0.41              |
| 3:I:820:GLU:HG3  | 3:I:836:VAL:CG2   | 2.49                     | 0.41              |
| 3:I:899:LEU:HD13 | 3:I:914:LEU:CD2   | 2.50                     | 0.41              |
| 1:L:48:ILE:HG22  | 1:L:173:PRO:HD2   | 2.01                     | 0.41              |
| 2:M:702:SER:OG   | 2:M:1000:MET:HE1  | 2.20                     | 0.41              |
| 2:M:174:LEU:HD21 | 2:M:184:MET:HG3   | 2.01                     | 0.41              |
| 2:M:267:TYR:O    | 2:M:268:ASP:C     | 2.59                     | 0.41              |
| 2:M:927:GLY:HA2  | 2:M:930:LYS:HD3   | 2.02                     | 0.41              |
| 3:N:992:ILE:CD1  | 3:N:1054:GLU:OE2  | 2.66                     | 0.41              |
| 2:M:449:ILE:CG2  | 3:N:1082:ALA:HA   | 2.46                     | 0.41              |
| 3:N:1109:GLU:HG3 | 3:N:1217:ILE:HD12 | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:374:GLU:O     | 3:N:375:GLU:HB3   | 2.19                     | 0.41              |
| 3:N:415:VAL:HG12  | 3:N:416:ALA:N     | 2.36                     | 0.41              |
| 3:N:550:ARG:NE    | 3:N:573:MET:HE2   | 2.36                     | 0.41              |
| 3:N:672:ALA:O     | 3:N:676:MET:N     | 2.49                     | 0.41              |
| 3:N:703:ASN:ND2   | 3:N:704:ARG:H     | 2.18                     | 0.41              |
| 4:O:43:GLU:O      | 4:O:44:GLU:CB     | 2.68                     | 0.41              |
| 4:O:60:ALA:O      | 4:O:63:TRP:HB2    | 2.20                     | 0.41              |
| 7:X:55:LYS:NZ     | 7:X:59:GLU:OE2    | 2.53                     | 0.41              |
| 1:A:111:ALA:HA    | 1:A:129:ILE:HD11  | 2.02                     | 0.41              |
| 1:A:144:VAL:HG12  | 1:A:145:ASP:N     | 2.35                     | 0.41              |
| 1:B:122:ILE:CD1   | 1:B:122:ILE:H     | 2.11                     | 0.41              |
| 2:C:428:ARG:HG3   | 2:C:451:LEU:HD21  | 2.03                     | 0.41              |
| 2:C:458:TYR:CB    | 2:C:470:PRO:HG3   | 2.50                     | 0.41              |
| 2:C:54:ILE:CD1    | 2:C:355:VAL:HG13  | 2.51                     | 0.41              |
| 2:C:676:ILE:HD12  | 2:C:871:LEU:HB2   | 2.03                     | 0.41              |
| 2:C:693:GLU:HG2   | 2:C:697:ARG:HH21  | 1.85                     | 0.41              |
| 2:C:758:ARG:CB    | 2:C:788:THR:O     | 2.62                     | 0.41              |
| 2:C:937:ASP:HB3   | 2:C:940:GLU:HG3   | 2.02                     | 0.41              |
| 2:C:94:LEU:O      | 2:C:115:LEU:HG    | 2.19                     | 0.41              |
| 3:D:963:TYR:HD2   | 3:D:1002:LYS:HD3  | 1.81                     | 0.41              |
| 3:D:952:ASP:HA    | 3:D:1062:ARG:HH11 | 1.85                     | 0.41              |
| 3:D:1274:ILE:C    | 3:D:1274:ILE:HD12 | 2.41                     | 0.41              |
| 3:D:1305:LEU:HD12 | 3:D:1309:ALA:HB1  | 2.03                     | 0.41              |
| 3:D:403:PHE:HD2   | 3:D:444:VAL:HG23  | 1.80                     | 0.41              |
| 3:D:479:GLU:C     | 3:D:483:HIS:HD1   | 2.21                     | 0.41              |
| 3:D:638:LYS:HD3   | 3:D:932:ASP:OD1   | 2.21                     | 0.41              |
| 3:D:761:ILE:O     | 3:D:767:HIS:HD2   | 2.03                     | 0.41              |
| 4:E:54:LEU:CD2    | 4:E:58:PRO:HD2    | 2.43                     | 0.41              |
| 1:F:92:PRO:C      | 1:F:94:LEU:N      | 2.73                     | 0.41              |
| 1:G:101:LEU:HD12  | 1:G:114:PHE:CA    | 2.51                     | 0.41              |
| 1:G:24:VAL:HG13   | 1:G:196:THR:HG22  | 2.03                     | 0.41              |
| 2:H:141:HIS:HB3   | 2:H:418:LEU:CD2   | 2.46                     | 0.41              |
| 2:H:242:LEU:HD11  | 2:H:254:VAL:CG1   | 2.49                     | 0.41              |
| 2:H:272:ALA:O     | 2:H:464:LEU:HD21  | 2.20                     | 0.41              |
| 2:H:350:ARG:O     | 2:H:353:ARG:HB3   | 2.20                     | 0.41              |
| 2:H:927:GLY:HA2   | 2:H:930:LYS:HD3   | 2.02                     | 0.41              |
| 3:I:1014:ASN:C    | 3:I:1016:PRO:HD3  | 2.41                     | 0.41              |
| 3:I:1052:THR:HG21 | 7:Y:57:ARG:HH11   | 1.86                     | 0.41              |
| 3:I:1375:MET:C    | 3:I:1376:MET:HG3  | 2.39                     | 0.41              |
| 3:I:32:ILE:HG23   | 3:I:33:ASN:N      | 2.36                     | 0.41              |
| 3:I:540:LEU:HA    | 3:I:543:LEU:CD1   | 2.31                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:761:ILE:O     | 3:I:767:HIS:HD2   | 2.03                     | 0.41              |
| 3:I:834:THR:CA    | 3:I:838:ARG:HD3   | 2.51                     | 0.41              |
| 1:L:105:GLY:O     | 1:L:132:LEU:HB3   | 2.21                     | 0.41              |
| 1:L:25:LEU:O      | 1:L:25:LEU:HD23   | 2.19                     | 0.41              |
| 2:M:1012:PRO:CD   | 2:M:1026:GLN:HG2  | 2.40                     | 0.41              |
| 2:M:557:ARG:NH1   | 2:M:557:ARG:HG3   | 2.34                     | 0.41              |
| 2:M:706:GLU:HA    | 2:M:706:GLU:OE2   | 2.20                     | 0.41              |
| 2:M:742:VAL:CG1   | 2:M:743:VAL:N     | 2.83                     | 0.41              |
| 2:M:787:ASP:OD1   | 2:M:791:ARG:NH2   | 2.53                     | 0.41              |
| 3:N:1014:ASN:C    | 3:N:1016:PRO:HD3  | 2.40                     | 0.41              |
| 3:N:127:LEU:N     | 3:N:127:LEU:HD12  | 2.33                     | 0.41              |
| 3:N:617:ASN:ND2   | 3:N:1466:VAL:HG12 | 2.33                     | 0.41              |
| 3:N:1488:ASP:C    | 3:N:1490:LYS:N    | 2.74                     | 0.41              |
| 3:N:198:ARG:O     | 3:N:199:LEU:HB2   | 2.20                     | 0.41              |
| 3:N:373:PRO:CA    | 3:N:376:GLU:CD    | 2.77                     | 0.41              |
| 3:N:857:ILE:HA    | 3:N:857:ILE:HD13  | 1.83                     | 0.41              |
| 4:O:63:TRP:O      | 4:O:64:ALA:C      | 2.58                     | 0.41              |
| 4:O:37:ASN:HD21   | 4:O:93:TYR:HB3    | 1.85                     | 0.41              |
| 5:P:17:DG:H2'     | 5:P:18:DC:H6      | 1.85                     | 0.41              |
| 7:Y:103:GLN:HE21  | 7:Y:105:VAL:HG11  | 1.85                     | 0.41              |
| 3:I:783:ARG:HD3   | 7:Y:41:ASP:OD2    | 2.20                     | 0.41              |
| 1:A:45:LEU:HD11   | 1:A:177:VAL:CG2   | 2.51                     | 0.41              |
| 1:B:142:VAL:HG23  | 1:B:142:VAL:O     | 2.21                     | 0.41              |
| 1:B:58:ILE:HB     | 1:B:61:VAL:HB     | 2.03                     | 0.41              |
| 2:C:1063:ARG:HE   | 2:C:1063:ARG:HB3  | 1.30                     | 0.41              |
| 2:C:304:LEU:O     | 2:C:308:ARG:N     | 2.50                     | 0.41              |
| 3:D:1146:GLY:HA3  | 3:D:1207:TYR:CB   | 2.41                     | 0.41              |
| 3:D:1209:LEU:O    | 3:D:1211:MET:O    | 2.37                     | 0.41              |
| 3:D:1273:VAL:HG21 | 3:D:1305:LEU:CD2  | 2.50                     | 0.41              |
| 3:D:28:LYS:CG     | 3:D:29:PRO:CD     | 2.90                     | 0.41              |
| 3:D:573:MET:O     | 3:D:576:GLU:HB2   | 2.20                     | 0.41              |
| 3:D:642:CYS:HB3   | 3:D:716:PHE:HB3   | 1.99                     | 0.41              |
| 3:D:844:ALA:O     | 3:D:867:ARG:HB3   | 2.20                     | 0.41              |
| 3:D:991:GLN:OE1   | 7:X:112:VAL:N     | 2.51                     | 0.41              |
| 1:F:186:LEU:C     | 1:F:186:LEU:CD2   | 2.86                     | 0.41              |
| 1:G:56:VAL:CG1    | 1:G:57:TYR:N      | 2.83                     | 0.41              |
| 2:H:17:PRO:O      | 2:H:20:GLU:HG2    | 2.20                     | 0.41              |
| 2:H:328:LEU:HB2   | 2:H:488:ALA:HB2   | 2.00                     | 0.41              |
| 2:H:677:MET:HA    | 2:H:678:PRO:HD3   | 1.89                     | 0.41              |
| 2:H:694:LEU:HD11  | 2:H:868:ASP:HB3   | 2.02                     | 0.41              |
| 3:I:1254:GLN:CG   | 3:I:1355:VAL:HG13 | 2.50                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:185:VAL:HG21  | 3:I:203:ALA:HB2   | 2.02                     | 0.41              |
| 3:I:434:ARG:HB2   | 3:I:449:SER:HG    | 1.86                     | 0.41              |
| 3:I:514:LEU:HD12  | 3:I:578:VAL:CG1   | 2.50                     | 0.41              |
| 3:I:590:PRO:O     | 3:I:600:LEU:HD12  | 2.20                     | 0.41              |
| 2:H:1070:ILE:HG23 | 3:I:656:PHE:CD1   | 2.56                     | 0.41              |
| 3:I:820:GLU:CD    | 3:I:820:GLU:C     | 2.79                     | 0.41              |
| 3:I:820:GLU:HB2   | 3:I:836:VAL:HG21  | 2.03                     | 0.41              |
| 3:I:857:ILE:HA    | 3:I:857:ILE:HD13  | 1.84                     | 0.41              |
| 3:I:956:ILE:HD11  | 3:I:1062:ARG:CG   | 2.50                     | 0.41              |
| 3:I:99:ALA:O      | 3:I:514:LEU:O     | 2.38                     | 0.41              |
| 3:I:693:GLU:CG    | 4:J:48:MET:HE1    | 2.50                     | 0.41              |
| 1:L:150:TYR:HE1   | 1:L:170:VAL:HG12  | 1.85                     | 0.41              |
| 2:M:343:GLN:HA    | 2:M:346:VAL:CG2   | 2.49                     | 0.41              |
| 2:M:472:ARG:HH11  | 2:M:481:ASP:HA    | 1.86                     | 0.41              |
| 3:N:908:LYS:CB    | 3:N:1027:GLY:HA3  | 2.48                     | 0.41              |
| 3:N:1029:ARG:HA   | 3:N:1029:ARG:NH1  | 2.36                     | 0.41              |
| 3:N:1155:VAL:CG1  | 3:N:1177:ALA:CB   | 2.99                     | 0.41              |
| 3:N:1278:ASP:HA   | 3:N:1319:VAL:O    | 2.20                     | 0.41              |
| 3:N:1370:ILE:H    | 3:N:1370:ILE:HG13 | 1.59                     | 0.41              |
| 3:N:1471:LEU:HD12 | 3:N:1471:LEU:HA   | 1.95                     | 0.41              |
| 3:N:185:VAL:O     | 3:N:200:ASP:OD1   | 2.39                     | 0.41              |
| 3:N:208:PRO:HG3   | 3:N:353:VAL:CG1   | 2.50                     | 0.41              |
| 3:N:561:GLY:O     | 3:N:563:PRO:CD    | 2.65                     | 0.41              |
| 3:N:749:VAL:HA    | 3:N:750:PRO:HD3   | 1.71                     | 0.41              |
| 3:N:793:THR:O     | 3:N:879:ARG:NH1   | 2.54                     | 0.41              |
| 7:X:11:GLY:CA     | 7:X:109:GLU:OE1   | 2.69                     | 0.41              |
| 7:X:37:MET:HG3    | 7:X:48:LEU:HD11   | 2.02                     | 0.41              |
| 7:Y:91:LEU:HD23   | 7:Y:91:LEU:N      | 2.35                     | 0.41              |
| 2:C:241:LEU:O     | 2:C:241:LEU:HD23  | 2.20                     | 0.41              |
| 2:C:36:PRO:O      | 2:C:39:ARG:CG     | 2.53                     | 0.41              |
| 2:C:49:ARG:O      | 2:C:53:PRO:HD2    | 2.20                     | 0.41              |
| 2:C:573:ARG:CB    | 2:C:670:GLN:NE2   | 2.83                     | 0.41              |
| 2:C:863:ASP:OD1   | 2:C:865:THR:CG2   | 2.67                     | 0.41              |
| 3:D:1148:VAL:O    | 3:D:1188:VAL:HG23 | 2.20                     | 0.41              |
| 3:D:1295:GLU:HB3  | 3:D:1300:SER:HB3  | 2.02                     | 0.41              |
| 3:D:1356:TYR:CD1  | 3:D:1356:TYR:N    | 2.88                     | 0.41              |
| 3:D:1447:LEU:HD12 | 3:D:1447:LEU:N    | 2.35                     | 0.41              |
| 3:D:451:ASP:C     | 3:D:451:ASP:OD1   | 2.59                     | 0.41              |
| 3:D:658:LEU:O     | 3:D:661:MET:CB    | 2.68                     | 0.41              |
| 3:D:683:ILE:CG2   | 3:D:683:ILE:O     | 2.67                     | 0.41              |
| 3:D:813:LEU:HD12  | 3:D:813:LEU:C     | 2.41                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:834:THR:CA    | 3:D:838:ARG:HD3   | 2.50                     | 0.41              |
| 1:F:117:VAL:HB    | 1:F:120:VAL:CG1   | 2.50                     | 0.41              |
| 2:H:261:ILE:HD12  | 2:H:262:ALA:N     | 2.34                     | 0.41              |
| 2:H:374:ASN:ND2   | 2:H:374:ASN:O     | 2.54                     | 0.41              |
| 2:H:39:ARG:O      | 2:H:40:GLU:O      | 2.38                     | 0.41              |
| 2:H:40:GLU:HG3    | 2:H:42:VAL:H      | 1.85                     | 0.41              |
| 2:H:835:VAL:HA    | 2:H:849:VAL:HG12  | 2.02                     | 0.41              |
| 2:H:874:LEU:O     | 3:I:1029:ARG:HD2  | 2.20                     | 0.41              |
| 3:I:1126:ASP:OD1  | 3:I:1127:GLU:N    | 2.53                     | 0.41              |
| 3:I:115:LEU:C     | 3:I:115:LEU:CD2   | 2.89                     | 0.41              |
| 3:I:1274:ILE:HD12 | 3:I:1274:ILE:C    | 2.41                     | 0.41              |
| 3:I:1278:ASP:HB3  | 3:I:1321:ALA:N    | 2.35                     | 0.41              |
| 3:I:510:GLU:O     | 3:I:513:ILE:CG1   | 2.63                     | 0.41              |
| 3:I:639:LEU:HD12  | 3:I:640:HIS:H     | 1.85                     | 0.41              |
| 3:I:879:ARG:HH11  | 3:I:879:ARG:CG    | 2.34                     | 0.41              |
| 3:I:901:GLN:HG2   | 3:I:901:GLN:H     | 1.77                     | 0.41              |
| 3:I:964:LEU:O     | 3:I:968:ASP:HB2   | 2.21                     | 0.41              |
| 3:I:978:TYR:C     | 3:I:980:MET:H     | 2.23                     | 0.41              |
| 4:J:69:LEU:C      | 4:J:69:LEU:HD23   | 2.40                     | 0.41              |
| 1:K:18:ARG:HH11   | 1:K:123:MET:CE    | 2.34                     | 0.41              |
| 1:K:176:ARG:NH1   | 2:M:865:THR:HB    | 2.36                     | 0.41              |
| 2:M:1084:SER:C    | 2:M:1087:VAL:HG12 | 2.41                     | 0.41              |
| 2:M:575:GLN:O     | 2:M:667:ALA:HB1   | 2.21                     | 0.41              |
| 2:M:677:MET:HA    | 2:M:678:PRO:HD3   | 1.89                     | 0.41              |
| 2:M:691:SER:C     | 2:M:693:GLU:N     | 2.72                     | 0.41              |
| 2:M:730:SER:O     | 2:M:734:LEU:CD1   | 2.67                     | 0.41              |
| 2:M:854:PRO:O     | 2:M:855:VAL:C     | 2.59                     | 0.41              |
| 2:M:957:LYS:CD    | 2:M:961:GLU:CB    | 2.95                     | 0.41              |
| 3:N:1434:TRP:HZ3  | 3:N:1455:LYS:O    | 2.04                     | 0.41              |
| 3:N:372:ASP:O     | 3:N:374:GLU:N     | 2.52                     | 0.41              |
| 3:N:632:VAL:CG2   | 3:N:725:SER:CB    | 2.99                     | 0.41              |
| 3:N:841:TYR:HB2   | 3:N:864:VAL:HG13  | 2.03                     | 0.41              |
| 3:N:899:LEU:HD13  | 3:N:914:LEU:CD2   | 2.50                     | 0.41              |
| 1:A:180:GLN:HE21  | 1:A:180:GLN:HB3   | 1.55                     | 0.41              |
| 1:B:80:LEU:HG     | 3:D:844:ALA:CB    | 2.51                     | 0.41              |
| 2:C:492:ASP:OD2   | 2:C:518:LYS:CG    | 2.66                     | 0.41              |
| 2:C:86:LYS:O      | 2:C:813:VAL:HG23  | 2.20                     | 0.41              |
| 2:C:89:THR:HG21   | 2:C:383:ARG:HH21  | 1.84                     | 0.41              |
| 3:D:115:LEU:CD2   | 3:D:115:LEU:C     | 2.89                     | 0.41              |
| 2:C:1098:ASP:CB   | 3:D:11:ALA:O      | 2.57                     | 0.41              |
| 3:D:1372:VAL:HG13 | 3:D:1373:ARG:N    | 2.34                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1403:LEU:O   | 3:D:1407:LEU:HD13 | 2.20                     | 0.41              |
| 3:D:177:ALA:HB3  | 3:D:390:PRO:HG2   | 2.02                     | 0.41              |
| 3:D:191:LEU:HD21 | 3:D:197:SER:OG    | 2.21                     | 0.41              |
| 3:D:361:VAL:HG12 | 3:D:383:GLY:H     | 1.84                     | 0.41              |
| 3:D:412:GLY:HA2  | 3:D:434:ARG:CZ    | 2.49                     | 0.41              |
| 2:C:885:ILE:HG21 | 3:D:950:GLY:HA2   | 2.02                     | 0.41              |
| 4:E:63:TRP:O     | 4:E:64:ALA:C      | 2.59                     | 0.41              |
| 2:H:831:ARG:NH1  | 2:H:1002:GLU:HB2  | 2.35                     | 0.41              |
| 2:H:292:ARG:HG2  | 2:H:299:LYS:CB    | 2.37                     | 0.41              |
| 2:H:366:SER:C    | 2:H:371:LYS:HZ1   | 2.24                     | 0.41              |
| 2:H:626:ARG:HB2  | 2:H:639:GLN:HE21  | 1.86                     | 0.41              |
| 2:H:691:SER:O    | 2:H:693:GLU:N     | 2.53                     | 0.41              |
| 2:H:79:PRO:HG2   | 2:H:82:GLU:HB2    | 2.02                     | 0.41              |
| 3:I:1491:THR:O   | 3:I:1495:ILE:HG12 | 2.21                     | 0.41              |
| 3:I:158:TYR:HE1  | 3:I:452:ILE:HD11  | 1.86                     | 0.41              |
| 3:I:521:PRO:CD   | 3:I:524:LEU:HD13  | 2.49                     | 0.41              |
| 3:I:562:ALA:CB   | 3:I:567:ILE:HD11  | 2.50                     | 0.41              |
| 3:I:793:THR:O    | 3:I:879:ARG:NH1   | 2.54                     | 0.41              |
| 3:I:975:GLU:HA   | 3:I:975:GLU:OE1   | 2.20                     | 0.41              |
| 2:M:704:HIS:HE2  | 2:M:998:TYR:HE1   | 1.66                     | 0.41              |
| 2:M:937:ASP:HB3  | 2:M:940:GLU:HG3   | 2.02                     | 0.41              |
| 3:N:1288:GLU:C   | 3:N:1289:LYS:HG3  | 2.38                     | 0.41              |
| 3:N:139:GLY:HA3  | 3:N:162:ARG:HE    | 1.85                     | 0.41              |
| 3:N:1452:ILE:CD1 | 3:N:1452:ILE:H    | 2.34                     | 0.41              |
| 3:N:34:TYR:CD2   | 3:N:34:TYR:N      | 2.89                     | 0.41              |
| 3:N:356:PRO:HA   | 3:N:440:VAL:O     | 2.21                     | 0.41              |
| 3:N:683:ILE:HG21 | 3:N:688:TRP:CZ2   | 2.55                     | 0.41              |
| 3:N:761:ILE:O    | 3:N:767:HIS:HD2   | 2.03                     | 0.41              |
| 2:M:1106:ASP:OD1 | 3:N:7:LYS:HD2     | 2.21                     | 0.41              |
| 3:N:814:ALA:HB1  | 3:N:818:ARG:NE    | 2.34                     | 0.41              |
| 3:N:834:THR:CA   | 3:N:838:ARG:HD3   | 2.51                     | 0.41              |
| 3:N:844:ALA:O    | 3:N:867:ARG:HB3   | 2.20                     | 0.41              |
| 7:X:16:MET:O     | 7:X:20:GLU:HG3    | 2.21                     | 0.41              |
| 7:Z:82:VAL:CG2   | 7:Z:133:ARG:HH21  | 2.34                     | 0.41              |
| 2:C:26:TYR:CE2   | 2:C:127:PHE:CE2   | 3.09                     | 0.41              |
| 2:C:181:VAL:HG13 | 2:C:220:GLY:HA2   | 1.88                     | 0.41              |
| 2:C:39:ARG:O     | 2:C:40:GLU:O      | 2.38                     | 0.41              |
| 2:C:441:VAL:HG12 | 2:C:559:LEU:CA    | 2.51                     | 0.41              |
| 2:C:73:LEU:HD13  | 2:C:92:ALA:HB1    | 2.03                     | 0.41              |
| 3:D:112:ILE:HG21 | 3:D:128:TYR:OH    | 2.21                     | 0.41              |
| 3:D:593:ASN:CB   | 3:D:594:PRO:HD2   | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:835:SER:C     | 3:D:837:GLY:N     | 2.69                     | 0.41              |
| 4:E:69:LEU:C      | 4:E:69:LEU:HD23   | 2.41                     | 0.41              |
| 1:G:112:ARG:CG    | 1:G:125:PRO:CA    | 2.98                     | 0.41              |
| 1:G:48:ILE:CD1    | 1:G:48:ILE:N      | 2.82                     | 0.41              |
| 2:H:65:VAL:O      | 2:H:100:LEU:HA    | 2.20                     | 0.41              |
| 2:H:191:PHE:HA    | 2:H:192:PRO:HD3   | 1.87                     | 0.41              |
| 2:H:236:ILE:HD12  | 2:H:236:ILE:H     | 1.85                     | 0.41              |
| 2:H:267:TYR:O     | 2:H:268:ASP:C     | 2.58                     | 0.41              |
| 2:H:314:THR:O     | 2:H:314:THR:HG22  | 2.21                     | 0.41              |
| 2:H:338:GLU:O     | 2:H:342:ASP:HB2   | 2.21                     | 0.41              |
| 2:H:573:ARG:HB3   | 2:H:670:GLN:NE2   | 2.36                     | 0.41              |
| 2:H:854:PRO:O     | 2:H:855:VAL:C     | 2.59                     | 0.41              |
| 2:H:937:ASP:HB3   | 2:H:940:GLU:HG3   | 2.02                     | 0.41              |
| 3:I:1346:ARG:HA   | 3:I:1346:ARG:HD2  | 1.84                     | 0.41              |
| 3:I:415:VAL:HG12  | 3:I:416:ALA:N     | 2.36                     | 0.41              |
| 3:I:521:PRO:CG    | 3:I:524:LEU:HD13  | 2.50                     | 0.41              |
| 1:L:101:LEU:HD12  | 1:L:114:PHE:CA    | 2.50                     | 0.41              |
| 1:K:224:TYR:CG    | 1:L:9:PRO:HG2     | 2.55                     | 0.41              |
| 2:M:1040:LEU:O    | 2:M:1041:GLU:C    | 2.56                     | 0.41              |
| 2:M:172:ILE:CD1   | 2:M:172:ILE:N     | 2.57                     | 0.41              |
| 2:M:397:GLU:H     | 2:M:633:GLN:HG2   | 1.85                     | 0.41              |
| 2:M:573:ARG:HB3   | 2:M:670:GLN:NE2   | 2.36                     | 0.41              |
| 2:M:583:LEU:N     | 2:M:583:LEU:HD12  | 2.34                     | 0.41              |
| 2:M:603:VAL:CG1   | 2:M:604:ALA:N     | 2.83                     | 0.41              |
| 3:N:1026:SER:C    | 3:N:1028:ALA:N    | 2.74                     | 0.41              |
| 3:N:1029:ARG:NH1  | 3:N:1029:ARG:CG   | 2.83                     | 0.41              |
| 3:N:123:LEU:HD21  | 3:N:151:GLN:HE22  | 1.86                     | 0.41              |
| 3:N:1313:VAL:HG21 | 3:N:1319:VAL:CG1  | 2.51                     | 0.41              |
| 3:N:1385:GLY:HA2  | 3:N:1413:THR:HG21 | 2.03                     | 0.41              |
| 3:N:209:ARG:HB2   | 3:N:389:GLU:O     | 2.21                     | 0.41              |
| 3:N:524:LEU:HD12  | 3:N:524:LEU:N     | 2.36                     | 0.41              |
| 3:N:660:LYS:HA    | 3:N:660:LYS:CE    | 2.50                     | 0.41              |
| 3:N:638:LYS:CA    | 3:N:932:ASP:OD1   | 2.66                     | 0.41              |
| 7:Y:84:GLY:HA2    | 7:Y:130:LEU:HD12  | 2.02                     | 0.41              |
| 1:A:35:THR:HG21   | 1:B:43:ILE:HG12   | 2.03                     | 0.41              |
| 2:C:1042:ALA:HB2  | 3:D:1223:ILE:CG2  | 2.50                     | 0.41              |
| 2:C:1099:VAL:HG22 | 3:D:10:ILE:HG13   | 1.92                     | 0.41              |
| 2:C:26:TYR:CD2    | 2:C:121:MET:HB2   | 2.49                     | 0.41              |
| 2:C:191:PHE:CE2   | 2:C:195:LEU:HB3   | 2.56                     | 0.41              |
| 2:C:335:THR:O     | 2:C:339:LEU:HG    | 2.21                     | 0.41              |
| 2:C:391:LEU:HD23  | 2:C:391:LEU:C     | 2.41                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1083:ASP:OD2  | 3:D:1237:THR:HG22 | 2.20                     | 0.41              |
| 3:D:1127:GLU:OE2  | 7:X:66:GLU:OE2    | 2.39                     | 0.41              |
| 3:D:149:LYS:HE3   | 3:D:149:LYS:H     | 1.85                     | 0.41              |
| 3:D:520:LEU:HD11  | 3:D:524:LEU:CD2   | 2.49                     | 0.41              |
| 3:D:554:LEU:CD1   | 3:D:570:GLU:HB3   | 2.50                     | 0.41              |
| 3:D:862:ASP:O     | 3:D:876:SER:HB2   | 2.21                     | 0.41              |
| 1:G:102:LYS:HB2   | 1:G:139:ASN:OD1   | 2.20                     | 0.41              |
| 1:G:76:VAL:O      | 1:G:79:ILE:HG13   | 2.21                     | 0.41              |
| 2:H:1012:PRO:CD   | 2:H:1026:GLN:HG2  | 2.45                     | 0.41              |
| 2:H:1047:HIS:O    | 2:H:1051:GLU:HB2  | 2.21                     | 0.41              |
| 2:H:274:ARG:HG3   | 2:H:285:LEU:HB3   | 2.01                     | 0.41              |
| 2:H:395:LYS:HE2   | 2:H:403:SER:HB2   | 2.02                     | 0.41              |
| 2:H:333:ILE:CG1   | 2:H:410:ILE:HD11  | 2.51                     | 0.41              |
| 2:H:78:PHE:N      | 2:H:78:PHE:CD1    | 2.88                     | 0.41              |
| 2:H:863:ASP:OD1   | 2:H:865:THR:CG2   | 2.67                     | 0.41              |
| 3:I:1101:VAL:CG1  | 3:I:1428:ALA:HB2  | 2.49                     | 0.41              |
| 3:I:31:THR:O      | 3:I:45:PHE:HD2    | 2.04                     | 0.41              |
| 3:I:481:MET:HE2   | 3:I:493:ARG:CA    | 2.49                     | 0.41              |
| 3:I:563:PRO:HB2   | 3:I:566:ILE:HG13  | 2.03                     | 0.41              |
| 3:I:586:ARG:HD3   | 3:I:586:ARG:HA    | 1.94                     | 0.41              |
| 3:I:814:ALA:HB1   | 3:I:818:ARG:NE    | 2.34                     | 0.41              |
| 3:I:841:TYR:HB2   | 3:I:864:VAL:HG13  | 2.03                     | 0.41              |
| 1:K:229:GLN:HB2   | 1:K:229:GLN:HE21  | 1.64                     | 0.41              |
| 1:L:73:GLU:HG3    | 1:L:130:ALA:CB    | 2.51                     | 0.41              |
| 2:M:1001:VAL:HG22 | 3:N:630:VAL:HG21  | 2.03                     | 0.41              |
| 2:M:115:LEU:O     | 2:M:378:LEU:HD23  | 2.20                     | 0.41              |
| 2:M:198:ARG:HH12  | 2:M:203:ASP:HA    | 1.85                     | 0.41              |
| 2:M:625:LEU:HD11  | 2:M:641:PRO:HG3   | 2.03                     | 0.41              |
| 2:M:907:ASP:CG    | 2:M:907:ASP:O     | 2.59                     | 0.41              |
| 2:M:967:PHE:CD1   | 2:M:972:VAL:HG12  | 2.56                     | 0.41              |
| 3:N:1312:LEU:HA   | 3:N:1312:LEU:HD23 | 1.86                     | 0.41              |
| 3:N:153:LEU:C     | 3:N:153:LEU:HD12  | 2.42                     | 0.41              |
| 3:N:407:VAL:HG13  | 3:N:408:GLU:N     | 2.36                     | 0.41              |
| 3:N:441:ARG:CD    | 3:N:445:ARG:HH22  | 2.34                     | 0.41              |
| 3:N:47:GLU:O      | 3:N:51:GLY:CA     | 2.68                     | 0.41              |
| 3:N:131:LYS:HE3   | 3:N:568:ARG:HH11  | 1.51                     | 0.41              |
| 3:N:656:PHE:HB3   | 3:N:694:VAL:CG1   | 2.50                     | 0.41              |
| 3:N:681:ARG:HG3   | 3:N:682:ASP:H     | 1.84                     | 0.41              |
| 3:N:887:ALA:HB1   | 3:N:893:GLU:HG3   | 2.01                     | 0.41              |
| 3:I:970:LYS:NZ    | 7:Y:113:LEU:HA    | 2.35                     | 0.41              |
| 1:B:172:SER:HA    | 1:B:173:PRO:HD3   | 1.92                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:265:ARG:HD3   | 2:C:267:TYR:CD1  | 2.55                     | 0.41              |
| 2:C:309:TYR:CE2   | 2:C:321:GLU:HG3  | 2.56                     | 0.41              |
| 2:C:575:GLN:O     | 2:C:667:ALA:HB1  | 2.21                     | 0.41              |
| 2:C:675:ALA:O     | 2:C:870:ILE:HA   | 2.21                     | 0.41              |
| 3:D:1150:ALA:HB3  | 3:D:1187:PRO:HB2 | 2.03                     | 0.41              |
| 3:D:1262:LEU:HD21 | 3:D:1351:GLU:HG3 | 2.03                     | 0.41              |
| 3:D:180:LYS:NZ    | 3:D:386:HIS:HA   | 2.36                     | 0.41              |
| 3:D:703:ASN:ND2   | 3:D:704:ARG:H    | 2.18                     | 0.41              |
| 3:D:706:PRO:HG3   | 6:Q:16:G:N2      | 2.36                     | 0.41              |
| 3:D:820:GLU:HB2   | 3:D:836:VAL:HG21 | 2.03                     | 0.41              |
| 4:E:40:LEU:CD2    | 4:E:67:GLU:HA    | 2.51                     | 0.41              |
| 1:G:104:GLU:CG    | 1:G:137:ARG:HD2  | 2.51                     | 0.41              |
| 1:G:44:LEU:CA     | 1:G:48:ILE:HD13  | 2.44                     | 0.41              |
| 2:H:1012:PRO:HD2  | 2:H:1026:GLN:HB2 | 2.01                     | 0.41              |
| 2:H:214:TYR:C     | 2:H:214:TYR:CD1  | 2.95                     | 0.41              |
| 2:H:289:THR:C     | 2:H:291:ALA:N    | 2.75                     | 0.41              |
| 2:H:31:GLN:HG2    | 2:H:34:VAL:HG23  | 2.01                     | 0.41              |
| 2:H:575:GLN:O     | 2:H:667:ALA:HB1  | 2.21                     | 0.41              |
| 2:H:71:TYR:CG     | 2:H:71:TYR:O     | 2.74                     | 0.41              |
| 2:H:90:TYR:CD1    | 2:H:120:LEU:HB2  | 2.55                     | 0.41              |
| 3:I:1106:VAL:HG11 | 3:I:1474:ALA:CB  | 2.51                     | 0.41              |
| 3:I:1294:VAL:O    | 3:I:1300:SER:HA  | 2.20                     | 0.41              |
| 3:I:464:LEU:HD23  | 3:I:464:LEU:HA   | 1.73                     | 0.41              |
| 3:I:925:GLU:O     | 3:I:928:ALA:HB3  | 2.21                     | 0.41              |
| 4:J:62:THR:O      | 4:J:66:LYS:HB2   | 2.21                     | 0.41              |
| 1:L:184:THR:O     | 1:L:192:LEU:HB2  | 2.21                     | 0.41              |
| 1:L:91:ASN:HB2    | 1:L:92:PRO:HD2   | 2.02                     | 0.41              |
| 2:M:1058:ASP:O    | 2:M:1060:ILE:N   | 2.53                     | 0.41              |
| 2:M:102:HIS:HD2   | 2:M:107:LEU:O    | 2.04                     | 0.41              |
| 2:M:144:PRO:O     | 2:M:276:LYS:CD   | 2.69                     | 0.41              |
| 2:M:145:GLY:HA2   | 2:M:276:LYS:HD3  | 2.03                     | 0.41              |
| 2:M:188:LYS:CA    | 2:M:188:LYS:HZ2  | 2.34                     | 0.41              |
| 2:M:194:VAL:O     | 2:M:195:LEU:C    | 2.59                     | 0.41              |
| 2:M:202:TYR:OH    | 2:M:304:LEU:HD23 | 2.21                     | 0.41              |
| 2:M:260:LEU:CD2   | 2:M:260:LEU:C    | 2.87                     | 0.41              |
| 2:M:28:ARG:HG2    | 2:M:42:VAL:CG2   | 2.51                     | 0.41              |
| 2:M:328:LEU:HD22  | 2:M:433:THR:HG22 | 2.03                     | 0.41              |
| 2:M:496:ILE:HA    | 2:M:531:PHE:O    | 2.20                     | 0.41              |
| 2:M:578:VAL:HA    | 2:M:900:ARG:CG   | 2.51                     | 0.41              |
| 3:N:1126:ASP:OD1  | 3:N:1129:THR:CA  | 2.69                     | 0.41              |
| 3:N:1375:MET:C    | 3:N:1376:MET:HG3 | 2.40                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1468:LEU:HD13 | 3:N:1470:ARG:CD   | 2.50                     | 0.41              |
| 3:N:184:GLU:OE1   | 3:N:202:VAL:HG22  | 2.21                     | 0.41              |
| 3:N:586:ARG:HA    | 3:N:586:ARG:HD3   | 1.94                     | 0.41              |
| 3:N:970:LYS:HA    | 3:N:973:GLN:HE21  | 1.86                     | 0.41              |
| 4:O:86:GLN:H      | 4:O:86:GLN:HG2    | 1.53                     | 0.41              |
| 7:X:105:VAL:O     | 7:X:121:ASP:N     | 2.54                     | 0.41              |
| 7:Y:15:LEU:HB2    | 7:Y:69:LEU:HD21   | 2.03                     | 0.41              |
| 7:Y:83:ILE:HD13   | 7:Y:129:LEU:HD22  | 2.03                     | 0.41              |
| 1:A:218:LEU:HD23  | 1:B:222:LEU:HD11  | 2.03                     | 0.41              |
| 1:A:229:GLN:HE21  | 1:A:229:GLN:HB2   | 1.58                     | 0.41              |
| 1:A:65:PHE:CD1    | 1:A:65:PHE:N      | 2.89                     | 0.41              |
| 2:C:182:VAL:HB    | 2:C:193:LEU:HB2   | 2.03                     | 0.41              |
| 2:C:341:THR:HG23  | 2:C:342:ASP:N     | 2.35                     | 0.41              |
| 2:C:42:VAL:O      | 2:C:43:GLY:O      | 2.39                     | 0.41              |
| 2:C:969:GLN:HE21  | 2:C:969:GLN:HB3   | 1.48                     | 0.41              |
| 3:D:1026:SER:C    | 3:D:1028:ALA:N    | 2.74                     | 0.41              |
| 3:D:1254:GLN:CA   | 3:D:1258:ARG:HB2  | 2.35                     | 0.41              |
| 2:C:1046:ALA:HB1  | 3:D:1471:LEU:HD11 | 2.03                     | 0.41              |
| 3:D:1472:ILE:HA   | 3:D:1473:PRO:HD3  | 1.80                     | 0.41              |
| 3:D:907:GLU:O     | 3:D:911:LEU:HD12  | 2.21                     | 0.41              |
| 1:G:98:THR:HG22   | 1:G:100:LEU:HD21  | 2.03                     | 0.41              |
| 2:H:208:ALA:CB    | 2:H:222:MET:SD    | 3.09                     | 0.41              |
| 2:H:139:GLN:O     | 2:H:333:ILE:HA    | 2.21                     | 0.41              |
| 2:H:341:THR:HG23  | 2:H:342:ASP:N     | 2.35                     | 0.41              |
| 2:H:480:THR:HG22  | 2:H:481:ASP:H     | 1.86                     | 0.41              |
| 2:H:577:PRO:HG3   | 2:H:993:PHE:CD1   | 2.56                     | 0.41              |
| 2:H:86:LYS:O      | 2:H:87:ASP:HB2    | 2.20                     | 0.41              |
| 2:H:928:LYS:HA    | 2:H:928:LYS:HD2   | 1.83                     | 0.41              |
| 3:I:1209:LEU:O    | 3:I:1211:MET:O    | 2.39                     | 0.41              |
| 3:I:1107:VAL:HG11 | 3:I:1217:ILE:HA   | 2.01                     | 0.41              |
| 3:I:1462:LEU:CD2  | 3:I:1472:ILE:HG22 | 2.46                     | 0.41              |
| 3:I:795:VAL:CG2   | 3:I:879:ARG:HH12  | 2.34                     | 0.41              |
| 4:J:26:ARG:NH2    | 4:J:67:GLU:OE2    | 2.54                     | 0.41              |
| 1:K:122:ILE:HD12  | 1:K:122:ILE:N     | 2.36                     | 0.41              |
| 1:K:175:ARG:HH22  | 2:M:697:ARG:HH22  | 1.67                     | 0.41              |
| 1:K:64:GLU:CD     | 2:M:830:LYS:HE2   | 2.41                     | 0.41              |
| 1:K:80:LEU:HD23   | 1:K:80:LEU:C      | 2.41                     | 0.41              |
| 1:K:83:LYS:HZ3    | 1:K:168:ASP:HB2   | 1.85                     | 0.41              |
| 1:L:117:VAL:HG12  | 1:L:118:ALA:N     | 2.36                     | 0.41              |
| 2:M:1004:LYS:HA   | 2:M:1004:LYS:HD3  | 1.93                     | 0.41              |
| 2:M:159:ILE:HD12  | 2:M:159:ILE:O     | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:39:ARG:CD     | 2:M:45:GLN:CG     | 2.99                     | 0.41              |
| 3:N:361:VAL:HG23  | 3:N:383:GLY:O     | 2.21                     | 0.41              |
| 3:N:845:ASN:O     | 3:N:848:GLU:HB2   | 2.20                     | 0.41              |
| 3:N:983:LEU:N     | 3:N:983:LEU:CD2   | 2.82                     | 0.41              |
| 4:O:3:GLU:O       | 4:O:6:ILE:HG22    | 2.21                     | 0.41              |
| 1:A:18:ARG:NH1    | 1:A:123:MET:CE    | 2.85                     | 0.40              |
| 1:A:19:GLU:O      | 1:A:207:PRO:HG3   | 2.21                     | 0.40              |
| 1:B:106:PRO:HG2   | 1:B:134:GLU:OE2   | 2.21                     | 0.40              |
| 2:C:1084:SER:C    | 2:C:1087:VAL:HG12 | 2.41                     | 0.40              |
| 2:C:197:LEU:HD13  | 2:C:207:LEU:CD1   | 2.31                     | 0.40              |
| 2:C:194:VAL:O     | 2:C:197:LEU:N     | 2.54                     | 0.40              |
| 2:C:199:VAL:CG1   | 2:C:235:LEU:HG    | 2.51                     | 0.40              |
| 2:C:418:LEU:CD1   | 2:C:418:LEU:N     | 2.84                     | 0.40              |
| 2:C:572:ILE:HG13  | 2:C:572:ILE:H     | 1.66                     | 0.40              |
| 2:C:575:GLN:HB2   | 2:C:670:GLN:HG2   | 2.03                     | 0.40              |
| 2:C:676:ILE:HG21  | 2:C:988:VAL:CG1   | 2.42                     | 0.40              |
| 2:C:742:VAL:CG1   | 2:C:743:VAL:N     | 2.83                     | 0.40              |
| 2:C:81:ASP:CA     | 2:C:84:ARG:NH1    | 2.84                     | 0.40              |
| 2:C:854:PRO:O     | 2:C:855:VAL:C     | 2.59                     | 0.40              |
| 2:C:928:LYS:HZ3   | 2:C:932:GLU:HG3   | 1.85                     | 0.40              |
| 3:D:1289:LYS:C    | 3:D:1290:LEU:HD12 | 2.41                     | 0.40              |
| 3:D:1313:VAL:HG21 | 3:D:1319:VAL:CG1  | 2.51                     | 0.40              |
| 3:D:1440:PHE:O    | 3:D:1441:GLN:O    | 2.38                     | 0.40              |
| 3:D:1491:THR:HA   | 3:D:1494:ALA:CB   | 2.52                     | 0.40              |
| 3:D:165:LYS:HG2   | 2:H:213:ALA:HB1   | 2.03                     | 0.40              |
| 3:D:54:LYS:HD2    | 3:D:55:ASP:N      | 2.30                     | 0.40              |
| 3:D:845:ASN:H     | 3:D:848:GLU:HG3   | 1.86                     | 0.40              |
| 3:D:964:LEU:O     | 3:D:968:ASP:HB2   | 2.21                     | 0.40              |
| 2:H:1056:LYS:HB3  | 3:I:624:ASP:H     | 1.85                     | 0.40              |
| 2:H:1084:SER:C    | 2:H:1087:VAL:HG12 | 2.41                     | 0.40              |
| 2:H:206:THR:O     | 2:H:209:ARG:HG2   | 2.21                     | 0.40              |
| 2:H:242:LEU:O     | 2:H:243:ARG:HB2   | 2.21                     | 0.40              |
| 2:H:252:LYS:O     | 2:H:253:ALA:C     | 2.59                     | 0.40              |
| 2:H:265:ARG:CG    | 2:H:267:TYR:CD1   | 3.04                     | 0.40              |
| 2:H:333:ILE:HG12  | 2:H:410:ILE:HD11  | 2.03                     | 0.40              |
| 2:H:424:GLY:O     | 2:H:425:PHE:C     | 2.60                     | 0.40              |
| 2:H:752:GLY:H     | 2:H:792:VAL:HB    | 1.85                     | 0.40              |
| 3:I:1313:VAL:HG21 | 3:I:1319:VAL:CG1  | 2.51                     | 0.40              |
| 3:I:135:LEU:HD22  | 3:I:148:GLU:O     | 2.22                     | 0.40              |
| 3:I:1374:GLN:OE1  | 3:I:1374:GLN:HA   | 2.22                     | 0.40              |
| 3:I:169:TYR:HA    | 3:I:170:PRO:HD3   | 1.90                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:I:199:LEU:HD23  | 3:I:200:ASP:O    | 2.21                     | 0.40              |
| 3:I:116:LEU:CD1   | 3:I:461:ILE:HG23 | 2.51                     | 0.40              |
| 3:I:632:VAL:CG2   | 3:I:725:SER:CB   | 2.99                     | 0.40              |
| 3:I:845:ASN:H     | 3:I:848:GLU:HG3  | 1.86                     | 0.40              |
| 3:I:980:MET:HA    | 7:Y:142:THR:HG23 | 2.02                     | 0.40              |
| 2:M:141:HIS:C     | 2:M:141:HIS:CD2  | 2.94                     | 0.40              |
| 2:M:207:LEU:HD22  | 2:M:221:LEU:HD13 | 2.02                     | 0.40              |
| 2:M:20:GLU:OE2    | 2:M:460:ARG:HD3  | 2.21                     | 0.40              |
| 2:M:305:PRO:CA    | 2:M:308:ARG:HB3  | 2.38                     | 0.40              |
| 2:M:141:HIS:O     | 2:M:331:ARG:HG2  | 2.21                     | 0.40              |
| 2:M:610:ARG:HG3   | 2:M:610:ARG:HH11 | 1.86                     | 0.40              |
| 2:M:794:PRO:CD    | 2:M:1025:ALA:HA  | 2.51                     | 0.40              |
| 2:M:797:GLY:C     | 2:M:827:VAL:HG11 | 2.42                     | 0.40              |
| 2:M:851:LYS:HG2   | 2:M:853:LEU:CD1  | 2.50                     | 0.40              |
| 1:K:42:ARG:CZ     | 2:M:857:ASP:HB3  | 2.51                     | 0.40              |
| 3:N:1262:LEU:HD21 | 3:N:1351:GLU:HG3 | 2.03                     | 0.40              |
| 3:N:1287:GLU:C    | 3:N:1289:LYS:H   | 2.25                     | 0.40              |
| 3:N:134:VAL:HB    | 3:N:135:LEU:H    | 1.72                     | 0.40              |
| 3:N:481:MET:SD    | 3:N:1388:ARG:HD3 | 2.61                     | 0.40              |
| 3:N:160:GLU:HB3   | 3:N:161:LEU:H    | 1.75                     | 0.40              |
| 3:N:361:VAL:HG12  | 3:N:379:ALA:HB1  | 2.03                     | 0.40              |
| 3:N:389:GLU:N     | 3:N:390:PRO:CD   | 2.84                     | 0.40              |
| 3:N:593:ASN:O     | 3:N:594:PRO:C    | 2.60                     | 0.40              |
| 3:N:620:GLY:O     | 3:N:621:LYS:HG2  | 2.20                     | 0.40              |
| 3:N:642:CYS:HB3   | 3:N:716:PHE:HB3  | 2.00                     | 0.40              |
| 3:N:783:ARG:HE    | 3:N:1029:ARG:HG2 | 1.86                     | 0.40              |
| 3:N:813:LEU:C     | 3:N:813:LEU:HD12 | 2.41                     | 0.40              |
| 3:N:820:GLU:HB2   | 3:N:836:VAL:HG21 | 2.03                     | 0.40              |
| 3:N:949:ILE:HD11  | 3:N:1023:MET:HE2 | 2.02                     | 0.40              |
| 3:N:964:LEU:O     | 3:N:968:ASP:HB2  | 2.21                     | 0.40              |
| 4:O:29:GLN:HB3    | 4:O:89:MET:HE3   | 2.04                     | 0.40              |
| 5:T:18:DC:C2'     | 5:T:19:DC:C5'    | 2.96                     | 0.40              |
| 7:Y:56:ALA:HA     | 7:Y:59:GLU:OE1   | 2.22                     | 0.40              |
| 7:Z:153:ALA:C     | 7:Z:154:ILE:HG13 | 2.39                     | 0.40              |
| 1:A:11:PHE:CD2    | 1:B:225:PHE:O    | 2.74                     | 0.40              |
| 1:B:91:ASN:HB2    | 1:B:92:PRO:HD2   | 2.02                     | 0.40              |
| 2:C:221:LEU:C     | 2:C:223:ASP:H    | 2.24                     | 0.40              |
| 2:C:54:ILE:HD11   | 2:C:356:ARG:CG   | 2.51                     | 0.40              |
| 2:C:591:SER:O     | 2:C:592:LEU:HB2  | 2.21                     | 0.40              |
| 2:C:64:LEU:HD22   | 2:C:359:MET:HG2  | 2.04                     | 0.40              |
| 2:C:657:ASP:OD1   | 2:C:662:GLU:C    | 2.60                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:573:ARG:HB3  | 2:C:670:GLN:NE2   | 2.36                     | 0.40              |
| 2:C:76:PRO:O     | 2:C:77:PRO:C      | 2.60                     | 0.40              |
| 2:C:679:PHE:CZ   | 2:C:853:LEU:HD21  | 2.55                     | 0.40              |
| 2:C:897:LEU:CD2  | 2:C:921:ALA:HA    | 2.49                     | 0.40              |
| 2:C:979:THR:HG23 | 2:C:981:GLU:N     | 2.23                     | 0.40              |
| 3:D:1095:THR:O   | 3:D:1099:VAL:CG2  | 2.67                     | 0.40              |
| 3:D:1169:ASP:O   | 3:D:1172:HIS:HB2  | 2.21                     | 0.40              |
| 3:D:1277:ILE:CD1 | 3:D:1277:ILE:N    | 2.85                     | 0.40              |
| 3:D:134:VAL:CG2  | 3:D:460:ALA:HB2   | 2.35                     | 0.40              |
| 1:F:45:LEU:HD11  | 1:F:177:VAL:CG2   | 2.51                     | 0.40              |
| 1:F:39:PRO:HG3   | 1:G:39:PRO:HG3    | 2.03                     | 0.40              |
| 1:G:184:THR:O    | 1:G:192:LEU:HB2   | 2.21                     | 0.40              |
| 1:G:72:LYS:HB3   | 1:G:131:THR:OG1   | 2.21                     | 0.40              |
| 1:G:91:ASN:HB2   | 1:G:92:PRO:HD2    | 2.02                     | 0.40              |
| 2:H:1090:LYS:HA  | 2:H:1093:GLN:CG   | 2.47                     | 0.40              |
| 2:H:1090:LYS:HA  | 2:H:1090:LYS:HD3  | 1.89                     | 0.40              |
| 2:H:206:THR:HG23 | 2:H:207:LEU:H     | 1.86                     | 0.40              |
| 3:D:166:GLN:CB   | 2:H:210:GLU:HG3   | 2.42                     | 0.40              |
| 2:H:265:ARG:O    | 2:H:288:ARG:HG2   | 2.21                     | 0.40              |
| 2:H:311:PHE:N    | 2:H:311:PHE:HD2   | 2.18                     | 0.40              |
| 2:H:332:ARG:NH1  | 2:H:338:GLU:CD    | 2.73                     | 0.40              |
| 2:H:575:GLN:HB2  | 2:H:670:GLN:HG2   | 2.03                     | 0.40              |
| 2:H:84:ARG:HG3   | 2:H:84:ARG:NH1    | 2.35                     | 0.40              |
| 3:I:119:SER:H    | 3:I:123:LEU:HD22  | 1.87                     | 0.40              |
| 3:I:1225:ALA:HB2 | 3:I:1370:ILE:CD1  | 2.52                     | 0.40              |
| 3:I:1273:VAL:O   | 3:I:1273:VAL:CG2  | 2.69                     | 0.40              |
| 3:I:1403:LEU:O   | 3:I:1407:LEU:HD13 | 2.20                     | 0.40              |
| 3:I:451:ASP:C    | 3:I:452:ILE:CG2   | 2.89                     | 0.40              |
| 3:I:549:ASN:HA   | 3:I:549:ASN:HD22  | 1.56                     | 0.40              |
| 3:I:907:GLU:O    | 3:I:911:LEU:HD12  | 2.21                     | 0.40              |
| 3:I:970:LYS:HA   | 3:I:973:GLN:HE21  | 1.86                     | 0.40              |
| 3:I:995:LEU:O    | 3:I:999:THR:HB    | 2.22                     | 0.40              |
| 1:K:121:GLU:HG2  | 1:K:122:ILE:N     | 2.36                     | 0.40              |
| 1:K:111:ALA:HA   | 1:K:129:ILE:HD11  | 2.02                     | 0.40              |
| 1:K:218:LEU:CD2  | 1:L:222:LEU:HD21  | 2.51                     | 0.40              |
| 1:L:48:ILE:HG21  | 1:L:173:PRO:HD2   | 2.03                     | 0.40              |
| 2:M:141:HIS:CD2  | 2:M:141:HIS:N     | 2.89                     | 0.40              |
| 2:M:346:VAL:O    | 2:M:350:ARG:HG3   | 2.21                     | 0.40              |
| 2:M:39:ARG:HD2   | 2:M:45:GLN:CD     | 2.36                     | 0.40              |
| 2:M:575:GLN:HB2  | 2:M:670:GLN:HG2   | 2.04                     | 0.40              |
| 2:M:604:ALA:HB3  | 2:M:612:VAL:O     | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:918:LEU:HD23  | 2:M:968:LEU:HA    | 2.02                     | 0.40              |
| 3:N:1151:ARG:HA   | 3:N:1162:GLU:HG3  | 2.03                     | 0.40              |
| 3:N:1286:THR:O    | 3:N:1287:GLU:HB2  | 2.21                     | 0.40              |
| 3:N:624:ASP:O     | 3:N:625:TYR:HB2   | 2.22                     | 0.40              |
| 2:M:681:GLY:HA3   | 3:N:635:PRO:HB3   | 2.03                     | 0.40              |
| 2:M:678:PRO:O     | 3:N:943:THR:HA    | 2.22                     | 0.40              |
| 4:O:37:ASN:N      | 4:O:37:ASN:ND2    | 2.69                     | 0.40              |
| 7:Y:123:SER:O     | 7:Y:126:GLY:N     | 2.54                     | 0.40              |
| 7:Y:152:VAL:O     | 7:Y:153:ALA:HB2   | 2.21                     | 0.40              |
| 3:I:1052:THR:CG2  | 7:Y:57:ARG:HH11   | 2.34                     | 0.40              |
| 7:Z:152:VAL:O     | 7:Z:153:ALA:HB2   | 2.21                     | 0.40              |
| 1:A:121:GLU:HG2   | 1:A:122:ILE:N     | 2.36                     | 0.40              |
| 1:B:99:LEU:HB2    | 1:B:142:VAL:HG23  | 2.03                     | 0.40              |
| 1:B:56:VAL:HG21   | 1:B:82:LEU:HD12   | 2.03                     | 0.40              |
| 2:C:103:LYS:HG2   | 2:C:103:LYS:H     | 1.70                     | 0.40              |
| 2:C:140:ILE:CG2   | 2:C:410:ILE:HG21  | 2.50                     | 0.40              |
| 2:C:191:PHE:CE2   | 2:C:192:PRO:O     | 2.74                     | 0.40              |
| 2:C:263:ASP:C     | 2:C:264:PRO:O     | 2.60                     | 0.40              |
| 2:C:368:THR:O     | 2:C:369:PRO:C     | 2.58                     | 0.40              |
| 2:C:541:SER:O     | 2:C:545:ASN:HB2   | 2.21                     | 0.40              |
| 2:C:626:ARG:HB2   | 2:C:639:GLN:HE21  | 1.86                     | 0.40              |
| 3:D:1084:THR:HA   | 3:D:1087:ARG:HH11 | 1.85                     | 0.40              |
| 3:D:1096:ARG:NE   | 3:D:1100:ASP:OD2  | 2.54                     | 0.40              |
| 3:D:483:HIS:CB    | 3:D:484:PRO:HD3   | 2.37                     | 0.40              |
| 3:D:29:PRO:HD3    | 3:D:548:ILE:CG2   | 2.50                     | 0.40              |
| 3:D:793:THR:O     | 3:D:879:ARG:NH1   | 2.54                     | 0.40              |
| 3:D:820:GLU:CD    | 3:D:820:GLU:C     | 2.79                     | 0.40              |
| 1:F:165:ILE:HA    | 1:F:166:PRO:HD3   | 1.90                     | 0.40              |
| 1:F:206:THR:HG22  | 1:F:209:GLU:HG2   | 2.03                     | 0.40              |
| 1:G:88:ARG:HD2    | 1:G:123:MET:CE    | 2.51                     | 0.40              |
| 1:G:99:LEU:HB2    | 1:G:142:VAL:HG23  | 2.02                     | 0.40              |
| 2:H:414:GLY:O     | 2:H:416:GLY:N     | 2.55                     | 0.40              |
| 2:H:494:TYR:CD1   | 2:H:494:TYR:N     | 2.89                     | 0.40              |
| 2:H:500:ASN:OD1   | 3:I:1067:VAL:HG23 | 2.21                     | 0.40              |
| 2:H:473:ARG:HA    | 2:H:531:PHE:CE1   | 2.56                     | 0.40              |
| 2:H:568:ALA:HB1   | 2:H:668:LEU:HB3   | 2.02                     | 0.40              |
| 2:H:625:LEU:HD11  | 2:H:641:PRO:HG3   | 2.03                     | 0.40              |
| 2:H:716:LYS:HB3   | 2:H:716:LYS:HE2   | 1.95                     | 0.40              |
| 3:I:1280:VAL:HG22 | 3:I:1295:GLU:O    | 2.22                     | 0.40              |
| 3:I:1468:LEU:HD22 | 3:I:1470:ARG:HD3  | 2.03                     | 0.40              |
| 3:I:632:VAL:O     | 3:I:727:GLN:HA    | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:25:LYS:HA     | 4:J:28:GLN:CD     | 2.41                     | 0.40              |
| 4:J:47:LYS:C      | 4:J:54:LEU:HD12   | 2.42                     | 0.40              |
| 4:J:54:LEU:CD2    | 4:J:58:PRO:CG     | 2.99                     | 0.40              |
| 1:K:30:ARG:NH1    | 1:K:30:ARG:HG2    | 2.36                     | 0.40              |
| 2:M:1047:HIS:N    | 2:M:1047:HIS:CD2  | 2.88                     | 0.40              |
| 2:M:10:ARG:HA     | 2:M:10:ARG:HD3    | 1.84                     | 0.40              |
| 2:M:178:PRO:C     | 2:M:180:GLY:H     | 2.25                     | 0.40              |
| 2:M:835:VAL:HG13  | 2:M:836:GLY:N     | 2.36                     | 0.40              |
| 3:N:1120:VAL:CG2  | 3:N:1188:VAL:HG11 | 2.51                     | 0.40              |
| 3:N:1274:ILE:HD12 | 3:N:1274:ILE:C    | 2.41                     | 0.40              |
| 3:N:160:GLU:HG2   | 3:N:165:LYS:CB    | 2.51                     | 0.40              |
| 3:N:845:ASN:H     | 3:N:848:GLU:HG3   | 1.86                     | 0.40              |
| 3:N:907:GLU:O     | 3:N:911:LEU:HD12  | 2.21                     | 0.40              |
| 3:N:995:LEU:O     | 3:N:999:THR:HB    | 2.22                     | 0.40              |
| 4:O:68:LEU:HD12   | 4:O:73:LEU:HD13   | 2.04                     | 0.40              |
| 7:X:102:VAL:CG1   | 7:X:103:GLN:N     | 2.83                     | 0.40              |
| 7:X:132:HIS:NE2   | 7:X:138:LEU:HD22  | 2.36                     | 0.40              |
| 1:B:13:VAL:HG13   | 1:B:23:PHE:CE1    | 2.57                     | 0.40              |
| 1:B:34:VAL:HG23   | 1:B:181:VAL:HG21  | 2.03                     | 0.40              |
| 1:B:52:ALA:HB1    | 1:B:170:VAL:N     | 2.36                     | 0.40              |
| 1:B:73:GLU:HB2    | 1:B:78:ILE:CG1    | 2.50                     | 0.40              |
| 2:C:1031:ARG:HG2  | 2:C:1033:GLY:H    | 1.86                     | 0.40              |
| 2:C:1040:LEU:HD23 | 2:C:1049:LEU:HA   | 2.03                     | 0.40              |
| 2:C:1085:PHE:CD2  | 3:D:1468:LEU:HA   | 2.57                     | 0.40              |
| 2:C:1096:ALA:O    | 2:C:1097:LEU:C    | 2.60                     | 0.40              |
| 2:C:266:ARG:CD    | 2:C:266:ARG:O     | 2.63                     | 0.40              |
| 2:C:141:HIS:HB3   | 2:C:418:LEU:HB3   | 2.03                     | 0.40              |
| 2:C:45:GLN:HG2    | 2:C:45:GLN:O      | 2.21                     | 0.40              |
| 2:C:572:ILE:HG13  | 2:C:701:THR:O     | 2.20                     | 0.40              |
| 2:C:69:LEU:HB2    | 2:C:97:ARG:O      | 2.21                     | 0.40              |
| 2:C:78:PHE:HB3    | 2:C:79:PRO:HD2    | 2.02                     | 0.40              |
| 3:D:1065:LEU:HD23 | 3:D:1070:TYR:CD2  | 2.56                     | 0.40              |
| 3:D:1122:LEU:CD1  | 3:D:1185:GLU:HA   | 2.45                     | 0.40              |
| 3:D:1327:ARG:HG3  | 3:D:1328:GLY:N    | 2.34                     | 0.40              |
| 2:C:1093:GLN:OE1  | 3:D:21:TRP:CE3    | 2.75                     | 0.40              |
| 3:D:524:LEU:N     | 3:D:524:LEU:HD12  | 2.36                     | 0.40              |
| 3:D:639:LEU:HD12  | 3:D:640:HIS:H     | 1.85                     | 0.40              |
| 3:D:749:VAL:HA    | 3:D:750:PRO:HD3   | 1.71                     | 0.40              |
| 3:D:995:LEU:O     | 3:D:999:THR:HB    | 2.22                     | 0.40              |
| 4:E:43:GLU:O      | 4:E:44:GLU:CB     | 2.68                     | 0.40              |
| 1:F:117:VAL:CG1   | 1:F:120:VAL:HG12  | 2.52                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:F:121:GLU:HG2   | 1:F:122:ILE:N    | 2.36                     | 0.40              |
| 1:F:65:PHE:CD1    | 1:F:65:PHE:N     | 2.89                     | 0.40              |
| 1:G:86:VAL:CG1    | 1:G:124:ASN:HB2  | 2.51                     | 0.40              |
| 2:H:309:TYR:CD1   | 2:H:313:LEU:CD1  | 2.97                     | 0.40              |
| 2:H:338:GLU:HA    | 2:H:341:THR:CG2  | 2.52                     | 0.40              |
| 2:H:729:LEU:C     | 2:H:729:LEU:HD23 | 2.41                     | 0.40              |
| 2:H:739:GLU:OE1   | 2:H:742:VAL:HB   | 2.22                     | 0.40              |
| 2:H:73:LEU:HD12   | 2:H:74:GLY:N     | 2.36                     | 0.40              |
| 2:H:90:TYR:CD1    | 2:H:90:TYR:O     | 2.74                     | 0.40              |
| 2:H:897:LEU:CD2   | 2:H:921:ALA:HA   | 2.49                     | 0.40              |
| 3:I:1047:LYS:CB   | 3:I:1048:PRO:CD  | 2.94                     | 0.40              |
| 3:I:1065:LEU:HD23 | 3:I:1070:TYR:CD2 | 2.57                     | 0.40              |
| 3:I:1331:ASP:HA   | 3:I:1332:PRO:HD3 | 1.90                     | 0.40              |
| 3:I:1105:ILE:HD11 | 3:I:1374:GLN:NE2 | 2.37                     | 0.40              |
| 3:I:497:GLU:O     | 3:I:500:ARG:HB3  | 2.21                     | 0.40              |
| 3:I:584:ASN:OD1   | 3:I:590:PRO:HG2  | 2.21                     | 0.40              |
| 3:I:866:VAL:HG11  | 3:I:880:ILE:HD11 | 2.04                     | 0.40              |
| 1:K:35:THR:O      | 1:K:39:PRO:HG2   | 2.22                     | 0.40              |
| 2:M:295:ASP:O     | 2:M:297:GLU:N    | 2.50                     | 0.40              |
| 2:M:328:LEU:HD13  | 2:M:433:THR:CB   | 2.27                     | 0.40              |
| 2:M:35:PRO:C      | 2:M:37:GLU:N     | 2.75                     | 0.40              |
| 2:M:399:ASN:HD22  | 2:M:668:LEU:HD23 | 1.86                     | 0.40              |
| 2:M:477:GLY:O     | 2:M:507:ARG:HA   | 2.21                     | 0.40              |
| 2:M:678:PRO:HG2   | 3:N:947:ILE:CD1  | 2.45                     | 0.40              |
| 2:M:874:LEU:O     | 3:N:1029:ARG:HD3 | 2.22                     | 0.40              |
| 3:N:1225:ALA:HB2  | 3:N:1370:ILE:CD1 | 2.52                     | 0.40              |
| 3:N:1293:PHE:CE1  | 3:N:1302:GLU:HA  | 2.57                     | 0.40              |
| 3:N:447:VAL:HG22  | 3:N:447:VAL:H    | 1.53                     | 0.40              |
| 3:N:502:PHE:CE1   | 3:N:509:PRO:HB3  | 2.56                     | 0.40              |
| 3:N:729:HIS:HB3   | 3:N:732:VAL:CG2  | 2.51                     | 0.40              |
| 3:N:820:GLU:CD    | 3:N:820:GLU:C    | 2.80                     | 0.40              |
| 7:Z:123:SER:O     | 7:Z:126:GLY:N    | 2.54                     | 0.40              |
| 7:Z:20:GLU:O      | 7:Z:23:ARG:HB2   | 2.21                     | 0.40              |
| 1:A:122:ILE:N     | 1:A:122:ILE:HD12 | 2.36                     | 0.40              |
| 2:C:99:GLN:NE2    | 2:C:101:ILE:HD11 | 2.36                     | 0.40              |
| 2:C:127:PHE:O     | 2:C:133:ASP:HA   | 2.20                     | 0.40              |
| 2:C:250:ARG:HG2   | 2:C:250:ARG:H    | 1.33                     | 0.40              |
| 2:C:267:TYR:O     | 2:C:268:ASP:C    | 2.60                     | 0.40              |
| 2:C:363:SER:O     | 2:C:366:SER:HB2  | 2.22                     | 0.40              |
| 2:C:395:LYS:HE2   | 2:C:397:GLU:CD   | 2.42                     | 0.40              |
| 2:C:395:LYS:O     | 2:C:397:GLU:HG3  | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:554:ASP:HA    | 3:D:1061:PHE:CZ   | 2.57                     | 0.40              |
| 2:C:739:GLU:OE1   | 2:C:742:VAL:HB    | 2.22                     | 0.40              |
| 3:D:1112:CYS:CB   | 3:D:1201:CYS:SG   | 3.09                     | 0.40              |
| 3:D:138:LYS:HG2   | 3:D:138:LYS:O     | 2.21                     | 0.40              |
| 3:D:1442:ASN:O    | 3:D:1446:VAL:HG23 | 2.21                     | 0.40              |
| 3:D:1476:THR:O    | 3:D:1476:THR:CG2  | 2.69                     | 0.40              |
| 3:D:409:VAL:O     | 3:D:410:SER:HB2   | 2.21                     | 0.40              |
| 3:D:704:ARG:HH12  | 3:D:743:ASP:CB    | 2.35                     | 0.40              |
| 3:D:843:PHE:CD2   | 3:D:849:ALA:HA    | 2.57                     | 0.40              |
| 3:D:845:ASN:O     | 3:D:848:GLU:HB2   | 2.20                     | 0.40              |
| 1:F:122:ILE:N     | 1:F:122:ILE:HD12  | 2.36                     | 0.40              |
| 1:F:216:GLU:CD    | 1:F:219:ARG:HH21  | 2.25                     | 0.40              |
| 1:F:8:ALA:O       | 1:F:9:PRO:C       | 2.60                     | 0.40              |
| 1:G:143:ARG:NH1   | 1:G:158:ILE:HG23  | 2.37                     | 0.40              |
| 1:G:65:PHE:N      | 1:G:65:PHE:CD1    | 2.89                     | 0.40              |
| 2:H:1035:MET:HB3  | 2:H:1036:GLU:OE1  | 2.21                     | 0.40              |
| 2:H:1046:ALA:HB2  | 3:I:1476:THR:HB   | 2.04                     | 0.40              |
| 2:H:165:LEU:CD2   | 2:H:418:LEU:HG    | 2.51                     | 0.40              |
| 2:H:277:ALA:O     | 2:H:278:GLU:C     | 2.60                     | 0.40              |
| 2:H:31:GLN:HE22   | 2:H:39:ARG:CB     | 2.35                     | 0.40              |
| 2:H:441:VAL:HG12  | 2:H:559:LEU:CA    | 2.51                     | 0.40              |
| 2:H:816:LYS:HB2   | 2:H:819:VAL:HG21  | 2.04                     | 0.40              |
| 3:I:1042:ARG:HB2  | 3:I:1042:ARG:NH1  | 2.36                     | 0.40              |
| 3:I:1061:PHE:CE1  | 3:I:1065:LEU:HD22 | 2.41                     | 0.40              |
| 3:I:1305:LEU:HD12 | 3:I:1311:LEU:CD2  | 2.31                     | 0.40              |
| 3:I:138:LYS:CD    | 3:I:138:LYS:N     | 2.85                     | 0.40              |
| 3:I:704:ARG:HH12  | 3:I:743:ASP:CB    | 2.35                     | 0.40              |
| 3:I:729:HIS:HB3   | 3:I:732:VAL:CG2   | 2.51                     | 0.40              |
| 3:I:813:LEU:C     | 3:I:813:LEU:HD12  | 2.41                     | 0.40              |
| 1:K:11:PHE:CB     | 1:K:25:LEU:HD13   | 2.48                     | 0.40              |
| 1:L:73:GLU:OE1    | 1:L:131:THR:N     | 2.54                     | 0.40              |
| 1:L:56:VAL:HG12   | 1:L:58:ILE:CD1    | 2.51                     | 0.40              |
| 2:M:202:TYR:CZ    | 2:M:304:LEU:CD2   | 3.04                     | 0.40              |
| 2:M:199:VAL:CG1   | 2:M:235:LEU:HD12  | 2.51                     | 0.40              |
| 2:M:348:LEU:HA    | 2:M:348:LEU:HD12  | 1.89                     | 0.40              |
| 2:M:465:GLY:O     | 2:M:466:PHE:C     | 2.59                     | 0.40              |
| 3:N:1042:ARG:NH1  | 3:N:1042:ARG:HB2  | 2.36                     | 0.40              |
| 3:N:1112:CYS:HB2  | 3:N:1195:GLN:OE1  | 2.21                     | 0.40              |
| 3:N:447:VAL:O     | 3:N:449:SER:N     | 2.54                     | 0.40              |
| 3:N:134:VAL:HG23  | 3:N:455:ARG:H     | 1.86                     | 0.40              |
| 7:Z:125:MET:SD    | 7:Z:125:MET:C     | 2.99                     | 0.40              |



All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1           | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------------|--------------------------|-------------------|
| 1:A:100:LEU:CD1  | 1:F:59:GLU:OE1[2_455]  | 1.51                     | 0.69              |
| 3:D:1182:GLU:OE2 | 1:G:112:ARG:NE[1_655]  | 1.61                     | 0.59              |
| 1:B:162:ILE:CG1  | 3:N:976:GLN:NE2[1_655] | 1.90                     | 0.30              |
| 1:A:100:LEU:CD1  | 1:F:59:GLU:CD[2_455]   | 1.97                     | 0.23              |
| 2:C:223:ASP:O    | 3:N:562:ALA:O[2_444]   | 2.02                     | 0.18              |
| 3:D:1182:GLU:OE2 | 1:G:112:ARG:CD[1_655]  | 2.05                     | 0.15              |
| 3:I:159:ARG:NH1  | 2:M:218:VAL:CG1[2_445] | 2.06                     | 0.14              |
| 3:D:1181:GLY:O   | 1:G:112:ARG:O[1_655]   | 2.14                     | 0.06              |
| 1:B:162:ILE:CD1  | 3:N:976:GLN:NE2[1_655] | 2.17                     | 0.03              |
| 1:A:115:LEU:CD2  | 1:F:161:ARG:CD[2_455]  | 2.18                     | 0.02              |

## 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     | 221/315 (70%)   | 191 (86%)  | 22 (10%)  | 8 (4%)   | 3           | 28 |
| 1   | B     | 221/315 (70%)   | 191 (86%)  | 27 (12%)  | 3 (1%)   | 11          | 47 |
| 1   | F     | 221/315 (70%)   | 191 (86%)  | 20 (9%)   | 10 (4%)  | 2           | 24 |
| 1   | G     | 222/315 (70%)   | 193 (87%)  | 26 (12%)  | 3 (1%)   | 11          | 47 |
| 1   | K     | 223/315 (71%)   | 193 (86%)  | 21 (9%)   | 9 (4%)   | 3           | 26 |
| 1   | L     | 221/315 (70%)   | 188 (85%)  | 28 (13%)  | 5 (2%)   | 6           | 37 |
| 2   | C     | 1077/1119 (96%) | 864 (80%)  | 150 (14%) | 63 (6%)  | 1           | 20 |
| 2   | H     | 1074/1119 (96%) | 867 (81%)  | 145 (14%) | 62 (6%)  | 1           | 20 |
| 2   | M     | 1078/1119 (96%) | 871 (81%)  | 149 (14%) | 58 (5%)  | 2           | 22 |
| 3   | D     | 1306/1524 (86%) | 1062 (81%) | 186 (14%) | 58 (4%)  | 2           | 25 |
| 3   | I     | 1252/1524 (82%) | 1012 (81%) | 177 (14%) | 63 (5%)  | 2           | 23 |
| 3   | N     | 1317/1524 (86%) | 1052 (80%) | 196 (15%) | 69 (5%)  | 2           | 22 |

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| Mol | Chain | Analysed         | Favoured   | Allowed    | Outliers | Percentiles |    |
|-----|-------|------------------|------------|------------|----------|-------------|----|
| 4   | E     | 91/99 (92%)      | 67 (74%)   | 17 (19%)   | 7 (8%)   | 1           | 15 |
| 4   | J     | 91/99 (92%)      | 70 (77%)   | 14 (15%)   | 7 (8%)   | 1           | 15 |
| 4   | O     | 91/99 (92%)      | 68 (75%)   | 16 (18%)   | 7 (8%)   | 1           | 15 |
| 7   | X     | 152/156 (97%)    | 132 (87%)  | 16 (10%)   | 4 (3%)   | 5           | 35 |
| 7   | Y     | 150/156 (96%)    | 135 (90%)  | 12 (8%)    | 3 (2%)   | 7           | 40 |
| 7   | Z     | 150/156 (96%)    | 131 (87%)  | 16 (11%)   | 3 (2%)   | 7           | 40 |
| All | All   | 9158/10584 (86%) | 7478 (82%) | 1238 (14%) | 442 (5%) | 2           | 23 |

All (442) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 187  | GLY  |
| 2   | C     | 23   | VAL  |
| 2   | C     | 40   | GLU  |
| 2   | C     | 44   | ILE  |
| 2   | C     | 152  | PRO  |
| 2   | C     | 164  | PRO  |
| 2   | C     | 231  | PRO  |
| 2   | C     | 250  | ARG  |
| 2   | C     | 253  | ALA  |
| 2   | C     | 264  | PRO  |
| 2   | C     | 364  | GLU  |
| 2   | C     | 808  | ARG  |
| 2   | C     | 809  | GLY  |
| 2   | C     | 864  | GLY  |
| 2   | C     | 905  | ILE  |
| 2   | C     | 1033 | GLY  |
| 2   | C     | 1106 | ASP  |
| 3   | D     | 136  | ASP  |
| 3   | D     | 594  | PRO  |
| 3   | D     | 683  | ILE  |
| 3   | D     | 696  | HIS  |
| 3   | D     | 705  | ALA  |
| 3   | D     | 832  | ARG  |
| 3   | D     | 1028 | ALA  |
| 3   | D     | 1125 | PRO  |
| 3   | D     | 1129 | THR  |
| 3   | D     | 1287 | GLU  |
| 3   | D     | 1432 | LYS  |
| 3   | D     | 1441 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | E     | 42   | PRO  |
| 4   | E     | 58   | PRO  |
| 1   | G     | 187  | GLY  |
| 2   | H     | 40   | GLU  |
| 2   | H     | 44   | ILE  |
| 2   | H     | 105  | THR  |
| 2   | H     | 152  | PRO  |
| 2   | H     | 181  | VAL  |
| 2   | H     | 231  | PRO  |
| 2   | H     | 243  | ARG  |
| 2   | H     | 250  | ARG  |
| 2   | H     | 253  | ALA  |
| 2   | H     | 364  | GLU  |
| 2   | H     | 727  | PRO  |
| 2   | H     | 808  | ARG  |
| 2   | H     | 809  | GLY  |
| 2   | H     | 864  | GLY  |
| 2   | H     | 905  | ILE  |
| 2   | H     | 1106 | ASP  |
| 3   | I     | 120  | ALA  |
| 3   | I     | 137  | PRO  |
| 3   | I     | 448  | GLU  |
| 3   | I     | 539  | ASP  |
| 3   | I     | 594  | PRO  |
| 3   | I     | 696  | HIS  |
| 3   | I     | 705  | ALA  |
| 3   | I     | 832  | ARG  |
| 3   | I     | 1028 | ALA  |
| 3   | I     | 1125 | PRO  |
| 3   | I     | 1287 | GLU  |
| 3   | I     | 1441 | GLN  |
| 3   | I     | 1454 | GLY  |
| 4   | J     | 42   | PRO  |
| 1   | L     | 187  | GLY  |
| 2   | M     | 50   | GLU  |
| 2   | M     | 152  | PRO  |
| 2   | M     | 179  | ASN  |
| 2   | M     | 181  | VAL  |
| 2   | M     | 231  | PRO  |
| 2   | M     | 244  | PRO  |
| 2   | M     | 250  | ARG  |
| 2   | M     | 253  | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 364  | GLU  |
| 2   | M     | 808  | ARG  |
| 2   | M     | 809  | GLY  |
| 2   | M     | 864  | GLY  |
| 2   | M     | 905  | ILE  |
| 2   | M     | 1055 | LEU  |
| 2   | M     | 1106 | ASP  |
| 3   | N     | 120  | ALA  |
| 3   | N     | 137  | PRO  |
| 3   | N     | 151  | GLN  |
| 3   | N     | 192  | ALA  |
| 3   | N     | 539  | ASP  |
| 3   | N     | 594  | PRO  |
| 3   | N     | 665  | GLY  |
| 3   | N     | 696  | HIS  |
| 3   | N     | 705  | ALA  |
| 3   | N     | 832  | ARG  |
| 3   | N     | 1028 | ALA  |
| 3   | N     | 1125 | PRO  |
| 3   | N     | 1287 | GLU  |
| 3   | N     | 1441 | GLN  |
| 4   | O     | 42   | PRO  |
| 1   | A     | 9    | PRO  |
| 1   | A     | 111  | ALA  |
| 2   | C     | 10   | ARG  |
| 2   | C     | 43   | GLY  |
| 2   | C     | 105  | THR  |
| 2   | C     | 129  | ILE  |
| 2   | C     | 156  | GLY  |
| 2   | C     | 213  | ALA  |
| 2   | C     | 218  | VAL  |
| 2   | C     | 252  | LYS  |
| 2   | C     | 278  | GLU  |
| 2   | C     | 290  | LEU  |
| 2   | C     | 396  | ASP  |
| 2   | C     | 450  | GLY  |
| 2   | C     | 466  | PHE  |
| 2   | C     | 684  | PHE  |
| 2   | C     | 740  | GLU  |
| 2   | C     | 908  | GLY  |
| 2   | C     | 998  | TYR  |
| 2   | C     | 1055 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 31   | THR  |
| 3   | D     | 458  | ALA  |
| 3   | D     | 639  | LEU  |
| 3   | D     | 665  | GLY  |
| 3   | D     | 737  | ASN  |
| 3   | D     | 803  | GLY  |
| 3   | D     | 808  | THR  |
| 3   | D     | 844  | ALA  |
| 3   | D     | 1111 | ASP  |
| 3   | D     | 1454 | GLY  |
| 4   | E     | 82   | GLU  |
| 1   | F     | 111  | ALA  |
| 2   | H     | 10   | ARG  |
| 2   | H     | 23   | VAL  |
| 2   | H     | 43   | GLY  |
| 2   | H     | 129  | ILE  |
| 2   | H     | 156  | GLY  |
| 2   | H     | 213  | ALA  |
| 2   | H     | 283  | ILE  |
| 2   | H     | 290  | LEU  |
| 2   | H     | 684  | PHE  |
| 2   | H     | 740  | GLU  |
| 2   | H     | 908  | GLY  |
| 2   | H     | 998  | TYR  |
| 2   | H     | 1033 | GLY  |
| 2   | H     | 1055 | LEU  |
| 3   | I     | 119  | SER  |
| 3   | I     | 151  | GLN  |
| 3   | I     | 458  | ALA  |
| 3   | I     | 639  | LEU  |
| 3   | I     | 665  | GLY  |
| 3   | I     | 737  | ASN  |
| 3   | I     | 844  | ALA  |
| 3   | I     | 1111 | ASP  |
| 3   | I     | 1129 | THR  |
| 3   | I     | 1208 | ASP  |
| 3   | I     | 1432 | LYS  |
| 4   | J     | 46   | PRO  |
| 4   | J     | 58   | PRO  |
| 4   | J     | 82   | GLU  |
| 1   | K     | 9    | PRO  |
| 1   | K     | 111  | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 156  | GLY  |
| 2   | M     | 164  | PRO  |
| 2   | M     | 262  | ALA  |
| 2   | M     | 278  | GLU  |
| 2   | M     | 450  | GLY  |
| 2   | M     | 466  | PHE  |
| 2   | M     | 684  | PHE  |
| 2   | M     | 727  | PRO  |
| 2   | M     | 740  | GLU  |
| 2   | M     | 908  | GLY  |
| 2   | M     | 998  | TYR  |
| 2   | M     | 1033 | GLY  |
| 3   | N     | 31   | THR  |
| 3   | N     | 119  | SER  |
| 3   | N     | 136  | ASP  |
| 3   | N     | 146  | PRO  |
| 3   | N     | 189  | GLN  |
| 3   | N     | 639  | LEU  |
| 3   | N     | 737  | ASN  |
| 3   | N     | 844  | ALA  |
| 3   | N     | 1111 | ASP  |
| 3   | N     | 1129 | THR  |
| 3   | N     | 1208 | ASP  |
| 3   | N     | 1252 | ILE  |
| 3   | N     | 1454 | GLY  |
| 4   | O     | 58   | PRO  |
| 4   | O     | 82   | GLU  |
| 7   | Y     | 47   | GLY  |
| 7   | Y     | 94   | PRO  |
| 1   | A     | 125  | PRO  |
| 1   | A     | 133  | GLU  |
| 1   | A     | 224  | TYR  |
| 1   | A     | 226  | SER  |
| 1   | B     | 125  | PRO  |
| 2   | C     | 50   | GLU  |
| 2   | C     | 80   | GLN  |
| 2   | C     | 277  | ALA  |
| 2   | C     | 517  | ARG  |
| 2   | C     | 545  | ASN  |
| 2   | C     | 727  | PRO  |
| 2   | C     | 859  | PRO  |
| 3   | D     | 96   | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 98   | PRO  |
| 3   | D     | 144  | GLY  |
| 3   | D     | 448  | GLU  |
| 3   | D     | 507  | ASN  |
| 3   | D     | 735  | ALA  |
| 3   | D     | 1085 | ALA  |
| 3   | D     | 1269 | LYS  |
| 3   | D     | 1410 | GLU  |
| 3   | D     | 1459 | LEU  |
| 4   | E     | 44   | GLU  |
| 4   | E     | 46   | PRO  |
| 1   | F     | 9    | PRO  |
| 1   | F     | 72   | LYS  |
| 1   | F     | 125  | PRO  |
| 1   | F     | 133  | GLU  |
| 1   | F     | 191  | ASP  |
| 1   | F     | 224  | TYR  |
| 1   | F     | 226  | SER  |
| 2   | H     | 50   | GLU  |
| 2   | H     | 80   | GLN  |
| 2   | H     | 164  | PRO  |
| 2   | H     | 179  | ASN  |
| 2   | H     | 252  | LYS  |
| 2   | H     | 261  | ILE  |
| 2   | H     | 278  | GLU  |
| 2   | H     | 396  | ASP  |
| 2   | H     | 466  | PHE  |
| 2   | H     | 517  | ARG  |
| 2   | H     | 545  | ASN  |
| 2   | H     | 859  | PRO  |
| 2   | H     | 1012 | PRO  |
| 2   | H     | 1046 | ALA  |
| 3   | I     | 96   | ALA  |
| 3   | I     | 98   | PRO  |
| 3   | I     | 117  | ASP  |
| 3   | I     | 136  | ASP  |
| 3   | I     | 144  | GLY  |
| 3   | I     | 146  | PRO  |
| 3   | I     | 507  | ASN  |
| 3   | I     | 735  | ALA  |
| 3   | I     | 807  | ALA  |
| 3   | I     | 808  | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | I     | 1269 | LYS  |
| 3   | I     | 1306 | PRO  |
| 3   | I     | 1410 | GLU  |
| 4   | J     | 44   | GLU  |
| 1   | K     | 125  | PRO  |
| 1   | K     | 133  | GLU  |
| 1   | K     | 224  | TYR  |
| 2   | M     | 23   | VAL  |
| 2   | M     | 141  | HIS  |
| 2   | M     | 144  | PRO  |
| 2   | M     | 213  | ALA  |
| 2   | M     | 261  | ILE  |
| 2   | M     | 290  | LEU  |
| 2   | M     | 517  | ARG  |
| 2   | M     | 545  | ASN  |
| 2   | M     | 859  | PRO  |
| 2   | M     | 1012 | PRO  |
| 3   | N     | 96   | ALA  |
| 3   | N     | 98   | PRO  |
| 3   | N     | 117  | ASP  |
| 3   | N     | 140  | ALA  |
| 3   | N     | 142  | LEU  |
| 3   | N     | 143  | ASN  |
| 3   | N     | 382  | GLU  |
| 3   | N     | 392  | SER  |
| 3   | N     | 507  | ASN  |
| 3   | N     | 735  | ALA  |
| 3   | N     | 802  | ALA  |
| 3   | N     | 808  | THR  |
| 3   | N     | 1269 | LYS  |
| 3   | N     | 1286 | THR  |
| 3   | N     | 1298 | GLY  |
| 3   | N     | 1306 | PRO  |
| 3   | N     | 1410 | GLU  |
| 3   | N     | 1432 | LYS  |
| 3   | N     | 1489 | GLN  |
| 4   | O     | 44   | GLU  |
| 4   | O     | 46   | PRO  |
| 7   | X     | 47   | GLY  |
| 7   | X     | 94   | PRO  |
| 7   | Z     | 47   | GLY  |
| 7   | Z     | 94   | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 72   | LYS  |
| 2   | C     | 53   | PRO  |
| 2   | C     | 144  | PRO  |
| 2   | C     | 283  | ILE  |
| 2   | C     | 295  | ASP  |
| 2   | C     | 457  | ALA  |
| 2   | C     | 680  | ASP  |
| 2   | C     | 932  | GLU  |
| 2   | C     | 1012 | PRO  |
| 3   | D     | 356  | PRO  |
| 3   | D     | 409  | VAL  |
| 3   | D     | 802  | ALA  |
| 3   | D     | 822  | ALA  |
| 3   | D     | 1265 | ALA  |
| 3   | D     | 1296 | SER  |
| 3   | D     | 1298 | GLY  |
| 3   | D     | 1385 | GLY  |
| 4   | E     | 24   | ALA  |
| 1   | G     | 125  | PRO  |
| 2   | H     | 53   | PRO  |
| 2   | H     | 144  | PRO  |
| 2   | H     | 216  | GLU  |
| 2   | H     | 262  | ALA  |
| 2   | H     | 272  | ALA  |
| 2   | H     | 457  | ALA  |
| 2   | H     | 680  | ASP  |
| 2   | H     | 932  | GLU  |
| 3   | I     | 140  | ALA  |
| 3   | I     | 407  | VAL  |
| 3   | I     | 802  | ALA  |
| 3   | I     | 822  | ALA  |
| 3   | I     | 1265 | ALA  |
| 3   | I     | 1286 | THR  |
| 3   | I     | 1296 | SER  |
| 3   | I     | 1298 | GLY  |
| 3   | I     | 1385 | GLY  |
| 4   | J     | 24   | ALA  |
| 1   | K     | 30   | ARG  |
| 1   | K     | 72   | LYS  |
| 1   | K     | 226  | SER  |
| 1   | L     | 118  | ALA  |
| 2   | M     | 53   | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 272  | ALA  |
| 2   | M     | 283  | ILE  |
| 2   | M     | 424  | GLY  |
| 2   | M     | 457  | ALA  |
| 2   | M     | 680  | ASP  |
| 2   | M     | 932  | GLU  |
| 3   | N     | 160  | GLU  |
| 3   | N     | 409  | VAL  |
| 3   | N     | 549  | ASN  |
| 3   | N     | 822  | ALA  |
| 3   | N     | 1265 | ALA  |
| 3   | N     | 1296 | SER  |
| 3   | N     | 1385 | GLY  |
| 4   | O     | 24   | ALA  |
| 7   | Y     | 151  | VAL  |
| 1   | B     | 44   | LEU  |
| 2   | C     | 31   | GLN  |
| 2   | C     | 272  | ALA  |
| 2   | C     | 424  | GLY  |
| 2   | C     | 538  | GLN  |
| 3   | D     | 572  | ARG  |
| 3   | D     | 766  | ALA  |
| 3   | D     | 1197 | ARG  |
| 3   | D     | 1286 | THR  |
| 3   | D     | 1389 | LEU  |
| 3   | D     | 1489 | GLN  |
| 4   | E     | 16   | LYS  |
| 1   | F     | 30   | ARG  |
| 2   | H     | 31   | GLN  |
| 2   | H     | 424  | GLY  |
| 2   | H     | 538  | GLN  |
| 3   | I     | 483  | HIS  |
| 3   | I     | 512  | MET  |
| 3   | I     | 766  | ALA  |
| 3   | I     | 1085 | ALA  |
| 3   | I     | 1086 | LEU  |
| 3   | I     | 1197 | ARG  |
| 1   | L     | 125  | PRO  |
| 2   | M     | 10   | ARG  |
| 2   | M     | 207  | LEU  |
| 2   | M     | 216  | GLU  |
| 2   | M     | 232  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 252  | LYS  |
| 2   | M     | 295  | ASP  |
| 2   | M     | 538  | GLN  |
| 2   | M     | 1046 | ALA  |
| 3   | N     | 356  | PRO  |
| 3   | N     | 483  | HIS  |
| 3   | N     | 766  | ALA  |
| 3   | N     | 1086 | LEU  |
| 3   | N     | 1197 | ARG  |
| 2   | C     | 21   | ILE  |
| 2   | C     | 181  | VAL  |
| 2   | C     | 261  | ILE  |
| 2   | C     | 263  | ASP  |
| 2   | C     | 627  | ARG  |
| 2   | C     | 1046 | ALA  |
| 3   | D     | 377  | VAL  |
| 3   | D     | 512  | MET  |
| 3   | D     | 1224 | VAL  |
| 2   | H     | 11   | GLU  |
| 2   | H     | 277  | ALA  |
| 2   | H     | 279  | GLU  |
| 2   | H     | 627  | ARG  |
| 3   | I     | 31   | THR  |
| 3   | I     | 580  | ALA  |
| 3   | I     | 1224 | VAL  |
| 3   | I     | 1412 | LYS  |
| 3   | I     | 1459 | LEU  |
| 4   | J     | 25   | LYS  |
| 1   | L     | 59   | GLU  |
| 2   | M     | 277  | ALA  |
| 2   | M     | 369  | PRO  |
| 2   | M     | 627  | ARG  |
| 3   | N     | 410  | SER  |
| 3   | N     | 512  | MET  |
| 3   | N     | 580  | ALA  |
| 3   | N     | 1478 | SER  |
| 4   | O     | 64   | ALA  |
| 7   | X     | 115  | THR  |
| 7   | Z     | 115  | THR  |
| 3   | D     | 1223 | ILE  |
| 3   | I     | 1027 | GLY  |
| 3   | I     | 1223 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 1223 | ILE  |
| 3   | N     | 1224 | VAL  |
| 7   | X     | 151  | VAL  |
| 2   | C     | 369  | PRO  |
| 2   | C     | 548  | PRO  |
| 3   | D     | 1371 | VAL  |
| 2   | H     | 548  | PRO  |
| 3   | I     | 1371 | VAL  |
| 2   | M     | 548  | PRO  |
| 3   | N     | 1371 | VAL  |
| 2   | C     | 42   | VAL  |
| 2   | C     | 74   | GLY  |
| 3   | D     | 29   | PRO  |
| 1   | G     | 157  | GLY  |
| 3   | I     | 484  | PRO  |
| 1   | L     | 157  | GLY  |
| 2   | M     | 74   | GLY  |
| 3   | N     | 349  | PRO  |
| 3   | N     | 484  | PRO  |
| 3   | D     | 146  | PRO  |
| 3   | D     | 407  | VAL  |
| 3   | D     | 1027 | GLY  |
| 3   | D     | 1050 | GLY  |
| 2   | H     | 296  | GLY  |
| 3   | I     | 409  | VAL  |
| 3   | I     | 1050 | GLY  |
| 3   | N     | 407  | VAL  |
| 3   | N     | 1050 | GLY  |
| 1   | A     | 21   | GLY  |
| 3   | D     | 208  | PRO  |
| 3   | D     | 1306 | PRO  |
| 1   | F     | 21   | GLY  |
| 2   | H     | 369  | PRO  |
| 1   | K     | 21   | GLY  |
| 2   | M     | 368  | THR  |

### 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     | 196/273 (72%)   | 164 (84%)  | 32 (16%)   | 2           | 14 |
| 1   | B     | 196/273 (72%)   | 166 (85%)  | 30 (15%)   | 2           | 16 |
| 1   | F     | 196/273 (72%)   | 167 (85%)  | 29 (15%)   | 3           | 17 |
| 1   | G     | 196/273 (72%)   | 164 (84%)  | 32 (16%)   | 2           | 14 |
| 1   | K     | 196/273 (72%)   | 164 (84%)  | 32 (16%)   | 2           | 14 |
| 1   | L     | 196/273 (72%)   | 164 (84%)  | 32 (16%)   | 2           | 14 |
| 2   | C     | 912/941 (97%)   | 737 (81%)  | 175 (19%)  | 1           | 9  |
| 2   | H     | 909/941 (97%)   | 736 (81%)  | 173 (19%)  | 1           | 9  |
| 2   | M     | 912/941 (97%)   | 746 (82%)  | 166 (18%)  | 1           | 11 |
| 3   | D     | 1113/1279 (87%) | 928 (83%)  | 185 (17%)  | 2           | 14 |
| 3   | I     | 1068/1279 (84%) | 878 (82%)  | 190 (18%)  | 2           | 12 |
| 3   | N     | 1124/1279 (88%) | 937 (83%)  | 187 (17%)  | 2           | 14 |
| 4   | E     | 82/88 (93%)     | 72 (88%)   | 10 (12%)   | 5           | 23 |
| 4   | J     | 82/88 (93%)     | 72 (88%)   | 10 (12%)   | 5           | 23 |
| 4   | O     | 82/88 (93%)     | 67 (82%)   | 15 (18%)   | 1           | 11 |
| 7   | X     | 130/131 (99%)   | 115 (88%)  | 15 (12%)   | 5           | 24 |
| 7   | Y     | 128/131 (98%)   | 104 (81%)  | 24 (19%)   | 1           | 10 |
| 7   | Z     | 128/131 (98%)   | 110 (86%)  | 18 (14%)   | 3           | 19 |
| All | All   | 7846/8955 (88%) | 6491 (83%) | 1355 (17%) | 2           | 13 |

All (1355) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | PRO  |
| 1   | A     | 15  | THR  |
| 1   | A     | 16  | GLN  |
| 1   | A     | 20  | TYR  |
| 1   | A     | 22  | GLU  |
| 1   | A     | 26  | GLU  |
| 1   | A     | 28  | LEU  |
| 1   | A     | 30  | ARG  |
| 1   | A     | 47  | SER  |
| 1   | A     | 62  | LEU  |
| 1   | A     | 65  | PHE  |
| 1   | A     | 74  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 92  | PRO  |
| 1   | A     | 96  | THR  |
| 1   | A     | 100 | LEU  |
| 1   | A     | 101 | LEU  |
| 1   | A     | 113 | ASP  |
| 1   | A     | 123 | MET  |
| 1   | A     | 126 | ASP  |
| 1   | A     | 141 | GLU  |
| 1   | A     | 143 | ARG  |
| 1   | A     | 161 | ARG  |
| 1   | A     | 163 | ASN  |
| 1   | A     | 165 | ILE  |
| 1   | A     | 175 | ARG  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 183 | ASP  |
| 1   | A     | 184 | THR  |
| 1   | A     | 186 | LEU  |
| 1   | A     | 189 | ARG  |
| 1   | A     | 206 | THR  |
| 1   | A     | 219 | ARG  |
| 1   | B     | 18  | ARG  |
| 1   | B     | 20  | TYR  |
| 1   | B     | 25  | LEU  |
| 1   | B     | 40  | LEU  |
| 1   | B     | 54  | THR  |
| 1   | B     | 62  | LEU  |
| 1   | B     | 65  | PHE  |
| 1   | B     | 66  | SER  |
| 1   | B     | 73  | GLU  |
| 1   | B     | 95  | GLN  |
| 1   | B     | 104 | GLU  |
| 1   | B     | 122 | ILE  |
| 1   | B     | 123 | MET  |
| 1   | B     | 138 | LEU  |
| 1   | B     | 141 | GLU  |
| 1   | B     | 145 | ASP  |
| 1   | B     | 159 | LYS  |
| 1   | B     | 161 | ARG  |
| 1   | B     | 162 | ILE  |
| 1   | B     | 165 | ILE  |
| 1   | B     | 167 | VAL  |
| 1   | B     | 179 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 180 | GLN  |
| 1   | B     | 184 | THR  |
| 1   | B     | 185 | ARG  |
| 1   | B     | 186 | LEU  |
| 1   | B     | 197 | LEU  |
| 1   | B     | 198 | ARG  |
| 1   | B     | 201 | THR  |
| 1   | B     | 206 | THR  |
| 2   | C     | 6   | PHE  |
| 2   | C     | 26  | TYR  |
| 2   | C     | 30  | LEU  |
| 2   | C     | 31  | GLN  |
| 2   | C     | 34  | VAL  |
| 2   | C     | 39  | ARG  |
| 2   | C     | 41  | ASN  |
| 2   | C     | 42  | VAL  |
| 2   | C     | 48  | PHE  |
| 2   | C     | 52  | PHE  |
| 2   | C     | 75  | GLU  |
| 2   | C     | 80  | GLN  |
| 2   | C     | 88  | LEU  |
| 2   | C     | 89  | THR  |
| 2   | C     | 94  | LEU  |
| 2   | C     | 95  | TYR  |
| 2   | C     | 98  | LEU  |
| 2   | C     | 104 | ASP  |
| 2   | C     | 105 | THR  |
| 2   | C     | 113 | VAL  |
| 2   | C     | 115 | LEU  |
| 2   | C     | 122 | THR  |
| 2   | C     | 124 | ASP  |
| 2   | C     | 133 | ASP  |
| 2   | C     | 137 | VAL  |
| 2   | C     | 138 | SER  |
| 2   | C     | 141 | HIS  |
| 2   | C     | 142 | ARG  |
| 2   | C     | 158 | TYR  |
| 2   | C     | 165 | LEU  |
| 2   | C     | 168 | ARG  |
| 2   | C     | 181 | VAL  |
| 2   | C     | 182 | VAL  |
| 2   | C     | 184 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 188 | LYS  |
| 2   | C     | 190 | LYS  |
| 2   | C     | 191 | PHE  |
| 2   | C     | 194 | VAL  |
| 2   | C     | 198 | ARG  |
| 2   | C     | 200 | LEU  |
| 2   | C     | 205 | GLU  |
| 2   | C     | 210 | GLU  |
| 2   | C     | 216 | GLU  |
| 2   | C     | 222 | MET  |
| 2   | C     | 224 | GLU  |
| 2   | C     | 230 | ARG  |
| 2   | C     | 235 | LEU  |
| 2   | C     | 237 | ARG  |
| 2   | C     | 238 | LEU  |
| 2   | C     | 241 | LEU  |
| 2   | C     | 243 | ARG  |
| 2   | C     | 264 | PRO  |
| 2   | C     | 267 | TYR  |
| 2   | C     | 268 | ASP  |
| 2   | C     | 283 | ILE  |
| 2   | C     | 285 | LEU  |
| 2   | C     | 290 | LEU  |
| 2   | C     | 292 | ARG  |
| 2   | C     | 293 | PHE  |
| 2   | C     | 294 | GLU  |
| 2   | C     | 297 | GLU  |
| 2   | C     | 309 | TYR  |
| 2   | C     | 310 | LEU  |
| 2   | C     | 314 | THR  |
| 2   | C     | 325 | ILE  |
| 2   | C     | 328 | LEU  |
| 2   | C     | 343 | GLN  |
| 2   | C     | 345 | ARG  |
| 2   | C     | 348 | LEU  |
| 2   | C     | 359 | MET  |
| 2   | C     | 360 | LEU  |
| 2   | C     | 365 | ASP  |
| 2   | C     | 368 | THR  |
| 2   | C     | 369 | PRO  |
| 2   | C     | 374 | ASN  |
| 2   | C     | 376 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 383 | ARG  |
| 2   | C     | 393 | GLN  |
| 2   | C     | 394 | PHE  |
| 2   | C     | 400 | PRO  |
| 2   | C     | 413 | LEU  |
| 2   | C     | 419 | THR  |
| 2   | C     | 421 | GLU  |
| 2   | C     | 422 | ARG  |
| 2   | C     | 425 | PHE  |
| 2   | C     | 433 | THR  |
| 2   | C     | 453 | THR  |
| 2   | C     | 455 | LEU  |
| 2   | C     | 462 | ASP  |
| 2   | C     | 466 | PHE  |
| 2   | C     | 474 | VAL  |
| 2   | C     | 480 | THR  |
| 2   | C     | 481 | ASP  |
| 2   | C     | 486 | MET  |
| 2   | C     | 498 | GLN  |
| 2   | C     | 500 | ASN  |
| 2   | C     | 503 | LEU  |
| 2   | C     | 507 | ARG  |
| 2   | C     | 523 | ILE  |
| 2   | C     | 533 | ASP  |
| 2   | C     | 545 | ASN  |
| 2   | C     | 554 | ASP  |
| 2   | C     | 557 | ARG  |
| 2   | C     | 579 | VAL  |
| 2   | C     | 609 | ASN  |
| 2   | C     | 614 | ARG  |
| 2   | C     | 621 | VAL  |
| 2   | C     | 631 | SER  |
| 2   | C     | 632 | ASN  |
| 2   | C     | 635 | THR  |
| 2   | C     | 640 | ARG  |
| 2   | C     | 642 | ARG  |
| 2   | C     | 645 | VAL  |
| 2   | C     | 654 | LEU  |
| 2   | C     | 657 | ASP  |
| 2   | C     | 662 | GLU  |
| 2   | C     | 668 | LEU  |
| 2   | C     | 679 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 685 | GLU  |
| 2   | C     | 691 | SER  |
| 2   | C     | 695 | LEU  |
| 2   | C     | 699 | PHE  |
| 2   | C     | 704 | HIS  |
| 2   | C     | 714 | ASP  |
| 2   | C     | 722 | ILE  |
| 2   | C     | 725 | ASP  |
| 2   | C     | 727 | PRO  |
| 2   | C     | 728 | HIS  |
| 2   | C     | 729 | LEU  |
| 2   | C     | 738 | ASP  |
| 2   | C     | 740 | GLU  |
| 2   | C     | 794 | PRO  |
| 2   | C     | 796 | GLU  |
| 2   | C     | 803 | THR  |
| 2   | C     | 805 | ARG  |
| 2   | C     | 807 | ARG  |
| 2   | C     | 829 | GLN  |
| 2   | C     | 839 | LEU  |
| 2   | C     | 863 | ASP  |
| 2   | C     | 869 | VAL  |
| 2   | C     | 870 | ILE  |
| 2   | C     | 881 | ASN  |
| 2   | C     | 884 | GLN  |
| 2   | C     | 904 | PRO  |
| 2   | C     | 920 | GLN  |
| 2   | C     | 923 | GLU  |
| 2   | C     | 929 | ARG  |
| 2   | C     | 938 | LYS  |
| 2   | C     | 939 | ARG  |
| 2   | C     | 942 | GLU  |
| 2   | C     | 946 | ARG  |
| 2   | C     | 950 | LEU  |
| 2   | C     | 952 | LEU  |
| 2   | C     | 958 | THR  |
| 2   | C     | 963 | LEU  |
| 2   | C     | 969 | GLN  |
| 2   | C     | 975 | TYR  |
| 2   | C     | 981 | GLU  |
| 2   | C     | 988 | VAL  |
| 2   | C     | 989 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 995  | MET  |
| 2   | C     | 999  | HIS  |
| 2   | C     | 1001 | VAL  |
| 2   | C     | 1004 | LYS  |
| 2   | C     | 1008 | ARG  |
| 2   | C     | 1010 | THR  |
| 2   | C     | 1012 | PRO  |
| 2   | C     | 1021 | LEU  |
| 2   | C     | 1052 | MET  |
| 2   | C     | 1063 | ARG  |
| 2   | C     | 1088 | LEU  |
| 2   | C     | 1092 | LEU  |
| 2   | C     | 1097 | LEU  |
| 2   | C     | 1105 | LYS  |
| 2   | C     | 1111 | ILE  |
| 3   | D     | 6    | ARG  |
| 3   | D     | 21   | TRP  |
| 3   | D     | 37   | LEU  |
| 3   | D     | 41   | ARG  |
| 3   | D     | 47   | GLU  |
| 3   | D     | 52   | PRO  |
| 3   | D     | 55   | ASP  |
| 3   | D     | 95   | LEU  |
| 3   | D     | 98   | PRO  |
| 3   | D     | 102  | ILE  |
| 3   | D     | 108  | VAL  |
| 3   | D     | 112  | ILE  |
| 3   | D     | 127  | LEU  |
| 3   | D     | 128  | TYR  |
| 3   | D     | 134  | VAL  |
| 3   | D     | 138  | LYS  |
| 3   | D     | 141  | ILE  |
| 3   | D     | 142  | LEU  |
| 3   | D     | 143  | ASN  |
| 3   | D     | 145  | VAL  |
| 3   | D     | 149  | LYS  |
| 3   | D     | 151  | GLN  |
| 3   | D     | 152  | LEU  |
| 3   | D     | 153  | LEU  |
| 3   | D     | 161  | LEU  |
| 3   | D     | 162  | ARG  |
| 3   | D     | 165  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 171 | LEU  |
| 3   | D     | 205 | TYR  |
| 3   | D     | 213 | VAL  |
| 3   | D     | 349 | PRO  |
| 3   | D     | 351 | MET  |
| 3   | D     | 361 | VAL  |
| 3   | D     | 387 | LEU  |
| 3   | D     | 392 | SER  |
| 3   | D     | 394 | LEU  |
| 3   | D     | 423 | ASP  |
| 3   | D     | 434 | ARG  |
| 3   | D     | 451 | ASP  |
| 3   | D     | 452 | ILE  |
| 3   | D     | 456 | MET  |
| 3   | D     | 465 | LEU  |
| 3   | D     | 469 | ASP  |
| 3   | D     | 470 | LEU  |
| 3   | D     | 471 | GLU  |
| 3   | D     | 486 | ARG  |
| 3   | D     | 489 | ARG  |
| 3   | D     | 504 | ASP  |
| 3   | D     | 511 | TRP  |
| 3   | D     | 512 | MET  |
| 3   | D     | 525 | ARG  |
| 3   | D     | 539 | ASP  |
| 3   | D     | 546 | ARG  |
| 3   | D     | 549 | ASN  |
| 3   | D     | 581 | LEU  |
| 3   | D     | 594 | PRO  |
| 3   | D     | 614 | PHE  |
| 3   | D     | 624 | ASP  |
| 3   | D     | 631 | ILE  |
| 3   | D     | 639 | LEU  |
| 3   | D     | 641 | GLN  |
| 3   | D     | 642 | CYS  |
| 3   | D     | 651 | GLU  |
| 3   | D     | 652 | LEU  |
| 3   | D     | 660 | LYS  |
| 3   | D     | 681 | ARG  |
| 3   | D     | 688 | TRP  |
| 3   | D     | 701 | LEU  |
| 3   | D     | 703 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 709 | HIS  |
| 3   | D     | 710 | ARG  |
| 3   | D     | 734 | GLU  |
| 3   | D     | 747 | VAL  |
| 3   | D     | 749 | VAL  |
| 3   | D     | 754 | PHE  |
| 3   | D     | 764 | LEU  |
| 3   | D     | 765 | SER  |
| 3   | D     | 772 | PRO  |
| 3   | D     | 778 | LEU  |
| 3   | D     | 783 | ARG  |
| 3   | D     | 785 | ILE  |
| 3   | D     | 791 | TYR  |
| 3   | D     | 799 | LYS  |
| 3   | D     | 804 | LEU  |
| 3   | D     | 805 | GLU  |
| 3   | D     | 808 | THR  |
| 3   | D     | 824 | ASN  |
| 3   | D     | 833 | GLU  |
| 3   | D     | 838 | ARG  |
| 3   | D     | 847 | ASP  |
| 3   | D     | 863 | VAL  |
| 3   | D     | 864 | VAL  |
| 3   | D     | 879 | ARG  |
| 3   | D     | 890 | VAL  |
| 3   | D     | 892 | ASP  |
| 3   | D     | 897 | TRP  |
| 3   | D     | 900 | ILE  |
| 3   | D     | 902 | LEU  |
| 3   | D     | 914 | LEU  |
| 3   | D     | 920 | LEU  |
| 3   | D     | 922 | LEU  |
| 3   | D     | 925 | GLU  |
| 3   | D     | 927 | THR  |
| 3   | D     | 947 | ILE  |
| 3   | D     | 953 | ASP  |
| 3   | D     | 964 | LEU  |
| 3   | D     | 970 | LYS  |
| 3   | D     | 982 | PHE  |
| 3   | D     | 983 | LEU  |
| 3   | D     | 988 | ARG  |
| 3   | D     | 991 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 999  | THR  |
| 3   | D     | 1001 | GLU  |
| 3   | D     | 1029 | ARG  |
| 3   | D     | 1031 | ASN  |
| 3   | D     | 1032 | PRO  |
| 3   | D     | 1033 | GLN  |
| 3   | D     | 1041 | LEU  |
| 3   | D     | 1042 | ARG  |
| 3   | D     | 1053 | PHE  |
| 3   | D     | 1062 | ARG  |
| 3   | D     | 1068 | LEU  |
| 3   | D     | 1078 | ARG  |
| 3   | D     | 1083 | ASP  |
| 3   | D     | 1087 | ARG  |
| 3   | D     | 1090 | ASP  |
| 3   | D     | 1093 | TYR  |
| 3   | D     | 1095 | THR  |
| 3   | D     | 1096 | ARG  |
| 3   | D     | 1103 | HIS  |
| 3   | D     | 1108 | ARG  |
| 3   | D     | 1109 | GLU  |
| 3   | D     | 1118 | ILE  |
| 3   | D     | 1122 | LEU  |
| 3   | D     | 1126 | ASP  |
| 3   | D     | 1127 | GLU  |
| 3   | D     | 1128 | VAL  |
| 3   | D     | 1130 | ARG  |
| 3   | D     | 1131 | SER  |
| 3   | D     | 1137 | ARG  |
| 3   | D     | 1161 | GLU  |
| 3   | D     | 1165 | TYR  |
| 3   | D     | 1166 | LEU  |
| 3   | D     | 1183 | ILE  |
| 3   | D     | 1184 | GLN  |
| 3   | D     | 1191 | PRO  |
| 3   | D     | 1194 | CYS  |
| 3   | D     | 1197 | ARG  |
| 3   | D     | 1207 | TYR  |
| 3   | D     | 1208 | ASP  |
| 3   | D     | 1210 | SER  |
| 3   | D     | 1236 | LEU  |
| 3   | D     | 1251 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1252 | ILE  |
| 3   | D     | 1254 | GLN  |
| 3   | D     | 1262 | LEU  |
| 3   | D     | 1278 | ASP  |
| 3   | D     | 1299 | PHE  |
| 3   | D     | 1306 | PRO  |
| 3   | D     | 1311 | LEU  |
| 3   | D     | 1314 | LYS  |
| 3   | D     | 1320 | GLU  |
| 3   | D     | 1325 | LEU  |
| 3   | D     | 1327 | ARG  |
| 3   | D     | 1337 | GLU  |
| 3   | D     | 1342 | GLU  |
| 3   | D     | 1355 | VAL  |
| 3   | D     | 1382 | THR  |
| 3   | D     | 1388 | ARG  |
| 3   | D     | 1396 | GLU  |
| 3   | D     | 1410 | GLU  |
| 3   | D     | 1415 | VAL  |
| 3   | D     | 1424 | VAL  |
| 3   | D     | 1434 | TRP  |
| 3   | D     | 1436 | SER  |
| 3   | D     | 1440 | PHE  |
| 3   | D     | 1441 | GLN  |
| 3   | D     | 1459 | LEU  |
| 3   | D     | 1465 | ASN  |
| 3   | D     | 1472 | ILE  |
| 3   | D     | 1476 | THR  |
| 3   | D     | 1483 | PHE  |
| 3   | D     | 1488 | ASP  |
| 3   | D     | 1492 | LEU  |
| 3   | D     | 1496 | GLU  |
| 4   | E     | 7    | ASP  |
| 4   | E     | 20   | THR  |
| 4   | E     | 32   | ARG  |
| 4   | E     | 35   | PHE  |
| 4   | E     | 36   | LYS  |
| 4   | E     | 44   | GLU  |
| 4   | E     | 51   | LEU  |
| 4   | E     | 52   | GLU  |
| 4   | E     | 62   | THR  |
| 4   | E     | 73   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 7   | LYS  |
| 1   | F     | 19  | GLU  |
| 1   | F     | 20  | TYR  |
| 1   | F     | 28  | LEU  |
| 1   | F     | 30  | ARG  |
| 1   | F     | 47  | SER  |
| 1   | F     | 62  | LEU  |
| 1   | F     | 65  | PHE  |
| 1   | F     | 74  | ASP  |
| 1   | F     | 80  | LEU  |
| 1   | F     | 92  | PRO  |
| 1   | F     | 96  | THR  |
| 1   | F     | 100 | LEU  |
| 1   | F     | 101 | LEU  |
| 1   | F     | 113 | ASP  |
| 1   | F     | 123 | MET  |
| 1   | F     | 126 | ASP  |
| 1   | F     | 141 | GLU  |
| 1   | F     | 143 | ARG  |
| 1   | F     | 161 | ARG  |
| 1   | F     | 163 | ASN  |
| 1   | F     | 165 | ILE  |
| 1   | F     | 175 | ARG  |
| 1   | F     | 180 | GLN  |
| 1   | F     | 183 | ASP  |
| 1   | F     | 184 | THR  |
| 1   | F     | 186 | LEU  |
| 1   | F     | 189 | ARG  |
| 1   | F     | 206 | THR  |
| 1   | G     | 18  | ARG  |
| 1   | G     | 20  | TYR  |
| 1   | G     | 25  | LEU  |
| 1   | G     | 34  | VAL  |
| 1   | G     | 42  | ARG  |
| 1   | G     | 51  | THR  |
| 1   | G     | 55  | SER  |
| 1   | G     | 60  | ASP  |
| 1   | G     | 62  | LEU  |
| 1   | G     | 65  | PHE  |
| 1   | G     | 67  | THR  |
| 1   | G     | 74  | ASP  |
| 1   | G     | 79  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 95  | GLN  |
| 1   | G     | 104 | GLU  |
| 1   | G     | 119 | ASP  |
| 1   | G     | 123 | MET  |
| 1   | G     | 126 | ASP  |
| 1   | G     | 137 | ARG  |
| 1   | G     | 145 | ASP  |
| 1   | G     | 159 | LYS  |
| 1   | G     | 162 | ILE  |
| 1   | G     | 165 | ILE  |
| 1   | G     | 179 | PHE  |
| 1   | G     | 180 | GLN  |
| 1   | G     | 184 | THR  |
| 1   | G     | 185 | ARG  |
| 1   | G     | 186 | LEU  |
| 1   | G     | 197 | LEU  |
| 1   | G     | 198 | ARG  |
| 1   | G     | 201 | THR  |
| 1   | G     | 206 | THR  |
| 2   | H     | 5   | ARG  |
| 2   | H     | 6   | PHE  |
| 2   | H     | 10  | ARG  |
| 2   | H     | 13  | ILE  |
| 2   | H     | 16  | PRO  |
| 2   | H     | 19  | THR  |
| 2   | H     | 21  | ILE  |
| 2   | H     | 26  | TYR  |
| 2   | H     | 30  | LEU  |
| 2   | H     | 31  | GLN  |
| 2   | H     | 34  | VAL  |
| 2   | H     | 39  | ARG  |
| 2   | H     | 41  | ASN  |
| 2   | H     | 48  | PHE  |
| 2   | H     | 52  | PHE  |
| 2   | H     | 56  | GLU  |
| 2   | H     | 77  | PRO  |
| 2   | H     | 78  | PHE  |
| 2   | H     | 88  | LEU  |
| 2   | H     | 91  | GLN  |
| 2   | H     | 94  | LEU  |
| 2   | H     | 95  | TYR  |
| 2   | H     | 98  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 105 | THR  |
| 2   | H     | 115 | LEU  |
| 2   | H     | 124 | ASP  |
| 2   | H     | 126 | SER  |
| 2   | H     | 137 | VAL  |
| 2   | H     | 142 | ARG  |
| 2   | H     | 158 | TYR  |
| 2   | H     | 177 | GLU  |
| 2   | H     | 178 | PRO  |
| 2   | H     | 188 | LYS  |
| 2   | H     | 189 | ARG  |
| 2   | H     | 190 | LYS  |
| 2   | H     | 191 | PHE  |
| 2   | H     | 193 | LEU  |
| 2   | H     | 194 | VAL  |
| 2   | H     | 198 | ARG  |
| 2   | H     | 203 | ASP  |
| 2   | H     | 205 | GLU  |
| 2   | H     | 206 | THR  |
| 2   | H     | 214 | TYR  |
| 2   | H     | 225 | SER  |
| 2   | H     | 230 | ARG  |
| 2   | H     | 237 | ARG  |
| 2   | H     | 238 | LEU  |
| 2   | H     | 241 | LEU  |
| 2   | H     | 250 | ARG  |
| 2   | H     | 265 | ARG  |
| 2   | H     | 266 | ARG  |
| 2   | H     | 267 | TYR  |
| 2   | H     | 278 | GLU  |
| 2   | H     | 281 | LEU  |
| 2   | H     | 283 | ILE  |
| 2   | H     | 285 | LEU  |
| 2   | H     | 288 | ARG  |
| 2   | H     | 289 | THR  |
| 2   | H     | 290 | LEU  |
| 2   | H     | 292 | ARG  |
| 2   | H     | 293 | PHE  |
| 2   | H     | 294 | GLU  |
| 2   | H     | 298 | PHE  |
| 2   | H     | 335 | THR  |
| 2   | H     | 343 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 345 | ARG  |
| 2   | H     | 356 | ARG  |
| 2   | H     | 358 | ARG  |
| 2   | H     | 359 | MET  |
| 2   | H     | 360 | LEU  |
| 2   | H     | 365 | ASP  |
| 2   | H     | 368 | THR  |
| 2   | H     | 369 | PRO  |
| 2   | H     | 371 | LYS  |
| 2   | H     | 374 | ASN  |
| 2   | H     | 376 | ARG  |
| 2   | H     | 383 | ARG  |
| 2   | H     | 388 | ARG  |
| 2   | H     | 390 | GLN  |
| 2   | H     | 393 | GLN  |
| 2   | H     | 394 | PHE  |
| 2   | H     | 419 | THR  |
| 2   | H     | 422 | ARG  |
| 2   | H     | 425 | PHE  |
| 2   | H     | 433 | THR  |
| 2   | H     | 453 | THR  |
| 2   | H     | 455 | LEU  |
| 2   | H     | 463 | GLU  |
| 2   | H     | 466 | PHE  |
| 2   | H     | 480 | THR  |
| 2   | H     | 489 | THR  |
| 2   | H     | 492 | ASP  |
| 2   | H     | 500 | ASN  |
| 2   | H     | 503 | LEU  |
| 2   | H     | 523 | ILE  |
| 2   | H     | 533 | ASP  |
| 2   | H     | 545 | ASN  |
| 2   | H     | 548 | PRO  |
| 2   | H     | 554 | ASP  |
| 2   | H     | 557 | ARG  |
| 2   | H     | 579 | VAL  |
| 2   | H     | 586 | ARG  |
| 2   | H     | 600 | ASP  |
| 2   | H     | 609 | ASN  |
| 2   | H     | 614 | ARG  |
| 2   | H     | 620 | LEU  |
| 2   | H     | 621 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 631 | SER  |
| 2   | H     | 632 | ASN  |
| 2   | H     | 635 | THR  |
| 2   | H     | 640 | ARG  |
| 2   | H     | 642 | ARG  |
| 2   | H     | 645 | VAL  |
| 2   | H     | 654 | LEU  |
| 2   | H     | 657 | ASP  |
| 2   | H     | 662 | GLU  |
| 2   | H     | 668 | LEU  |
| 2   | H     | 679 | PHE  |
| 2   | H     | 685 | GLU  |
| 2   | H     | 691 | SER  |
| 2   | H     | 695 | LEU  |
| 2   | H     | 701 | THR  |
| 2   | H     | 704 | HIS  |
| 2   | H     | 714 | ASP  |
| 2   | H     | 722 | ILE  |
| 2   | H     | 727 | PRO  |
| 2   | H     | 729 | LEU  |
| 2   | H     | 738 | ASP  |
| 2   | H     | 740 | GLU  |
| 2   | H     | 794 | PRO  |
| 2   | H     | 796 | GLU  |
| 2   | H     | 803 | THR  |
| 2   | H     | 805 | ARG  |
| 2   | H     | 807 | ARG  |
| 2   | H     | 839 | LEU  |
| 2   | H     | 863 | ASP  |
| 2   | H     | 869 | VAL  |
| 2   | H     | 870 | ILE  |
| 2   | H     | 881 | ASN  |
| 2   | H     | 884 | GLN  |
| 2   | H     | 904 | PRO  |
| 2   | H     | 920 | GLN  |
| 2   | H     | 923 | GLU  |
| 2   | H     | 929 | ARG  |
| 2   | H     | 938 | LYS  |
| 2   | H     | 939 | ARG  |
| 2   | H     | 942 | GLU  |
| 2   | H     | 946 | ARG  |
| 2   | H     | 950 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | H     | 952  | LEU  |
| 2   | H     | 958  | THR  |
| 2   | H     | 963  | LEU  |
| 2   | H     | 969  | GLN  |
| 2   | H     | 975  | TYR  |
| 2   | H     | 981  | GLU  |
| 2   | H     | 988  | VAL  |
| 2   | H     | 989  | VAL  |
| 2   | H     | 995  | MET  |
| 2   | H     | 999  | HIS  |
| 2   | H     | 1004 | LYS  |
| 2   | H     | 1012 | PRO  |
| 2   | H     | 1014 | SER  |
| 2   | H     | 1026 | GLN  |
| 2   | H     | 1050 | GLN  |
| 2   | H     | 1060 | ILE  |
| 2   | H     | 1063 | ARG  |
| 2   | H     | 1088 | LEU  |
| 2   | H     | 1092 | LEU  |
| 2   | H     | 1097 | LEU  |
| 2   | H     | 1105 | LYS  |
| 2   | H     | 1110 | ASP  |
| 2   | H     | 1111 | ILE  |
| 2   | H     | 1112 | PHE  |
| 3   | I     | 3    | LYS  |
| 3   | I     | 5    | VAL  |
| 3   | I     | 6    | ARG  |
| 3   | I     | 10   | ILE  |
| 3   | I     | 21   | TRP  |
| 3   | I     | 32   | ILE  |
| 3   | I     | 37   | LEU  |
| 3   | I     | 40   | GLU  |
| 3   | I     | 41   | ARG  |
| 3   | I     | 47   | GLU  |
| 3   | I     | 84   | ILE  |
| 3   | I     | 85   | VAL  |
| 3   | I     | 87   | ARG  |
| 3   | I     | 89   | ARG  |
| 3   | I     | 95   | LEU  |
| 3   | I     | 98   | PRO  |
| 3   | I     | 102  | ILE  |
| 3   | I     | 108  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 112 | ILE  |
| 3   | I     | 127 | LEU  |
| 3   | I     | 128 | TYR  |
| 3   | I     | 134 | VAL  |
| 3   | I     | 138 | LYS  |
| 3   | I     | 141 | ILE  |
| 3   | I     | 142 | LEU  |
| 3   | I     | 143 | ASN  |
| 3   | I     | 148 | GLU  |
| 3   | I     | 151 | GLN  |
| 3   | I     | 152 | LEU  |
| 3   | I     | 153 | LEU  |
| 3   | I     | 154 | THR  |
| 3   | I     | 157 | GLU  |
| 3   | I     | 160 | GLU  |
| 3   | I     | 163 | TYR  |
| 3   | I     | 181 | ASP  |
| 3   | I     | 199 | LEU  |
| 3   | I     | 205 | TYR  |
| 3   | I     | 206 | ARG  |
| 3   | I     | 207 | PHE  |
| 3   | I     | 390 | PRO  |
| 3   | I     | 394 | LEU  |
| 3   | I     | 405 | ASP  |
| 3   | I     | 406 | ASP  |
| 3   | I     | 419 | ASP  |
| 3   | I     | 434 | ARG  |
| 3   | I     | 438 | ASP  |
| 3   | I     | 451 | ASP  |
| 3   | I     | 452 | ILE  |
| 3   | I     | 456 | MET  |
| 3   | I     | 465 | LEU  |
| 3   | I     | 469 | ASP  |
| 3   | I     | 471 | GLU  |
| 3   | I     | 489 | ARG  |
| 3   | I     | 504 | ASP  |
| 3   | I     | 511 | TRP  |
| 3   | I     | 512 | MET  |
| 3   | I     | 522 | PRO  |
| 3   | I     | 524 | LEU  |
| 3   | I     | 525 | ARG  |
| 3   | I     | 539 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 551 | ASN  |
| 3   | I     | 564 | GLU  |
| 3   | I     | 594 | PRO  |
| 3   | I     | 598 | ARG  |
| 3   | I     | 600 | LEU  |
| 3   | I     | 602 | SER  |
| 3   | I     | 614 | PHE  |
| 3   | I     | 618 | LEU  |
| 3   | I     | 619 | LEU  |
| 3   | I     | 621 | LYS  |
| 3   | I     | 622 | ARG  |
| 3   | I     | 631 | ILE  |
| 3   | I     | 639 | LEU  |
| 3   | I     | 641 | GLN  |
| 3   | I     | 642 | CYS  |
| 3   | I     | 651 | GLU  |
| 3   | I     | 652 | LEU  |
| 3   | I     | 660 | LYS  |
| 3   | I     | 685 | ASP  |
| 3   | I     | 686 | GLU  |
| 3   | I     | 688 | TRP  |
| 3   | I     | 701 | LEU  |
| 3   | I     | 703 | ASN  |
| 3   | I     | 709 | HIS  |
| 3   | I     | 710 | ARG  |
| 3   | I     | 734 | GLU  |
| 3   | I     | 747 | VAL  |
| 3   | I     | 749 | VAL  |
| 3   | I     | 754 | PHE  |
| 3   | I     | 764 | LEU  |
| 3   | I     | 765 | SER  |
| 3   | I     | 772 | PRO  |
| 3   | I     | 778 | LEU  |
| 3   | I     | 781 | PRO  |
| 3   | I     | 783 | ARG  |
| 3   | I     | 784 | ASP  |
| 3   | I     | 791 | TYR  |
| 3   | I     | 795 | VAL  |
| 3   | I     | 799 | LYS  |
| 3   | I     | 804 | LEU  |
| 3   | I     | 824 | ASN  |
| 3   | I     | 833 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | I     | 838  | ARG  |
| 3   | I     | 847  | ASP  |
| 3   | I     | 863  | VAL  |
| 3   | I     | 864  | VAL  |
| 3   | I     | 879  | ARG  |
| 3   | I     | 890  | VAL  |
| 3   | I     | 892  | ASP  |
| 3   | I     | 897  | TRP  |
| 3   | I     | 900  | ILE  |
| 3   | I     | 902  | LEU  |
| 3   | I     | 914  | LEU  |
| 3   | I     | 920  | LEU  |
| 3   | I     | 922  | LEU  |
| 3   | I     | 925  | GLU  |
| 3   | I     | 927  | THR  |
| 3   | I     | 964  | LEU  |
| 3   | I     | 970  | LYS  |
| 3   | I     | 982  | PHE  |
| 3   | I     | 983  | LEU  |
| 3   | I     | 988  | ARG  |
| 3   | I     | 991  | GLN  |
| 3   | I     | 999  | THR  |
| 3   | I     | 1001 | GLU  |
| 3   | I     | 1025 | GLN  |
| 3   | I     | 1029 | ARG  |
| 3   | I     | 1031 | ASN  |
| 3   | I     | 1041 | LEU  |
| 3   | I     | 1042 | ARG  |
| 3   | I     | 1053 | PHE  |
| 3   | I     | 1062 | ARG  |
| 3   | I     | 1068 | LEU  |
| 3   | I     | 1078 | ARG  |
| 3   | I     | 1083 | ASP  |
| 3   | I     | 1087 | ARG  |
| 3   | I     | 1088 | THR  |
| 3   | I     | 1090 | ASP  |
| 3   | I     | 1096 | ARG  |
| 3   | I     | 1097 | LYS  |
| 3   | I     | 1100 | ASP  |
| 3   | I     | 1101 | VAL  |
| 3   | I     | 1102 | THR  |
| 3   | I     | 1103 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | I     | 1108 | ARG  |
| 3   | I     | 1109 | GLU  |
| 3   | I     | 1119 | SER  |
| 3   | I     | 1126 | ASP  |
| 3   | I     | 1130 | ARG  |
| 3   | I     | 1151 | ARG  |
| 3   | I     | 1161 | GLU  |
| 3   | I     | 1166 | LEU  |
| 3   | I     | 1183 | ILE  |
| 3   | I     | 1191 | PRO  |
| 3   | I     | 1194 | CYS  |
| 3   | I     | 1197 | ARG  |
| 3   | I     | 1207 | TYR  |
| 3   | I     | 1208 | ASP  |
| 3   | I     | 1237 | THR  |
| 3   | I     | 1262 | LEU  |
| 3   | I     | 1286 | THR  |
| 3   | I     | 1293 | PHE  |
| 3   | I     | 1299 | PHE  |
| 3   | I     | 1304 | LYS  |
| 3   | I     | 1305 | LEU  |
| 3   | I     | 1307 | LYS  |
| 3   | I     | 1308 | GLU  |
| 3   | I     | 1311 | LEU  |
| 3   | I     | 1314 | LYS  |
| 3   | I     | 1320 | GLU  |
| 3   | I     | 1325 | LEU  |
| 3   | I     | 1327 | ARG  |
| 3   | I     | 1337 | GLU  |
| 3   | I     | 1342 | GLU  |
| 3   | I     | 1355 | VAL  |
| 3   | I     | 1382 | THR  |
| 3   | I     | 1387 | SER  |
| 3   | I     | 1388 | ARG  |
| 3   | I     | 1389 | LEU  |
| 3   | I     | 1396 | GLU  |
| 3   | I     | 1410 | GLU  |
| 3   | I     | 1415 | VAL  |
| 3   | I     | 1424 | VAL  |
| 3   | I     | 1425 | THR  |
| 3   | I     | 1434 | TRP  |
| 3   | I     | 1440 | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | I     | 1466 | VAL  |
| 3   | I     | 1472 | ILE  |
| 3   | I     | 1485 | GLN  |
| 3   | I     | 1492 | LEU  |
| 4   | J     | 18   | ARG  |
| 4   | J     | 20   | THR  |
| 4   | J     | 35   | PHE  |
| 4   | J     | 37   | ASN  |
| 4   | J     | 43   | GLU  |
| 4   | J     | 44   | GLU  |
| 4   | J     | 52   | GLU  |
| 4   | J     | 62   | THR  |
| 4   | J     | 77   | GLU  |
| 4   | J     | 86   | GLN  |
| 1   | K     | 12   | THR  |
| 1   | K     | 16   | GLN  |
| 1   | K     | 20   | TYR  |
| 1   | K     | 22   | GLU  |
| 1   | K     | 26   | GLU  |
| 1   | K     | 30   | ARG  |
| 1   | K     | 47   | SER  |
| 1   | K     | 62   | LEU  |
| 1   | K     | 65   | PHE  |
| 1   | K     | 74   | ASP  |
| 1   | K     | 79   | ILE  |
| 1   | K     | 92   | PRO  |
| 1   | K     | 96   | THR  |
| 1   | K     | 100  | LEU  |
| 1   | K     | 101  | LEU  |
| 1   | K     | 113  | ASP  |
| 1   | K     | 123  | MET  |
| 1   | K     | 126  | ASP  |
| 1   | K     | 141  | GLU  |
| 1   | K     | 143  | ARG  |
| 1   | K     | 161  | ARG  |
| 1   | K     | 163  | ASN  |
| 1   | K     | 165  | ILE  |
| 1   | K     | 175  | ARG  |
| 1   | K     | 180  | GLN  |
| 1   | K     | 181  | VAL  |
| 1   | K     | 183  | ASP  |
| 1   | K     | 188  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 189 | ARG  |
| 1   | K     | 206 | THR  |
| 1   | K     | 219 | ARG  |
| 1   | K     | 229 | GLN  |
| 1   | L     | 18  | ARG  |
| 1   | L     | 20  | TYR  |
| 1   | L     | 25  | LEU  |
| 1   | L     | 35  | THR  |
| 1   | L     | 54  | THR  |
| 1   | L     | 60  | ASP  |
| 1   | L     | 62  | LEU  |
| 1   | L     | 65  | PHE  |
| 1   | L     | 66  | SER  |
| 1   | L     | 67  | THR  |
| 1   | L     | 73  | GLU  |
| 1   | L     | 79  | ILE  |
| 1   | L     | 80  | LEU  |
| 1   | L     | 84  | GLU  |
| 1   | L     | 95  | GLN  |
| 1   | L     | 104 | GLU  |
| 1   | L     | 115 | LEU  |
| 1   | L     | 123 | MET  |
| 1   | L     | 154 | GLU  |
| 1   | L     | 159 | LYS  |
| 1   | L     | 161 | ARG  |
| 1   | L     | 162 | ILE  |
| 1   | L     | 165 | ILE  |
| 1   | L     | 179 | PHE  |
| 1   | L     | 180 | GLN  |
| 1   | L     | 184 | THR  |
| 1   | L     | 185 | ARG  |
| 1   | L     | 186 | LEU  |
| 1   | L     | 197 | LEU  |
| 1   | L     | 198 | ARG  |
| 1   | L     | 201 | THR  |
| 1   | L     | 206 | THR  |
| 2   | M     | 6   | PHE  |
| 2   | M     | 26  | TYR  |
| 2   | M     | 33  | ASP  |
| 2   | M     | 48  | PHE  |
| 2   | M     | 52  | PHE  |
| 2   | M     | 56  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 72  | ARG  |
| 2   | M     | 75  | GLU  |
| 2   | M     | 84  | ARG  |
| 2   | M     | 88  | LEU  |
| 2   | M     | 89  | THR  |
| 2   | M     | 94  | LEU  |
| 2   | M     | 97  | ARG  |
| 2   | M     | 115 | LEU  |
| 2   | M     | 124 | ASP  |
| 2   | M     | 126 | SER  |
| 2   | M     | 141 | HIS  |
| 2   | M     | 142 | ARG  |
| 2   | M     | 158 | TYR  |
| 2   | M     | 172 | ILE  |
| 2   | M     | 177 | GLU  |
| 2   | M     | 187 | ASN  |
| 2   | M     | 188 | LYS  |
| 2   | M     | 190 | LYS  |
| 2   | M     | 192 | PRO  |
| 2   | M     | 193 | LEU  |
| 2   | M     | 196 | LEU  |
| 2   | M     | 203 | ASP  |
| 2   | M     | 205 | GLU  |
| 2   | M     | 207 | LEU  |
| 2   | M     | 209 | ARG  |
| 2   | M     | 214 | TYR  |
| 2   | M     | 225 | SER  |
| 2   | M     | 235 | LEU  |
| 2   | M     | 236 | ILE  |
| 2   | M     | 237 | ARG  |
| 2   | M     | 238 | LEU  |
| 2   | M     | 239 | PHE  |
| 2   | M     | 241 | LEU  |
| 2   | M     | 242 | LEU  |
| 2   | M     | 252 | LYS  |
| 2   | M     | 257 | VAL  |
| 2   | M     | 261 | ILE  |
| 2   | M     | 263 | ASP  |
| 2   | M     | 267 | TYR  |
| 2   | M     | 281 | LEU  |
| 2   | M     | 283 | ILE  |
| 2   | M     | 290 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 293 | PHE  |
| 2   | M     | 298 | PHE  |
| 2   | M     | 304 | LEU  |
| 2   | M     | 313 | LEU  |
| 2   | M     | 314 | THR  |
| 2   | M     | 321 | GLU  |
| 2   | M     | 323 | ASP  |
| 2   | M     | 331 | ARG  |
| 2   | M     | 335 | THR  |
| 2   | M     | 343 | GLN  |
| 2   | M     | 345 | ARG  |
| 2   | M     | 359 | MET  |
| 2   | M     | 361 | MET  |
| 2   | M     | 365 | ASP  |
| 2   | M     | 367 | LEU  |
| 2   | M     | 368 | THR  |
| 2   | M     | 369 | PRO  |
| 2   | M     | 374 | ASN  |
| 2   | M     | 375 | SER  |
| 2   | M     | 376 | ARG  |
| 2   | M     | 383 | ARG  |
| 2   | M     | 388 | ARG  |
| 2   | M     | 392 | SER  |
| 2   | M     | 394 | PHE  |
| 2   | M     | 419 | THR  |
| 2   | M     | 422 | ARG  |
| 2   | M     | 433 | THR  |
| 2   | M     | 453 | THR  |
| 2   | M     | 455 | LEU  |
| 2   | M     | 460 | ARG  |
| 2   | M     | 469 | THR  |
| 2   | M     | 480 | THR  |
| 2   | M     | 481 | ASP  |
| 2   | M     | 489 | THR  |
| 2   | M     | 523 | ILE  |
| 2   | M     | 533 | ASP  |
| 2   | M     | 545 | ASN  |
| 2   | M     | 554 | ASP  |
| 2   | M     | 557 | ARG  |
| 2   | M     | 579 | VAL  |
| 2   | M     | 586 | ARG  |
| 2   | M     | 587 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 590 | ASP  |
| 2   | M     | 592 | LEU  |
| 2   | M     | 600 | ASP  |
| 2   | M     | 607 | ASP  |
| 2   | M     | 611 | ILE  |
| 2   | M     | 617 | ASP  |
| 2   | M     | 620 | LEU  |
| 2   | M     | 621 | VAL  |
| 2   | M     | 631 | SER  |
| 2   | M     | 632 | ASN  |
| 2   | M     | 635 | THR  |
| 2   | M     | 640 | ARG  |
| 2   | M     | 642 | ARG  |
| 2   | M     | 645 | VAL  |
| 2   | M     | 654 | LEU  |
| 2   | M     | 657 | ASP  |
| 2   | M     | 662 | GLU  |
| 2   | M     | 668 | LEU  |
| 2   | M     | 679 | PHE  |
| 2   | M     | 685 | GLU  |
| 2   | M     | 691 | SER  |
| 2   | M     | 695 | LEU  |
| 2   | M     | 699 | PHE  |
| 2   | M     | 701 | THR  |
| 2   | M     | 702 | SER  |
| 2   | M     | 704 | HIS  |
| 2   | M     | 714 | ASP  |
| 2   | M     | 722 | ILE  |
| 2   | M     | 727 | PRO  |
| 2   | M     | 729 | LEU  |
| 2   | M     | 738 | ASP  |
| 2   | M     | 740 | GLU  |
| 2   | M     | 788 | THR  |
| 2   | M     | 794 | PRO  |
| 2   | M     | 796 | GLU  |
| 2   | M     | 803 | THR  |
| 2   | M     | 805 | ARG  |
| 2   | M     | 807 | ARG  |
| 2   | M     | 825 | VAL  |
| 2   | M     | 839 | LEU  |
| 2   | M     | 863 | ASP  |
| 2   | M     | 869 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 870  | ILE  |
| 2   | M     | 881  | ASN  |
| 2   | M     | 884  | GLN  |
| 2   | M     | 904  | PRO  |
| 2   | M     | 920  | GLN  |
| 2   | M     | 923  | GLU  |
| 2   | M     | 929  | ARG  |
| 2   | M     | 938  | LYS  |
| 2   | M     | 939  | ARG  |
| 2   | M     | 942  | GLU  |
| 2   | M     | 946  | ARG  |
| 2   | M     | 950  | LEU  |
| 2   | M     | 952  | LEU  |
| 2   | M     | 958  | THR  |
| 2   | M     | 963  | LEU  |
| 2   | M     | 969  | GLN  |
| 2   | M     | 975  | TYR  |
| 2   | M     | 981  | GLU  |
| 2   | M     | 988  | VAL  |
| 2   | M     | 989  | VAL  |
| 2   | M     | 995  | MET  |
| 2   | M     | 999  | HIS  |
| 2   | M     | 1004 | LYS  |
| 2   | M     | 1005 | MET  |
| 2   | M     | 1006 | HIS  |
| 2   | M     | 1012 | PRO  |
| 2   | M     | 1050 | GLN  |
| 2   | M     | 1058 | ASP  |
| 2   | M     | 1064 | ASN  |
| 2   | M     | 1088 | LEU  |
| 2   | M     | 1092 | LEU  |
| 2   | M     | 1097 | LEU  |
| 2   | M     | 1105 | LYS  |
| 2   | M     | 1111 | ILE  |
| 3   | N     | 6    | ARG  |
| 3   | N     | 21   | TRP  |
| 3   | N     | 34   | TYR  |
| 3   | N     | 37   | LEU  |
| 3   | N     | 41   | ARG  |
| 3   | N     | 47   | GLU  |
| 3   | N     | 53   | ILE  |
| 3   | N     | 55   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | N     | 82  | LYS  |
| 3   | N     | 86  | ARG  |
| 3   | N     | 87  | ARG  |
| 3   | N     | 88  | TYR  |
| 3   | N     | 95  | LEU  |
| 3   | N     | 98  | PRO  |
| 3   | N     | 102 | ILE  |
| 3   | N     | 108 | VAL  |
| 3   | N     | 112 | ILE  |
| 3   | N     | 127 | LEU  |
| 3   | N     | 128 | TYR  |
| 3   | N     | 129 | PHE  |
| 3   | N     | 130 | SER  |
| 3   | N     | 131 | LYS  |
| 3   | N     | 135 | LEU  |
| 3   | N     | 138 | LYS  |
| 3   | N     | 141 | ILE  |
| 3   | N     | 145 | VAL  |
| 3   | N     | 149 | LYS  |
| 3   | N     | 150 | ARG  |
| 3   | N     | 152 | LEU  |
| 3   | N     | 153 | LEU  |
| 3   | N     | 154 | THR  |
| 3   | N     | 161 | LEU  |
| 3   | N     | 163 | TYR  |
| 3   | N     | 169 | TYR  |
| 3   | N     | 176 | ASP  |
| 3   | N     | 178 | LEU  |
| 3   | N     | 189 | GLN  |
| 3   | N     | 199 | LEU  |
| 3   | N     | 205 | TYR  |
| 3   | N     | 216 | VAL  |
| 3   | N     | 340 | THR  |
| 3   | N     | 344 | ASP  |
| 3   | N     | 349 | PRO  |
| 3   | N     | 351 | MET  |
| 3   | N     | 357 | GLU  |
| 3   | N     | 372 | ASP  |
| 3   | N     | 387 | LEU  |
| 3   | N     | 394 | LEU  |
| 3   | N     | 405 | ASP  |
| 3   | N     | 419 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | N     | 434 | ARG  |
| 3   | N     | 438 | ASP  |
| 3   | N     | 450 | TYR  |
| 3   | N     | 452 | ILE  |
| 3   | N     | 465 | LEU  |
| 3   | N     | 469 | ASP  |
| 3   | N     | 471 | GLU  |
| 3   | N     | 489 | ARG  |
| 3   | N     | 504 | ASP  |
| 3   | N     | 511 | TRP  |
| 3   | N     | 512 | MET  |
| 3   | N     | 525 | ARG  |
| 3   | N     | 538 | SER  |
| 3   | N     | 544 | TYR  |
| 3   | N     | 594 | PRO  |
| 3   | N     | 614 | PHE  |
| 3   | N     | 631 | ILE  |
| 3   | N     | 639 | LEU  |
| 3   | N     | 641 | GLN  |
| 3   | N     | 642 | CYS  |
| 3   | N     | 651 | GLU  |
| 3   | N     | 652 | LEU  |
| 3   | N     | 660 | LYS  |
| 3   | N     | 678 | GLU  |
| 3   | N     | 679 | ARG  |
| 3   | N     | 685 | ASP  |
| 3   | N     | 686 | GLU  |
| 3   | N     | 688 | TRP  |
| 3   | N     | 701 | LEU  |
| 3   | N     | 703 | ASN  |
| 3   | N     | 709 | HIS  |
| 3   | N     | 710 | ARG  |
| 3   | N     | 734 | GLU  |
| 3   | N     | 747 | VAL  |
| 3   | N     | 749 | VAL  |
| 3   | N     | 754 | PHE  |
| 3   | N     | 764 | LEU  |
| 3   | N     | 765 | SER  |
| 3   | N     | 772 | PRO  |
| 3   | N     | 778 | LEU  |
| 3   | N     | 781 | PRO  |
| 3   | N     | 783 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 784  | ASP  |
| 3   | N     | 791  | TYR  |
| 3   | N     | 804  | LEU  |
| 3   | N     | 805  | GLU  |
| 3   | N     | 824  | ASN  |
| 3   | N     | 833  | GLU  |
| 3   | N     | 838  | ARG  |
| 3   | N     | 847  | ASP  |
| 3   | N     | 863  | VAL  |
| 3   | N     | 864  | VAL  |
| 3   | N     | 879  | ARG  |
| 3   | N     | 890  | VAL  |
| 3   | N     | 892  | ASP  |
| 3   | N     | 897  | TRP  |
| 3   | N     | 900  | ILE  |
| 3   | N     | 902  | LEU  |
| 3   | N     | 914  | LEU  |
| 3   | N     | 920  | LEU  |
| 3   | N     | 922  | LEU  |
| 3   | N     | 925  | GLU  |
| 3   | N     | 927  | THR  |
| 3   | N     | 952  | ASP  |
| 3   | N     | 964  | LEU  |
| 3   | N     | 970  | LYS  |
| 3   | N     | 982  | PHE  |
| 3   | N     | 983  | LEU  |
| 3   | N     | 988  | ARG  |
| 3   | N     | 991  | GLN  |
| 3   | N     | 999  | THR  |
| 3   | N     | 1001 | GLU  |
| 3   | N     | 1025 | GLN  |
| 3   | N     | 1029 | ARG  |
| 3   | N     | 1041 | LEU  |
| 3   | N     | 1042 | ARG  |
| 3   | N     | 1053 | PHE  |
| 3   | N     | 1062 | ARG  |
| 3   | N     | 1068 | LEU  |
| 3   | N     | 1078 | ARG  |
| 3   | N     | 1083 | ASP  |
| 3   | N     | 1087 | ARG  |
| 3   | N     | 1090 | ASP  |
| 3   | N     | 1093 | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 1095 | THR  |
| 3   | N     | 1096 | ARG  |
| 3   | N     | 1108 | ARG  |
| 3   | N     | 1109 | GLU  |
| 3   | N     | 1126 | ASP  |
| 3   | N     | 1127 | GLU  |
| 3   | N     | 1128 | VAL  |
| 3   | N     | 1135 | ARG  |
| 3   | N     | 1151 | ARG  |
| 3   | N     | 1152 | GLU  |
| 3   | N     | 1166 | LEU  |
| 3   | N     | 1183 | ILE  |
| 3   | N     | 1191 | PRO  |
| 3   | N     | 1194 | CYS  |
| 3   | N     | 1197 | ARG  |
| 3   | N     | 1207 | TYR  |
| 3   | N     | 1208 | ASP  |
| 3   | N     | 1251 | ASP  |
| 3   | N     | 1254 | GLN  |
| 3   | N     | 1262 | LEU  |
| 3   | N     | 1282 | ARG  |
| 3   | N     | 1286 | THR  |
| 3   | N     | 1297 | GLU  |
| 3   | N     | 1299 | PHE  |
| 3   | N     | 1304 | LYS  |
| 3   | N     | 1305 | LEU  |
| 3   | N     | 1307 | LYS  |
| 3   | N     | 1308 | GLU  |
| 3   | N     | 1311 | LEU  |
| 3   | N     | 1314 | LYS  |
| 3   | N     | 1320 | GLU  |
| 3   | N     | 1325 | LEU  |
| 3   | N     | 1327 | ARG  |
| 3   | N     | 1337 | GLU  |
| 3   | N     | 1342 | GLU  |
| 3   | N     | 1355 | VAL  |
| 3   | N     | 1382 | THR  |
| 3   | N     | 1386 | ASP  |
| 3   | N     | 1388 | ARG  |
| 3   | N     | 1396 | GLU  |
| 3   | N     | 1410 | GLU  |
| 3   | N     | 1415 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 1424 | VAL  |
| 3   | N     | 1425 | THR  |
| 3   | N     | 1433 | SER  |
| 3   | N     | 1434 | TRP  |
| 3   | N     | 1440 | PHE  |
| 3   | N     | 1449 | GLU  |
| 3   | N     | 1465 | ASN  |
| 3   | N     | 1472 | ILE  |
| 3   | N     | 1476 | THR  |
| 3   | N     | 1488 | ASP  |
| 3   | N     | 1493 | LYS  |
| 4   | O     | 6    | ILE  |
| 4   | O     | 7    | ASP  |
| 4   | O     | 14   | ASP  |
| 4   | O     | 15   | SER  |
| 4   | O     | 18   | ARG  |
| 4   | O     | 31   | LEU  |
| 4   | O     | 32   | ARG  |
| 4   | O     | 41   | GLU  |
| 4   | O     | 43   | GLU  |
| 4   | O     | 44   | GLU  |
| 4   | O     | 48   | MET  |
| 4   | O     | 62   | THR  |
| 4   | O     | 73   | LEU  |
| 4   | O     | 81   | PRO  |
| 4   | O     | 86   | GLN  |
| 7   | X     | 8    | THR  |
| 7   | X     | 37   | MET  |
| 7   | X     | 41   | ASP  |
| 7   | X     | 43   | TYR  |
| 7   | X     | 48   | LEU  |
| 7   | X     | 62   | ILE  |
| 7   | X     | 77   | GLU  |
| 7   | X     | 94   | PRO  |
| 7   | X     | 102  | VAL  |
| 7   | X     | 105  | VAL  |
| 7   | X     | 113  | LEU  |
| 7   | X     | 114  | ASP  |
| 7   | X     | 115  | THR  |
| 7   | X     | 138  | LEU  |
| 7   | X     | 139  | SER  |
| 7   | Y     | 7    | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | Y     | 21  | ARG  |
| 7   | Y     | 30  | THR  |
| 7   | Y     | 37  | MET  |
| 7   | Y     | 41  | ASP  |
| 7   | Y     | 45  | ASP  |
| 7   | Y     | 54  | GLU  |
| 7   | Y     | 61  | ARG  |
| 7   | Y     | 67  | ASP  |
| 7   | Y     | 70  | SER  |
| 7   | Y     | 74  | ILE  |
| 7   | Y     | 76  | GLU  |
| 7   | Y     | 95  | LEU  |
| 7   | Y     | 98  | GLU  |
| 7   | Y     | 113 | LEU  |
| 7   | Y     | 114 | ASP  |
| 7   | Y     | 115 | THR  |
| 7   | Y     | 117 | MET  |
| 7   | Y     | 124 | PRO  |
| 7   | Y     | 138 | LEU  |
| 7   | Y     | 143 | PRO  |
| 7   | Y     | 148 | GLU  |
| 7   | Y     | 150 | ARG  |
| 7   | Y     | 154 | ILE  |
| 7   | Z     | 8   | THR  |
| 7   | Z     | 14  | ARG  |
| 7   | Z     | 21  | ARG  |
| 7   | Z     | 37  | MET  |
| 7   | Z     | 40  | SER  |
| 7   | Z     | 48  | LEU  |
| 7   | Z     | 57  | ARG  |
| 7   | Z     | 71  | ARG  |
| 7   | Z     | 77  | GLU  |
| 7   | Z     | 94  | PRO  |
| 7   | Z     | 98  | GLU  |
| 7   | Z     | 113 | LEU  |
| 7   | Z     | 114 | ASP  |
| 7   | Z     | 115 | THR  |
| 7   | Z     | 125 | MET  |
| 7   | Z     | 138 | LEU  |
| 7   | Z     | 139 | SER  |
| 7   | Z     | 154 | ILE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (252) such

sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 63  | HIS  |
| 1   | A     | 91  | ASN  |
| 1   | A     | 124 | ASN  |
| 1   | A     | 128 | HIS  |
| 1   | A     | 139 | ASN  |
| 1   | A     | 156 | HIS  |
| 1   | A     | 163 | ASN  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 188 | GLN  |
| 1   | A     | 229 | GLN  |
| 1   | B     | 16  | GLN  |
| 1   | B     | 38  | ASN  |
| 1   | B     | 95  | GLN  |
| 1   | B     | 124 | ASN  |
| 1   | B     | 163 | ASN  |
| 1   | B     | 180 | GLN  |
| 1   | B     | 227 | ASN  |
| 2   | C     | 22  | GLN  |
| 2   | C     | 41  | ASN  |
| 2   | C     | 80  | GLN  |
| 2   | C     | 91  | GLN  |
| 2   | C     | 102 | HIS  |
| 2   | C     | 117 | HIS  |
| 2   | C     | 139 | GLN  |
| 2   | C     | 343 | GLN  |
| 2   | C     | 374 | ASN  |
| 2   | C     | 390 | GLN  |
| 2   | C     | 393 | GLN  |
| 2   | C     | 406 | HIS  |
| 2   | C     | 431 | HIS  |
| 2   | C     | 434 | HIS  |
| 2   | C     | 498 | GLN  |
| 2   | C     | 556 | ASN  |
| 2   | C     | 575 | GLN  |
| 2   | C     | 633 | GLN  |
| 2   | C     | 639 | GLN  |
| 2   | C     | 670 | GLN  |
| 2   | C     | 834 | GLN  |
| 2   | C     | 860 | HIS  |
| 2   | C     | 872 | ASN  |
| 2   | C     | 899 | GLN  |
| 2   | C     | 969 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1047 | HIS  |
| 2   | C     | 1100 | GLN  |
| 2   | C     | 1107 | ASN  |
| 3   | D     | 33   | ASN  |
| 3   | D     | 151  | GLN  |
| 3   | D     | 166  | GLN  |
| 3   | D     | 463  | GLN  |
| 3   | D     | 541  | ASN  |
| 3   | D     | 549  | ASN  |
| 3   | D     | 560  | GLN  |
| 3   | D     | 569  | ASN  |
| 3   | D     | 703  | ASN  |
| 3   | D     | 727  | GLN  |
| 3   | D     | 744  | GLN  |
| 3   | D     | 762  | GLN  |
| 3   | D     | 824  | ASN  |
| 3   | D     | 855  | HIS  |
| 3   | D     | 909  | ASN  |
| 3   | D     | 973  | GLN  |
| 3   | D     | 976  | GLN  |
| 3   | D     | 1025 | GLN  |
| 3   | D     | 1033 | GLN  |
| 3   | D     | 1034 | GLN  |
| 3   | D     | 1184 | GLN  |
| 3   | D     | 1202 | GLN  |
| 3   | D     | 1323 | GLN  |
| 3   | D     | 1359 | GLN  |
| 3   | D     | 1367 | HIS  |
| 3   | D     | 1441 | GLN  |
| 3   | D     | 1442 | ASN  |
| 4   | E     | 28   | GLN  |
| 4   | E     | 33   | HIS  |
| 4   | E     | 37   | ASN  |
| 4   | E     | 86   | GLN  |
| 1   | F     | 38   | ASN  |
| 1   | F     | 63   | HIS  |
| 1   | F     | 91   | ASN  |
| 1   | F     | 124  | ASN  |
| 1   | F     | 128  | HIS  |
| 1   | F     | 139  | ASN  |
| 1   | F     | 156  | HIS  |
| 1   | F     | 163  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 180  | GLN  |
| 1   | F     | 188  | GLN  |
| 1   | F     | 229  | GLN  |
| 1   | G     | 16   | GLN  |
| 1   | G     | 38   | ASN  |
| 1   | G     | 95   | GLN  |
| 1   | G     | 124  | ASN  |
| 1   | G     | 180  | GLN  |
| 1   | G     | 227  | ASN  |
| 2   | H     | 31   | GLN  |
| 2   | H     | 41   | ASN  |
| 2   | H     | 45   | GLN  |
| 2   | H     | 80   | GLN  |
| 2   | H     | 99   | GLN  |
| 2   | H     | 102  | HIS  |
| 2   | H     | 187  | ASN  |
| 2   | H     | 327  | HIS  |
| 2   | H     | 343  | GLN  |
| 2   | H     | 374  | ASN  |
| 2   | H     | 390  | GLN  |
| 2   | H     | 393  | GLN  |
| 2   | H     | 431  | HIS  |
| 2   | H     | 498  | GLN  |
| 2   | H     | 552  | HIS  |
| 2   | H     | 575  | GLN  |
| 2   | H     | 609  | ASN  |
| 2   | H     | 633  | GLN  |
| 2   | H     | 639  | GLN  |
| 2   | H     | 670  | GLN  |
| 2   | H     | 834  | GLN  |
| 2   | H     | 860  | HIS  |
| 2   | H     | 872  | ASN  |
| 2   | H     | 899  | GLN  |
| 2   | H     | 969  | GLN  |
| 2   | H     | 1030 | GLN  |
| 2   | H     | 1047 | HIS  |
| 2   | H     | 1064 | ASN  |
| 2   | H     | 1100 | GLN  |
| 2   | H     | 1107 | ASN  |
| 3   | I     | 125  | GLN  |
| 3   | I     | 151  | GLN  |
| 3   | I     | 166  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | I     | 189  | GLN  |
| 3   | I     | 463  | GLN  |
| 3   | I     | 549  | ASN  |
| 3   | I     | 552  | ASN  |
| 3   | I     | 560  | GLN  |
| 3   | I     | 593  | ASN  |
| 3   | I     | 611  | GLN  |
| 3   | I     | 703  | ASN  |
| 3   | I     | 727  | GLN  |
| 3   | I     | 744  | GLN  |
| 3   | I     | 762  | GLN  |
| 3   | I     | 767  | HIS  |
| 3   | I     | 768  | ASN  |
| 3   | I     | 824  | ASN  |
| 3   | I     | 909  | ASN  |
| 3   | I     | 973  | GLN  |
| 3   | I     | 976  | GLN  |
| 3   | I     | 991  | GLN  |
| 3   | I     | 1025 | GLN  |
| 3   | I     | 1034 | GLN  |
| 3   | I     | 1116 | ASN  |
| 3   | I     | 1202 | GLN  |
| 3   | I     | 1235 | GLN  |
| 3   | I     | 1323 | GLN  |
| 3   | I     | 1359 | GLN  |
| 3   | I     | 1367 | HIS  |
| 3   | I     | 1441 | GLN  |
| 3   | I     | 1442 | ASN  |
| 3   | I     | 1465 | ASN  |
| 3   | I     | 1485 | GLN  |
| 4   | J     | 28   | GLN  |
| 4   | J     | 33   | HIS  |
| 4   | J     | 37   | ASN  |
| 4   | J     | 86   | GLN  |
| 1   | K     | 38   | ASN  |
| 1   | K     | 63   | HIS  |
| 1   | K     | 91   | ASN  |
| 1   | K     | 124  | ASN  |
| 1   | K     | 128  | HIS  |
| 1   | K     | 139  | ASN  |
| 1   | K     | 156  | HIS  |
| 1   | K     | 163  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K     | 180  | GLN  |
| 1   | K     | 229  | GLN  |
| 1   | L     | 16   | GLN  |
| 1   | L     | 95   | GLN  |
| 1   | L     | 180  | GLN  |
| 1   | L     | 227  | ASN  |
| 2   | M     | 22   | GLN  |
| 2   | M     | 31   | GLN  |
| 2   | M     | 102  | HIS  |
| 2   | M     | 219  | GLN  |
| 2   | M     | 343  | GLN  |
| 2   | M     | 374  | ASN  |
| 2   | M     | 390  | GLN  |
| 2   | M     | 393  | GLN  |
| 2   | M     | 406  | HIS  |
| 2   | M     | 431  | HIS  |
| 2   | M     | 552  | HIS  |
| 2   | M     | 556  | ASN  |
| 2   | M     | 575  | GLN  |
| 2   | M     | 633  | GLN  |
| 2   | M     | 639  | GLN  |
| 2   | M     | 670  | GLN  |
| 2   | M     | 834  | GLN  |
| 2   | M     | 860  | HIS  |
| 2   | M     | 872  | ASN  |
| 2   | M     | 899  | GLN  |
| 2   | M     | 969  | GLN  |
| 2   | M     | 1006 | HIS  |
| 2   | M     | 1030 | GLN  |
| 2   | M     | 1047 | HIS  |
| 2   | M     | 1064 | ASN  |
| 2   | M     | 1100 | GLN  |
| 2   | M     | 1107 | ASN  |
| 3   | N     | 151  | GLN  |
| 3   | N     | 166  | GLN  |
| 3   | N     | 189  | GLN  |
| 3   | N     | 463  | GLN  |
| 3   | N     | 549  | ASN  |
| 3   | N     | 560  | GLN  |
| 3   | N     | 617  | ASN  |
| 3   | N     | 669  | ASN  |
| 3   | N     | 703  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 724  | GLN  |
| 3   | N     | 727  | GLN  |
| 3   | N     | 744  | GLN  |
| 3   | N     | 762  | GLN  |
| 3   | N     | 767  | HIS  |
| 3   | N     | 824  | ASN  |
| 3   | N     | 909  | ASN  |
| 3   | N     | 973  | GLN  |
| 3   | N     | 976  | GLN  |
| 3   | N     | 994  | GLN  |
| 3   | N     | 1025 | GLN  |
| 3   | N     | 1034 | GLN  |
| 3   | N     | 1103 | HIS  |
| 3   | N     | 1116 | ASN  |
| 3   | N     | 1202 | GLN  |
| 3   | N     | 1235 | GLN  |
| 3   | N     | 1254 | GLN  |
| 3   | N     | 1323 | GLN  |
| 3   | N     | 1359 | GLN  |
| 3   | N     | 1367 | HIS  |
| 3   | N     | 1441 | GLN  |
| 3   | N     | 1442 | ASN  |
| 3   | N     | 1465 | ASN  |
| 4   | O     | 28   | GLN  |
| 4   | O     | 33   | HIS  |
| 4   | O     | 37   | ASN  |
| 4   | O     | 59   | ASN  |
| 4   | O     | 86   | GLN  |
| 7   | X     | 27   | GLN  |
| 7   | X     | 34   | GLN  |
| 7   | X     | 53   | GLN  |
| 7   | X     | 103  | GLN  |
| 7   | Y     | 17   | GLN  |
| 7   | Y     | 18   | GLN  |
| 7   | Y     | 27   | GLN  |
| 7   | Y     | 103  | GLN  |
| 7   | Y     | 132  | HIS  |
| 7   | Z     | 17   | GLN  |
| 7   | Z     | 18   | GLN  |
| 7   | Z     | 27   | GLN  |
| 7   | Z     | 34   | GLN  |
| 7   | Z     | 132  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 6   | Q     | 6/32 (18%)  | 1 (16%)           | 0               |
| 6   | S     | 7/32 (21%)  | 2 (28%)           | 0               |
| 6   | U     | 6/32 (18%)  | 2 (33%)           | 0               |
| All | All   | 19/96 (19%) | 5 (26%)           | 0               |

All (5) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | Q     | 11  | C    |
| 6   | S     | 13  | G    |
| 6   | S     | 16  | G    |
| 6   | U     | 11  | C    |
| 6   | U     | 12  | G    |

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 223/315 (70%)   | -0.18  | 1 (0%) 92 87  | 82, 143, 203, 231     | 0     |
| 1   | B     | 223/315 (70%)   | -0.25  | 1 (0%) 92 87  | 86, 150, 211, 231     | 0     |
| 1   | F     | 223/315 (70%)   | -0.04  | 4 (1%) 68 60  | 88, 145, 202, 231     | 0     |
| 1   | G     | 224/315 (71%)   | -0.22  | 0 100 100     | 74, 150, 204, 231     | 0     |
| 1   | K     | 225/315 (71%)   | 0.03   | 4 (1%) 68 60  | 77, 152, 205, 231     | 0     |
| 1   | L     | 223/315 (70%)   | -0.24  | 1 (0%) 92 87  | 71, 146, 208, 231     | 0     |
| 2   | C     | 1083/1119 (96%) | -0.17  | 11 (1%) 82 74 | 46, 150, 225, 231     | 0     |
| 2   | H     | 1080/1119 (96%) | -0.18  | 15 (1%) 75 66 | 32, 148, 226, 231     | 0     |
| 2   | M     | 1084/1119 (96%) | -0.07  | 20 (1%) 68 60 | 51, 150, 227, 231     | 0     |
| 3   | D     | 1316/1524 (86%) | -0.08  | 25 (1%) 66 58 | 91, 161, 249, 285     | 0     |
| 3   | I     | 1262/1524 (82%) | 0.04   | 45 (3%) 42 34 | 91, 160, 246, 285     | 0     |
| 3   | N     | 1327/1524 (87%) | -0.01  | 24 (1%) 68 60 | 91, 162, 250, 284     | 0     |
| 4   | E     | 93/99 (93%)     | 0.06   | 2 (2%) 62 52  | 91, 182, 231, 231     | 0     |
| 4   | J     | 93/99 (93%)     | -0.01  | 3 (3%) 47 37  | 98, 176, 231, 231     | 0     |
| 4   | O     | 93/99 (93%)     | -0.06  | 3 (3%) 47 37  | 90, 172, 231, 231     | 0     |
| 5   | P     | 7/27 (25%)      | 0.31   | 0 100 100     | 199, 200, 200, 200    | 0     |
| 5   | R     | 6/27 (22%)      | 0.80   | 0 100 100     | 200, 200, 200, 200    | 0     |
| 5   | T     | 5/27 (18%)      | 0.57   | 0 100 100     | 199, 200, 200, 200    | 0     |
| 6   | Q     | 7/32 (21%)      | 0.94   | 0 100 100     | 195, 200, 200, 200    | 0     |
| 6   | S     | 8/32 (25%)      | 2.18   | 4 (50%) 0 0   | 200, 200, 200, 200    | 0     |
| 6   | U     | 7/32 (21%)      | 1.24   | 1 (14%) 2 3   | 194, 200, 200, 200    | 0     |
| 7   | X     | 154/156 (98%)   | 0.11   | 4 (2%) 56 46  | 97, 175, 229, 231     | 0     |
| 7   | Y     | 152/156 (97%)   | 0.11   | 6 (3%) 39 31  | 88, 174, 228, 231     | 0     |
| 7   | Z     | 152/156 (97%)   | 0.18   | 6 (3%) 39 31  | 95, 172, 228, 231     | 0     |

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| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|----------------|-----------------------|-------|
| All | All   | 9270/10761 (86%) | -0.07  | 180 (1%) 66 58 | 32, 156, 231, 285     | 0     |

All (180) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | E     | 56   | ASP  | 6.1  |
| 3   | I     | 1301 | LYS  | 5.9  |
| 3   | I     | 191  | LEU  | 5.5  |
| 3   | I     | 1292 | VAL  | 5.3  |
| 2   | C     | 270  | GLY  | 4.9  |
| 2   | H     | 270  | GLY  | 4.4  |
| 4   | E     | 57   | ASP  | 4.4  |
| 4   | O     | 56   | ASP  | 4.1  |
| 6   | S     | 10   | G    | 4.1  |
| 4   | J     | 56   | ASP  | 4.0  |
| 2   | H     | 812  | GLY  | 3.8  |
| 2   | C     | 757  | GLY  | 3.7  |
| 3   | I     | 1302 | GLU  | 3.7  |
| 3   | N     | 191  | LEU  | 3.7  |
| 3   | I     | 1313 | VAL  | 3.6  |
| 3   | I     | 560  | GLN  | 3.6  |
| 3   | D     | 38   | LYS  | 3.6  |
| 3   | N     | 165  | LYS  | 3.5  |
| 3   | D     | 355  | VAL  | 3.5  |
| 2   | C     | 268  | ASP  | 3.5  |
| 2   | M     | 269  | LEU  | 3.5  |
| 7   | X     | 118  | LYS  | 3.4  |
| 3   | D     | 1313 | VAL  | 3.4  |
| 4   | J     | 33   | HIS  | 3.4  |
| 3   | I     | 1380 | GLU  | 3.4  |
| 3   | I     | 488  | ARG  | 3.3  |
| 3   | N     | 1313 | VAL  | 3.3  |
| 3   | D     | 369  | ALA  | 3.2  |
| 1   | K     | 7    | LYS  | 3.2  |
| 3   | I     | 1294 | VAL  | 3.2  |
| 3   | I     | 176  | ASP  | 3.2  |
| 3   | I     | 48   | ARG  | 3.2  |
| 3   | D     | 801  | GLY  | 3.2  |
| 3   | I     | 801  | GLY  | 3.2  |
| 6   | S     | 13   | G    | 3.2  |
| 2   | M     | 268  | ASP  | 3.2  |
| 3   | D     | 560  | GLN  | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | N     | 801  | GLY  | 3.1  |
| 3   | D     | 212  | ARG  | 3.1  |
| 3   | N     | 1308 | GLU  | 3.1  |
| 3   | I     | 409  | VAL  | 3.1  |
| 2   | M     | 70   | GLU  | 3.1  |
| 3   | N     | 482  | LYS  | 3.1  |
| 7   | Y     | 83   | ILE  | 3.1  |
| 3   | I     | 1304 | LYS  | 3.1  |
| 3   | I     | 184  | GLU  | 3.0  |
| 3   | N     | 808  | THR  | 3.0  |
| 3   | I     | 1414 | PRO  | 3.0  |
| 1   | F     | 146  | ARG  | 3.0  |
| 2   | C     | 805  | ARG  | 3.0  |
| 3   | I     | 1412 | LYS  | 3.0  |
| 3   | N     | 1090 | ASP  | 3.0  |
| 4   | J     | 57   | ASP  | 3.0  |
| 3   | N     | 802  | ALA  | 3.0  |
| 2   | M     | 736  | ASP  | 2.9  |
| 2   | M     | 167  | LYS  | 2.9  |
| 3   | D     | 444  | VAL  | 2.9  |
| 2   | M     | 266  | ARG  | 2.9  |
| 3   | D     | 802  | ALA  | 2.9  |
| 3   | N     | 594  | PRO  | 2.9  |
| 2   | H     | 417  | GLY  | 2.9  |
| 3   | N     | 340  | THR  | 2.9  |
| 3   | N     | 397  | LYS  | 2.8  |
| 3   | D     | 421  | LEU  | 2.8  |
| 3   | I     | 1319 | VAL  | 2.8  |
| 3   | I     | 430  | ASP  | 2.8  |
| 3   | N     | 666  | ILE  | 2.8  |
| 3   | D     | 368  | VAL  | 2.8  |
| 3   | I     | 165  | LYS  | 2.8  |
| 2   | M     | 785  | VAL  | 2.8  |
| 3   | I     | 174  | GLY  | 2.8  |
| 2   | C     | 807  | ARG  | 2.8  |
| 6   | S     | 12   | G    | 2.8  |
| 6   | S     | 11   | C    | 2.7  |
| 3   | I     | 177  | ALA  | 2.7  |
| 2   | M     | 415  | PRO  | 2.7  |
| 2   | M     | 758  | ARG  | 2.7  |
| 2   | H     | 821  | GLU  | 2.7  |
| 7   | Z     | 83   | ILE  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | D     | 85   | VAL  | 2.6  |
| 3   | I     | 190  | GLU  | 2.6  |
| 3   | N     | 1339 | LYS  | 2.6  |
| 7   | Z     | 117  | MET  | 2.6  |
| 3   | N     | 811  | GLU  | 2.6  |
| 7   | X     | 139  | SER  | 2.6  |
| 3   | D     | 177  | ALA  | 2.5  |
| 2   | H     | 805  | ARG  | 2.5  |
| 1   | L     | 119  | ASP  | 2.5  |
| 3   | I     | 1308 | GLU  | 2.5  |
| 7   | Y     | 156  | GLY  | 2.5  |
| 3   | I     | 49   | ILE  | 2.5  |
| 2   | M     | 786  | LYS  | 2.5  |
| 3   | N     | 1302 | GLU  | 2.5  |
| 2   | C     | 269  | LEU  | 2.5  |
| 1   | F     | 122  | ILE  | 2.5  |
| 3   | I     | 192  | ALA  | 2.5  |
| 2   | H     | 808  | ARG  | 2.5  |
| 1   | K     | 182  | GLU  | 2.4  |
| 3   | N     | 39   | PRO  | 2.4  |
| 2   | M     | 714  | ASP  | 2.4  |
| 2   | M     | 418  | LEU  | 2.4  |
| 3   | I     | 86   | ARG  | 2.4  |
| 2   | M     | 244  | PRO  | 2.4  |
| 2   | M     | 248  | PRO  | 2.4  |
| 7   | Y     | 129  | LEU  | 2.4  |
| 7   | Z     | 104  | VAL  | 2.4  |
| 3   | I     | 1276 | GLU  | 2.4  |
| 2   | H     | 271  | GLU  | 2.4  |
| 2   | H     | 823  | VAL  | 2.4  |
| 2   | H     | 733  | ALA  | 2.4  |
| 1   | F     | 17   | GLY  | 2.4  |
| 3   | I     | 1305 | LEU  | 2.3  |
| 7   | Z     | 146  | ARG  | 2.3  |
| 2   | C     | 99   | GLN  | 2.3  |
| 2   | M     | 243  | ARG  | 2.3  |
| 2   | H     | 1022 | GLY  | 2.3  |
| 3   | N     | 610  | LYS  | 2.3  |
| 1   | K     | 186  | LEU  | 2.2  |
| 3   | I     | 1300 | SER  | 2.2  |
| 3   | D     | 448  | GLU  | 2.2  |
| 3   | I     | 484  | PRO  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | I     | 182  | GLY  | 2.2  |
| 7   | X     | 85   | LEU  | 2.2  |
| 7   | X     | 150  | ARG  | 2.2  |
| 3   | I     | 485  | SER  | 2.2  |
| 2   | H     | 1023 | GLY  | 2.2  |
| 1   | B     | 134  | GLU  | 2.2  |
| 3   | D     | 211  | VAL  | 2.2  |
| 3   | N     | 54   | LYS  | 2.2  |
| 3   | D     | 1319 | VAL  | 2.2  |
| 3   | N     | 1412 | LYS  | 2.2  |
| 6   | U     | 12   | G    | 2.2  |
| 3   | I     | 189  | GLN  | 2.2  |
| 3   | D     | 1276 | GLU  | 2.2  |
| 2   | H     | 648  | ARG  | 2.1  |
| 4   | O     | 94   | PRO  | 2.1  |
| 3   | D     | 1304 | LYS  | 2.1  |
| 3   | D     | 37   | LEU  | 2.1  |
| 7   | Y     | 78   | GLY  | 2.1  |
| 3   | I     | 834  | THR  | 2.1  |
| 7   | Y     | 130  | LEU  | 2.1  |
| 1   | A     | 185  | ARG  | 2.1  |
| 3   | I     | 50   | PHE  | 2.1  |
| 3   | N     | 189  | GLN  | 2.1  |
| 2   | H     | 807  | ARG  | 2.1  |
| 3   | D     | 1294 | VAL  | 2.1  |
| 2   | H     | 167  | LYS  | 2.1  |
| 2   | M     | 1023 | GLY  | 2.1  |
| 3   | I     | 483  | HIS  | 2.1  |
| 2   | C     | 754  | ILE  | 2.1  |
| 3   | I     | 610  | LYS  | 2.1  |
| 3   | D     | 39   | PRO  | 2.1  |
| 3   | I     | 44   | LEU  | 2.1  |
| 3   | D     | 796  | ARG  | 2.1  |
| 3   | N     | 509  | PRO  | 2.1  |
| 4   | O     | 57   | ASP  | 2.1  |
| 3   | N     | 212  | ARG  | 2.1  |
| 7   | Z     | 102  | VAL  | 2.1  |
| 7   | Z     | 131  | GLY  | 2.1  |
| 3   | I     | 1421 | LEU  | 2.1  |
| 2   | C     | 721  | ARG  | 2.1  |
| 2   | M     | 930  | LYS  | 2.1  |
| 3   | I     | 421  | LEU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | Y     | 81   | GLU  | 2.1  |
| 3   | I     | 161  | LEU  | 2.1  |
| 3   | N     | 120  | ALA  | 2.1  |
| 2   | M     | 270  | GLY  | 2.1  |
| 2   | M     | 247  | PRO  | 2.0  |
| 3   | I     | 802  | ALA  | 2.0  |
| 2   | C     | 808  | ARG  | 2.0  |
| 2   | H     | 757  | GLY  | 2.0  |
| 3   | D     | 378  | ILE  | 2.0  |
| 1   | F     | 229  | GLN  | 2.0  |
| 1   | K     | 22   | GLU  | 2.0  |
| 2   | M     | 757  | GLY  | 2.0  |
| 3   | I     | 1303 | TYR  | 2.0  |
| 3   | I     | 1311 | LEU  | 2.0  |
| 2   | C     | 423  | ALA  | 2.0  |
| 3   | D     | 1301 | LYS  | 2.0  |
| 3   | D     | 1154 | GLU  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 8   | ZN   | N     | 2001 | 1/1   | 0.91 | 0.07 | 115,115,115,115             | 0     |
| 8   | ZN   | D     | 2002 | 1/1   | 0.96 | 0.03 | 115,115,115,115             | 0     |
| 9   | MG   | N     | 2006 | 1/1   | 0.96 | 0.45 | 115,115,115,115             | 0     |
| 9   | MG   | S     | 2005 | 1/1   | 0.97 | 0.86 | 115,115,115,115             | 0     |
| 8   | ZN   | I     | 2003 | 1/1   | 0.99 | 0.09 | 115,115,115,115             | 0     |
| 9   | MG   | D     | 2004 | 1/1   | 0.99 | 0.11 | 115,115,115,115             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.