



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 14, 2017 – 10:47 AM EST

PDB ID : 5WQ9  
EMDB ID: : EMD-6677  
Title : CryoEM structure of type II secretion system secretin GspD G453A mutant  
in *Vibrio cholerae*  
Authors : Yan, Z.; Yin, M.; Li, X.  
Deposited on : 2016-11-23  
Resolution : 4.22 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

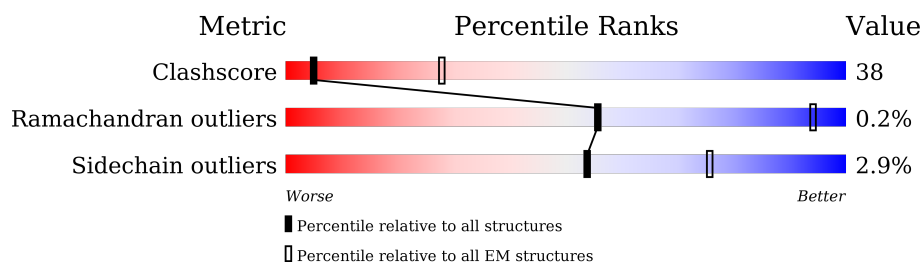
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.22 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 114402                      | 924                         |
| Ramachandran outliers | 111179                      | 726                         |
| Sidechain outliers    | 111093                      | 686                         |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 650    | 41% 33% • 24%    |
| 1   | B     | 650    | 40% 33% • 24%    |
| 1   | C     | 650    | 40% 33% • 24%    |
| 1   | D     | 650    | 41% 33% • 24%    |
| 1   | E     | 650    | 41% 33% • 24%    |
| 1   | F     | 650    | 41% 33% • 24%    |
| 1   | G     | 650    | 40% 33% • 24%    |
| 1   | H     | 650    | 40% 33% • 24%    |
| 1   | I     | 650    | 41% 33% • 24%    |

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| Mol | Chain | Length | Quality of chain                           |
|-----|-------|--------|--|
| 1   | J     | 650    | <div><div></div><div>41%33%24%</div></div> |
| 1   | K     | 650    | <div><div></div><div>41%33%24%</div></div> |
| 1   | L     | 650    | <div><div></div><div>40%33%24%</div></div> |
| 1   | M     | 650    | <div><div></div><div>40%33%24%</div></div> |
| 1   | N     | 650    | <div><div></div><div>40%33%24%</div></div> |
| 1   | O     | 650    | <div><div></div><div>41%33%24%</div></div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 56340 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Type II secretion system protein D.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | B     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | C     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | D     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | E     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | F     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | G     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | H     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | I     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | J     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | K     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | L     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | M     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | N     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |
| 1   | O     | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2347 | 656 | 740 | 13 |         |       |

There are 15 discrepancies between the modelled and reference sequences:

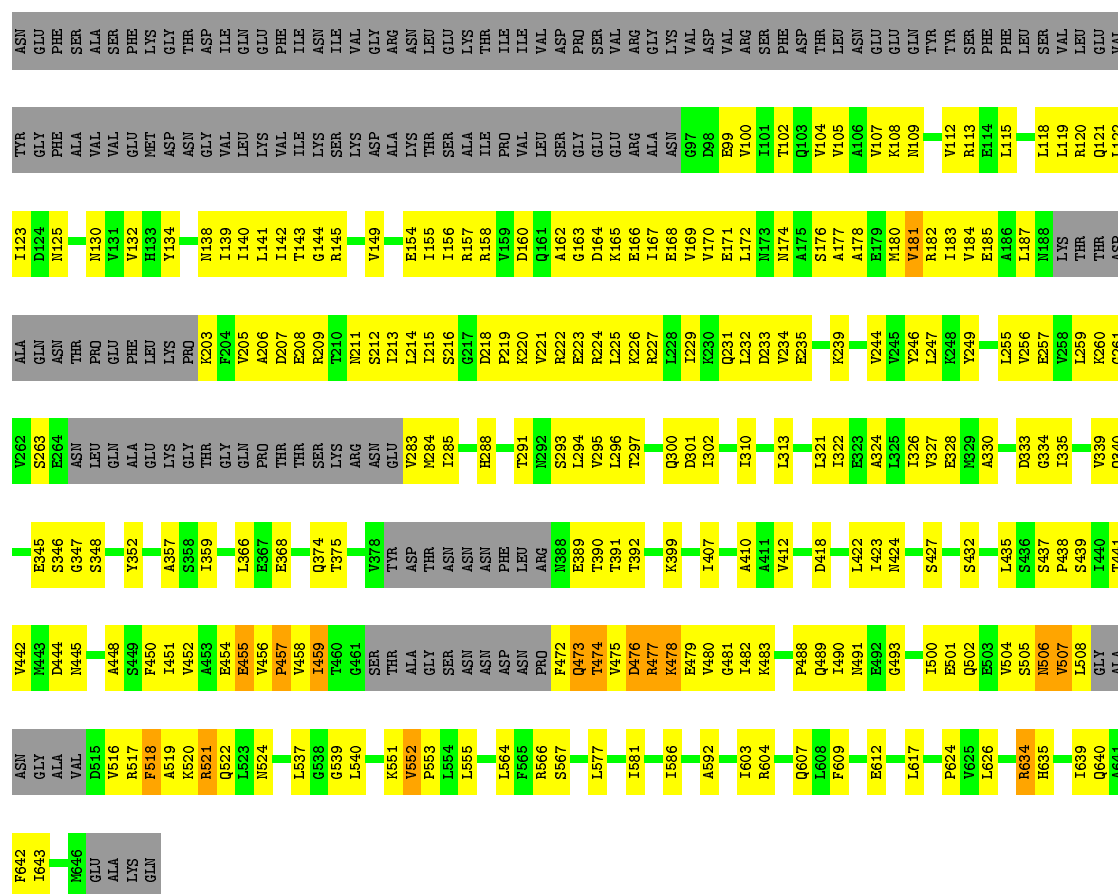
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| B     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| C     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| D     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| E     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| F     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| G     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| H     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| I     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| J     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| K     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| L     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| M     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| N     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |
| O     | 453     | ALA      | GLY    | engineered mutation | UNP P45779 |

### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

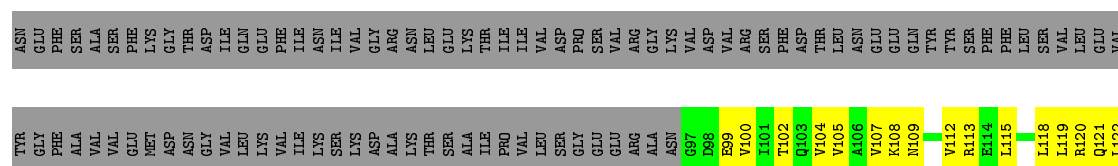
- Molecule 1: Type II secretion system protein D

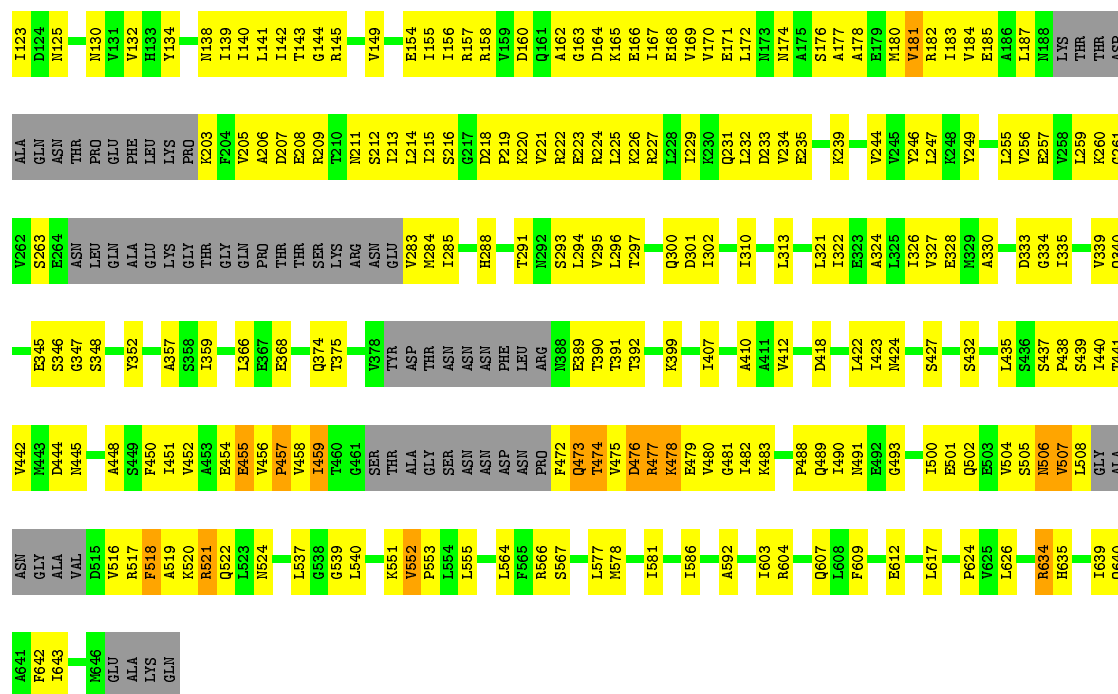
Chain A: 



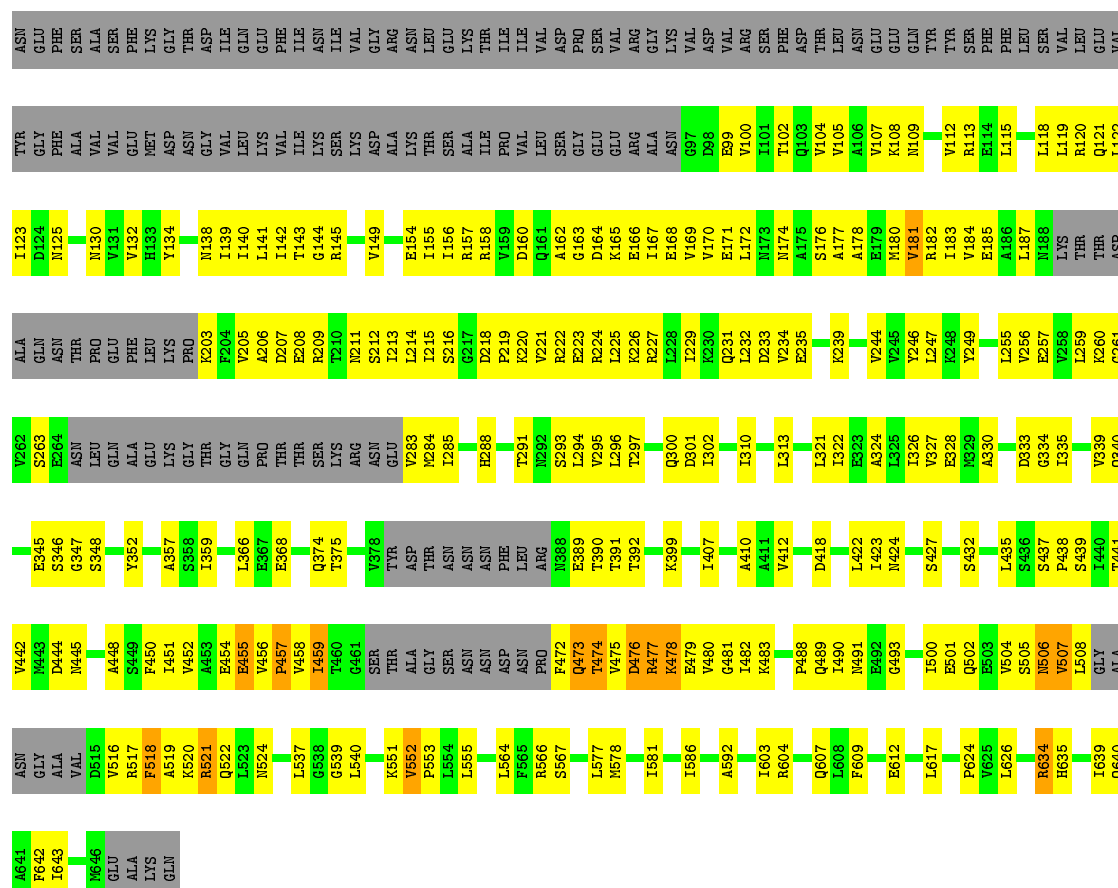
- Molecule 1: Type II secretion system protein D

Chain B: 





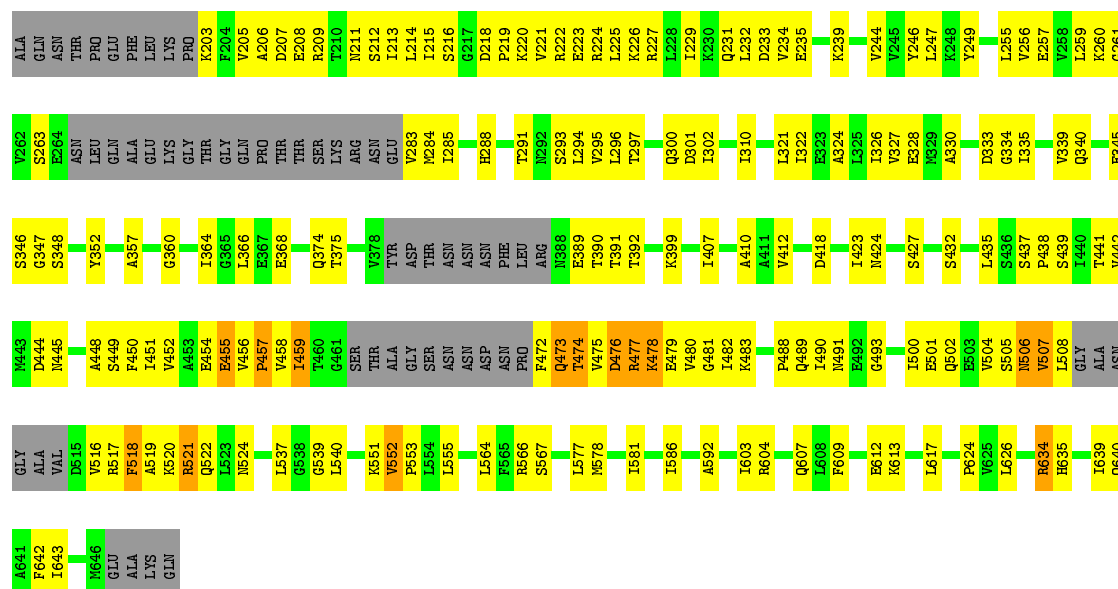
• Molecule 1: Type II secretion system protein D



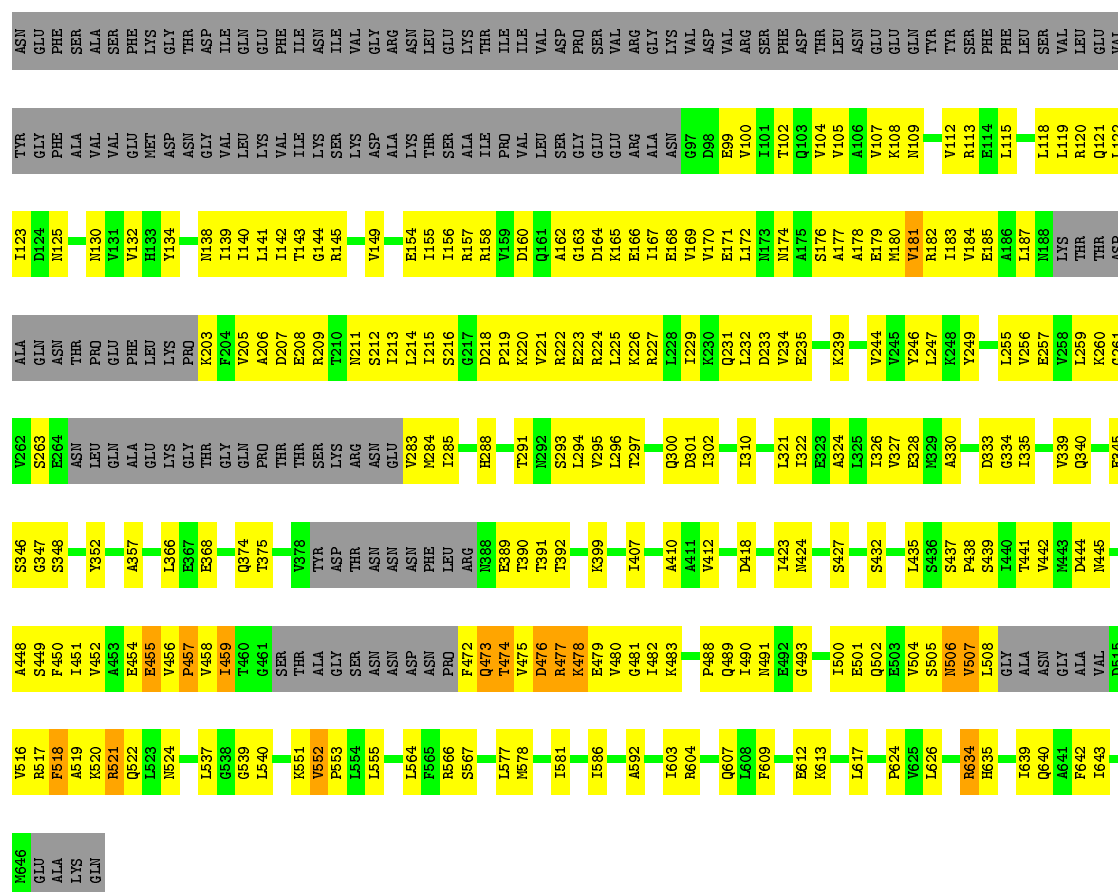








• Molecule 1: Type II secretion system protein D



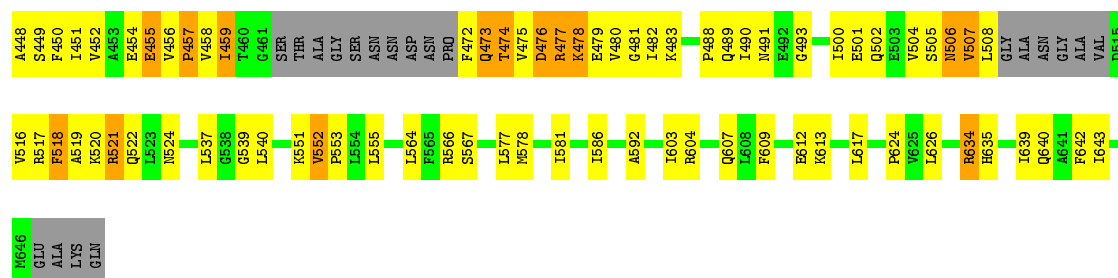
• Molecule 1: Type II secretion system protein D

| Category  | Percentage |
|-----------|------------|
| Very good | 41%        |
| Good      | 33%        |
| Not good  | 1%         |
| Very bad  | 24%        |



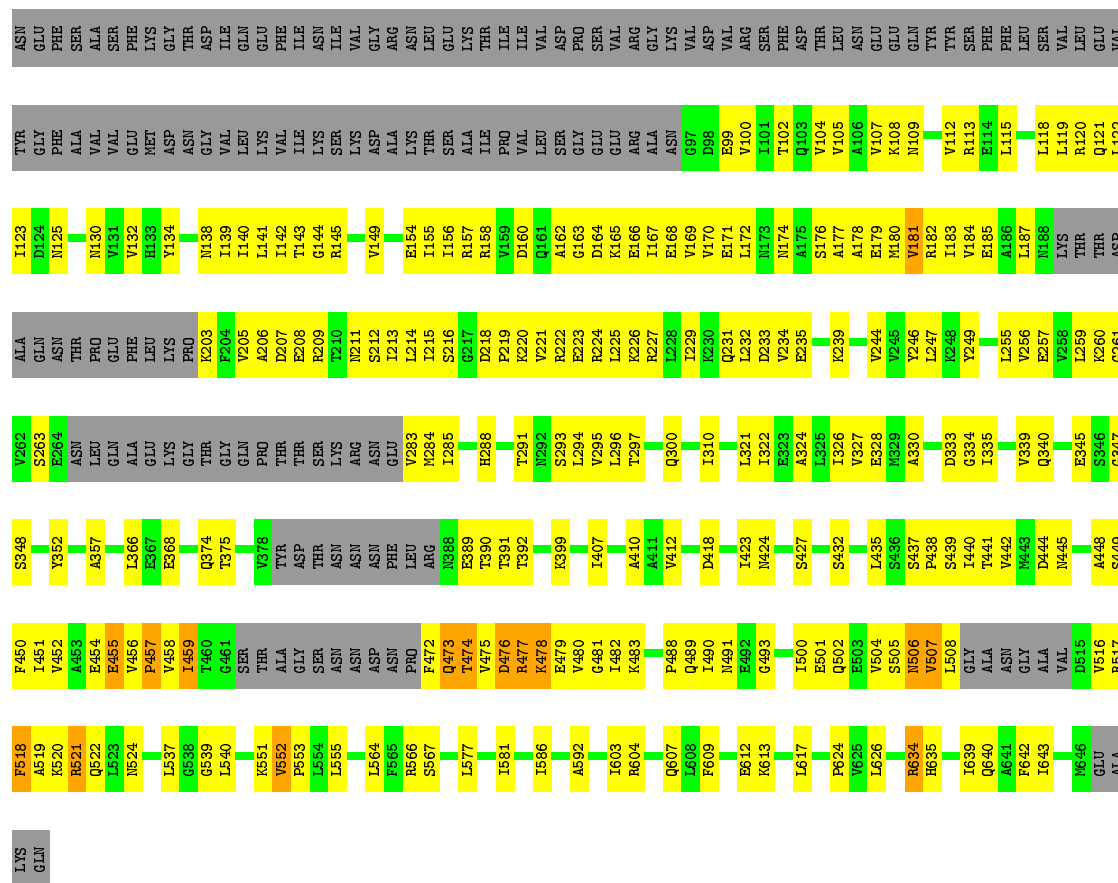
| Response             | Percentage |
|----------------------|------------|
| Doing a good job     | 41%        |
| Not doing a good job | 33%        |
| Don't know           | 24%        |





• Molecule 1: Type II secretion system protein D

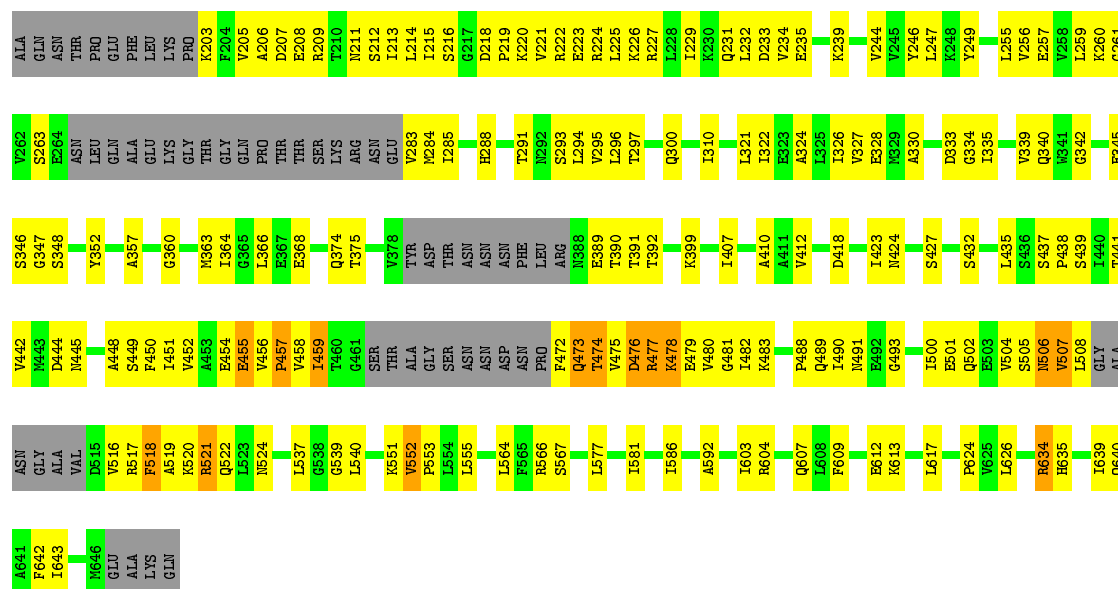
Chain K: 41% 33% 24%



• Molecule 1: Type II secretion system protein D

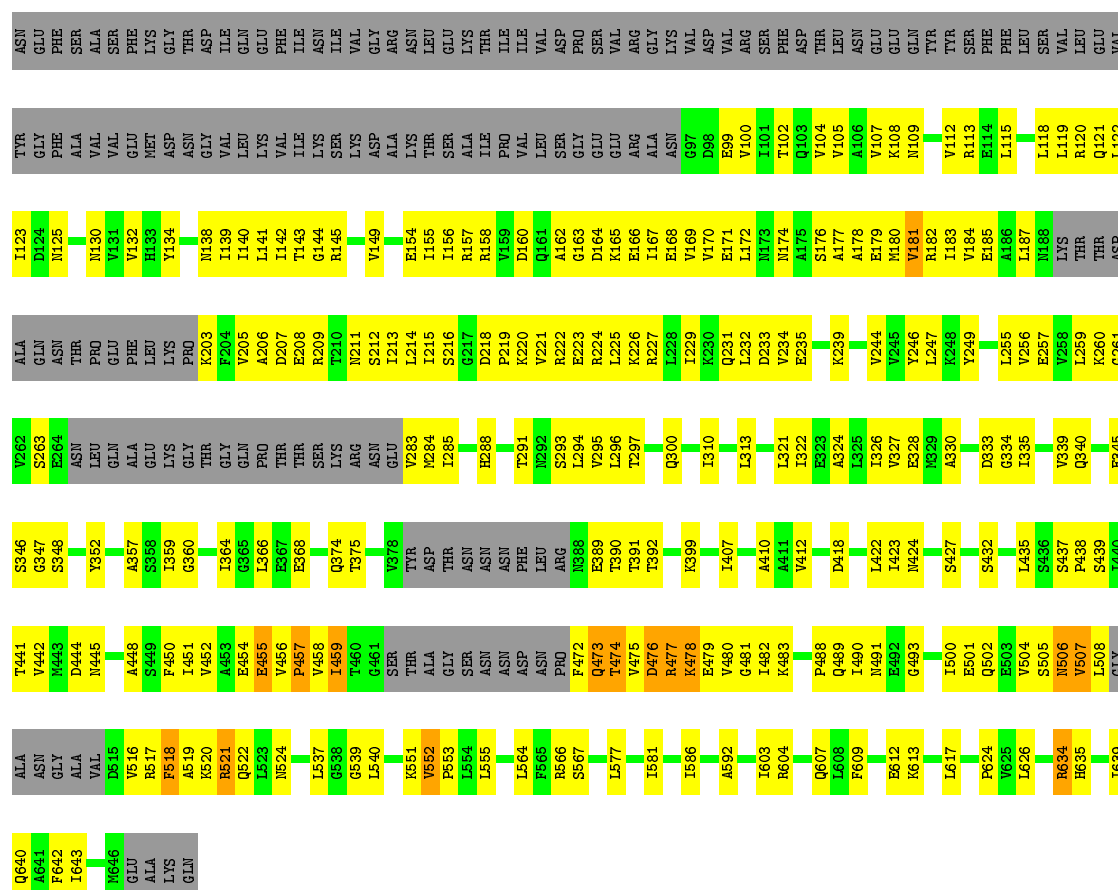
Chain L: 40% 33% 24%





- Molecule 1: Type II secretion system protein D

Chain M:



- Molecule 1: Type II secretion system protein D





## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, Not provided | Depositor |
| Number of particles used             | 26955               | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF   | Depositor |
| CTF correction method                | Not provided        | Depositor |
| Microscope                           | FEI TITAN KRIOS     | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | Not provided        | Depositor |
| Minimum defocus (nm)                 | Not provided        | Depositor |
| Maximum defocus (nm)                 | Not provided        | Depositor |
| Magnification                        | Not provided        | Depositor |
| Image detector                       | Not provided        | Depositor |



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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         | $\# Z  > 2$     | RMSZ        | $\# Z  > 2$     |
| 1   | A     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | B     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | C     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | D     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | E     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | F     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | G     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | H     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | I     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | J     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | K     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | L     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | M     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | N     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| 1   | O     | 0.41         | 1/3786 (0.0%)   | 0.64        | 4/5117 (0.1%)   |
| All | All   | 0.41         | 15/56790 (0.0%) | 0.64        | 60/76755 (0.1%) |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | M     | 457 | PRO  | N-CD  | 5.24 | 1.55        | 1.47     |
| 1   | E     | 457 | PRO  | N-CD  | 5.23 | 1.55        | 1.47     |
| 1   | J     | 457 | PRO  | N-CD  | 5.23 | 1.55        | 1.47     |
| 1   | C     | 457 | PRO  | N-CD  | 5.21 | 1.55        | 1.47     |
| 1   | B     | 457 | PRO  | N-CD  | 5.21 | 1.55        | 1.47     |
| 1   | L     | 457 | PRO  | N-CD  | 5.21 | 1.55        | 1.47     |
| 1   | A     | 457 | PRO  | N-CD  | 5.21 | 1.55        | 1.47     |
| 1   | G     | 457 | PRO  | N-CD  | 5.21 | 1.55        | 1.47     |
| 1   | H     | 457 | PRO  | N-CD  | 5.21 | 1.55        | 1.47     |
| 1   | F     | 457 | PRO  | N-CD  | 5.20 | 1.55        | 1.47     |
| 1   | O     | 457 | PRO  | N-CD  | 5.20 | 1.55        | 1.47     |
| 1   | K     | 457 | PRO  | N-CD  | 5.20 | 1.55        | 1.47     |
| 1   | D     | 457 | PRO  | N-CD  | 5.19 | 1.55        | 1.47     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | N     | 457 | PRO  | N-CD  | 5.19 | 1.55        | 1.47     |
| 1   | I     | 457 | PRO  | N-CD  | 5.19 | 1.55        | 1.47     |

All (60) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | B     | 507 | VAL  | CB-CA-C | -10.70 | 91.07       | 111.40   |
| 1   | E     | 507 | VAL  | CB-CA-C | -10.70 | 91.07       | 111.40   |
| 1   | C     | 507 | VAL  | CB-CA-C | -10.70 | 91.07       | 111.40   |
| 1   | I     | 507 | VAL  | CB-CA-C | -10.70 | 91.08       | 111.40   |
| 1   | M     | 507 | VAL  | CB-CA-C | -10.70 | 91.08       | 111.40   |
| 1   | G     | 507 | VAL  | CB-CA-C | -10.69 | 91.08       | 111.40   |
| 1   | A     | 507 | VAL  | CB-CA-C | -10.69 | 91.09       | 111.40   |
| 1   | O     | 507 | VAL  | CB-CA-C | -10.69 | 91.09       | 111.40   |
| 1   | H     | 507 | VAL  | CB-CA-C | -10.69 | 91.09       | 111.40   |
| 1   | L     | 507 | VAL  | CB-CA-C | -10.69 | 91.09       | 111.40   |
| 1   | K     | 507 | VAL  | CB-CA-C | -10.69 | 91.09       | 111.40   |
| 1   | F     | 507 | VAL  | CB-CA-C | -10.68 | 91.10       | 111.40   |
| 1   | J     | 507 | VAL  | CB-CA-C | -10.68 | 91.10       | 111.40   |
| 1   | D     | 507 | VAL  | CB-CA-C | -10.68 | 91.11       | 111.40   |
| 1   | N     | 507 | VAL  | CB-CA-C | -10.68 | 91.11       | 111.40   |
| 1   | I     | 552 | VAL  | C-N-CD  | -6.92  | 105.38      | 120.60   |
| 1   | D     | 552 | VAL  | C-N-CD  | -6.92  | 105.39      | 120.60   |
| 1   | N     | 552 | VAL  | C-N-CD  | -6.91  | 105.40      | 120.60   |
| 1   | C     | 552 | VAL  | C-N-CD  | -6.90  | 105.41      | 120.60   |
| 1   | F     | 552 | VAL  | C-N-CD  | -6.90  | 105.42      | 120.60   |
| 1   | J     | 552 | VAL  | C-N-CD  | -6.90  | 105.41      | 120.60   |
| 1   | K     | 552 | VAL  | C-N-CD  | -6.90  | 105.42      | 120.60   |
| 1   | A     | 552 | VAL  | C-N-CD  | -6.90  | 105.42      | 120.60   |
| 1   | O     | 552 | VAL  | C-N-CD  | -6.90  | 105.42      | 120.60   |
| 1   | M     | 552 | VAL  | C-N-CD  | -6.90  | 105.43      | 120.60   |
| 1   | B     | 552 | VAL  | C-N-CD  | -6.89  | 105.43      | 120.60   |
| 1   | G     | 552 | VAL  | C-N-CD  | -6.89  | 105.43      | 120.60   |
| 1   | E     | 552 | VAL  | C-N-CD  | -6.89  | 105.44      | 120.60   |
| 1   | H     | 552 | VAL  | C-N-CD  | -6.88  | 105.46      | 120.60   |
| 1   | L     | 552 | VAL  | C-N-CD  | -6.88  | 105.46      | 120.60   |
| 1   | D     | 634 | ARG  | N-CA-C  | 5.34   | 125.43      | 111.00   |
| 1   | B     | 634 | ARG  | N-CA-C  | 5.34   | 125.43      | 111.00   |
| 1   | C     | 634 | ARG  | N-CA-C  | 5.33   | 125.40      | 111.00   |
| 1   | E     | 634 | ARG  | N-CA-C  | 5.33   | 125.40      | 111.00   |
| 1   | F     | 634 | ARG  | N-CA-C  | 5.33   | 125.40      | 111.00   |
| 1   | K     | 634 | ARG  | N-CA-C  | 5.33   | 125.39      | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | J     | 634 | ARG  | N-CA-C | 5.33 | 125.38      | 111.00   |
| 1   | M     | 634 | ARG  | N-CA-C | 5.33 | 125.38      | 111.00   |
| 1   | A     | 634 | ARG  | N-CA-C | 5.32 | 125.38      | 111.00   |
| 1   | H     | 634 | ARG  | N-CA-C | 5.32 | 125.37      | 111.00   |
| 1   | O     | 634 | ARG  | N-CA-C | 5.32 | 125.37      | 111.00   |
| 1   | G     | 634 | ARG  | N-CA-C | 5.32 | 125.37      | 111.00   |
| 1   | N     | 634 | ARG  | N-CA-C | 5.32 | 125.37      | 111.00   |
| 1   | L     | 634 | ARG  | N-CA-C | 5.32 | 125.36      | 111.00   |
| 1   | I     | 634 | ARG  | N-CA-C | 5.31 | 125.35      | 111.00   |
| 1   | D     | 552 | VAL  | C-N-CA | 5.25 | 144.05      | 122.00   |
| 1   | F     | 552 | VAL  | C-N-CA | 5.25 | 144.04      | 122.00   |
| 1   | E     | 552 | VAL  | C-N-CA | 5.25 | 144.04      | 122.00   |
| 1   | I     | 552 | VAL  | C-N-CA | 5.25 | 144.03      | 122.00   |
| 1   | J     | 552 | VAL  | C-N-CA | 5.25 | 144.03      | 122.00   |
| 1   | B     | 552 | VAL  | C-N-CA | 5.24 | 144.02      | 122.00   |
| 1   | K     | 552 | VAL  | C-N-CA | 5.24 | 144.03      | 122.00   |
| 1   | N     | 552 | VAL  | C-N-CA | 5.24 | 144.03      | 122.00   |
| 1   | A     | 552 | VAL  | C-N-CA | 5.24 | 144.02      | 122.00   |
| 1   | C     | 552 | VAL  | C-N-CA | 5.24 | 144.02      | 122.00   |
| 1   | G     | 552 | VAL  | C-N-CA | 5.24 | 144.01      | 122.00   |
| 1   | O     | 552 | VAL  | C-N-CA | 5.24 | 143.99      | 122.00   |
| 1   | H     | 552 | VAL  | C-N-CA | 5.23 | 143.98      | 122.00   |
| 1   | L     | 552 | VAL  | C-N-CA | 5.23 | 143.98      | 122.00   |
| 1   | M     | 552 | VAL  | C-N-CA | 5.23 | 143.98      | 122.00   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3756  | 0        | 3858     | 323     | 0            |
| 1   | B     | 3756  | 0        | 3858     | 327     | 0            |
| 1   | C     | 3756  | 0        | 3858     | 320     | 0            |
| 1   | D     | 3756  | 0        | 3858     | 317     | 0            |
| 1   | E     | 3756  | 0        | 3858     | 319     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | F     | 3756  | 0        | 3858     | 319     | 0            |
| 1   | G     | 3756  | 0        | 3858     | 318     | 0            |
| 1   | H     | 3756  | 0        | 3858     | 319     | 0            |
| 1   | I     | 3756  | 0        | 3858     | 318     | 0            |
| 1   | J     | 3756  | 0        | 3858     | 324     | 0            |
| 1   | K     | 3756  | 0        | 3858     | 322     | 0            |
| 1   | L     | 3756  | 0        | 3858     | 320     | 0            |
| 1   | M     | 3756  | 0        | 3858     | 317     | 0            |
| 1   | N     | 3756  | 0        | 3858     | 321     | 0            |
| 1   | O     | 3756  | 0        | 3858     | 324     | 0            |
| All | All   | 56340 | 0        | 57870    | 4309    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (4309) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:G:481:GLY:H  | 1:G:505:SER:CB | 1.22                     | 1.53              |
| 1:I:481:GLY:H  | 1:I:505:SER:CB | 1.22                     | 1.53              |
| 1:L:481:GLY:H  | 1:L:505:SER:CB | 1.22                     | 1.52              |
| 1:N:481:GLY:H  | 1:N:505:SER:CB | 1.22                     | 1.52              |
| 1:K:481:GLY:H  | 1:K:505:SER:CB | 1.22                     | 1.52              |
| 1:D:481:GLY:H  | 1:D:505:SER:CB | 1.22                     | 1.52              |
| 1:E:481:GLY:H  | 1:E:505:SER:CB | 1.22                     | 1.51              |
| 1:B:481:GLY:H  | 1:B:505:SER:CB | 1.22                     | 1.51              |
| 1:F:481:GLY:H  | 1:F:505:SER:CB | 1.22                     | 1.51              |
| 1:J:481:GLY:H  | 1:J:505:SER:CB | 1.22                     | 1.50              |
| 1:A:481:GLY:H  | 1:A:505:SER:CB | 1.22                     | 1.50              |
| 1:M:481:GLY:H  | 1:M:505:SER:CB | 1.22                     | 1.49              |
| 1:O:481:GLY:H  | 1:O:505:SER:CB | 1.22                     | 1.49              |
| 1:H:481:GLY:H  | 1:H:505:SER:CB | 1.22                     | 1.48              |
| 1:C:481:GLY:H  | 1:C:505:SER:CB | 1.22                     | 1.47              |
| 1:H:480:VAL:CB | 1:H:505:SER:OG | 1.65                     | 1.45              |
| 1:D:480:VAL:CB | 1:D:505:SER:OG | 1.65                     | 1.45              |
| 1:N:480:VAL:CB | 1:N:505:SER:OG | 1.65                     | 1.45              |
| 1:O:480:VAL:CB | 1:O:505:SER:OG | 1.65                     | 1.45              |
| 1:I:480:VAL:CB | 1:I:505:SER:OG | 1.65                     | 1.45              |
| 1:C:480:VAL:CB | 1:C:505:SER:OG | 1.65                     | 1.44              |
| 1:G:480:VAL:CB | 1:G:505:SER:OG | 1.65                     | 1.44              |
| 1:M:480:VAL:CB | 1:M:505:SER:OG | 1.65                     | 1.44              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:A:480:VAL:CB | 1:A:505:SER:OG  | 1.65                     | 1.43              |
| 1:L:480:VAL:CB | 1:L:505:SER:OG  | 1.65                     | 1.43              |
| 1:E:480:VAL:CB | 1:E:505:SER:OG  | 1.65                     | 1.43              |
| 1:K:481:GLY:N  | 1:K:505:SER:HB3 | 1.12                     | 1.43              |
| 1:J:481:GLY:N  | 1:J:505:SER:HB3 | 1.12                     | 1.43              |
| 1:B:480:VAL:CB | 1:B:505:SER:OG  | 1.65                     | 1.42              |
| 1:J:480:VAL:CB | 1:J:505:SER:OG  | 1.65                     | 1.42              |
| 1:K:480:VAL:CB | 1:K:505:SER:OG  | 1.65                     | 1.42              |
| 1:L:481:GLY:N  | 1:L:505:SER:HB3 | 1.12                     | 1.42              |
| 1:I:481:GLY:N  | 1:I:505:SER:HB3 | 1.12                     | 1.42              |
| 1:F:480:VAL:CB | 1:F:505:SER:OG  | 1.65                     | 1.42              |
| 1:M:481:GLY:N  | 1:M:505:SER:HB3 | 1.12                     | 1.40              |
| 1:H:481:GLY:N  | 1:H:505:SER:HB3 | 1.12                     | 1.40              |
| 1:D:481:GLY:N  | 1:D:505:SER:HB3 | 1.12                     | 1.39              |
| 1:C:481:GLY:N  | 1:C:505:SER:HB3 | 1.12                     | 1.39              |
| 1:E:481:GLY:N  | 1:E:505:SER:HB3 | 1.12                     | 1.39              |
| 1:F:481:GLY:N  | 1:F:505:SER:HB3 | 1.12                     | 1.38              |
| 1:B:481:GLY:N  | 1:B:505:SER:HB3 | 1.12                     | 1.38              |
| 1:N:481:GLY:N  | 1:N:505:SER:HB3 | 1.12                     | 1.37              |
| 1:G:481:GLY:N  | 1:G:505:SER:HB3 | 1.12                     | 1.37              |
| 1:O:481:GLY:N  | 1:O:505:SER:HB3 | 1.12                     | 1.37              |
| 1:A:481:GLY:N  | 1:A:505:SER:HB3 | 1.12                     | 1.37              |
| 1:C:480:VAL:CA | 1:C:505:SER:OG  | 1.74                     | 1.36              |
| 1:B:480:VAL:CA | 1:B:505:SER:OG  | 1.74                     | 1.35              |
| 1:D:480:VAL:CA | 1:D:505:SER:OG  | 1.74                     | 1.35              |
| 1:G:480:VAL:CA | 1:G:505:SER:OG  | 1.74                     | 1.35              |
| 1:M:480:VAL:CA | 1:M:505:SER:OG  | 1.74                     | 1.35              |
| 1:F:480:VAL:CA | 1:F:505:SER:OG  | 1.74                     | 1.34              |
| 1:J:480:VAL:CA | 1:J:505:SER:OG  | 1.74                     | 1.34              |
| 1:I:480:VAL:CA | 1:I:505:SER:OG  | 1.74                     | 1.34              |
| 1:L:480:VAL:CA | 1:L:505:SER:OG  | 1.74                     | 1.34              |
| 1:H:480:VAL:CA | 1:H:505:SER:OG  | 1.74                     | 1.34              |
| 1:N:480:VAL:CA | 1:N:505:SER:OG  | 1.74                     | 1.34              |
| 1:A:480:VAL:CA | 1:A:505:SER:OG  | 1.74                     | 1.33              |
| 1:E:480:VAL:CA | 1:E:505:SER:OG  | 1.74                     | 1.33              |
| 1:K:480:VAL:CA | 1:K:505:SER:OG  | 1.74                     | 1.33              |
| 1:O:480:VAL:CA | 1:O:505:SER:OG  | 1.74                     | 1.32              |
| 1:G:480:VAL:HB | 1:G:505:SER:OG  | 1.15                     | 1.31              |
| 1:H:480:VAL:HB | 1:H:505:SER:OG  | 1.15                     | 1.31              |
| 1:I:480:VAL:HB | 1:I:505:SER:OG  | 1.15                     | 1.31              |
| 1:F:480:VAL:HB | 1:F:505:SER:OG  | 1.15                     | 1.30              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:E:480:VAL:HB   | 1:E:505:SER:OG  | 1.15                     | 1.29              |
| 1:J:459:ILE:HG23 | 1:J:474:THR:O   | 1.31                     | 1.28              |
| 1:D:459:ILE:HG23 | 1:D:474:THR:O   | 1.31                     | 1.27              |
| 1:D:480:VAL:HB   | 1:D:505:SER:OG  | 1.15                     | 1.27              |
| 1:B:459:ILE:HG23 | 1:B:474:THR:O   | 1.31                     | 1.26              |
| 1:I:459:ILE:HG23 | 1:I:474:THR:O   | 1.31                     | 1.26              |
| 1:M:480:VAL:HB   | 1:M:505:SER:OG  | 1.15                     | 1.26              |
| 1:B:481:GLY:N    | 1:B:505:SER:CB  | 1.88                     | 1.25              |
| 1:M:459:ILE:HG23 | 1:M:474:THR:O   | 1.31                     | 1.25              |
| 1:N:480:VAL:HB   | 1:N:505:SER:OG  | 1.15                     | 1.25              |
| 1:A:459:ILE:HG23 | 1:A:474:THR:O   | 1.31                     | 1.25              |
| 1:K:459:ILE:HG23 | 1:K:474:THR:O   | 1.31                     | 1.25              |
| 1:O:481:GLY:N    | 1:O:505:SER:CB  | 1.88                     | 1.25              |
| 1:C:481:GLY:N    | 1:C:505:SER:CB  | 1.88                     | 1.24              |
| 1:L:459:ILE:HG23 | 1:L:474:THR:O   | 1.31                     | 1.24              |
| 1:O:480:VAL:HB   | 1:O:505:SER:OG  | 1.15                     | 1.24              |
| 1:F:459:ILE:HG23 | 1:F:474:THR:O   | 1.31                     | 1.24              |
| 1:C:480:VAL:HB   | 1:C:505:SER:OG  | 1.15                     | 1.24              |
| 1:G:459:ILE:HG23 | 1:G:474:THR:O   | 1.31                     | 1.24              |
| 1:C:459:ILE:HG23 | 1:C:474:THR:O   | 1.31                     | 1.24              |
| 1:N:459:ILE:HG23 | 1:N:474:THR:O   | 1.31                     | 1.24              |
| 1:A:481:GLY:N    | 1:A:505:SER:CB  | 1.88                     | 1.23              |
| 1:O:459:ILE:HG23 | 1:O:474:THR:O   | 1.31                     | 1.23              |
| 1:D:481:GLY:N    | 1:D:505:SER:CB  | 1.88                     | 1.22              |
| 1:H:459:ILE:HG23 | 1:H:474:THR:O   | 1.31                     | 1.22              |
| 1:N:481:GLY:N    | 1:N:505:SER:CB  | 1.88                     | 1.22              |
| 1:A:234:VAL:O    | 1:B:209:ARG:NH1 | 1.72                     | 1.22              |
| 1:B:234:VAL:O    | 1:C:209:ARG:NH1 | 1.72                     | 1.22              |
| 1:M:234:VAL:O    | 1:N:209:ARG:NH1 | 1.72                     | 1.21              |
| 1:E:481:GLY:N    | 1:E:505:SER:CB  | 1.88                     | 1.21              |
| 1:E:459:ILE:HG23 | 1:E:474:THR:O   | 1.31                     | 1.21              |
| 1:I:234:VAL:O    | 1:J:209:ARG:NH1 | 1.72                     | 1.21              |
| 1:N:234:VAL:O    | 1:O:209:ARG:NH1 | 1.72                     | 1.21              |
| 1:B:480:VAL:HB   | 1:B:505:SER:OG  | 1.15                     | 1.21              |
| 1:F:234:VAL:O    | 1:G:209:ARG:NH1 | 1.72                     | 1.20              |
| 1:H:234:VAL:O    | 1:I:209:ARG:NH1 | 1.72                     | 1.20              |
| 1:M:481:GLY:N    | 1:M:505:SER:CB  | 1.88                     | 1.20              |
| 1:J:234:VAL:O    | 1:K:209:ARG:NH1 | 1.72                     | 1.20              |
| 1:L:480:VAL:HB   | 1:L:505:SER:OG  | 1.15                     | 1.20              |
| 1:C:234:VAL:O    | 1:D:209:ARG:NH1 | 1.72                     | 1.20              |
| 1:E:234:VAL:O    | 1:F:209:ARG:NH1 | 1.72                     | 1.20              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:L:234:VAL:O    | 1:M:209:ARG:NH1 | 1.72                     | 1.20              |
| 1:A:209:ARG:NH1  | 1:O:234:VAL:O   | 1.72                     | 1.20              |
| 1:G:234:VAL:O    | 1:H:209:ARG:NH1 | 1.72                     | 1.19              |
| 1:A:480:VAL:HB   | 1:A:505:SER:OG  | 1.15                     | 1.19              |
| 1:D:234:VAL:O    | 1:E:209:ARG:NH1 | 1.72                     | 1.19              |
| 1:L:481:GLY:N    | 1:L:505:SER:CB  | 1.88                     | 1.18              |
| 1:K:480:VAL:HB   | 1:K:505:SER:OG  | 1.15                     | 1.18              |
| 1:F:481:GLY:N    | 1:F:505:SER:CB  | 1.88                     | 1.17              |
| 1:E:459:ILE:HG21 | 1:E:473:GLN:HB2 | 1.27                     | 1.17              |
| 1:K:234:VAL:O    | 1:L:209:ARG:NH1 | 1.72                     | 1.17              |
| 1:G:481:GLY:N    | 1:G:505:SER:CB  | 1.88                     | 1.17              |
| 1:G:459:ILE:HG21 | 1:G:473:GLN:HB2 | 1.27                     | 1.17              |
| 1:J:480:VAL:HB   | 1:J:505:SER:OG  | 1.15                     | 1.16              |
| 1:J:481:GLY:N    | 1:J:505:SER:CB  | 1.88                     | 1.15              |
| 1:H:481:GLY:N    | 1:H:505:SER:CB  | 1.88                     | 1.15              |
| 1:K:481:GLY:N    | 1:K:505:SER:CB  | 1.88                     | 1.15              |
| 1:B:459:ILE:HG21 | 1:B:473:GLN:HB2 | 1.27                     | 1.14              |
| 1:C:459:ILE:HG21 | 1:C:473:GLN:HB2 | 1.27                     | 1.14              |
| 1:I:481:GLY:N    | 1:I:505:SER:CB  | 1.88                     | 1.14              |
| 1:I:459:ILE:HG21 | 1:I:473:GLN:HB2 | 1.27                     | 1.14              |
| 1:H:459:ILE:HG21 | 1:H:473:GLN:HB2 | 1.27                     | 1.13              |
| 1:J:167:ILE:HA   | 1:J:215:ILE:O   | 1.49                     | 1.12              |
| 1:J:459:ILE:HG21 | 1:J:473:GLN:HB2 | 1.27                     | 1.12              |
| 1:O:459:ILE:HG21 | 1:O:473:GLN:HB2 | 1.27                     | 1.12              |
| 1:D:459:ILE:HG21 | 1:D:473:GLN:HB2 | 1.27                     | 1.12              |
| 1:I:167:ILE:HA   | 1:I:215:ILE:O   | 1.49                     | 1.12              |
| 1:K:167:ILE:HA   | 1:K:215:ILE:O   | 1.49                     | 1.12              |
| 1:D:167:ILE:HA   | 1:D:215:ILE:O   | 1.49                     | 1.12              |
| 1:C:167:ILE:HA   | 1:C:215:ILE:O   | 1.49                     | 1.11              |
| 1:A:459:ILE:HG21 | 1:A:473:GLN:HB2 | 1.27                     | 1.11              |
| 1:E:167:ILE:HA   | 1:E:215:ILE:O   | 1.49                     | 1.11              |
| 1:K:459:ILE:HG21 | 1:K:473:GLN:HB2 | 1.27                     | 1.10              |
| 1:H:167:ILE:HA   | 1:H:215:ILE:O   | 1.49                     | 1.10              |
| 1:B:167:ILE:HA   | 1:B:215:ILE:O   | 1.49                     | 1.10              |
| 1:L:167:ILE:HA   | 1:L:215:ILE:O   | 1.49                     | 1.10              |
| 1:M:459:ILE:HG21 | 1:M:473:GLN:HB2 | 1.27                     | 1.10              |
| 1:L:459:ILE:HG21 | 1:L:473:GLN:HB2 | 1.27                     | 1.10              |
| 1:A:167:ILE:HA   | 1:A:215:ILE:O   | 1.49                     | 1.09              |
| 1:N:459:ILE:HG21 | 1:N:473:GLN:HB2 | 1.27                     | 1.09              |
| 1:F:167:ILE:HA   | 1:F:215:ILE:O   | 1.49                     | 1.09              |
| 1:F:459:ILE:HG21 | 1:F:473:GLN:HB2 | 1.27                     | 1.09              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:612:GLU:HG3  | 1:I:642:PHE:CE2  | 1.88                     | 1.09              |
| 1:K:612:GLU:HG3  | 1:L:642:PHE:CE2  | 1.88                     | 1.09              |
| 1:M:612:GLU:HG3  | 1:N:642:PHE:CE2  | 1.88                     | 1.09              |
| 1:G:507:VAL:O    | 1:G:507:VAL:HG13 | 1.53                     | 1.09              |
| 1:L:612:GLU:HG3  | 1:M:642:PHE:CE2  | 1.88                     | 1.09              |
| 1:I:612:GLU:HG3  | 1:J:642:PHE:CE2  | 1.88                     | 1.08              |
| 1:O:167:ILE:HA   | 1:O:215:ILE:O    | 1.49                     | 1.08              |
| 1:N:167:ILE:HA   | 1:N:215:ILE:O    | 1.49                     | 1.08              |
| 1:G:167:ILE:HA   | 1:G:215:ILE:O    | 1.49                     | 1.08              |
| 1:J:612:GLU:HG3  | 1:K:642:PHE:CE2  | 1.88                     | 1.08              |
| 1:M:167:ILE:HA   | 1:M:215:ILE:O    | 1.49                     | 1.08              |
| 1:A:642:PHE:CE2  | 1:O:612:GLU:HG3  | 1.88                     | 1.08              |
| 1:F:507:VAL:HG13 | 1:F:507:VAL:O    | 1.53                     | 1.08              |
| 1:M:507:VAL:O    | 1:M:507:VAL:HG13 | 1.53                     | 1.08              |
| 1:D:612:GLU:HG3  | 1:E:642:PHE:CE2  | 1.88                     | 1.08              |
| 1:C:612:GLU:HG3  | 1:D:642:PHE:CE2  | 1.88                     | 1.08              |
| 1:G:612:GLU:HG3  | 1:H:642:PHE:CE2  | 1.88                     | 1.08              |
| 1:L:507:VAL:HG13 | 1:L:507:VAL:O    | 1.53                     | 1.08              |
| 1:F:612:GLU:HG3  | 1:G:642:PHE:CE2  | 1.88                     | 1.08              |
| 1:N:612:GLU:HG3  | 1:O:642:PHE:CE2  | 1.88                     | 1.08              |
| 1:A:612:GLU:HG3  | 1:B:642:PHE:CE2  | 1.88                     | 1.07              |
| 1:A:458:VAL:O    | 1:A:476:ASP:N    | 1.87                     | 1.07              |
| 1:B:507:VAL:O    | 1:B:507:VAL:HG13 | 1.53                     | 1.07              |
| 1:C:458:VAL:O    | 1:C:476:ASP:N    | 1.87                     | 1.07              |
| 1:D:458:VAL:O    | 1:D:476:ASP:N    | 1.87                     | 1.07              |
| 1:H:507:VAL:HG13 | 1:H:507:VAL:O    | 1.53                     | 1.07              |
| 1:D:479:GLU:OE1  | 1:D:479:GLU:N    | 1.88                     | 1.07              |
| 1:F:479:GLU:N    | 1:F:479:GLU:OE1  | 1.88                     | 1.07              |
| 1:E:612:GLU:HG3  | 1:F:642:PHE:CE2  | 1.88                     | 1.07              |
| 1:J:458:VAL:O    | 1:J:476:ASP:N    | 1.87                     | 1.07              |
| 1:B:612:GLU:HG3  | 1:C:642:PHE:CE2  | 1.88                     | 1.07              |
| 1:I:458:VAL:O    | 1:I:476:ASP:N    | 1.87                     | 1.07              |
| 1:B:479:GLU:OE1  | 1:B:479:GLU:N    | 1.88                     | 1.06              |
| 1:F:458:VAL:O    | 1:F:476:ASP:N    | 1.87                     | 1.06              |
| 1:K:459:ILE:CG2  | 1:K:474:THR:O    | 2.03                     | 1.06              |
| 1:M:459:ILE:CG2  | 1:M:474:THR:O    | 2.03                     | 1.06              |
| 1:H:459:ILE:CG2  | 1:H:474:THR:O    | 2.03                     | 1.06              |
| 1:N:507:VAL:HG13 | 1:N:507:VAL:O    | 1.53                     | 1.06              |
| 1:B:458:VAL:O    | 1:B:476:ASP:N    | 1.87                     | 1.06              |
| 1:C:507:VAL:HG13 | 1:C:507:VAL:O    | 1.53                     | 1.06              |
| 1:K:507:VAL:O    | 1:K:507:VAL:HG13 | 1.53                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:507:VAL:HG13 | 1:A:507:VAL:O    | 1.53                     | 1.06              |
| 1:F:459:ILE:CG2  | 1:F:474:THR:O    | 2.03                     | 1.06              |
| 1:I:459:ILE:CG2  | 1:I:474:THR:O    | 2.03                     | 1.06              |
| 1:N:458:VAL:O    | 1:N:476:ASP:N    | 1.87                     | 1.06              |
| 1:G:459:ILE:CG2  | 1:G:474:THR:O    | 2.03                     | 1.06              |
| 1:H:479:GLU:N    | 1:H:479:GLU:OE1  | 1.88                     | 1.06              |
| 1:J:459:ILE:CG2  | 1:J:474:THR:O    | 2.03                     | 1.06              |
| 1:A:235:GLU:OE1  | 1:A:235:GLU:N    | 1.89                     | 1.06              |
| 1:M:458:VAL:O    | 1:M:476:ASP:N    | 1.87                     | 1.06              |
| 1:E:235:GLU:OE1  | 1:E:235:GLU:N    | 1.89                     | 1.06              |
| 1:E:459:ILE:CG2  | 1:E:474:THR:O    | 2.03                     | 1.06              |
| 1:L:459:ILE:CG2  | 1:L:474:THR:O    | 2.03                     | 1.06              |
| 1:O:459:ILE:CG2  | 1:O:474:THR:O    | 2.03                     | 1.06              |
| 1:I:479:GLU:N    | 1:I:479:GLU:OE1  | 1.88                     | 1.06              |
| 1:N:459:ILE:CG2  | 1:N:474:THR:O    | 2.03                     | 1.06              |
| 1:A:459:ILE:CG2  | 1:A:474:THR:O    | 2.03                     | 1.06              |
| 1:B:235:GLU:N    | 1:B:235:GLU:OE1  | 1.89                     | 1.06              |
| 1:C:459:ILE:CG2  | 1:C:474:THR:O    | 2.03                     | 1.06              |
| 1:G:479:GLU:OE1  | 1:G:479:GLU:N    | 1.88                     | 1.05              |
| 1:K:458:VAL:O    | 1:K:476:ASP:N    | 1.87                     | 1.05              |
| 1:L:458:VAL:O    | 1:L:476:ASP:N    | 1.87                     | 1.05              |
| 1:M:235:GLU:OE1  | 1:M:235:GLU:N    | 1.89                     | 1.05              |
| 1:E:458:VAL:O    | 1:E:476:ASP:N    | 1.87                     | 1.05              |
| 1:E:479:GLU:OE1  | 1:E:479:GLU:N    | 1.88                     | 1.05              |
| 1:L:235:GLU:N    | 1:L:235:GLU:OE1  | 1.89                     | 1.05              |
| 1:F:235:GLU:OE1  | 1:F:235:GLU:N    | 1.89                     | 1.05              |
| 1:D:235:GLU:N    | 1:D:235:GLU:OE1  | 1.89                     | 1.05              |
| 1:D:459:ILE:CG2  | 1:D:474:THR:O    | 2.03                     | 1.05              |
| 1:H:458:VAL:O    | 1:H:476:ASP:N    | 1.87                     | 1.05              |
| 1:O:235:GLU:OE1  | 1:O:235:GLU:N    | 1.89                     | 1.05              |
| 1:M:479:GLU:OE1  | 1:M:479:GLU:N    | 1.88                     | 1.05              |
| 1:E:507:VAL:O    | 1:E:507:VAL:HG13 | 1.53                     | 1.05              |
| 1:K:479:GLU:OE1  | 1:K:479:GLU:N    | 1.88                     | 1.05              |
| 1:N:479:GLU:N    | 1:N:479:GLU:OE1  | 1.88                     | 1.05              |
| 1:O:458:VAL:O    | 1:O:476:ASP:N    | 1.87                     | 1.05              |
| 1:G:458:VAL:O    | 1:G:476:ASP:N    | 1.87                     | 1.04              |
| 1:N:235:GLU:N    | 1:N:235:GLU:OE1  | 1.89                     | 1.04              |
| 1:B:459:ILE:CG2  | 1:B:474:THR:O    | 2.03                     | 1.04              |
| 1:I:235:GLU:N    | 1:I:235:GLU:OE1  | 1.89                     | 1.04              |
| 1:A:479:GLU:N    | 1:A:479:GLU:OE1  | 1.88                     | 1.04              |
| 1:C:235:GLU:N    | 1:C:235:GLU:OE1  | 1.89                     | 1.04              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:479:GLU:OE1  | 1:C:479:GLU:N    | 1.88                     | 1.04              |
| 1:H:235:GLU:OE1  | 1:H:235:GLU:N    | 1.89                     | 1.04              |
| 1:J:479:GLU:OE1  | 1:J:479:GLU:N    | 1.88                     | 1.04              |
| 1:O:479:GLU:OE1  | 1:O:479:GLU:N    | 1.88                     | 1.04              |
| 1:I:507:VAL:HG13 | 1:I:507:VAL:O    | 1.53                     | 1.04              |
| 1:J:507:VAL:O    | 1:J:507:VAL:HG13 | 1.53                     | 1.04              |
| 1:D:507:VAL:HG13 | 1:D:507:VAL:O    | 1.53                     | 1.04              |
| 1:J:235:GLU:OE1  | 1:J:235:GLU:N    | 1.89                     | 1.04              |
| 1:K:235:GLU:N    | 1:K:235:GLU:OE1  | 1.89                     | 1.03              |
| 1:L:479:GLU:OE1  | 1:L:479:GLU:N    | 1.88                     | 1.03              |
| 1:O:507:VAL:O    | 1:O:507:VAL:HG13 | 1.53                     | 1.03              |
| 1:G:235:GLU:OE1  | 1:G:235:GLU:N    | 1.89                     | 1.03              |
| 1:O:324:ALA:O    | 1:O:437:SER:HB2  | 1.60                     | 1.01              |
| 1:A:324:ALA:O    | 1:A:437:SER:HB2  | 1.60                     | 1.01              |
| 1:K:324:ALA:O    | 1:K:437:SER:HB2  | 1.60                     | 1.01              |
| 1:N:324:ALA:O    | 1:N:437:SER:HB2  | 1.60                     | 1.01              |
| 1:B:324:ALA:O    | 1:B:437:SER:HB2  | 1.60                     | 1.01              |
| 1:G:324:ALA:O    | 1:G:437:SER:HB2  | 1.60                     | 1.01              |
| 1:L:105:VAL:O    | 1:L:140:ILE:HB   | 1.61                     | 1.01              |
| 1:H:105:VAL:O    | 1:H:140:ILE:HB   | 1.61                     | 1.01              |
| 1:J:324:ALA:O    | 1:J:437:SER:HB2  | 1.60                     | 1.01              |
| 1:M:324:ALA:O    | 1:M:437:SER:HB2  | 1.60                     | 1.01              |
| 1:I:105:VAL:O    | 1:I:140:ILE:HB   | 1.61                     | 1.01              |
| 1:C:324:ALA:O    | 1:C:437:SER:HB2  | 1.60                     | 1.00              |
| 1:F:105:VAL:O    | 1:F:140:ILE:HB   | 1.61                     | 1.00              |
| 1:M:105:VAL:O    | 1:M:140:ILE:HB   | 1.61                     | 1.00              |
| 1:E:105:VAL:O    | 1:E:140:ILE:HB   | 1.61                     | 1.00              |
| 1:F:324:ALA:O    | 1:F:437:SER:HB2  | 1.60                     | 1.00              |
| 1:D:612:GLU:HG3  | 1:E:642:PHE:HE2  | 1.23                     | 1.00              |
| 1:G:105:VAL:O    | 1:G:140:ILE:HB   | 1.61                     | 1.00              |
| 1:L:324:ALA:O    | 1:L:437:SER:HB2  | 1.60                     | 1.00              |
| 1:N:105:VAL:O    | 1:N:140:ILE:HB   | 1.61                     | 1.00              |
| 1:D:105:VAL:O    | 1:D:140:ILE:HB   | 1.61                     | 1.00              |
| 1:F:612:GLU:HG3  | 1:G:642:PHE:HE2  | 1.22                     | 1.00              |
| 1:K:105:VAL:O    | 1:K:140:ILE:HB   | 1.61                     | 1.00              |
| 1:D:324:ALA:O    | 1:D:437:SER:HB2  | 1.60                     | 0.99              |
| 1:O:105:VAL:O    | 1:O:140:ILE:HB   | 1.61                     | 0.99              |
| 1:E:612:GLU:HG3  | 1:F:642:PHE:HE2  | 1.22                     | 0.99              |
| 1:C:105:VAL:O    | 1:C:140:ILE:HB   | 1.61                     | 0.99              |
| 1:H:324:ALA:O    | 1:H:437:SER:HB2  | 1.60                     | 0.99              |
| 1:A:105:VAL:O    | 1:A:140:ILE:HB   | 1.61                     | 0.99              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:105:VAL:O    | 1:B:140:ILE:HB  | 1.61                     | 0.99              |
| 1:I:324:ALA:O    | 1:I:437:SER:HB2 | 1.60                     | 0.98              |
| 1:J:105:VAL:O    | 1:J:140:ILE:HB  | 1.61                     | 0.98              |
| 1:I:612:GLU:HG3  | 1:J:642:PHE:HE2 | 1.22                     | 0.98              |
| 1:I:456:VAL:HG23 | 1:I:457:PRO:HD2 | 1.46                     | 0.98              |
| 1:J:456:VAL:HG23 | 1:J:457:PRO:HD2 | 1.46                     | 0.98              |
| 1:E:324:ALA:O    | 1:E:437:SER:HB2 | 1.60                     | 0.98              |
| 1:K:456:VAL:HG23 | 1:K:457:PRO:HD2 | 1.46                     | 0.98              |
| 1:H:456:VAL:HG23 | 1:H:457:PRO:HD2 | 1.46                     | 0.98              |
| 1:L:456:VAL:HG23 | 1:L:457:PRO:HD2 | 1.46                     | 0.98              |
| 1:O:456:VAL:HG23 | 1:O:457:PRO:HD2 | 1.46                     | 0.98              |
| 1:B:612:GLU:HG3  | 1:C:642:PHE:HE2 | 1.22                     | 0.97              |
| 1:M:456:VAL:HG23 | 1:M:457:PRO:HD2 | 1.46                     | 0.97              |
| 1:N:456:VAL:HG23 | 1:N:457:PRO:HD2 | 1.46                     | 0.97              |
| 1:A:456:VAL:HG23 | 1:A:457:PRO:HD2 | 1.46                     | 0.97              |
| 1:G:456:VAL:HG23 | 1:G:457:PRO:HD2 | 1.46                     | 0.97              |
| 1:G:612:GLU:HG3  | 1:H:642:PHE:HE2 | 1.23                     | 0.97              |
| 1:B:456:VAL:HG23 | 1:B:457:PRO:HD2 | 1.46                     | 0.97              |
| 1:L:612:GLU:HG3  | 1:M:642:PHE:HE2 | 1.22                     | 0.96              |
| 1:C:456:VAL:HG23 | 1:C:457:PRO:HD2 | 1.46                     | 0.96              |
| 1:F:456:VAL:HG23 | 1:F:457:PRO:HD2 | 1.46                     | 0.96              |
| 1:D:456:VAL:HG23 | 1:D:457:PRO:HD2 | 1.46                     | 0.96              |
| 1:N:612:GLU:HG3  | 1:O:642:PHE:HE2 | 1.22                     | 0.96              |
| 1:A:480:VAL:C    | 1:A:505:SER:OG  | 2.05                     | 0.96              |
| 1:E:456:VAL:HG23 | 1:E:457:PRO:HD2 | 1.46                     | 0.95              |
| 1:O:480:VAL:C    | 1:O:505:SER:OG  | 2.05                     | 0.95              |
| 1:B:480:VAL:C    | 1:B:505:SER:OG  | 2.05                     | 0.95              |
| 1:E:480:VAL:C    | 1:E:505:SER:OG  | 2.05                     | 0.95              |
| 1:D:480:VAL:C    | 1:D:505:SER:OG  | 2.05                     | 0.95              |
| 1:F:480:VAL:C    | 1:F:505:SER:OG  | 2.05                     | 0.95              |
| 1:K:612:GLU:HG3  | 1:L:642:PHE:HE2 | 1.22                     | 0.94              |
| 1:N:480:VAL:C    | 1:N:505:SER:OG  | 2.05                     | 0.94              |
| 1:C:480:VAL:C    | 1:C:505:SER:OG  | 2.05                     | 0.94              |
| 1:L:480:VAL:C    | 1:L:505:SER:OG  | 2.05                     | 0.94              |
| 1:H:480:VAL:C    | 1:H:505:SER:OG  | 2.05                     | 0.94              |
| 1:K:480:VAL:C    | 1:K:505:SER:OG  | 2.05                     | 0.94              |
| 1:G:480:VAL:C    | 1:G:505:SER:OG  | 2.05                     | 0.94              |
| 1:J:612:GLU:HG3  | 1:K:642:PHE:HE2 | 1.22                     | 0.94              |
| 1:M:480:VAL:C    | 1:M:505:SER:OG  | 2.05                     | 0.94              |
| 1:J:480:VAL:C    | 1:J:505:SER:OG  | 2.05                     | 0.93              |
| 1:M:612:GLU:HG3  | 1:N:642:PHE:HE2 | 1.23                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:480:VAL:C    | 1:I:505:SER:OG   | 2.05                     | 0.93              |
| 1:J:609:PHE:CG   | 1:K:639:ILE:CD1  | 2.52                     | 0.93              |
| 1:A:612:GLU:HG3  | 1:B:642:PHE:HE2  | 1.23                     | 0.93              |
| 1:H:609:PHE:CG   | 1:I:639:ILE:CD1  | 2.52                     | 0.93              |
| 1:L:609:PHE:CG   | 1:M:639:ILE:CD1  | 2.52                     | 0.93              |
| 1:N:218:ASP:HB2  | 1:N:221:VAL:H    | 1.34                     | 0.93              |
| 1:C:609:PHE:CD2  | 1:D:639:ILE:HD11 | 2.04                     | 0.93              |
| 1:H:612:GLU:HG3  | 1:I:642:PHE:HE2  | 1.23                     | 0.93              |
| 1:O:218:ASP:HB2  | 1:O:221:VAL:H    | 1.34                     | 0.93              |
| 1:A:642:PHE:HE2  | 1:O:612:GLU:HG3  | 1.23                     | 0.93              |
| 1:M:218:ASP:HB2  | 1:M:221:VAL:H    | 1.34                     | 0.93              |
| 1:A:218:ASP:HB2  | 1:A:221:VAL:H    | 1.34                     | 0.93              |
| 1:C:609:PHE:CG   | 1:D:639:ILE:CD1  | 2.52                     | 0.93              |
| 1:K:609:PHE:CG   | 1:L:639:ILE:CD1  | 2.52                     | 0.93              |
| 1:A:609:PHE:CD2  | 1:B:639:ILE:HD11 | 2.04                     | 0.92              |
| 1:A:609:PHE:CG   | 1:B:639:ILE:CD1  | 2.52                     | 0.92              |
| 1:F:609:PHE:CD2  | 1:G:639:ILE:HD11 | 2.04                     | 0.92              |
| 1:L:218:ASP:HB2  | 1:L:221:VAL:H    | 1.34                     | 0.92              |
| 1:K:609:PHE:CD2  | 1:L:639:ILE:HD11 | 2.04                     | 0.92              |
| 1:M:609:PHE:CG   | 1:N:639:ILE:CD1  | 2.52                     | 0.92              |
| 1:B:609:PHE:CG   | 1:C:639:ILE:CD1  | 2.52                     | 0.92              |
| 1:J:609:PHE:CD2  | 1:K:639:ILE:HD11 | 2.04                     | 0.92              |
| 1:I:609:PHE:CG   | 1:J:639:ILE:CD1  | 2.52                     | 0.92              |
| 1:A:639:ILE:HD11 | 1:O:609:PHE:CD2  | 2.04                     | 0.92              |
| 1:D:609:PHE:CD2  | 1:E:639:ILE:HD11 | 2.04                     | 0.92              |
| 1:D:609:PHE:CG   | 1:E:639:ILE:CD1  | 2.52                     | 0.92              |
| 1:E:609:PHE:CG   | 1:F:639:ILE:CD1  | 2.52                     | 0.92              |
| 1:C:612:GLU:HG3  | 1:D:642:PHE:HE2  | 1.23                     | 0.92              |
| 1:N:609:PHE:CG   | 1:O:639:ILE:CD1  | 2.52                     | 0.92              |
| 1:A:639:ILE:CD1  | 1:O:609:PHE:CG   | 2.52                     | 0.92              |
| 1:B:218:ASP:HB2  | 1:B:221:VAL:H    | 1.34                     | 0.92              |
| 1:B:609:PHE:CD2  | 1:C:639:ILE:HD11 | 2.04                     | 0.92              |
| 1:E:609:PHE:CD2  | 1:F:639:ILE:HD11 | 2.04                     | 0.92              |
| 1:F:609:PHE:CG   | 1:G:639:ILE:CD1  | 2.52                     | 0.92              |
| 1:N:506:ASN:HD22 | 1:N:507:VAL:N    | 1.68                     | 0.92              |
| 1:K:218:ASP:HB2  | 1:K:221:VAL:H    | 1.34                     | 0.92              |
| 1:K:506:ASN:HD22 | 1:K:507:VAL:N    | 1.68                     | 0.92              |
| 1:D:218:ASP:HB2  | 1:D:221:VAL:H    | 1.34                     | 0.92              |
| 1:I:609:PHE:CD2  | 1:J:639:ILE:HD11 | 2.04                     | 0.92              |
| 1:G:218:ASP:HB2  | 1:G:221:VAL:H    | 1.34                     | 0.92              |
| 1:B:506:ASN:HD22 | 1:B:507:VAL:N    | 1.68                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:218:ASP:HB2  | 1:F:221:VAL:H    | 1.34                     | 0.91              |
| 1:N:458:VAL:O    | 1:N:475:VAL:HA   | 1.70                     | 0.91              |
| 1:O:458:VAL:O    | 1:O:475:VAL:HA   | 1.70                     | 0.91              |
| 1:D:458:VAL:O    | 1:D:475:VAL:HA   | 1.70                     | 0.91              |
| 1:H:506:ASN:HD22 | 1:H:507:VAL:N    | 1.68                     | 0.91              |
| 1:I:458:VAL:O    | 1:I:475:VAL:HA   | 1.70                     | 0.91              |
| 1:I:506:ASN:HD22 | 1:I:507:VAL:N    | 1.68                     | 0.91              |
| 1:L:506:ASN:HD22 | 1:L:507:VAL:N    | 1.68                     | 0.91              |
| 1:I:218:ASP:HB2  | 1:I:221:VAL:H    | 1.34                     | 0.91              |
| 1:M:609:PHE:CD2  | 1:N:639:ILE:HD11 | 2.04                     | 0.91              |
| 1:O:506:ASN:HD22 | 1:O:507:VAL:N    | 1.68                     | 0.91              |
| 1:G:609:PHE:CG   | 1:H:639:ILE:CD1  | 2.52                     | 0.91              |
| 1:H:218:ASP:HB2  | 1:H:221:VAL:H    | 1.34                     | 0.91              |
| 1:G:609:PHE:CD2  | 1:H:639:ILE:HD11 | 2.04                     | 0.91              |
| 1:H:458:VAL:O    | 1:H:475:VAL:HA   | 1.70                     | 0.91              |
| 1:H:609:PHE:CD2  | 1:I:639:ILE:HD11 | 2.04                     | 0.91              |
| 1:J:458:VAL:O    | 1:J:475:VAL:HA   | 1.70                     | 0.91              |
| 1:L:609:PHE:CD2  | 1:M:639:ILE:HD11 | 2.04                     | 0.91              |
| 1:B:458:VAL:O    | 1:B:475:VAL:HA   | 1.70                     | 0.91              |
| 1:E:218:ASP:HB2  | 1:E:221:VAL:H    | 1.34                     | 0.91              |
| 1:E:506:ASN:HD22 | 1:E:507:VAL:N    | 1.68                     | 0.91              |
| 1:G:458:VAL:O    | 1:G:475:VAL:HA   | 1.70                     | 0.91              |
| 1:C:218:ASP:HB2  | 1:C:221:VAL:H    | 1.34                     | 0.91              |
| 1:C:506:ASN:HD22 | 1:C:507:VAL:N    | 1.68                     | 0.91              |
| 1:N:455:GLU:N    | 1:N:455:GLU:OE1  | 2.04                     | 0.91              |
| 1:E:455:GLU:OE1  | 1:E:455:GLU:N    | 2.04                     | 0.90              |
| 1:E:458:VAL:O    | 1:E:475:VAL:HA   | 1.70                     | 0.90              |
| 1:F:506:ASN:HD22 | 1:F:507:VAL:N    | 1.68                     | 0.90              |
| 1:J:218:ASP:HB2  | 1:J:221:VAL:H    | 1.34                     | 0.90              |
| 1:M:458:VAL:O    | 1:M:475:VAL:HA   | 1.70                     | 0.90              |
| 1:O:455:GLU:N    | 1:O:455:GLU:OE1  | 2.04                     | 0.90              |
| 1:A:506:ASN:HD22 | 1:A:507:VAL:N    | 1.68                     | 0.90              |
| 1:F:455:GLU:OE1  | 1:F:455:GLU:N    | 2.04                     | 0.90              |
| 1:M:506:ASN:HD22 | 1:M:507:VAL:N    | 1.68                     | 0.90              |
| 1:N:609:PHE:CD2  | 1:O:639:ILE:HD11 | 2.04                     | 0.90              |
| 1:A:458:VAL:O    | 1:A:475:VAL:HA   | 1.70                     | 0.90              |
| 1:D:455:GLU:OE1  | 1:D:455:GLU:N    | 2.04                     | 0.90              |
| 1:F:458:VAL:O    | 1:F:475:VAL:HA   | 1.70                     | 0.90              |
| 1:I:455:GLU:OE1  | 1:I:455:GLU:N    | 2.04                     | 0.90              |
| 1:M:455:GLU:OE1  | 1:M:455:GLU:N    | 2.04                     | 0.90              |
| 1:J:455:GLU:OE1  | 1:J:455:GLU:N    | 2.04                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:458:VAL:O    | 1:K:475:VAL:HA   | 1.70                     | 0.90              |
| 1:J:506:ASN:HD22 | 1:J:507:VAL:N    | 1.68                     | 0.90              |
| 1:C:455:GLU:N    | 1:C:455:GLU:OE1  | 2.04                     | 0.90              |
| 1:H:455:GLU:OE1  | 1:H:455:GLU:N    | 2.04                     | 0.90              |
| 1:A:205:VAL:HB   | 1:A:214:LEU:HB2  | 1.54                     | 0.90              |
| 1:A:455:GLU:N    | 1:A:455:GLU:OE1  | 2.04                     | 0.90              |
| 1:B:205:VAL:HB   | 1:B:214:LEU:HB2  | 1.54                     | 0.90              |
| 1:D:506:ASN:HD22 | 1:D:507:VAL:N    | 1.68                     | 0.89              |
| 1:G:506:ASN:HD22 | 1:G:507:VAL:N    | 1.68                     | 0.89              |
| 1:K:455:GLU:N    | 1:K:455:GLU:OE1  | 2.04                     | 0.89              |
| 1:C:205:VAL:HB   | 1:C:214:LEU:HB2  | 1.54                     | 0.89              |
| 1:C:458:VAL:O    | 1:C:475:VAL:HA   | 1.70                     | 0.89              |
| 1:O:205:VAL:HB   | 1:O:214:LEU:HB2  | 1.54                     | 0.89              |
| 1:G:455:GLU:OE1  | 1:G:455:GLU:N    | 2.04                     | 0.89              |
| 1:L:458:VAL:O    | 1:L:475:VAL:HA   | 1.70                     | 0.89              |
| 1:L:455:GLU:OE1  | 1:L:455:GLU:N    | 2.04                     | 0.89              |
| 1:N:205:VAL:HB   | 1:N:214:LEU:HB2  | 1.54                     | 0.89              |
| 1:A:328:GLU:OE1  | 1:A:521:ARG:NH1  | 2.06                     | 0.89              |
| 1:B:455:GLU:N    | 1:B:455:GLU:OE1  | 2.04                     | 0.89              |
| 1:L:328:GLU:OE1  | 1:L:521:ARG:NH1  | 2.06                     | 0.89              |
| 1:D:205:VAL:HB   | 1:D:214:LEU:HB2  | 1.54                     | 0.88              |
| 1:D:328:GLU:OE1  | 1:D:521:ARG:NH1  | 2.06                     | 0.88              |
| 1:O:328:GLU:OE1  | 1:O:521:ARG:NH1  | 2.06                     | 0.88              |
| 1:B:169:VAL:HG22 | 1:B:214:LEU:HD22 | 1.56                     | 0.88              |
| 1:I:205:VAL:HB   | 1:I:214:LEU:HB2  | 1.54                     | 0.88              |
| 1:M:328:GLU:OE1  | 1:M:521:ARG:NH1  | 2.06                     | 0.88              |
| 1:H:205:VAL:HB   | 1:H:214:LEU:HB2  | 1.54                     | 0.88              |
| 1:J:480:VAL:HA   | 1:J:505:SER:OG   | 1.74                     | 0.88              |
| 1:M:205:VAL:HB   | 1:M:214:LEU:HB2  | 1.54                     | 0.88              |
| 1:N:480:VAL:HA   | 1:N:505:SER:OG   | 1.73                     | 0.88              |
| 1:E:328:GLU:OE1  | 1:E:521:ARG:NH1  | 2.06                     | 0.88              |
| 1:K:328:GLU:OE1  | 1:K:521:ARG:NH1  | 2.06                     | 0.88              |
| 1:D:169:VAL:HG22 | 1:D:214:LEU:HD22 | 1.56                     | 0.88              |
| 1:O:480:VAL:HA   | 1:O:505:SER:OG   | 1.74                     | 0.88              |
| 1:B:328:GLU:OE1  | 1:B:521:ARG:NH1  | 2.06                     | 0.88              |
| 1:H:328:GLU:OE1  | 1:H:521:ARG:NH1  | 2.06                     | 0.88              |
| 1:J:205:VAL:HB   | 1:J:214:LEU:HB2  | 1.54                     | 0.88              |
| 1:K:122:LEU:HD23 | 1:K:125:ASN:HD22 | 1.39                     | 0.88              |
| 1:O:169:VAL:HG22 | 1:O:214:LEU:HD22 | 1.56                     | 0.88              |
| 1:C:169:VAL:HG22 | 1:C:214:LEU:HD22 | 1.56                     | 0.88              |
| 1:C:328:GLU:OE1  | 1:C:521:ARG:NH1  | 2.06                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:169:VAL:HG22 | 1:E:214:LEU:HD22 | 1.56                     | 0.88              |
| 1:G:205:VAL:HB   | 1:G:214:LEU:HB2  | 1.54                     | 0.88              |
| 1:I:328:GLU:OE1  | 1:I:521:ARG:NH1  | 2.06                     | 0.88              |
| 1:L:122:LEU:HD23 | 1:L:125:ASN:HD22 | 1.39                     | 0.88              |
| 1:A:169:VAL:HG22 | 1:A:214:LEU:HD22 | 1.56                     | 0.88              |
| 1:E:480:VAL:HA   | 1:E:505:SER:OG   | 1.74                     | 0.88              |
| 1:K:480:VAL:HA   | 1:K:505:SER:OG   | 1.74                     | 0.88              |
| 1:L:205:VAL:HB   | 1:L:214:LEU:HB2  | 1.54                     | 0.88              |
| 1:D:480:VAL:HA   | 1:D:505:SER:OG   | 1.74                     | 0.87              |
| 1:E:205:VAL:HB   | 1:E:214:LEU:HB2  | 1.54                     | 0.87              |
| 1:C:480:VAL:HA   | 1:C:505:SER:OG   | 1.73                     | 0.87              |
| 1:F:480:VAL:HA   | 1:F:505:SER:OG   | 1.74                     | 0.87              |
| 1:I:480:VAL:HA   | 1:I:505:SER:OG   | 1.74                     | 0.87              |
| 1:N:169:VAL:HG22 | 1:N:214:LEU:HD22 | 1.56                     | 0.87              |
| 1:N:328:GLU:OE1  | 1:N:521:ARG:NH1  | 2.06                     | 0.87              |
| 1:C:122:LEU:HD23 | 1:C:125:ASN:HD22 | 1.39                     | 0.87              |
| 1:J:122:LEU:HD23 | 1:J:125:ASN:HD22 | 1.39                     | 0.87              |
| 1:K:205:VAL:HB   | 1:K:214:LEU:HB2  | 1.54                     | 0.87              |
| 1:F:122:LEU:HD23 | 1:F:125:ASN:HD22 | 1.39                     | 0.87              |
| 1:G:328:GLU:OE1  | 1:G:521:ARG:NH1  | 2.06                     | 0.87              |
| 1:E:122:LEU:HD23 | 1:E:125:ASN:HD22 | 1.39                     | 0.87              |
| 1:J:328:GLU:OE1  | 1:J:521:ARG:NH1  | 2.06                     | 0.87              |
| 1:D:122:LEU:HD23 | 1:D:125:ASN:HD22 | 1.39                     | 0.87              |
| 1:F:328:GLU:OE1  | 1:F:521:ARG:NH1  | 2.06                     | 0.87              |
| 1:G:480:VAL:HA   | 1:G:505:SER:OG   | 1.74                     | 0.87              |
| 1:M:480:VAL:HA   | 1:M:505:SER:OG   | 1.74                     | 0.87              |
| 1:A:480:VAL:HA   | 1:A:505:SER:OG   | 1.74                     | 0.87              |
| 1:F:205:VAL:HB   | 1:F:214:LEU:HB2  | 1.54                     | 0.87              |
| 1:F:169:VAL:HG22 | 1:F:214:LEU:HD22 | 1.56                     | 0.87              |
| 1:G:122:LEU:HD23 | 1:G:125:ASN:HD22 | 1.39                     | 0.87              |
| 1:G:169:VAL:HG22 | 1:G:214:LEU:HD22 | 1.56                     | 0.87              |
| 1:M:122:LEU:HD23 | 1:M:125:ASN:HD22 | 1.39                     | 0.86              |
| 1:B:122:LEU:HD23 | 1:B:125:ASN:HD22 | 1.39                     | 0.86              |
| 1:B:480:VAL:HA   | 1:B:505:SER:OG   | 1.74                     | 0.86              |
| 1:M:169:VAL:HG22 | 1:M:214:LEU:HD22 | 1.56                     | 0.86              |
| 1:A:122:LEU:HD23 | 1:A:125:ASN:HD22 | 1.39                     | 0.86              |
| 1:H:169:VAL:HG22 | 1:H:214:LEU:HD22 | 1.56                     | 0.86              |
| 1:L:169:VAL:HG22 | 1:L:214:LEU:HD22 | 1.56                     | 0.86              |
| 1:L:480:VAL:HA   | 1:L:505:SER:OG   | 1.74                     | 0.86              |
| 1:B:473:GLN:OE1  | 1:B:473:GLN:N    | 2.09                     | 0.86              |
| 1:I:122:LEU:HD23 | 1:I:125:ASN:HD22 | 1.39                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:473:GLN:N    | 1:K:473:GLN:OE1  | 2.09                     | 0.86              |
| 1:A:473:GLN:OE1  | 1:A:473:GLN:N    | 2.09                     | 0.85              |
| 1:H:122:LEU:HD23 | 1:H:125:ASN:HD22 | 1.39                     | 0.85              |
| 1:J:169:VAL:HG22 | 1:J:214:LEU:HD22 | 1.56                     | 0.85              |
| 1:K:169:VAL:HG22 | 1:K:214:LEU:HD22 | 1.56                     | 0.85              |
| 1:H:480:VAL:HA   | 1:H:505:SER:OG   | 1.74                     | 0.85              |
| 1:L:473:GLN:N    | 1:L:473:GLN:OE1  | 2.09                     | 0.85              |
| 1:O:122:LEU:HD23 | 1:O:125:ASN:HD22 | 1.39                     | 0.85              |
| 1:J:473:GLN:N    | 1:J:473:GLN:OE1  | 2.09                     | 0.85              |
| 1:C:473:GLN:OE1  | 1:C:473:GLN:N    | 2.09                     | 0.85              |
| 1:F:473:GLN:OE1  | 1:F:473:GLN:N    | 2.09                     | 0.85              |
| 1:N:122:LEU:HD23 | 1:N:125:ASN:HD22 | 1.39                     | 0.85              |
| 1:O:473:GLN:N    | 1:O:473:GLN:OE1  | 2.09                     | 0.85              |
| 1:H:480:VAL:CA   | 1:H:505:SER:CB   | 2.55                     | 0.85              |
| 1:N:480:VAL:CA   | 1:N:505:SER:CB   | 2.55                     | 0.85              |
| 1:A:480:VAL:CA   | 1:A:505:SER:CB   | 2.55                     | 0.85              |
| 1:I:169:VAL:HG22 | 1:I:214:LEU:HD22 | 1.56                     | 0.85              |
| 1:K:480:VAL:CA   | 1:K:505:SER:CB   | 2.55                     | 0.85              |
| 1:M:480:VAL:CA   | 1:M:505:SER:CB   | 2.55                     | 0.85              |
| 1:G:473:GLN:N    | 1:G:473:GLN:OE1  | 2.09                     | 0.85              |
| 1:J:480:VAL:CA   | 1:J:505:SER:CB   | 2.55                     | 0.85              |
| 1:M:473:GLN:OE1  | 1:M:473:GLN:N    | 2.09                     | 0.84              |
| 1:F:480:VAL:CA   | 1:F:505:SER:CB   | 2.55                     | 0.84              |
| 1:I:480:VAL:CA   | 1:I:505:SER:CB   | 2.55                     | 0.84              |
| 1:N:473:GLN:N    | 1:N:473:GLN:OE1  | 2.09                     | 0.84              |
| 1:C:480:VAL:CA   | 1:C:505:SER:CB   | 2.55                     | 0.84              |
| 1:H:473:GLN:N    | 1:H:473:GLN:OE1  | 2.09                     | 0.84              |
| 1:O:480:VAL:CA   | 1:O:505:SER:CB   | 2.55                     | 0.84              |
| 1:D:473:GLN:N    | 1:D:473:GLN:OE1  | 2.09                     | 0.84              |
| 1:L:480:VAL:CA   | 1:L:505:SER:CB   | 2.55                     | 0.84              |
| 1:B:480:VAL:CA   | 1:B:505:SER:CB   | 2.55                     | 0.84              |
| 1:D:480:VAL:CA   | 1:D:505:SER:CB   | 2.55                     | 0.84              |
| 1:E:480:VAL:CA   | 1:E:505:SER:CB   | 2.55                     | 0.84              |
| 1:G:480:VAL:CA   | 1:G:505:SER:CB   | 2.55                     | 0.84              |
| 1:B:203:LYS:N    | 1:B:216:SER:O    | 2.11                     | 0.83              |
| 1:H:203:LYS:N    | 1:H:216:SER:O    | 2.11                     | 0.83              |
| 1:J:203:LYS:N    | 1:J:216:SER:O    | 2.11                     | 0.83              |
| 1:K:203:LYS:N    | 1:K:216:SER:O    | 2.11                     | 0.83              |
| 1:L:203:LYS:N    | 1:L:216:SER:O    | 2.11                     | 0.83              |
| 1:O:203:LYS:N    | 1:O:216:SER:O    | 2.11                     | 0.83              |
| 1:I:203:LYS:N    | 1:I:216:SER:O    | 2.11                     | 0.83              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:I:473:GLN:N   | 1:I:473:GLN:OE1 | 2.09                     | 0.83              |
| 1:L:168:GLU:O   | 1:L:214:LEU:HA  | 1.79                     | 0.83              |
| 1:C:203:LYS:N   | 1:C:216:SER:O   | 2.11                     | 0.83              |
| 1:G:168:GLU:O   | 1:G:214:LEU:HA  | 1.79                     | 0.83              |
| 1:G:203:LYS:N   | 1:G:216:SER:O   | 2.11                     | 0.83              |
| 1:D:203:LYS:N   | 1:D:216:SER:O   | 2.11                     | 0.82              |
| 1:I:168:GLU:O   | 1:I:214:LEU:HA  | 1.79                     | 0.82              |
| 1:J:168:GLU:O   | 1:J:214:LEU:HA  | 1.79                     | 0.82              |
| 1:E:203:LYS:N   | 1:E:216:SER:O   | 2.11                     | 0.82              |
| 1:E:473:GLN:N   | 1:E:473:GLN:OE1 | 2.09                     | 0.82              |
| 1:O:168:GLU:O   | 1:O:214:LEU:HA  | 1.79                     | 0.82              |
| 1:F:168:GLU:O   | 1:F:214:LEU:HA  | 1.79                     | 0.82              |
| 1:M:203:LYS:N   | 1:M:216:SER:O   | 2.11                     | 0.82              |
| 1:M:168:GLU:O   | 1:M:214:LEU:HA  | 1.79                     | 0.82              |
| 1:N:203:LYS:N   | 1:N:216:SER:O   | 2.11                     | 0.82              |
| 1:H:480:VAL:HA  | 1:H:505:SER:CB  | 2.10                     | 0.82              |
| 1:A:504:VAL:CG1 | 1:A:521:ARG:HG2 | 2.10                     | 0.82              |
| 1:D:168:GLU:O   | 1:D:214:LEU:HA  | 1.79                     | 0.82              |
| 1:D:507:VAL:CG1 | 1:D:507:VAL:O   | 2.28                     | 0.82              |
| 1:F:203:LYS:N   | 1:F:216:SER:O   | 2.11                     | 0.81              |
| 1:G:480:VAL:HA  | 1:G:505:SER:CB  | 2.10                     | 0.81              |
| 1:M:504:VAL:CG1 | 1:M:521:ARG:HG2 | 2.10                     | 0.81              |
| 1:O:480:VAL:HA  | 1:O:505:SER:CB  | 2.10                     | 0.81              |
| 1:A:203:LYS:N   | 1:A:216:SER:O   | 2.11                     | 0.81              |
| 1:A:480:VAL:HA  | 1:A:505:SER:CB  | 2.10                     | 0.81              |
| 1:C:168:GLU:O   | 1:C:214:LEU:HA  | 1.79                     | 0.81              |
| 1:E:168:GLU:O   | 1:E:214:LEU:HA  | 1.79                     | 0.81              |
| 1:I:480:VAL:HA  | 1:I:505:SER:CB  | 2.10                     | 0.81              |
| 1:J:480:VAL:HA  | 1:J:505:SER:CB  | 2.10                     | 0.81              |
| 1:C:480:VAL:HA  | 1:C:505:SER:CB  | 2.10                     | 0.81              |
| 1:D:504:VAL:CG1 | 1:D:521:ARG:HG2 | 2.10                     | 0.81              |
| 1:D:480:VAL:HA  | 1:D:505:SER:CB  | 2.10                     | 0.81              |
| 1:E:480:VAL:HA  | 1:E:505:SER:CB  | 2.10                     | 0.81              |
| 1:E:504:VAL:CG1 | 1:E:521:ARG:HG2 | 2.10                     | 0.81              |
| 1:G:504:VAL:CG1 | 1:G:521:ARG:HG2 | 2.10                     | 0.81              |
| 1:H:504:VAL:CG1 | 1:H:521:ARG:HG2 | 2.10                     | 0.81              |
| 1:I:504:VAL:CG1 | 1:I:521:ARG:HG2 | 2.10                     | 0.81              |
| 1:J:504:VAL:CG1 | 1:J:521:ARG:HG2 | 2.10                     | 0.81              |
| 1:K:168:GLU:O   | 1:K:214:LEU:HA  | 1.79                     | 0.81              |
| 1:L:504:VAL:CG1 | 1:L:521:ARG:HG2 | 2.10                     | 0.81              |
| 1:N:504:VAL:CG1 | 1:N:521:ARG:HG2 | 2.10                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:480:VAL:HA   | 1:B:505:SER:CB   | 2.10                     | 0.81              |
| 1:D:459:ILE:HA   | 1:D:474:THR:O    | 1.81                     | 0.81              |
| 1:F:504:VAL:CG1  | 1:F:521:ARG:HG2  | 2.10                     | 0.81              |
| 1:K:504:VAL:CG1  | 1:K:521:ARG:HG2  | 2.10                     | 0.81              |
| 1:N:168:GLU:O    | 1:N:214:LEU:HA   | 1.79                     | 0.81              |
| 1:A:168:GLU:O    | 1:A:214:LEU:HA   | 1.79                     | 0.81              |
| 1:E:507:VAL:O    | 1:E:507:VAL:CG1  | 2.28                     | 0.81              |
| 1:F:480:VAL:HA   | 1:F:505:SER:CB   | 2.10                     | 0.81              |
| 1:K:172:LEU:HD11 | 1:K:213:ILE:HG13 | 1.63                     | 0.81              |
| 1:B:504:VAL:CG1  | 1:B:521:ARG:HG2  | 2.10                     | 0.81              |
| 1:M:172:LEU:HD11 | 1:M:213:ILE:HG13 | 1.63                     | 0.81              |
| 1:C:459:ILE:HA   | 1:C:474:THR:O    | 1.81                     | 0.81              |
| 1:H:168:GLU:O    | 1:H:214:LEU:HA   | 1.79                     | 0.81              |
| 1:O:504:VAL:CG1  | 1:O:521:ARG:HG2  | 2.10                     | 0.81              |
| 1:E:459:ILE:HA   | 1:E:474:THR:O    | 1.81                     | 0.81              |
| 1:K:480:VAL:HA   | 1:K:505:SER:CB   | 2.10                     | 0.81              |
| 1:L:480:VAL:HA   | 1:L:505:SER:CB   | 2.10                     | 0.81              |
| 1:C:640:GLN:O    | 1:C:643:ILE:HG22 | 1.81                     | 0.81              |
| 1:D:640:GLN:O    | 1:D:643:ILE:HG22 | 1.81                     | 0.81              |
| 1:N:480:VAL:HA   | 1:N:505:SER:CB   | 2.10                     | 0.81              |
| 1:M:480:VAL:HA   | 1:M:505:SER:CB   | 2.10                     | 0.81              |
| 1:F:459:ILE:HA   | 1:F:474:THR:O    | 1.81                     | 0.80              |
| 1:N:640:GLN:O    | 1:N:643:ILE:HG22 | 1.81                     | 0.80              |
| 1:I:172:LEU:HD11 | 1:I:213:ILE:HG13 | 1.63                     | 0.80              |
| 1:L:640:GLN:O    | 1:L:643:ILE:HG22 | 1.81                     | 0.80              |
| 1:O:172:LEU:HD11 | 1:O:213:ILE:HG13 | 1.63                     | 0.80              |
| 1:B:168:GLU:O    | 1:B:214:LEU:HA   | 1.79                     | 0.80              |
| 1:B:459:ILE:HA   | 1:B:474:THR:O    | 1.81                     | 0.80              |
| 1:M:481:GLY:CA   | 1:M:505:SER:HB3  | 2.11                     | 0.80              |
| 1:N:481:GLY:CA   | 1:N:505:SER:HB3  | 2.11                     | 0.80              |
| 1:N:507:VAL:CG1  | 1:N:507:VAL:O    | 2.28                     | 0.80              |
| 1:F:507:VAL:CG1  | 1:F:507:VAL:O    | 2.28                     | 0.80              |
| 1:J:459:ILE:HA   | 1:J:474:THR:O    | 1.81                     | 0.80              |
| 1:L:481:GLY:CA   | 1:L:505:SER:HB3  | 2.11                     | 0.80              |
| 1:B:640:GLN:O    | 1:B:643:ILE:HG22 | 1.81                     | 0.80              |
| 1:C:504:VAL:CG1  | 1:C:521:ARG:HG2  | 2.10                     | 0.80              |
| 1:G:459:ILE:HA   | 1:G:474:THR:O    | 1.81                     | 0.80              |
| 1:H:481:GLY:CA   | 1:H:505:SER:HB3  | 2.11                     | 0.80              |
| 1:I:459:ILE:HA   | 1:I:474:THR:O    | 1.81                     | 0.80              |
| 1:I:481:GLY:CA   | 1:I:505:SER:HB3  | 2.11                     | 0.80              |
| 1:K:640:GLN:O    | 1:K:643:ILE:HG22 | 1.81                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:481:GLY:CA   | 1:O:505:SER:HB3  | 2.11                     | 0.80              |
| 1:D:481:GLY:CA   | 1:D:505:SER:HB3  | 2.11                     | 0.80              |
| 1:H:640:GLN:O    | 1:H:643:ILE:HG22 | 1.81                     | 0.80              |
| 1:J:640:GLN:O    | 1:J:643:ILE:HG22 | 1.81                     | 0.80              |
| 1:E:481:GLY:CA   | 1:E:505:SER:HB3  | 2.11                     | 0.80              |
| 1:E:640:GLN:O    | 1:E:643:ILE:HG22 | 1.81                     | 0.80              |
| 1:H:459:ILE:HA   | 1:H:474:THR:O    | 1.81                     | 0.80              |
| 1:I:640:GLN:O    | 1:I:643:ILE:HG22 | 1.81                     | 0.80              |
| 1:J:480:VAL:C    | 1:J:505:SER:CB   | 2.50                     | 0.80              |
| 1:K:368:GLU:HG3  | 1:K:399:LYS:HD2  | 1.64                     | 0.80              |
| 1:K:459:ILE:HA   | 1:K:474:THR:O    | 1.81                     | 0.80              |
| 1:K:481:GLY:CA   | 1:K:505:SER:HB3  | 2.11                     | 0.80              |
| 1:L:480:VAL:C    | 1:L:505:SER:CB   | 2.50                     | 0.80              |
| 1:F:481:GLY:CA   | 1:F:505:SER:HB3  | 2.11                     | 0.80              |
| 1:I:480:VAL:C    | 1:I:505:SER:CB   | 2.50                     | 0.80              |
| 1:J:481:GLY:CA   | 1:J:505:SER:HB3  | 2.11                     | 0.80              |
| 1:L:459:ILE:HA   | 1:L:474:THR:O    | 1.81                     | 0.80              |
| 1:A:481:GLY:CA   | 1:A:505:SER:HB3  | 2.11                     | 0.80              |
| 1:A:640:GLN:O    | 1:A:643:ILE:HG22 | 1.81                     | 0.80              |
| 1:M:459:ILE:HA   | 1:M:474:THR:O    | 1.81                     | 0.80              |
| 1:A:172:LEU:HD11 | 1:A:213:ILE:HG13 | 1.63                     | 0.80              |
| 1:G:480:VAL:C    | 1:G:505:SER:CB   | 2.50                     | 0.80              |
| 1:G:640:GLN:O    | 1:G:643:ILE:HG22 | 1.81                     | 0.80              |
| 1:M:640:GLN:O    | 1:M:643:ILE:HG22 | 1.81                     | 0.80              |
| 1:N:459:ILE:HA   | 1:N:474:THR:O    | 1.81                     | 0.80              |
| 1:O:507:VAL:CG1  | 1:O:507:VAL:O    | 2.28                     | 0.80              |
| 1:A:459:ILE:HA   | 1:A:474:THR:O    | 1.81                     | 0.79              |
| 1:G:481:GLY:CA   | 1:G:505:SER:HB3  | 2.11                     | 0.79              |
| 1:C:480:VAL:C    | 1:C:505:SER:CB   | 2.50                     | 0.79              |
| 1:O:459:ILE:HA   | 1:O:474:THR:O    | 1.81                     | 0.79              |
| 1:B:481:GLY:CA   | 1:B:505:SER:HB3  | 2.11                     | 0.79              |
| 1:H:172:LEU:HD11 | 1:H:213:ILE:HG13 | 1.63                     | 0.79              |
| 1:J:507:VAL:O    | 1:J:507:VAL:CG1  | 2.28                     | 0.79              |
| 1:L:459:ILE:CG2  | 1:L:473:GLN:HB2  | 2.12                     | 0.79              |
| 1:C:172:LEU:HD11 | 1:C:213:ILE:HG13 | 1.63                     | 0.79              |
| 1:J:368:GLU:HG3  | 1:J:399:LYS:HD2  | 1.64                     | 0.79              |
| 1:L:368:GLU:HG3  | 1:L:399:LYS:HD2  | 1.64                     | 0.79              |
| 1:M:480:VAL:C    | 1:M:505:SER:CB   | 2.50                     | 0.79              |
| 1:N:172:LEU:HD11 | 1:N:213:ILE:HG13 | 1.63                     | 0.79              |
| 1:B:480:VAL:C    | 1:B:505:SER:CB   | 2.50                     | 0.79              |
| 1:F:172:LEU:HD11 | 1:F:213:ILE:HG13 | 1.63                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:640:GLN:O    | 1:O:643:ILE:HG22 | 1.81                     | 0.79              |
| 1:H:368:GLU:HG3  | 1:H:399:LYS:HD2  | 1.64                     | 0.79              |
| 1:L:172:LEU:HD11 | 1:L:213:ILE:HG13 | 1.63                     | 0.79              |
| 1:N:368:GLU:HG3  | 1:N:399:LYS:HD2  | 1.64                     | 0.79              |
| 1:B:368:GLU:HG3  | 1:B:399:LYS:HD2  | 1.64                     | 0.79              |
| 1:C:481:GLY:CA   | 1:C:505:SER:HB3  | 2.11                     | 0.79              |
| 1:H:480:VAL:C    | 1:H:505:SER:CB   | 2.50                     | 0.79              |
| 1:J:172:LEU:HD11 | 1:J:213:ILE:HG13 | 1.63                     | 0.79              |
| 1:O:480:VAL:C    | 1:O:505:SER:CB   | 2.50                     | 0.79              |
| 1:A:507:VAL:CG1  | 1:A:507:VAL:O    | 2.28                     | 0.79              |
| 1:E:368:GLU:HG3  | 1:E:399:LYS:HD2  | 1.64                     | 0.79              |
| 1:E:480:VAL:C    | 1:E:505:SER:CB   | 2.50                     | 0.79              |
| 1:F:640:GLN:O    | 1:F:643:ILE:HG22 | 1.81                     | 0.79              |
| 1:G:507:VAL:CG1  | 1:G:507:VAL:O    | 2.28                     | 0.78              |
| 1:K:459:ILE:CG2  | 1:K:473:GLN:HB2  | 2.12                     | 0.78              |
| 1:A:480:VAL:C    | 1:A:505:SER:CB   | 2.50                     | 0.78              |
| 1:C:368:GLU:HG3  | 1:C:399:LYS:HD2  | 1.64                     | 0.78              |
| 1:D:368:GLU:HG3  | 1:D:399:LYS:HD2  | 1.64                     | 0.78              |
| 1:A:624:PRO:HB2  | 1:O:435:LEU:HD13 | 1.65                     | 0.78              |
| 1:G:368:GLU:HG3  | 1:G:399:LYS:HD2  | 1.64                     | 0.78              |
| 1:O:368:GLU:HG3  | 1:O:399:LYS:HD2  | 1.64                     | 0.78              |
| 1:O:459:ILE:CG2  | 1:O:473:GLN:HB2  | 2.12                     | 0.78              |
| 1:K:480:VAL:C    | 1:K:505:SER:CB   | 2.50                     | 0.78              |
| 1:D:480:VAL:C    | 1:D:505:SER:CB   | 2.50                     | 0.78              |
| 1:E:172:LEU:HD11 | 1:E:213:ILE:HG13 | 1.63                     | 0.78              |
| 1:F:480:VAL:C    | 1:F:505:SER:CB   | 2.50                     | 0.78              |
| 1:F:552:VAL:HG21 | 1:F:555:LEU:HB2  | 1.66                     | 0.78              |
| 1:H:435:LEU:HD13 | 1:I:624:PRO:HB2  | 1.65                     | 0.78              |
| 1:M:368:GLU:HG3  | 1:M:399:LYS:HD2  | 1.64                     | 0.78              |
| 1:B:435:LEU:HD13 | 1:C:624:PRO:HB2  | 1.65                     | 0.78              |
| 1:I:368:GLU:HG3  | 1:I:399:LYS:HD2  | 1.64                     | 0.78              |
| 1:D:172:LEU:HD11 | 1:D:213:ILE:HG13 | 1.63                     | 0.78              |
| 1:G:172:LEU:HD11 | 1:G:213:ILE:HG13 | 1.63                     | 0.78              |
| 1:I:435:LEU:HD13 | 1:J:624:PRO:HB2  | 1.65                     | 0.78              |
| 1:D:552:VAL:HG21 | 1:D:555:LEU:HB2  | 1.66                     | 0.78              |
| 1:G:552:VAL:HG21 | 1:G:555:LEU:HB2  | 1.66                     | 0.78              |
| 1:M:435:LEU:HD13 | 1:N:624:PRO:HB2  | 1.65                     | 0.78              |
| 1:B:172:LEU:HD11 | 1:B:213:ILE:HG13 | 1.63                     | 0.78              |
| 1:C:552:VAL:HG21 | 1:C:555:LEU:HB2  | 1.66                     | 0.78              |
| 1:F:435:LEU:HD13 | 1:G:624:PRO:HB2  | 1.65                     | 0.78              |
| 1:K:507:VAL:O    | 1:K:507:VAL:CG1  | 2.28                     | 0.78              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:139:ILE:HG22 | 1:D:140:ILE:H   | 1.50                     | 0.77              |
| 1:G:435:LEU:HD13 | 1:H:624:PRO:HB2 | 1.65                     | 0.77              |
| 1:I:139:ILE:HG22 | 1:I:140:ILE:H   | 1.49                     | 0.77              |
| 1:C:435:LEU:HD13 | 1:D:624:PRO:HB2 | 1.65                     | 0.77              |
| 1:H:459:ILE:CG2  | 1:H:473:GLN:HB2 | 2.12                     | 0.77              |
| 1:B:459:ILE:CG2  | 1:B:473:GLN:HB2 | 2.12                     | 0.77              |
| 1:B:507:VAL:O    | 1:B:507:VAL:CG1 | 2.28                     | 0.77              |
| 1:C:459:ILE:CG2  | 1:C:473:GLN:HB2 | 2.12                     | 0.77              |
| 1:E:504:VAL:HG13 | 1:E:521:ARG:HD3 | 1.67                     | 0.77              |
| 1:E:552:VAL:HG21 | 1:E:555:LEU:HB2 | 1.66                     | 0.77              |
| 1:C:504:VAL:HG13 | 1:C:521:ARG:HD3 | 1.67                     | 0.77              |
| 1:H:139:ILE:HG22 | 1:H:140:ILE:H   | 1.50                     | 0.77              |
| 1:L:504:VAL:HG13 | 1:L:521:ARG:HD3 | 1.67                     | 0.77              |
| 1:N:504:VAL:HG13 | 1:N:521:ARG:HD3 | 1.67                     | 0.77              |
| 1:N:480:VAL:C    | 1:N:505:SER:CB  | 2.50                     | 0.77              |
| 1:O:504:VAL:HG13 | 1:O:521:ARG:HD3 | 1.67                     | 0.77              |
| 1:A:368:GLU:HG3  | 1:A:399:LYS:HD2 | 1.64                     | 0.77              |
| 1:B:504:VAL:HG13 | 1:B:521:ARG:HD3 | 1.67                     | 0.77              |
| 1:D:504:VAL:HG13 | 1:D:521:ARG:HD3 | 1.67                     | 0.77              |
| 1:F:368:GLU:HG3  | 1:F:399:LYS:HD2 | 1.64                     | 0.77              |
| 1:H:552:VAL:HG21 | 1:H:555:LEU:HB2 | 1.66                     | 0.77              |
| 1:J:459:ILE:CG2  | 1:J:473:GLN:HB2 | 2.12                     | 0.77              |
| 1:M:504:VAL:HG13 | 1:M:521:ARG:HD3 | 1.67                     | 0.77              |
| 1:A:435:LEU:HD13 | 1:B:624:PRO:HB2 | 1.65                     | 0.77              |
| 1:B:139:ILE:HG22 | 1:B:140:ILE:H   | 1.49                     | 0.77              |
| 1:I:459:ILE:CG2  | 1:I:473:GLN:HB2 | 2.12                     | 0.77              |
| 1:N:139:ILE:HG22 | 1:N:140:ILE:H   | 1.49                     | 0.77              |
| 1:G:459:ILE:CG2  | 1:G:473:GLN:HB2 | 2.12                     | 0.77              |
| 1:I:552:VAL:HG21 | 1:I:555:LEU:HB2 | 1.66                     | 0.77              |
| 1:J:139:ILE:HG22 | 1:J:140:ILE:H   | 1.49                     | 0.77              |
| 1:M:139:ILE:HG22 | 1:M:140:ILE:H   | 1.49                     | 0.77              |
| 1:A:139:ILE:HG22 | 1:A:140:ILE:H   | 1.49                     | 0.77              |
| 1:A:459:ILE:CG2  | 1:A:473:GLN:HB2 | 2.12                     | 0.77              |
| 1:D:459:ILE:CG2  | 1:D:473:GLN:HB2 | 2.12                     | 0.77              |
| 1:F:139:ILE:HG22 | 1:F:140:ILE:H   | 1.50                     | 0.77              |
| 1:F:504:VAL:HG13 | 1:F:521:ARG:HD3 | 1.67                     | 0.77              |
| 1:E:435:LEU:HD13 | 1:F:624:PRO:HB2 | 1.65                     | 0.77              |
| 1:J:435:LEU:HD13 | 1:K:624:PRO:HB2 | 1.65                     | 0.77              |
| 1:K:504:VAL:HG13 | 1:K:521:ARG:HD3 | 1.67                     | 0.77              |
| 1:N:552:VAL:HG21 | 1:N:555:LEU:HB2 | 1.66                     | 0.77              |
| 1:N:435:LEU:HD13 | 1:O:624:PRO:HB2 | 1.65                     | 0.77              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:504:VAL:HG13 | 1:A:521:ARG:HD3 | 1.67                     | 0.77              |
| 1:H:504:VAL:HG13 | 1:H:521:ARG:HD3 | 1.67                     | 0.77              |
| 1:K:435:LEU:HD13 | 1:L:624:PRO:HB2 | 1.65                     | 0.77              |
| 1:M:130:ASN:HA   | 1:M:143:THR:O   | 1.85                     | 0.77              |
| 1:L:435:LEU:HD13 | 1:M:624:PRO:HB2 | 1.65                     | 0.77              |
| 1:O:139:ILE:HG22 | 1:O:140:ILE:H   | 1.49                     | 0.77              |
| 1:B:552:VAL:HG21 | 1:B:555:LEU:HB2 | 1.66                     | 0.76              |
| 1:I:504:VAL:HG13 | 1:I:521:ARG:HD3 | 1.67                     | 0.76              |
| 1:N:130:ASN:HA   | 1:N:143:THR:O   | 1.85                     | 0.76              |
| 1:G:139:ILE:HG22 | 1:G:140:ILE:H   | 1.50                     | 0.76              |
| 1:G:504:VAL:HG13 | 1:G:521:ARG:HD3 | 1.67                     | 0.76              |
| 1:D:130:ASN:HA   | 1:D:143:THR:O   | 1.85                     | 0.76              |
| 1:L:552:VAL:HG21 | 1:L:555:LEU:HB2 | 1.66                     | 0.76              |
| 1:E:130:ASN:HA   | 1:E:143:THR:O   | 1.85                     | 0.76              |
| 1:K:130:ASN:HA   | 1:K:143:THR:O   | 1.85                     | 0.76              |
| 1:K:552:VAL:HG21 | 1:K:555:LEU:HB2 | 1.66                     | 0.76              |
| 1:A:552:VAL:HG21 | 1:A:555:LEU:HB2 | 1.66                     | 0.76              |
| 1:D:435:LEU:HD13 | 1:E:624:PRO:HB2 | 1.65                     | 0.76              |
| 1:J:130:ASN:HA   | 1:J:143:THR:O   | 1.85                     | 0.76              |
| 1:J:552:VAL:HG21 | 1:J:555:LEU:HB2 | 1.66                     | 0.76              |
| 1:M:552:VAL:HG21 | 1:M:555:LEU:HB2 | 1.65                     | 0.76              |
| 1:H:507:VAL:O    | 1:H:507:VAL:CG1 | 2.28                     | 0.76              |
| 1:J:504:VAL:HG13 | 1:J:521:ARG:HD3 | 1.67                     | 0.76              |
| 1:O:130:ASN:HA   | 1:O:143:THR:O   | 1.85                     | 0.76              |
| 1:F:130:ASN:HA   | 1:F:143:THR:O   | 1.85                     | 0.76              |
| 1:L:130:ASN:HA   | 1:L:143:THR:O   | 1.85                     | 0.76              |
| 1:L:139:ILE:HG22 | 1:L:140:ILE:H   | 1.50                     | 0.76              |
| 1:C:130:ASN:HA   | 1:C:143:THR:O   | 1.85                     | 0.76              |
| 1:O:507:VAL:HA   | 1:O:518:PHE:HB3 | 1.67                     | 0.76              |
| 1:A:507:VAL:HA   | 1:A:518:PHE:HB3 | 1.67                     | 0.76              |
| 1:C:507:VAL:CG1  | 1:C:507:VAL:O   | 2.28                     | 0.76              |
| 1:F:459:ILE:CG2  | 1:F:473:GLN:HB2 | 2.12                     | 0.76              |
| 1:K:507:VAL:HA   | 1:K:518:PHE:HB3 | 1.67                     | 0.76              |
| 1:O:552:VAL:HG21 | 1:O:555:LEU:HB2 | 1.66                     | 0.76              |
| 1:C:139:ILE:HG22 | 1:C:140:ILE:H   | 1.49                     | 0.75              |
| 1:E:459:ILE:CG2  | 1:E:473:GLN:HB2 | 2.12                     | 0.75              |
| 1:I:130:ASN:HA   | 1:I:143:THR:O   | 1.85                     | 0.75              |
| 1:K:139:ILE:HG22 | 1:K:140:ILE:H   | 1.50                     | 0.75              |
| 1:L:507:VAL:CG1  | 1:L:507:VAL:O   | 2.28                     | 0.75              |
| 1:A:130:ASN:HA   | 1:A:143:THR:O   | 1.85                     | 0.75              |
| 1:G:130:ASN:HA   | 1:G:143:THR:O   | 1.85                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:507:VAL:HA   | 1:J:518:PHE:HB3  | 1.67                     | 0.75              |
| 1:E:507:VAL:HA   | 1:E:518:PHE:HB3  | 1.67                     | 0.75              |
| 1:L:507:VAL:HA   | 1:L:518:PHE:HB3  | 1.67                     | 0.75              |
| 1:B:130:ASN:HA   | 1:B:143:THR:O    | 1.85                     | 0.75              |
| 1:F:507:VAL:HA   | 1:F:518:PHE:HB3  | 1.67                     | 0.75              |
| 1:N:507:VAL:HA   | 1:N:518:PHE:HB3  | 1.67                     | 0.75              |
| 1:B:507:VAL:HA   | 1:B:518:PHE:HB3  | 1.67                     | 0.75              |
| 1:G:507:VAL:HA   | 1:G:518:PHE:HB3  | 1.67                     | 0.75              |
| 1:E:221:VAL:O    | 1:E:225:LEU:HB2  | 1.87                     | 0.75              |
| 1:E:139:ILE:HG22 | 1:E:140:ILE:H    | 1.49                     | 0.75              |
| 1:H:507:VAL:HA   | 1:H:518:PHE:HB3  | 1.67                     | 0.75              |
| 1:L:221:VAL:O    | 1:L:225:LEU:HB2  | 1.87                     | 0.75              |
| 1:F:410:ALA:O    | 1:F:424:ASN:HA   | 1.87                     | 0.74              |
| 1:I:507:VAL:HA   | 1:I:518:PHE:HB3  | 1.67                     | 0.74              |
| 1:J:221:VAL:O    | 1:J:225:LEU:HB2  | 1.87                     | 0.74              |
| 1:D:507:VAL:HA   | 1:D:518:PHE:HB3  | 1.67                     | 0.74              |
| 1:E:410:ALA:O    | 1:E:424:ASN:HA   | 1.87                     | 0.74              |
| 1:H:130:ASN:HA   | 1:H:143:THR:O    | 1.85                     | 0.74              |
| 1:I:221:VAL:O    | 1:I:225:LEU:HB2  | 1.87                     | 0.74              |
| 1:K:221:VAL:O    | 1:K:225:LEU:HB2  | 1.87                     | 0.74              |
| 1:K:410:ALA:O    | 1:K:424:ASN:HA   | 1.87                     | 0.74              |
| 1:A:221:VAL:O    | 1:A:225:LEU:HB2  | 1.87                     | 0.74              |
| 1:C:507:VAL:HA   | 1:C:518:PHE:HB3  | 1.67                     | 0.74              |
| 1:D:221:VAL:O    | 1:D:225:LEU:HB2  | 1.87                     | 0.74              |
| 1:D:410:ALA:O    | 1:D:424:ASN:HA   | 1.87                     | 0.74              |
| 1:F:221:VAL:O    | 1:F:225:LEU:HB2  | 1.87                     | 0.74              |
| 1:M:221:VAL:O    | 1:M:225:LEU:HB2  | 1.87                     | 0.74              |
| 1:G:410:ALA:O    | 1:G:424:ASN:HA   | 1.88                     | 0.74              |
| 1:H:221:VAL:O    | 1:H:225:LEU:HB2  | 1.87                     | 0.74              |
| 1:M:507:VAL:HA   | 1:M:518:PHE:HB3  | 1.67                     | 0.74              |
| 1:N:459:ILE:CG2  | 1:N:473:GLN:HB2  | 2.12                     | 0.74              |
| 1:I:221:VAL:HG13 | 1:I:225:LEU:HD12 | 1.69                     | 0.74              |
| 1:H:410:ALA:O    | 1:H:424:ASN:HA   | 1.88                     | 0.74              |
| 1:O:410:ALA:O    | 1:O:424:ASN:HA   | 1.87                     | 0.74              |
| 1:C:410:ALA:O    | 1:C:424:ASN:HA   | 1.88                     | 0.74              |
| 1:H:221:VAL:HG13 | 1:H:225:LEU:HD12 | 1.69                     | 0.74              |
| 1:J:221:VAL:HG13 | 1:J:225:LEU:HD12 | 1.69                     | 0.74              |
| 1:L:410:ALA:O    | 1:L:424:ASN:HA   | 1.87                     | 0.74              |
| 1:N:410:ALA:O    | 1:N:424:ASN:HA   | 1.87                     | 0.74              |
| 1:B:410:ALA:O    | 1:B:424:ASN:HA   | 1.87                     | 0.74              |
| 1:K:221:VAL:HG13 | 1:K:225:LEU:HD12 | 1.69                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:221:VAL:HG13 | 1:L:225:LEU:HD12 | 1.69                     | 0.74              |
| 1:F:456:VAL:CG2  | 1:F:457:PRO:HD2  | 2.18                     | 0.74              |
| 1:G:221:VAL:O    | 1:G:225:LEU:HB2  | 1.87                     | 0.74              |
| 1:O:221:VAL:O    | 1:O:225:LEU:HB2  | 1.87                     | 0.74              |
| 1:B:221:VAL:O    | 1:B:225:LEU:HB2  | 1.87                     | 0.74              |
| 1:E:456:VAL:CG2  | 1:E:457:PRO:HD2  | 2.18                     | 0.74              |
| 1:I:410:ALA:O    | 1:I:424:ASN:HA   | 1.88                     | 0.74              |
| 1:N:456:VAL:CG2  | 1:N:457:PRO:HD2  | 2.18                     | 0.74              |
| 1:O:456:VAL:CG2  | 1:O:457:PRO:HD2  | 2.18                     | 0.74              |
| 1:A:410:ALA:O    | 1:A:424:ASN:HA   | 1.87                     | 0.73              |
| 1:D:219:PRO:HA   | 1:D:222:ARG:HB2  | 1.70                     | 0.73              |
| 1:E:219:PRO:HA   | 1:E:222:ARG:HB2  | 1.70                     | 0.73              |
| 1:E:221:VAL:HG13 | 1:E:225:LEU:HD12 | 1.69                     | 0.73              |
| 1:G:221:VAL:HG13 | 1:G:225:LEU:HD12 | 1.69                     | 0.73              |
| 1:M:221:VAL:HG13 | 1:M:225:LEU:HD12 | 1.69                     | 0.73              |
| 1:D:221:VAL:HG13 | 1:D:225:LEU:HD12 | 1.69                     | 0.73              |
| 1:J:410:ALA:O    | 1:J:424:ASN:HA   | 1.87                     | 0.73              |
| 1:O:221:VAL:HG13 | 1:O:225:LEU:HD12 | 1.69                     | 0.73              |
| 1:D:456:VAL:CG2  | 1:D:457:PRO:HD2  | 2.18                     | 0.73              |
| 1:G:456:VAL:CG2  | 1:G:457:PRO:HD2  | 2.18                     | 0.73              |
| 1:F:219:PRO:HA   | 1:F:222:ARG:HB2  | 1.70                     | 0.73              |
| 1:A:456:VAL:CG2  | 1:A:457:PRO:HD2  | 2.18                     | 0.73              |
| 1:A:221:VAL:HG13 | 1:A:225:LEU:HD12 | 1.69                     | 0.73              |
| 1:K:219:PRO:HA   | 1:K:222:ARG:HB2  | 1.70                     | 0.73              |
| 1:M:410:ALA:O    | 1:M:424:ASN:HA   | 1.87                     | 0.73              |
| 1:M:507:VAL:O    | 1:M:507:VAL:CG1  | 2.28                     | 0.73              |
| 1:F:221:VAL:HG13 | 1:F:225:LEU:HD12 | 1.69                     | 0.73              |
| 1:J:219:PRO:HA   | 1:J:222:ARG:HB2  | 1.70                     | 0.73              |
| 1:N:221:VAL:HG13 | 1:N:225:LEU:HD12 | 1.69                     | 0.73              |
| 1:N:221:VAL:O    | 1:N:225:LEU:HB2  | 1.87                     | 0.73              |
| 1:C:219:PRO:HA   | 1:C:222:ARG:HB2  | 1.70                     | 0.73              |
| 1:C:221:VAL:O    | 1:C:225:LEU:HB2  | 1.87                     | 0.73              |
| 1:C:456:VAL:CG2  | 1:C:457:PRO:HD2  | 2.18                     | 0.73              |
| 1:G:219:PRO:HA   | 1:G:222:ARG:HB2  | 1.70                     | 0.73              |
| 1:H:456:VAL:CG2  | 1:H:457:PRO:HD2  | 2.18                     | 0.73              |
| 1:C:221:VAL:HG13 | 1:C:225:LEU:HD12 | 1.69                     | 0.73              |
| 1:I:507:VAL:CG1  | 1:I:507:VAL:O    | 2.28                     | 0.73              |
| 1:M:459:ILE:CG2  | 1:M:473:GLN:HB2  | 2.12                     | 0.73              |
| 1:O:219:PRO:HA   | 1:O:222:ARG:HB2  | 1.70                     | 0.72              |
| 1:B:456:VAL:CG2  | 1:B:457:PRO:HD2  | 2.18                     | 0.72              |
| 1:C:438:PRO:HG3  | 1:C:482:ILE:HG21 | 1.72                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:221:VAL:HG13 | 1:B:225:LEU:HD12 | 1.69                     | 0.72              |
| 1:I:219:PRO:HA   | 1:I:222:ARG:HB2  | 1.70                     | 0.72              |
| 1:D:438:PRO:HG3  | 1:D:482:ILE:HG21 | 1.72                     | 0.72              |
| 1:I:456:VAL:CG2  | 1:I:457:PRO:HD2  | 2.18                     | 0.72              |
| 1:I:438:PRO:HG3  | 1:I:482:ILE:HG21 | 1.72                     | 0.72              |
| 1:J:438:PRO:HG3  | 1:J:482:ILE:HG21 | 1.72                     | 0.72              |
| 1:L:219:PRO:HA   | 1:L:222:ARG:HB2  | 1.70                     | 0.72              |
| 1:L:438:PRO:HG3  | 1:L:482:ILE:HG21 | 1.72                     | 0.72              |
| 1:M:438:PRO:HG3  | 1:M:482:ILE:HG21 | 1.72                     | 0.72              |
| 1:A:219:PRO:HA   | 1:A:222:ARG:HB2  | 1.70                     | 0.72              |
| 1:B:438:PRO:HG3  | 1:B:482:ILE:HG21 | 1.72                     | 0.72              |
| 1:H:438:PRO:HG3  | 1:H:482:ILE:HG21 | 1.72                     | 0.72              |
| 1:N:219:PRO:HA   | 1:N:222:ARG:HB2  | 1.70                     | 0.72              |
| 1:O:438:PRO:HG3  | 1:O:482:ILE:HG21 | 1.72                     | 0.72              |
| 1:E:438:PRO:HG3  | 1:E:482:ILE:HG21 | 1.72                     | 0.72              |
| 1:G:438:PRO:HG3  | 1:G:482:ILE:HG21 | 1.72                     | 0.72              |
| 1:H:219:PRO:HA   | 1:H:222:ARG:HB2  | 1.71                     | 0.72              |
| 1:M:458:VAL:HG23 | 1:M:476:ASP:O    | 1.90                     | 0.72              |
| 1:N:458:VAL:HG23 | 1:N:476:ASP:O    | 1.90                     | 0.72              |
| 1:A:438:PRO:HG3  | 1:A:482:ILE:HG21 | 1.72                     | 0.72              |
| 1:F:438:PRO:HG3  | 1:F:482:ILE:HG21 | 1.72                     | 0.72              |
| 1:K:438:PRO:HG3  | 1:K:482:ILE:HG21 | 1.72                     | 0.72              |
| 1:O:458:VAL:HG23 | 1:O:476:ASP:O    | 1.90                     | 0.71              |
| 1:E:609:PHE:CD1  | 1:F:639:ILE:HD13 | 2.25                     | 0.71              |
| 1:H:458:VAL:HG23 | 1:H:476:ASP:O    | 1.90                     | 0.71              |
| 1:H:609:PHE:CD1  | 1:I:639:ILE:HD13 | 2.26                     | 0.71              |
| 1:L:609:PHE:CD1  | 1:M:639:ILE:HD13 | 2.26                     | 0.71              |
| 1:G:458:VAL:HG23 | 1:G:476:ASP:O    | 1.90                     | 0.71              |
| 1:J:458:VAL:HG23 | 1:J:476:ASP:O    | 1.90                     | 0.71              |
| 1:N:438:PRO:HG3  | 1:N:482:ILE:HG21 | 1.72                     | 0.71              |
| 1:B:207:ASP:O    | 1:B:211:ASN:N    | 2.24                     | 0.71              |
| 1:B:219:PRO:HA   | 1:B:222:ARG:HB2  | 1.70                     | 0.71              |
| 1:I:458:VAL:HG23 | 1:I:476:ASP:O    | 1.90                     | 0.71              |
| 1:A:639:ILE:HD13 | 1:O:609:PHE:CD1  | 2.25                     | 0.71              |
| 1:I:609:PHE:CD1  | 1:J:639:ILE:HD13 | 2.26                     | 0.71              |
| 1:K:609:PHE:CD1  | 1:L:639:ILE:HD13 | 2.26                     | 0.71              |
| 1:M:207:ASP:O    | 1:M:211:ASN:N    | 2.24                     | 0.71              |
| 1:M:609:PHE:CD1  | 1:N:639:ILE:HD13 | 2.26                     | 0.71              |
| 1:F:609:PHE:CD1  | 1:G:639:ILE:HD13 | 2.26                     | 0.71              |
| 1:G:609:PHE:CD1  | 1:H:639:ILE:HD13 | 2.26                     | 0.71              |
| 1:I:207:ASP:O    | 1:I:211:ASN:N    | 2.24                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:456:VAL:CG2  | 1:J:457:PRO:HD2  | 2.18                     | 0.71              |
| 1:L:458:VAL:HG23 | 1:L:476:ASP:O    | 1.90                     | 0.71              |
| 1:A:458:VAL:HG23 | 1:A:476:ASP:O    | 1.90                     | 0.71              |
| 1:B:609:PHE:CD1  | 1:C:639:ILE:HD13 | 2.25                     | 0.71              |
| 1:K:458:VAL:HG23 | 1:K:476:ASP:O    | 1.90                     | 0.71              |
| 1:N:609:PHE:CD1  | 1:O:639:ILE:HD13 | 2.26                     | 0.71              |
| 1:F:458:VAL:HG23 | 1:F:476:ASP:O    | 1.90                     | 0.71              |
| 1:C:609:PHE:CD1  | 1:D:639:ILE:HD13 | 2.26                     | 0.71              |
| 1:F:207:ASP:O    | 1:F:211:ASN:N    | 2.24                     | 0.71              |
| 1:G:207:ASP:O    | 1:G:211:ASN:N    | 2.24                     | 0.71              |
| 1:K:481:GLY:N    | 1:K:505:SER:OG   | 2.23                     | 0.71              |
| 1:N:207:ASP:O    | 1:N:211:ASN:N    | 2.24                     | 0.71              |
| 1:A:207:ASP:O    | 1:A:211:ASN:N    | 2.24                     | 0.71              |
| 1:C:207:ASP:O    | 1:C:211:ASN:N    | 2.24                     | 0.70              |
| 1:E:458:VAL:HG23 | 1:E:476:ASP:O    | 1.90                     | 0.70              |
| 1:K:207:ASP:O    | 1:K:211:ASN:N    | 2.24                     | 0.70              |
| 1:L:207:ASP:O    | 1:L:211:ASN:N    | 2.24                     | 0.70              |
| 1:L:456:VAL:CG2  | 1:L:457:PRO:HD2  | 2.18                     | 0.70              |
| 1:D:207:ASP:O    | 1:D:211:ASN:N    | 2.24                     | 0.70              |
| 1:C:609:PHE:CD2  | 1:D:639:ILE:CD1  | 2.75                     | 0.70              |
| 1:J:609:PHE:CD1  | 1:K:639:ILE:HD13 | 2.25                     | 0.70              |
| 1:K:456:VAL:CG2  | 1:K:457:PRO:HD2  | 2.18                     | 0.70              |
| 1:L:481:GLY:N    | 1:L:505:SER:OG   | 2.23                     | 0.70              |
| 1:E:458:VAL:O    | 1:E:475:VAL:CA   | 2.39                     | 0.70              |
| 1:H:207:ASP:O    | 1:H:211:ASN:N    | 2.24                     | 0.70              |
| 1:M:456:VAL:CG2  | 1:M:457:PRO:HD2  | 2.18                     | 0.70              |
| 1:A:609:PHE:CD1  | 1:B:639:ILE:HD13 | 2.26                     | 0.70              |
| 1:D:458:VAL:HG23 | 1:D:476:ASP:O    | 1.90                     | 0.70              |
| 1:M:219:PRO:HA   | 1:M:222:ARG:HB2  | 1.71                     | 0.70              |
| 1:B:458:VAL:HG23 | 1:B:476:ASP:O    | 1.90                     | 0.70              |
| 1:E:207:ASP:O    | 1:E:211:ASN:N    | 2.24                     | 0.70              |
| 1:D:609:PHE:CD1  | 1:E:639:ILE:HD13 | 2.26                     | 0.70              |
| 1:B:609:PHE:CD2  | 1:C:639:ILE:CD1  | 2.75                     | 0.70              |
| 1:D:458:VAL:O    | 1:D:475:VAL:CA   | 2.39                     | 0.70              |
| 1:F:458:VAL:O    | 1:F:475:VAL:CA   | 2.40                     | 0.70              |
| 1:C:458:VAL:HG23 | 1:C:476:ASP:O    | 1.90                     | 0.70              |
| 1:M:328:GLU:CD   | 1:M:521:ARG:NH1  | 2.45                     | 0.70              |
| 1:N:328:GLU:CD   | 1:N:521:ARG:NH1  | 2.45                     | 0.70              |
| 1:O:207:ASP:O    | 1:O:211:ASN:N    | 2.24                     | 0.70              |
| 1:L:328:GLU:CD   | 1:L:521:ARG:NH1  | 2.45                     | 0.70              |
| 1:J:207:ASP:O    | 1:J:211:ASN:N    | 2.24                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:458:VAL:O    | 1:A:475:VAL:CA   | 2.39                     | 0.69              |
| 1:I:609:PHE:CD2  | 1:J:639:ILE:CD1  | 2.75                     | 0.69              |
| 1:K:328:GLU:CD   | 1:K:521:ARG:NH1  | 2.45                     | 0.69              |
| 1:L:458:VAL:O    | 1:L:475:VAL:CA   | 2.40                     | 0.69              |
| 1:M:458:VAL:O    | 1:M:475:VAL:CA   | 2.40                     | 0.69              |
| 1:O:328:GLU:CD   | 1:O:521:ARG:NH1  | 2.45                     | 0.69              |
| 1:M:481:GLY:N    | 1:M:505:SER:OG   | 2.23                     | 0.69              |
| 1:N:458:VAL:O    | 1:N:475:VAL:CA   | 2.39                     | 0.69              |
| 1:O:458:VAL:O    | 1:O:475:VAL:CA   | 2.39                     | 0.69              |
| 1:F:328:GLU:CD   | 1:F:521:ARG:NH1  | 2.45                     | 0.69              |
| 1:G:328:GLU:CD   | 1:G:521:ARG:NH1  | 2.45                     | 0.69              |
| 1:M:609:PHE:CD2  | 1:N:639:ILE:CD1  | 2.75                     | 0.69              |
| 1:A:328:GLU:CD   | 1:A:521:ARG:NH1  | 2.45                     | 0.69              |
| 1:B:458:VAL:O    | 1:B:475:VAL:CA   | 2.39                     | 0.69              |
| 1:C:458:VAL:O    | 1:C:475:VAL:CA   | 2.40                     | 0.69              |
| 1:G:458:VAL:O    | 1:G:475:VAL:CA   | 2.40                     | 0.69              |
| 1:K:458:VAL:O    | 1:K:475:VAL:CA   | 2.40                     | 0.69              |
| 1:J:328:GLU:CD   | 1:J:521:ARG:NH1  | 2.45                     | 0.69              |
| 1:B:328:GLU:CD   | 1:B:521:ARG:NH1  | 2.45                     | 0.69              |
| 1:J:458:VAL:O    | 1:J:475:VAL:CA   | 2.39                     | 0.69              |
| 1:I:328:GLU:CD   | 1:I:521:ARG:NH1  | 2.45                     | 0.69              |
| 1:C:328:GLU:CD   | 1:C:521:ARG:NH1  | 2.45                     | 0.68              |
| 1:N:481:GLY:N    | 1:N:505:SER:OG   | 2.23                     | 0.68              |
| 1:D:328:GLU:CD   | 1:D:521:ARG:NH1  | 2.45                     | 0.68              |
| 1:E:328:GLU:CD   | 1:E:521:ARG:NH1  | 2.45                     | 0.68              |
| 1:H:328:GLU:CD   | 1:H:521:ARG:NH1  | 2.45                     | 0.68              |
| 1:I:458:VAL:O    | 1:I:475:VAL:CA   | 2.40                     | 0.68              |
| 1:H:458:VAL:O    | 1:H:475:VAL:CA   | 2.40                     | 0.68              |
| 1:I:375:THR:HG23 | 1:I:390:THR:HG22 | 1.77                     | 0.67              |
| 1:J:375:THR:HG23 | 1:J:390:THR:HG22 | 1.77                     | 0.67              |
| 1:H:375:THR:HG23 | 1:H:390:THR:HG22 | 1.77                     | 0.67              |
| 1:G:375:THR:HG23 | 1:G:390:THR:HG22 | 1.77                     | 0.67              |
| 1:K:375:THR:HG23 | 1:K:390:THR:HG22 | 1.77                     | 0.67              |
| 1:C:500:ILE:HD13 | 1:C:537:LEU:HD21 | 1.76                     | 0.67              |
| 1:D:500:ILE:HD13 | 1:D:537:LEU:HD21 | 1.77                     | 0.67              |
| 1:J:609:PHE:CD1  | 1:K:639:ILE:CD1  | 2.78                     | 0.67              |
| 1:B:609:PHE:CD1  | 1:C:639:ILE:CD1  | 2.78                     | 0.67              |
| 1:J:500:ILE:HD13 | 1:J:537:LEU:HD21 | 1.76                     | 0.67              |
| 1:K:500:ILE:HD13 | 1:K:537:LEU:HD21 | 1.76                     | 0.67              |
| 1:K:609:PHE:CD1  | 1:L:639:ILE:CD1  | 2.78                     | 0.67              |
| 1:E:500:ILE:HD13 | 1:E:537:LEU:HD21 | 1.76                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:609:PHE:CD1  | 1:G:639:ILE:CD1  | 2.78                     | 0.67              |
| 1:I:500:ILE:HD13 | 1:I:537:LEU:HD21 | 1.77                     | 0.66              |
| 1:K:321:LEU:HD13 | 1:K:441:THR:OG1  | 1.96                     | 0.66              |
| 1:G:609:PHE:CD1  | 1:H:639:ILE:CD1  | 2.78                     | 0.66              |
| 1:I:609:PHE:CD1  | 1:J:639:ILE:CD1  | 2.78                     | 0.66              |
| 1:A:639:ILE:CD1  | 1:O:609:PHE:CD1  | 2.78                     | 0.66              |
| 1:B:375:THR:HG23 | 1:B:390:THR:HG22 | 1.77                     | 0.66              |
| 1:B:481:GLY:N    | 1:B:505:SER:OG   | 2.23                     | 0.66              |
| 1:J:321:LEU:HD13 | 1:J:441:THR:OG1  | 1.96                     | 0.66              |
| 1:A:609:PHE:CD1  | 1:B:639:ILE:CD1  | 2.78                     | 0.66              |
| 1:C:375:THR:HG23 | 1:C:390:THR:HG22 | 1.77                     | 0.66              |
| 1:F:375:THR:HG23 | 1:F:390:THR:HG22 | 1.77                     | 0.66              |
| 1:E:609:PHE:CD1  | 1:F:639:ILE:CD1  | 2.78                     | 0.66              |
| 1:L:178:ALA:N    | 1:L:208:GLU:OE2  | 2.28                     | 0.66              |
| 1:L:321:LEU:HD13 | 1:L:441:THR:OG1  | 1.96                     | 0.66              |
| 1:L:500:ILE:HD13 | 1:L:537:LEU:HD21 | 1.76                     | 0.66              |
| 1:N:609:PHE:CD1  | 1:O:639:ILE:CD1  | 2.78                     | 0.66              |
| 1:A:375:THR:HG23 | 1:A:390:THR:HG22 | 1.77                     | 0.66              |
| 1:B:500:ILE:HD13 | 1:B:537:LEU:HD21 | 1.77                     | 0.66              |
| 1:D:609:PHE:CD2  | 1:E:639:ILE:CD1  | 2.75                     | 0.66              |
| 1:C:609:PHE:CD1  | 1:D:639:ILE:CD1  | 2.78                     | 0.66              |
| 1:J:178:ALA:N    | 1:J:208:GLU:OE2  | 2.28                     | 0.66              |
| 1:L:375:THR:HG23 | 1:L:390:THR:HG22 | 1.77                     | 0.66              |
| 1:L:609:PHE:CD1  | 1:M:639:ILE:CD1  | 2.78                     | 0.66              |
| 1:N:609:PHE:CD2  | 1:O:639:ILE:CD1  | 2.75                     | 0.66              |
| 1:O:140:ILE:HD13 | 1:O:156:ILE:HG23 | 1.78                     | 0.66              |
| 1:H:500:ILE:HD13 | 1:H:537:LEU:HD21 | 1.76                     | 0.66              |
| 1:L:140:ILE:HD13 | 1:L:156:ILE:HG23 | 1.78                     | 0.66              |
| 1:M:140:ILE:HD13 | 1:M:156:ILE:HG23 | 1.78                     | 0.66              |
| 1:M:500:ILE:HD13 | 1:M:537:LEU:HD21 | 1.77                     | 0.66              |
| 1:N:327:VAL:HG11 | 1:O:603:ILE:HG21 | 1.78                     | 0.66              |
| 1:M:327:VAL:HG11 | 1:N:603:ILE:HG21 | 1.78                     | 0.66              |
| 1:A:172:LEU:O    | 1:A:211:ASN:ND2  | 2.29                     | 0.66              |
| 1:A:321:LEU:HD13 | 1:A:441:THR:OG1  | 1.96                     | 0.66              |
| 1:B:442:VAL:HG21 | 1:B:488:PRO:HG3  | 1.78                     | 0.66              |
| 1:D:375:THR:HG23 | 1:D:390:THR:HG22 | 1.77                     | 0.66              |
| 1:F:500:ILE:HD13 | 1:F:537:LEU:HD21 | 1.77                     | 0.66              |
| 1:G:458:VAL:HG21 | 1:G:478:LYS:HG2  | 1.78                     | 0.66              |
| 1:H:609:PHE:CD2  | 1:I:639:ILE:CD1  | 2.75                     | 0.66              |
| 1:M:321:LEU:HD13 | 1:M:441:THR:OG1  | 1.96                     | 0.66              |
| 1:N:140:ILE:HD13 | 1:N:156:ILE:HG23 | 1.78                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:500:ILE:HD13 | 1:N:537:LEU:HD21 | 1.76                     | 0.66              |
| 1:B:321:LEU:HD13 | 1:B:441:THR:OG1  | 1.96                     | 0.66              |
| 1:C:172:LEU:O    | 1:C:211:ASN:ND2  | 2.29                     | 0.66              |
| 1:H:458:VAL:HG21 | 1:H:478:LYS:HG2  | 1.78                     | 0.66              |
| 1:I:321:LEU:HD13 | 1:I:441:THR:OG1  | 1.96                     | 0.66              |
| 1:O:172:LEU:O    | 1:O:211:ASN:ND2  | 2.29                     | 0.66              |
| 1:A:603:ILE:HG21 | 1:O:327:VAL:HG11 | 1.78                     | 0.66              |
| 1:O:375:THR:HG23 | 1:O:390:THR:HG22 | 1.77                     | 0.66              |
| 1:A:518:PHE:O    | 1:B:455:GLU:OE1  | 2.14                     | 0.66              |
| 1:D:172:LEU:O    | 1:D:211:ASN:ND2  | 2.29                     | 0.66              |
| 1:H:609:PHE:CD1  | 1:I:639:ILE:CD1  | 2.78                     | 0.66              |
| 1:I:518:PHE:O    | 1:J:455:GLU:OE1  | 2.14                     | 0.66              |
| 1:L:172:LEU:O    | 1:L:211:ASN:ND2  | 2.29                     | 0.66              |
| 1:M:518:PHE:O    | 1:N:455:GLU:OE1  | 2.14                     | 0.66              |
| 1:N:172:LEU:O    | 1:N:211:ASN:ND2  | 2.29                     | 0.66              |
| 1:C:321:LEU:HD13 | 1:C:441:THR:OG1  | 1.96                     | 0.66              |
| 1:B:518:PHE:O    | 1:C:455:GLU:OE1  | 2.14                     | 0.66              |
| 1:H:348:SER:HB2  | 1:I:412:VAL:HA   | 1.78                     | 0.66              |
| 1:K:172:LEU:O    | 1:K:211:ASN:ND2  | 2.29                     | 0.66              |
| 1:J:348:SER:HB2  | 1:K:412:VAL:HA   | 1.78                     | 0.66              |
| 1:L:327:VAL:HG11 | 1:M:603:ILE:HG21 | 1.78                     | 0.66              |
| 1:L:518:PHE:O    | 1:M:455:GLU:OE1  | 2.14                     | 0.66              |
| 1:B:140:ILE:HD13 | 1:B:156:ILE:HG23 | 1.78                     | 0.65              |
| 1:B:172:LEU:O    | 1:B:211:ASN:ND2  | 2.29                     | 0.65              |
| 1:D:458:VAL:HG21 | 1:D:478:LYS:HG2  | 1.78                     | 0.65              |
| 1:D:609:PHE:CD1  | 1:E:639:ILE:CD1  | 2.78                     | 0.65              |
| 1:E:458:VAL:HG21 | 1:E:478:LYS:HG2  | 1.78                     | 0.65              |
| 1:E:518:PHE:O    | 1:F:455:GLU:OE1  | 2.14                     | 0.65              |
| 1:F:458:VAL:HG21 | 1:F:478:LYS:HG2  | 1.78                     | 0.65              |
| 1:J:140:ILE:HD13 | 1:J:156:ILE:HG23 | 1.78                     | 0.65              |
| 1:K:140:ILE:HD13 | 1:K:156:ILE:HG23 | 1.78                     | 0.65              |
| 1:O:321:LEU:HD13 | 1:O:441:THR:OG1  | 1.96                     | 0.65              |
| 1:C:178:ALA:N    | 1:C:208:GLU:OE2  | 2.28                     | 0.65              |
| 1:D:321:LEU:HD13 | 1:D:441:THR:OG1  | 1.96                     | 0.65              |
| 1:D:442:VAL:HG21 | 1:D:488:PRO:HG3  | 1.78                     | 0.65              |
| 1:E:321:LEU:HD13 | 1:E:441:THR:OG1  | 1.96                     | 0.65              |
| 1:D:518:PHE:O    | 1:E:455:GLU:OE1  | 2.14                     | 0.65              |
| 1:G:172:LEU:O    | 1:G:211:ASN:ND2  | 2.29                     | 0.65              |
| 1:A:140:ILE:HD13 | 1:A:156:ILE:HG23 | 1.78                     | 0.65              |
| 1:E:375:THR:HG23 | 1:E:390:THR:HG22 | 1.77                     | 0.65              |
| 1:F:172:LEU:O    | 1:F:211:ASN:ND2  | 2.29                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:322:ILE:O    | 1:G:439:SER:HA   | 1.97                     | 0.65              |
| 1:J:518:PHE:O    | 1:K:455:GLU:OE1  | 2.14                     | 0.65              |
| 1:L:348:SER:HB2  | 1:M:412:VAL:HA   | 1.78                     | 0.65              |
| 1:M:172:LEU:O    | 1:M:211:ASN:ND2  | 2.29                     | 0.65              |
| 1:N:375:THR:HG23 | 1:N:390:THR:HG22 | 1.77                     | 0.65              |
| 1:O:442:VAL:HG21 | 1:O:488:PRO:HG3  | 1.78                     | 0.65              |
| 1:C:458:VAL:HG21 | 1:C:478:LYS:HG2  | 1.78                     | 0.65              |
| 1:D:322:ILE:O    | 1:D:439:SER:HA   | 1.97                     | 0.65              |
| 1:H:327:VAL:HG11 | 1:I:603:ILE:HG21 | 1.78                     | 0.65              |
| 1:G:609:PHE:CD2  | 1:H:639:ILE:CD1  | 2.75                     | 0.65              |
| 1:M:609:PHE:CD1  | 1:N:639:ILE:CD1  | 2.78                     | 0.65              |
| 1:O:500:ILE:HD13 | 1:O:537:LEU:HD21 | 1.76                     | 0.65              |
| 1:A:327:VAL:HG11 | 1:B:603:ILE:HG21 | 1.78                     | 0.65              |
| 1:A:481:GLY:N    | 1:A:505:SER:OG   | 2.23                     | 0.65              |
| 1:A:328:GLU:CD   | 1:A:521:ARG:HH11 | 2.00                     | 0.65              |
| 1:A:500:ILE:HD13 | 1:A:537:LEU:HD21 | 1.77                     | 0.65              |
| 1:C:140:ILE:HD13 | 1:C:156:ILE:HG23 | 1.78                     | 0.65              |
| 1:F:321:LEU:HD13 | 1:F:441:THR:OG1  | 1.96                     | 0.65              |
| 1:F:518:PHE:O    | 1:G:455:GLU:OE1  | 2.14                     | 0.65              |
| 1:G:500:ILE:HD13 | 1:G:537:LEU:HD21 | 1.77                     | 0.65              |
| 1:I:140:ILE:HD13 | 1:I:156:ILE:HG23 | 1.78                     | 0.65              |
| 1:H:518:PHE:O    | 1:I:455:GLU:OE1  | 2.14                     | 0.65              |
| 1:I:458:VAL:HG21 | 1:I:478:LYS:HG2  | 1.78                     | 0.65              |
| 1:J:458:VAL:HG21 | 1:J:478:LYS:HG2  | 1.78                     | 0.65              |
| 1:C:322:ILE:O    | 1:C:439:SER:HA   | 1.97                     | 0.65              |
| 1:D:178:ALA:N    | 1:D:208:GLU:OE2  | 2.28                     | 0.65              |
| 1:E:442:VAL:HG21 | 1:E:488:PRO:HG3  | 1.78                     | 0.65              |
| 1:H:321:LEU:HD13 | 1:H:441:THR:OG1  | 1.96                     | 0.65              |
| 1:G:327:VAL:HG11 | 1:H:603:ILE:HG21 | 1.78                     | 0.65              |
| 1:I:328:GLU:CD   | 1:I:521:ARG:HH11 | 2.00                     | 0.65              |
| 1:J:442:VAL:HG21 | 1:J:488:PRO:HG3  | 1.78                     | 0.65              |
| 1:O:322:ILE:O    | 1:O:439:SER:HA   | 1.97                     | 0.65              |
| 1:A:609:PHE:CD2  | 1:B:639:ILE:CD1  | 2.75                     | 0.65              |
| 1:A:639:ILE:CD1  | 1:O:609:PHE:CD2  | 2.75                     | 0.65              |
| 1:C:328:GLU:CD   | 1:C:521:ARG:HH11 | 2.00                     | 0.65              |
| 1:F:348:SER:HB2  | 1:G:412:VAL:HA   | 1.78                     | 0.65              |
| 1:H:172:LEU:O    | 1:H:211:ASN:ND2  | 2.29                     | 0.65              |
| 1:H:322:ILE:O    | 1:H:439:SER:HA   | 1.97                     | 0.65              |
| 1:K:348:SER:HB2  | 1:L:412:VAL:HA   | 1.78                     | 0.65              |
| 1:K:328:GLU:CD   | 1:K:521:ARG:HH11 | 2.00                     | 0.65              |
| 1:C:442:VAL:HG21 | 1:C:488:PRO:HG3  | 1.78                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:328:GLU:CD   | 1:F:521:ARG:HH11 | 2.00                     | 0.65              |
| 1:I:348:SER:HB2  | 1:J:412:VAL:HA   | 1.78                     | 0.65              |
| 1:I:327:VAL:HG11 | 1:J:603:ILE:HG21 | 1.78                     | 0.65              |
| 1:K:327:VAL:HG11 | 1:L:603:ILE:HG21 | 1.78                     | 0.65              |
| 1:K:442:VAL:HG21 | 1:K:488:PRO:HG3  | 1.78                     | 0.65              |
| 1:N:321:LEU:HD13 | 1:N:441:THR:OG1  | 1.96                     | 0.65              |
| 1:N:328:GLU:CD   | 1:N:521:ARG:HH11 | 2.00                     | 0.65              |
| 1:N:518:PHE:O    | 1:O:455:GLU:OE1  | 2.14                     | 0.65              |
| 1:A:455:GLU:OE1  | 1:O:518:PHE:O    | 2.14                     | 0.65              |
| 1:F:609:PHE:CD2  | 1:G:639:ILE:CD1  | 2.75                     | 0.65              |
| 1:M:375:THR:HG23 | 1:M:390:THR:HG22 | 1.77                     | 0.65              |
| 1:N:348:SER:HB2  | 1:O:412:VAL:HA   | 1.78                     | 0.65              |
| 1:A:178:ALA:N    | 1:A:208:GLU:OE2  | 2.28                     | 0.65              |
| 1:B:178:ALA:N    | 1:B:208:GLU:OE2  | 2.28                     | 0.65              |
| 1:C:518:PHE:O    | 1:D:455:GLU:OE1  | 2.14                     | 0.65              |
| 1:D:328:GLU:CD   | 1:D:521:ARG:HH11 | 2.00                     | 0.65              |
| 1:F:327:VAL:HG11 | 1:G:603:ILE:HG21 | 1.78                     | 0.65              |
| 1:H:442:VAL:HG21 | 1:H:488:PRO:HG3  | 1.78                     | 0.65              |
| 1:I:442:VAL:HG21 | 1:I:488:PRO:HG3  | 1.78                     | 0.65              |
| 1:J:172:LEU:O    | 1:J:211:ASN:ND2  | 2.29                     | 0.65              |
| 1:K:458:VAL:HG21 | 1:K:478:LYS:HG2  | 1.78                     | 0.65              |
| 1:K:518:PHE:O    | 1:L:455:GLU:OE1  | 2.14                     | 0.65              |
| 1:N:322:ILE:O    | 1:N:439:SER:HA   | 1.97                     | 0.65              |
| 1:A:322:ILE:O    | 1:A:439:SER:HA   | 1.97                     | 0.64              |
| 1:F:322:ILE:O    | 1:F:439:SER:HA   | 1.97                     | 0.64              |
| 1:I:172:LEU:O    | 1:I:211:ASN:ND2  | 2.29                     | 0.64              |
| 1:L:328:GLU:CD   | 1:L:521:ARG:HH11 | 2.00                     | 0.64              |
| 1:N:442:VAL:HG21 | 1:N:488:PRO:HG3  | 1.78                     | 0.64              |
| 1:O:178:ALA:N    | 1:O:208:GLU:OE2  | 2.28                     | 0.64              |
| 1:A:442:VAL:HG21 | 1:A:488:PRO:HG3  | 1.78                     | 0.64              |
| 1:G:328:GLU:CD   | 1:G:521:ARG:HH11 | 2.00                     | 0.64              |
| 1:G:348:SER:HB2  | 1:H:412:VAL:HA   | 1.78                     | 0.64              |
| 1:A:521:ARG:H    | 1:A:521:ARG:HD3  | 1.63                     | 0.64              |
| 1:E:172:LEU:O    | 1:E:211:ASN:ND2  | 2.29                     | 0.64              |
| 1:F:178:ALA:N    | 1:F:208:GLU:OE2  | 2.28                     | 0.64              |
| 1:E:327:VAL:HG11 | 1:F:603:ILE:HG21 | 1.78                     | 0.64              |
| 1:G:321:LEU:HD13 | 1:G:441:THR:OG1  | 1.96                     | 0.64              |
| 1:J:327:VAL:HG11 | 1:K:603:ILE:HG21 | 1.78                     | 0.64              |
| 1:M:348:SER:HB2  | 1:N:412:VAL:HA   | 1.78                     | 0.64              |
| 1:O:458:VAL:HG21 | 1:O:478:LYS:HG2  | 1.78                     | 0.64              |
| 1:O:521:ARG:H    | 1:O:521:ARG:HD3  | 1.63                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:458:VAL:HG21 | 1:B:478:LYS:HG2  | 1.78                     | 0.64              |
| 1:D:327:VAL:HG11 | 1:E:603:ILE:HG21 | 1.78                     | 0.64              |
| 1:E:322:ILE:O    | 1:E:439:SER:HA   | 1.97                     | 0.64              |
| 1:E:521:ARG:H    | 1:E:521:ARG:HD3  | 1.63                     | 0.64              |
| 1:G:442:VAL:HG21 | 1:G:488:PRO:HG3  | 1.78                     | 0.64              |
| 1:H:140:ILE:HD13 | 1:H:156:ILE:HG23 | 1.78                     | 0.64              |
| 1:N:521:ARG:HD3  | 1:N:521:ARG:H    | 1.63                     | 0.64              |
| 1:A:458:VAL:HG21 | 1:A:478:LYS:HG2  | 1.78                     | 0.64              |
| 1:D:140:ILE:HD13 | 1:D:156:ILE:HG23 | 1.78                     | 0.64              |
| 1:D:521:ARG:HD3  | 1:D:521:ARG:H    | 1.63                     | 0.64              |
| 1:F:140:ILE:HD13 | 1:F:156:ILE:HG23 | 1.78                     | 0.64              |
| 1:F:442:VAL:HG21 | 1:F:488:PRO:HG3  | 1.78                     | 0.64              |
| 1:G:140:ILE:HD13 | 1:G:156:ILE:HG23 | 1.78                     | 0.64              |
| 1:L:540:LEU:HD22 | 1:M:452:VAL:HG21 | 1.80                     | 0.64              |
| 1:M:458:VAL:HG21 | 1:M:478:LYS:HG2  | 1.78                     | 0.64              |
| 1:E:140:ILE:HD13 | 1:E:156:ILE:HG23 | 1.78                     | 0.64              |
| 1:E:178:ALA:N    | 1:E:208:GLU:OE2  | 2.28                     | 0.64              |
| 1:G:176:SER:OG   | 1:G:208:GLU:OE2  | 2.16                     | 0.64              |
| 1:I:322:ILE:O    | 1:I:439:SER:HA   | 1.97                     | 0.64              |
| 1:M:322:ILE:O    | 1:M:439:SER:HA   | 1.97                     | 0.64              |
| 1:M:442:VAL:HG21 | 1:M:488:PRO:HG3  | 1.78                     | 0.64              |
| 1:M:521:ARG:HD3  | 1:M:521:ARG:H    | 1.63                     | 0.64              |
| 1:B:327:VAL:HG11 | 1:C:603:ILE:HG21 | 1.78                     | 0.64              |
| 1:A:348:SER:HB2  | 1:B:412:VAL:HA   | 1.78                     | 0.64              |
| 1:B:521:ARG:H    | 1:B:521:ARG:HD3  | 1.63                     | 0.64              |
| 1:B:328:GLU:CD   | 1:B:521:ARG:HH11 | 2.00                     | 0.64              |
| 1:J:328:GLU:CD   | 1:J:521:ARG:HH11 | 2.00                     | 0.64              |
| 1:L:442:VAL:HG21 | 1:L:488:PRO:HG3  | 1.78                     | 0.64              |
| 1:M:540:LEU:HD22 | 1:N:452:VAL:HG21 | 1.80                     | 0.64              |
| 1:C:327:VAL:HG11 | 1:D:603:ILE:HG21 | 1.78                     | 0.64              |
| 1:E:348:SER:HB2  | 1:F:412:VAL:HA   | 1.78                     | 0.64              |
| 1:K:322:ILE:O    | 1:K:439:SER:HA   | 1.97                     | 0.64              |
| 1:A:176:SER:OG   | 1:A:208:GLU:OE2  | 2.16                     | 0.64              |
| 1:B:348:SER:HB2  | 1:C:412:VAL:HA   | 1.78                     | 0.64              |
| 1:G:518:PHE:O    | 1:H:455:GLU:OE1  | 2.14                     | 0.64              |
| 1:G:540:LEU:HD22 | 1:H:452:VAL:HG21 | 1.80                     | 0.64              |
| 1:K:540:LEU:HD22 | 1:L:452:VAL:HG21 | 1.80                     | 0.64              |
| 1:L:458:VAL:HG21 | 1:L:478:LYS:HG2  | 1.78                     | 0.64              |
| 1:L:521:ARG:H    | 1:L:521:ARG:HD3  | 1.63                     | 0.64              |
| 1:B:322:ILE:O    | 1:B:439:SER:HA   | 1.97                     | 0.64              |
| 1:C:348:SER:HB2  | 1:D:412:VAL:HA   | 1.78                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:348:SER:HB2  | 1:E:412:VAL:HA   | 1.78                     | 0.64              |
| 1:G:178:ALA:N    | 1:G:208:GLU:OE2  | 2.28                     | 0.64              |
| 1:M:504:VAL:HG11 | 1:M:521:ARG:HG2  | 1.80                     | 0.64              |
| 1:N:178:ALA:N    | 1:N:208:GLU:OE2  | 2.28                     | 0.64              |
| 1:D:504:VAL:HG11 | 1:D:521:ARG:HG2  | 1.80                     | 0.63              |
| 1:G:521:ARG:H    | 1:G:521:ARG:HD3  | 1.63                     | 0.63              |
| 1:I:521:ARG:HD3  | 1:I:521:ARG:H    | 1.63                     | 0.63              |
| 1:L:504:VAL:HG11 | 1:L:521:ARG:HG2  | 1.81                     | 0.63              |
| 1:A:412:VAL:HA   | 1:O:348:SER:HB2  | 1.78                     | 0.63              |
| 1:B:176:SER:OG   | 1:B:208:GLU:OE2  | 2.16                     | 0.63              |
| 1:E:504:VAL:HG11 | 1:E:521:ARG:HG2  | 1.80                     | 0.63              |
| 1:G:507:VAL:HA   | 1:G:518:PHE:CB   | 2.28                     | 0.63              |
| 1:H:540:LEU:HD22 | 1:I:452:VAL:HG21 | 1.80                     | 0.63              |
| 1:J:521:ARG:HD3  | 1:J:521:ARG:H    | 1.63                     | 0.63              |
| 1:K:504:VAL:HG11 | 1:K:521:ARG:HG2  | 1.81                     | 0.63              |
| 1:N:458:VAL:HG21 | 1:N:478:LYS:HG2  | 1.78                     | 0.63              |
| 1:A:639:ILE:HD12 | 1:O:609:PHE:CG   | 2.34                     | 0.63              |
| 1:C:521:ARG:H    | 1:C:521:ARG:HD3  | 1.63                     | 0.63              |
| 1:E:609:PHE:CG   | 1:F:639:ILE:HD12 | 2.34                     | 0.63              |
| 1:F:521:ARG:H    | 1:F:521:ARG:HD3  | 1.63                     | 0.63              |
| 1:F:609:PHE:CG   | 1:G:639:ILE:HD12 | 2.34                     | 0.63              |
| 1:H:176:SER:OG   | 1:H:208:GLU:OE2  | 2.16                     | 0.63              |
| 1:H:521:ARG:H    | 1:H:521:ARG:HD3  | 1.63                     | 0.63              |
| 1:I:257:GLU:HA   | 1:I:257:GLU:OE1  | 1.99                     | 0.63              |
| 1:J:322:ILE:O    | 1:J:439:SER:HA   | 1.97                     | 0.63              |
| 1:L:322:ILE:O    | 1:L:439:SER:HA   | 1.97                     | 0.63              |
| 1:O:176:SER:OG   | 1:O:208:GLU:OE2  | 2.16                     | 0.63              |
| 1:O:481:GLY:N    | 1:O:505:SER:OG   | 2.23                     | 0.63              |
| 1:A:609:PHE:CG   | 1:B:639:ILE:HD12 | 2.34                     | 0.63              |
| 1:C:504:VAL:HG11 | 1:C:521:ARG:HG2  | 1.80                     | 0.63              |
| 1:E:507:VAL:HA   | 1:E:518:PHE:CB   | 2.28                     | 0.63              |
| 1:F:257:GLU:HA   | 1:F:257:GLU:OE1  | 1.99                     | 0.63              |
| 1:K:521:ARG:HD3  | 1:K:521:ARG:H    | 1.63                     | 0.63              |
| 1:M:507:VAL:HA   | 1:M:518:PHE:CB   | 2.28                     | 0.63              |
| 1:N:540:LEU:HD22 | 1:O:452:VAL:HG21 | 1.80                     | 0.63              |
| 1:N:609:PHE:CG   | 1:O:639:ILE:HD12 | 2.34                     | 0.63              |
| 1:A:519:ALA:HB2  | 1:B:454:GLU:HG3  | 1.81                     | 0.63              |
| 1:F:540:LEU:HD22 | 1:G:452:VAL:HG21 | 1.80                     | 0.63              |
| 1:B:519:ALA:HB2  | 1:C:454:GLU:HG3  | 1.81                     | 0.63              |
| 1:E:257:GLU:HA   | 1:E:257:GLU:OE1  | 1.99                     | 0.63              |
| 1:H:244:VAL:HG22 | 1:H:295:VAL:HG22 | 1.81                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:504:VAL:HG11 | 1:J:521:ARG:HG2  | 1.80                     | 0.63              |
| 1:J:540:LEU:HD22 | 1:K:452:VAL:HG21 | 1.80                     | 0.63              |
| 1:M:178:ALA:N    | 1:M:208:GLU:OE2  | 2.28                     | 0.63              |
| 1:O:507:VAL:HA   | 1:O:518:PHE:CB   | 2.28                     | 0.63              |
| 1:C:519:ALA:HB2  | 1:D:454:GLU:HG3  | 1.81                     | 0.63              |
| 1:F:504:VAL:HG11 | 1:F:521:ARG:HG2  | 1.80                     | 0.63              |
| 1:G:244:VAL:HG22 | 1:G:295:VAL:HG22 | 1.81                     | 0.63              |
| 1:I:507:VAL:HA   | 1:I:518:PHE:CB   | 2.28                     | 0.63              |
| 1:K:326:ILE:HD11 | 1:K:502:GLN:HE21 | 1.64                     | 0.63              |
| 1:C:176:SER:OG   | 1:C:208:GLU:OE2  | 2.16                     | 0.63              |
| 1:E:164:ASP:O    | 1:E:218:ASP:HA   | 1.99                     | 0.63              |
| 1:E:326:ILE:HD11 | 1:E:502:GLN:HE21 | 1.64                     | 0.63              |
| 1:E:328:GLU:CD   | 1:E:521:ARG:HH11 | 2.00                     | 0.63              |
| 1:D:609:PHE:CG   | 1:E:639:ILE:HD12 | 2.34                     | 0.63              |
| 1:G:164:ASP:O    | 1:G:218:ASP:HA   | 1.99                     | 0.63              |
| 1:J:257:GLU:OE1  | 1:J:257:GLU:HA   | 1.99                     | 0.63              |
| 1:K:178:ALA:N    | 1:K:208:GLU:OE2  | 2.28                     | 0.63              |
| 1:N:504:VAL:HG11 | 1:N:521:ARG:HG2  | 1.80                     | 0.63              |
| 1:O:326:ILE:HD11 | 1:O:502:GLN:HE21 | 1.64                     | 0.63              |
| 1:O:458:VAL:CG2  | 1:O:476:ASP:O    | 2.47                     | 0.63              |
| 1:A:454:GLU:HG3  | 1:O:519:ALA:HB2  | 1.81                     | 0.63              |
| 1:O:328:GLU:CD   | 1:O:521:ARG:HH11 | 2.00                     | 0.63              |
| 1:A:326:ILE:HD11 | 1:A:502:GLN:HE21 | 1.64                     | 0.63              |
| 1:A:458:VAL:CG2  | 1:A:476:ASP:O    | 2.47                     | 0.63              |
| 1:A:507:VAL:HA   | 1:A:518:PHE:CB   | 2.28                     | 0.63              |
| 1:B:164:ASP:O    | 1:B:218:ASP:HA   | 1.99                     | 0.63              |
| 1:B:260:LYS:O    | 1:B:263:SER:OG   | 2.17                     | 0.63              |
| 1:E:540:LEU:HD22 | 1:F:452:VAL:HG21 | 1.80                     | 0.63              |
| 1:I:540:LEU:HD22 | 1:J:452:VAL:HG21 | 1.80                     | 0.63              |
| 1:J:458:VAL:CG2  | 1:J:476:ASP:O    | 2.47                     | 0.63              |
| 1:L:326:ILE:HD11 | 1:L:502:GLN:HE21 | 1.64                     | 0.63              |
| 1:C:507:VAL:HA   | 1:C:518:PHE:CB   | 2.28                     | 0.62              |
| 1:D:326:ILE:HD11 | 1:D:502:GLN:HE21 | 1.64                     | 0.62              |
| 1:D:519:ALA:HB2  | 1:E:454:GLU:HG3  | 1.81                     | 0.62              |
| 1:F:244:VAL:HG22 | 1:F:295:VAL:HG22 | 1.81                     | 0.62              |
| 1:H:178:ALA:N    | 1:H:208:GLU:OE2  | 2.28                     | 0.62              |
| 1:I:244:VAL:HG22 | 1:I:295:VAL:HG22 | 1.81                     | 0.62              |
| 1:I:458:VAL:CG2  | 1:I:476:ASP:O    | 2.47                     | 0.62              |
| 1:K:164:ASP:O    | 1:K:218:ASP:HA   | 1.99                     | 0.62              |
| 1:O:164:ASP:O    | 1:O:218:ASP:HA   | 1.99                     | 0.62              |
| 1:B:609:PHE:CG   | 1:C:639:ILE:HD12 | 2.33                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:540:LEU:HD22 | 1:D:452:VAL:HG21 | 1.80                     | 0.62              |
| 1:E:458:VAL:CG2  | 1:E:476:ASP:O    | 2.47                     | 0.62              |
| 1:I:164:ASP:O    | 1:I:218:ASP:HA   | 1.99                     | 0.62              |
| 1:J:326:ILE:HD11 | 1:J:502:GLN:HE21 | 1.64                     | 0.62              |
| 1:K:176:SER:OG   | 1:K:208:GLU:OE2  | 2.16                     | 0.62              |
| 1:N:489:GLN:NE2  | 1:O:249:TYR:O    | 2.32                     | 0.62              |
| 1:B:257:GLU:OE1  | 1:B:257:GLU:HA   | 1.99                     | 0.62              |
| 1:C:260:LYS:O    | 1:C:263:SER:OG   | 2.17                     | 0.62              |
| 1:H:507:VAL:HA   | 1:H:518:PHE:CB   | 2.28                     | 0.62              |
| 1:I:489:GLN:NE2  | 1:J:249:TYR:O    | 2.32                     | 0.62              |
| 1:L:507:VAL:HA   | 1:L:518:PHE:CB   | 2.28                     | 0.62              |
| 1:N:164:ASP:O    | 1:N:218:ASP:HA   | 1.99                     | 0.62              |
| 1:N:458:VAL:CG2  | 1:N:476:ASP:O    | 2.47                     | 0.62              |
| 1:B:504:VAL:HG11 | 1:B:521:ARG:HG2  | 1.81                     | 0.62              |
| 1:C:164:ASP:O    | 1:C:218:ASP:HA   | 1.99                     | 0.62              |
| 1:D:458:VAL:CG2  | 1:D:476:ASP:O    | 2.47                     | 0.62              |
| 1:E:244:VAL:HG22 | 1:E:295:VAL:HG22 | 1.81                     | 0.62              |
| 1:F:458:VAL:CG2  | 1:F:476:ASP:O    | 2.47                     | 0.62              |
| 1:F:489:GLN:NE2  | 1:G:249:TYR:O    | 2.32                     | 0.62              |
| 1:F:507:VAL:HA   | 1:F:518:PHE:CB   | 2.28                     | 0.62              |
| 1:G:489:GLN:NE2  | 1:H:249:TYR:O    | 2.33                     | 0.62              |
| 1:I:504:VAL:HG11 | 1:I:521:ARG:HG2  | 1.80                     | 0.62              |
| 1:K:244:VAL:HG22 | 1:K:295:VAL:HG22 | 1.81                     | 0.62              |
| 1:K:458:VAL:CG2  | 1:K:476:ASP:O    | 2.47                     | 0.62              |
| 1:K:489:GLN:NE2  | 1:L:249:TYR:O    | 2.32                     | 0.62              |
| 1:L:489:GLN:NE2  | 1:M:249:TYR:O    | 2.32                     | 0.62              |
| 1:M:519:ALA:HB2  | 1:N:454:GLU:HG3  | 1.81                     | 0.62              |
| 1:N:519:ALA:HB2  | 1:O:454:GLU:HG3  | 1.81                     | 0.62              |
| 1:A:489:GLN:NE2  | 1:B:249:TYR:O    | 2.32                     | 0.62              |
| 1:D:244:VAL:HG22 | 1:D:295:VAL:HG22 | 1.81                     | 0.62              |
| 1:E:489:GLN:NE2  | 1:F:249:TYR:O    | 2.32                     | 0.62              |
| 1:G:504:VAL:HG11 | 1:G:521:ARG:HG2  | 1.80                     | 0.62              |
| 1:H:257:GLU:HA   | 1:H:257:GLU:OE1  | 1.99                     | 0.62              |
| 1:H:458:VAL:CG2  | 1:H:476:ASP:O    | 2.47                     | 0.62              |
| 1:H:328:GLU:CD   | 1:H:521:ARG:HH11 | 2.00                     | 0.62              |
| 1:I:178:ALA:N    | 1:I:208:GLU:OE2  | 2.28                     | 0.62              |
| 1:J:244:VAL:HG22 | 1:J:295:VAL:HG22 | 1.81                     | 0.62              |
| 1:K:507:VAL:HA   | 1:K:518:PHE:CB   | 2.28                     | 0.62              |
| 1:L:176:SER:OG   | 1:L:208:GLU:OE2  | 2.16                     | 0.62              |
| 1:L:459:ILE:HG23 | 1:L:474:THR:C    | 2.16                     | 0.62              |
| 1:A:452:VAL:HG21 | 1:O:540:LEU:HD22 | 1.80                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:540:LEU:HD22 | 1:C:452:VAL:HG21 | 1.80                     | 0.62              |
| 1:C:489:GLN:NE2  | 1:D:249:TYR:O    | 2.32                     | 0.62              |
| 1:E:539:GLY:HA2  | 1:E:577:LEU:O    | 2.00                     | 0.62              |
| 1:G:257:GLU:OE1  | 1:G:257:GLU:HA   | 1.99                     | 0.62              |
| 1:J:459:ILE:HG23 | 1:J:474:THR:C    | 2.16                     | 0.62              |
| 1:L:164:ASP:O    | 1:L:218:ASP:HA   | 1.99                     | 0.62              |
| 1:M:176:SER:OG   | 1:M:208:GLU:OE2  | 2.16                     | 0.62              |
| 1:M:257:GLU:OE1  | 1:M:257:GLU:HA   | 1.99                     | 0.62              |
| 1:B:458:VAL:CG2  | 1:B:476:ASP:O    | 2.47                     | 0.62              |
| 1:C:257:GLU:OE1  | 1:C:257:GLU:HA   | 1.99                     | 0.62              |
| 1:D:260:LYS:O    | 1:D:263:SER:OG   | 2.17                     | 0.62              |
| 1:D:489:GLN:NE2  | 1:E:249:TYR:O    | 2.32                     | 0.62              |
| 1:F:326:ILE:HD11 | 1:F:502:GLN:HE21 | 1.64                     | 0.62              |
| 1:I:539:GLY:HA2  | 1:I:577:LEU:O    | 2.00                     | 0.62              |
| 1:J:507:VAL:HA   | 1:J:518:PHE:CB   | 2.28                     | 0.62              |
| 1:L:458:VAL:CG2  | 1:L:476:ASP:O    | 2.47                     | 0.62              |
| 1:M:164:ASP:O    | 1:M:218:ASP:HA   | 1.99                     | 0.62              |
| 1:L:519:ALA:HB2  | 1:M:454:GLU:HG3  | 1.81                     | 0.62              |
| 1:M:489:GLN:NE2  | 1:N:249:TYR:O    | 2.32                     | 0.62              |
| 1:A:244:VAL:HG22 | 1:A:295:VAL:HG22 | 1.81                     | 0.62              |
| 1:A:540:LEU:HD22 | 1:B:452:VAL:HG21 | 1.80                     | 0.62              |
| 1:B:539:GLY:HA2  | 1:B:577:LEU:O    | 2.00                     | 0.62              |
| 1:C:458:VAL:CG2  | 1:C:476:ASP:O    | 2.47                     | 0.62              |
| 1:C:326:ILE:HD11 | 1:C:502:GLN:HE21 | 1.64                     | 0.62              |
| 1:C:539:GLY:HA2  | 1:C:577:LEU:O    | 2.00                     | 0.62              |
| 1:D:164:ASP:O    | 1:D:218:ASP:HA   | 1.99                     | 0.62              |
| 1:D:257:GLU:OE1  | 1:D:257:GLU:HA   | 1.99                     | 0.62              |
| 1:C:609:PHE:CG   | 1:D:639:ILE:HD12 | 2.34                     | 0.62              |
| 1:D:540:LEU:HD22 | 1:E:452:VAL:HG21 | 1.80                     | 0.62              |
| 1:E:519:ALA:HB2  | 1:F:454:GLU:HG3  | 1.81                     | 0.62              |
| 1:F:539:GLY:HA2  | 1:F:577:LEU:O    | 2.00                     | 0.62              |
| 1:I:176:SER:OG   | 1:I:208:GLU:OE2  | 2.16                     | 0.62              |
| 1:I:459:ILE:HG23 | 1:I:474:THR:C    | 2.16                     | 0.62              |
| 1:J:539:GLY:HA2  | 1:J:577:LEU:O    | 2.00                     | 0.62              |
| 1:N:244:VAL:HG22 | 1:N:295:VAL:HG22 | 1.81                     | 0.62              |
| 1:C:226:LYS:HA   | 1:C:229:ILE:HD12 | 1.82                     | 0.62              |
| 1:D:507:VAL:HA   | 1:D:518:PHE:CB   | 2.28                     | 0.62              |
| 1:H:489:GLN:NE2  | 1:I:249:TYR:O    | 2.32                     | 0.62              |
| 1:I:326:ILE:HD11 | 1:I:502:GLN:HE21 | 1.64                     | 0.62              |
| 1:K:459:ILE:HG23 | 1:K:474:THR:C    | 2.16                     | 0.62              |
| 1:M:328:GLU:CD   | 1:M:521:ARG:HH11 | 2.00                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:507:VAL:HA   | 1:N:518:PHE:CB   | 2.28                     | 0.62              |
| 1:A:164:ASP:O    | 1:A:218:ASP:HA   | 1.99                     | 0.62              |
| 1:A:257:GLU:HA   | 1:A:257:GLU:OE1  | 1.99                     | 0.62              |
| 1:B:489:GLN:NE2  | 1:C:249:TYR:O    | 2.32                     | 0.62              |
| 1:D:176:SER:OG   | 1:D:208:GLU:OE2  | 2.16                     | 0.62              |
| 1:D:539:GLY:HA2  | 1:D:577:LEU:O    | 2.00                     | 0.62              |
| 1:E:481:GLY:O    | 1:E:505:SER:N    | 2.33                     | 0.62              |
| 1:F:481:GLY:O    | 1:F:505:SER:N    | 2.33                     | 0.62              |
| 1:G:458:VAL:CG2  | 1:G:476:ASP:O    | 2.47                     | 0.62              |
| 1:G:481:GLY:O    | 1:G:505:SER:N    | 2.33                     | 0.62              |
| 1:L:257:GLU:HA   | 1:L:257:GLU:OE1  | 1.99                     | 0.62              |
| 1:M:458:VAL:CG2  | 1:M:476:ASP:O    | 2.47                     | 0.62              |
| 1:A:249:TYR:O    | 1:O:489:GLN:NE2  | 2.32                     | 0.62              |
| 1:O:504:VAL:HG11 | 1:O:521:ARG:HG2  | 1.80                     | 0.62              |
| 1:B:507:VAL:HA   | 1:B:518:PHE:CB   | 2.28                     | 0.61              |
| 1:B:506:ASN:O    | 1:B:518:PHE:HB2  | 2.00                     | 0.61              |
| 1:D:481:GLY:O    | 1:D:505:SER:N    | 2.33                     | 0.61              |
| 1:E:260:LYS:O    | 1:E:263:SER:OG   | 2.17                     | 0.61              |
| 1:G:519:ALA:HB2  | 1:H:454:GLU:HG3  | 1.81                     | 0.61              |
| 1:G:522:GLN:HG2  | 1:H:451:ILE:CG2  | 2.30                     | 0.61              |
| 1:H:519:ALA:HB2  | 1:I:454:GLU:HG3  | 1.81                     | 0.61              |
| 1:J:176:SER:OG   | 1:J:208:GLU:OE2  | 2.16                     | 0.61              |
| 1:K:257:GLU:OE1  | 1:K:257:GLU:HA   | 1.99                     | 0.61              |
| 1:J:609:PHE:CG   | 1:K:639:ILE:HD12 | 2.34                     | 0.61              |
| 1:N:176:SER:OG   | 1:N:208:GLU:OE2  | 2.16                     | 0.61              |
| 1:M:522:GLN:HG2  | 1:N:451:ILE:CG2  | 2.30                     | 0.61              |
| 1:N:326:ILE:HD11 | 1:N:502:GLN:HE21 | 1.64                     | 0.61              |
| 1:A:504:VAL:HG11 | 1:A:521:ARG:HG2  | 1.80                     | 0.61              |
| 1:A:506:ASN:O    | 1:A:518:PHE:HB2  | 2.00                     | 0.61              |
| 1:A:539:GLY:HA2  | 1:A:577:LEU:O    | 2.00                     | 0.61              |
| 1:D:226:LYS:HA   | 1:D:229:ILE:HD12 | 1.82                     | 0.61              |
| 1:H:164:ASP:O    | 1:H:218:ASP:HA   | 1.99                     | 0.61              |
| 1:H:481:GLY:O    | 1:H:505:SER:N    | 2.33                     | 0.61              |
| 1:H:539:GLY:HA2  | 1:H:577:LEU:O    | 2.00                     | 0.61              |
| 1:I:226:LYS:HA   | 1:I:229:ILE:HD12 | 1.82                     | 0.61              |
| 1:J:226:LYS:HA   | 1:J:229:ILE:HD12 | 1.82                     | 0.61              |
| 1:J:522:GLN:HG2  | 1:K:451:ILE:CG2  | 2.30                     | 0.61              |
| 1:K:519:ALA:HB2  | 1:L:454:GLU:HG3  | 1.81                     | 0.61              |
| 1:L:244:VAL:HG22 | 1:L:295:VAL:HG22 | 1.81                     | 0.61              |
| 1:A:522:GLN:HG2  | 1:B:451:ILE:CG2  | 2.30                     | 0.61              |
| 1:B:326:ILE:HD11 | 1:B:502:GLN:HE21 | 1.64                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:604:ARG:NH2  | 1:B:626:LEU:O    | 2.34                     | 0.61              |
| 1:C:244:VAL:HG22 | 1:C:295:VAL:HG22 | 1.81                     | 0.61              |
| 1:C:481:GLY:O    | 1:C:505:SER:N    | 2.33                     | 0.61              |
| 1:C:506:ASN:O    | 1:C:518:PHE:HB2  | 2.01                     | 0.61              |
| 1:D:604:ARG:NH2  | 1:D:626:LEU:O    | 2.34                     | 0.61              |
| 1:H:506:ASN:O    | 1:H:518:PHE:HB2  | 2.01                     | 0.61              |
| 1:I:519:ALA:HB2  | 1:J:454:GLU:HG3  | 1.81                     | 0.61              |
| 1:I:609:PHE:CG   | 1:J:639:ILE:HD12 | 2.34                     | 0.61              |
| 1:K:539:GLY:HA2  | 1:K:577:LEU:O    | 2.00                     | 0.61              |
| 1:M:326:ILE:HD11 | 1:M:502:GLN:HE21 | 1.64                     | 0.61              |
| 1:A:451:ILE:CG2  | 1:O:522:GLN:HG2  | 2.30                     | 0.61              |
| 1:B:481:GLY:O    | 1:B:505:SER:N    | 2.33                     | 0.61              |
| 1:B:522:GLN:HG2  | 1:C:451:ILE:CG2  | 2.30                     | 0.61              |
| 1:D:506:ASN:O    | 1:D:518:PHE:HB2  | 2.01                     | 0.61              |
| 1:F:519:ALA:HB2  | 1:G:454:GLU:HG3  | 1.81                     | 0.61              |
| 1:I:481:GLY:O    | 1:I:505:SER:N    | 2.33                     | 0.61              |
| 1:I:604:ARG:NH2  | 1:I:626:LEU:O    | 2.34                     | 0.61              |
| 1:J:489:GLN:NE2  | 1:K:249:TYR:O    | 2.32                     | 0.61              |
| 1:J:604:ARG:NH2  | 1:J:626:LEU:O    | 2.34                     | 0.61              |
| 1:K:506:ASN:O    | 1:K:518:PHE:HB2  | 2.00                     | 0.61              |
| 1:O:506:ASN:O    | 1:O:518:PHE:HB2  | 2.01                     | 0.61              |
| 1:A:481:GLY:O    | 1:A:505:SER:N    | 2.33                     | 0.61              |
| 1:B:477:ARG:HH11 | 1:B:477:ARG:CG   | 2.14                     | 0.61              |
| 1:E:226:LYS:HA   | 1:E:229:ILE:HD12 | 1.82                     | 0.61              |
| 1:F:452:VAL:O    | 1:F:481:GLY:HA3  | 2.01                     | 0.61              |
| 1:F:604:ARG:NH2  | 1:F:626:LEU:O    | 2.34                     | 0.61              |
| 1:H:504:VAL:HG11 | 1:H:521:ARG:HG2  | 1.80                     | 0.61              |
| 1:J:477:ARG:HH11 | 1:J:477:ARG:CG   | 2.14                     | 0.61              |
| 1:J:481:GLY:O    | 1:J:505:SER:N    | 2.33                     | 0.61              |
| 1:J:519:ALA:HB2  | 1:K:454:GLU:HG3  | 1.81                     | 0.61              |
| 1:K:226:LYS:HA   | 1:K:229:ILE:HD12 | 1.83                     | 0.61              |
| 1:K:481:GLY:O    | 1:K:505:SER:N    | 2.33                     | 0.61              |
| 1:N:184:VAL:HG13 | 1:N:187:LEU:HD12 | 1.82                     | 0.61              |
| 1:N:257:GLU:OE1  | 1:N:257:GLU:HA   | 1.99                     | 0.61              |
| 1:O:184:VAL:HG13 | 1:O:187:LEU:HD12 | 1.82                     | 0.61              |
| 1:N:522:GLN:HG2  | 1:O:451:ILE:CG2  | 2.30                     | 0.61              |
| 1:B:226:LYS:HA   | 1:B:229:ILE:HD12 | 1.83                     | 0.61              |
| 1:C:452:VAL:O    | 1:C:481:GLY:HA3  | 2.01                     | 0.61              |
| 1:F:164:ASP:O    | 1:F:218:ASP:HA   | 1.99                     | 0.61              |
| 1:F:260:LYS:O    | 1:F:263:SER:OG   | 2.17                     | 0.61              |
| 1:H:477:ARG:HH11 | 1:H:477:ARG:CG   | 2.14                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:481:GLY:O    | 1:N:505:SER:N    | 2.33                     | 0.61              |
| 1:N:506:ASN:O    | 1:N:518:PHE:HB2  | 2.01                     | 0.61              |
| 1:O:481:GLY:O    | 1:O:505:SER:N    | 2.33                     | 0.61              |
| 1:O:539:GLY:HA2  | 1:O:577:LEU:O    | 2.00                     | 0.61              |
| 1:E:604:ARG:NH2  | 1:E:626:LEU:O    | 2.34                     | 0.61              |
| 1:G:506:ASN:O    | 1:G:518:PHE:HB2  | 2.01                     | 0.61              |
| 1:H:452:VAL:O    | 1:H:481:GLY:HA3  | 2.01                     | 0.61              |
| 1:H:604:ARG:NH2  | 1:H:626:LEU:O    | 2.34                     | 0.61              |
| 1:H:522:GLN:HG2  | 1:I:451:ILE:CG2  | 2.31                     | 0.61              |
| 1:I:452:VAL:O    | 1:I:481:GLY:HA3  | 2.01                     | 0.61              |
| 1:J:164:ASP:O    | 1:J:218:ASP:HA   | 1.99                     | 0.61              |
| 1:K:452:VAL:O    | 1:K:481:GLY:HA3  | 2.01                     | 0.61              |
| 1:L:452:VAL:O    | 1:L:481:GLY:HA3  | 2.01                     | 0.61              |
| 1:L:477:ARG:HH11 | 1:L:477:ARG:CG   | 2.14                     | 0.61              |
| 1:L:481:GLY:O    | 1:L:505:SER:N    | 2.33                     | 0.61              |
| 1:L:506:ASN:O    | 1:L:518:PHE:HB2  | 2.01                     | 0.61              |
| 1:L:539:GLY:HA2  | 1:L:577:LEU:O    | 2.00                     | 0.61              |
| 1:A:508:LEU:HD12 | 1:A:508:LEU:N    | 2.16                     | 0.61              |
| 1:C:604:ARG:NH2  | 1:C:626:LEU:O    | 2.34                     | 0.61              |
| 1:E:506:ASN:O    | 1:E:518:PHE:HB2  | 2.00                     | 0.61              |
| 1:E:522:GLN:HG2  | 1:F:451:ILE:CG2  | 2.30                     | 0.61              |
| 1:G:452:VAL:O    | 1:G:481:GLY:HA3  | 2.01                     | 0.61              |
| 1:H:226:LYS:HA   | 1:H:229:ILE:HD12 | 1.82                     | 0.61              |
| 1:H:326:ILE:HD11 | 1:H:502:GLN:HE21 | 1.64                     | 0.61              |
| 1:L:226:LYS:HA   | 1:L:229:ILE:HD12 | 1.82                     | 0.61              |
| 1:L:508:LEU:N    | 1:L:508:LEU:HD12 | 2.16                     | 0.61              |
| 1:M:184:VAL:HG13 | 1:M:187:LEU:HD12 | 1.82                     | 0.61              |
| 1:L:522:GLN:HG2  | 1:M:451:ILE:CG2  | 2.30                     | 0.61              |
| 1:M:506:ASN:O    | 1:M:518:PHE:HB2  | 2.00                     | 0.61              |
| 1:N:477:ARG:CG   | 1:N:477:ARG:HH11 | 2.14                     | 0.61              |
| 1:A:184:VAL:HG13 | 1:A:187:LEU:HD12 | 1.82                     | 0.61              |
| 1:A:604:ARG:NH2  | 1:A:626:LEU:O    | 2.34                     | 0.61              |
| 1:B:477:ARG:HH11 | 1:B:477:ARG:HG2  | 1.66                     | 0.61              |
| 1:C:477:ARG:HH11 | 1:C:477:ARG:HG2  | 1.66                     | 0.61              |
| 1:C:522:GLN:HG2  | 1:D:451:ILE:CG2  | 2.31                     | 0.61              |
| 1:E:184:VAL:HG13 | 1:E:187:LEU:HD12 | 1.82                     | 0.61              |
| 1:E:477:ARG:HH11 | 1:E:477:ARG:CG   | 2.14                     | 0.61              |
| 1:G:326:ILE:HD11 | 1:G:502:GLN:HE21 | 1.64                     | 0.61              |
| 1:G:539:GLY:HA2  | 1:G:577:LEU:O    | 2.00                     | 0.61              |
| 1:K:508:LEU:HD12 | 1:K:508:LEU:N    | 2.16                     | 0.61              |
| 1:K:522:GLN:HG2  | 1:L:451:ILE:CG2  | 2.30                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:481:GLY:O    | 1:M:505:SER:N    | 2.33                     | 0.61              |
| 1:L:609:PHE:CG   | 1:M:639:ILE:HD12 | 2.34                     | 0.61              |
| 1:N:452:VAL:O    | 1:N:481:GLY:HA3  | 2.01                     | 0.61              |
| 1:O:452:VAL:O    | 1:O:481:GLY:HA3  | 2.01                     | 0.61              |
| 1:B:244:VAL:HG22 | 1:B:295:VAL:HG22 | 1.81                     | 0.61              |
| 1:C:504:VAL:HG13 | 1:C:521:ARG:CD   | 2.31                     | 0.61              |
| 1:D:477:ARG:HG2  | 1:D:477:ARG:HH11 | 1.66                     | 0.61              |
| 1:D:522:GLN:HG2  | 1:E:451:ILE:CG2  | 2.30                     | 0.61              |
| 1:F:184:VAL:HG13 | 1:F:187:LEU:HD12 | 1.82                     | 0.61              |
| 1:F:508:LEU:HD12 | 1:F:508:LEU:N    | 2.16                     | 0.61              |
| 1:G:604:ARG:NH2  | 1:G:626:LEU:O    | 2.34                     | 0.61              |
| 1:I:184:VAL:HG13 | 1:I:187:LEU:HD12 | 1.82                     | 0.61              |
| 1:J:184:VAL:HG13 | 1:J:187:LEU:HD12 | 1.82                     | 0.61              |
| 1:J:452:VAL:O    | 1:J:481:GLY:HA3  | 2.01                     | 0.61              |
| 1:K:480:VAL:HA   | 1:K:505:SER:HB2  | 1.83                     | 0.61              |
| 1:M:244:VAL:HG22 | 1:M:295:VAL:HG22 | 1.81                     | 0.61              |
| 1:M:508:LEU:HD12 | 1:M:508:LEU:N    | 2.16                     | 0.61              |
| 1:M:604:ARG:NH2  | 1:M:626:LEU:O    | 2.34                     | 0.61              |
| 1:N:604:ARG:NH2  | 1:N:626:LEU:O    | 2.34                     | 0.61              |
| 1:O:458:VAL:HB   | 1:O:476:ASP:O    | 2.01                     | 0.61              |
| 1:O:604:ARG:NH2  | 1:O:626:LEU:O    | 2.34                     | 0.61              |
| 1:A:477:ARG:HH11 | 1:A:477:ARG:HG2  | 1.66                     | 0.60              |
| 1:D:458:VAL:HB   | 1:D:476:ASP:O    | 2.01                     | 0.60              |
| 1:F:477:ARG:HH11 | 1:F:477:ARG:CG   | 2.14                     | 0.60              |
| 1:F:506:ASN:O    | 1:F:518:PHE:HB2  | 2.01                     | 0.60              |
| 1:I:508:LEU:N    | 1:I:508:LEU:HD12 | 2.16                     | 0.60              |
| 1:J:508:LEU:N    | 1:J:508:LEU:HD12 | 2.16                     | 0.60              |
| 1:K:604:ARG:NH2  | 1:K:626:LEU:O    | 2.34                     | 0.60              |
| 1:M:226:LYS:HA   | 1:M:229:ILE:HD12 | 1.82                     | 0.60              |
| 1:M:459:ILE:HG23 | 1:M:474:THR:C    | 2.16                     | 0.60              |
| 1:M:477:ARG:HH11 | 1:M:477:ARG:CG   | 2.14                     | 0.60              |
| 1:N:539:GLY:HA2  | 1:N:577:LEU:O    | 2.00                     | 0.60              |
| 1:O:477:ARG:HH11 | 1:O:477:ARG:CG   | 2.14                     | 0.60              |
| 1:A:226:LYS:HA   | 1:A:229:ILE:HD12 | 1.82                     | 0.60              |
| 1:D:184:VAL:HG13 | 1:D:187:LEU:HD12 | 1.82                     | 0.60              |
| 1:D:452:VAL:O    | 1:D:481:GLY:HA3  | 2.01                     | 0.60              |
| 1:E:176:SER:OG   | 1:E:208:GLU:OE2  | 2.16                     | 0.60              |
| 1:G:260:LYS:O    | 1:G:263:SER:OG   | 2.17                     | 0.60              |
| 1:G:459:ILE:HG23 | 1:G:474:THR:C    | 2.16                     | 0.60              |
| 1:H:184:VAL:HG13 | 1:H:187:LEU:HD12 | 1.82                     | 0.60              |
| 1:H:480:VAL:HA   | 1:H:505:SER:HB2  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:506:ASN:O    | 1:I:518:PHE:HB2  | 2.00                     | 0.60              |
| 1:J:506:ASN:O    | 1:J:518:PHE:HB2  | 2.01                     | 0.60              |
| 1:L:480:VAL:HA   | 1:L:505:SER:HB2  | 1.83                     | 0.60              |
| 1:M:539:GLY:HA2  | 1:M:577:LEU:O    | 2.00                     | 0.60              |
| 1:N:459:ILE:HG23 | 1:N:474:THR:C    | 2.16                     | 0.60              |
| 1:N:480:VAL:HA   | 1:N:505:SER:HB2  | 1.83                     | 0.60              |
| 1:B:142:ILE:HD11 | 1:B:156:ILE:HD12 | 1.84                     | 0.60              |
| 1:C:184:VAL:HG13 | 1:C:187:LEU:HD12 | 1.82                     | 0.60              |
| 1:C:477:ARG:CG   | 1:C:477:ARG:HH11 | 2.14                     | 0.60              |
| 1:D:142:ILE:HD11 | 1:D:156:ILE:HD12 | 1.84                     | 0.60              |
| 1:D:508:LEU:N    | 1:D:508:LEU:HD12 | 2.16                     | 0.60              |
| 1:E:458:VAL:HB   | 1:E:476:ASP:O    | 2.01                     | 0.60              |
| 1:E:452:VAL:O    | 1:E:481:GLY:HA3  | 2.01                     | 0.60              |
| 1:F:438:PRO:HG3  | 1:F:482:ILE:CG2  | 2.32                     | 0.60              |
| 1:F:522:GLN:HG2  | 1:G:451:ILE:CG2  | 2.31                     | 0.60              |
| 1:G:184:VAL:HG13 | 1:G:187:LEU:HD12 | 1.82                     | 0.60              |
| 1:G:477:ARG:CG   | 1:G:477:ARG:HH11 | 2.14                     | 0.60              |
| 1:G:508:LEU:N    | 1:G:508:LEU:HD12 | 2.16                     | 0.60              |
| 1:N:458:VAL:HB   | 1:N:476:ASP:O    | 2.01                     | 0.60              |
| 1:N:508:LEU:N    | 1:N:508:LEU:HD12 | 2.16                     | 0.60              |
| 1:O:477:ARG:HG2  | 1:O:477:ARG:HH11 | 1.66                     | 0.60              |
| 1:O:504:VAL:HG13 | 1:O:521:ARG:CD   | 2.31                     | 0.60              |
| 1:O:480:VAL:HA   | 1:O:505:SER:HB2  | 1.83                     | 0.60              |
| 1:A:458:VAL:HB   | 1:A:476:ASP:O    | 2.01                     | 0.60              |
| 1:A:477:ARG:HH11 | 1:A:477:ARG:CG   | 2.14                     | 0.60              |
| 1:C:508:LEU:N    | 1:C:508:LEU:HD12 | 2.16                     | 0.60              |
| 1:D:477:ARG:CG   | 1:D:477:ARG:HH11 | 2.14                     | 0.60              |
| 1:F:226:LYS:HA   | 1:F:229:ILE:HD12 | 1.83                     | 0.60              |
| 1:F:504:VAL:HG13 | 1:F:521:ARG:CD   | 2.31                     | 0.60              |
| 1:H:459:ILE:HG23 | 1:H:474:THR:C    | 2.16                     | 0.60              |
| 1:I:522:GLN:HG2  | 1:J:451:ILE:CG2  | 2.31                     | 0.60              |
| 1:K:184:VAL:HG13 | 1:K:187:LEU:HD12 | 1.82                     | 0.60              |
| 1:A:142:ILE:HD11 | 1:A:156:ILE:HD12 | 1.84                     | 0.60              |
| 1:B:452:VAL:O    | 1:B:481:GLY:HA3  | 2.01                     | 0.60              |
| 1:E:477:ARG:HG2  | 1:E:477:ARG:HH11 | 1.66                     | 0.60              |
| 1:F:154:GLU:O    | 1:F:158:ARG:HB2  | 2.02                     | 0.60              |
| 1:I:260:LYS:O    | 1:I:263:SER:OG   | 2.17                     | 0.60              |
| 1:I:477:ARG:HG2  | 1:I:477:ARG:HH11 | 1.66                     | 0.60              |
| 1:I:438:PRO:HG3  | 1:I:482:ILE:CG2  | 2.32                     | 0.60              |
| 1:J:477:ARG:HH11 | 1:J:477:ARG:HG2  | 1.66                     | 0.60              |
| 1:L:166:GLU:HB2  | 1:L:222:ARG:HH21 | 1.67                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:604:ARG:NH2  | 1:L:626:LEU:O    | 2.34                     | 0.60              |
| 1:O:166:GLU:HB2  | 1:O:222:ARG:HH21 | 1.67                     | 0.60              |
| 1:O:257:GLU:HA   | 1:O:257:GLU:OE1  | 1.99                     | 0.60              |
| 1:B:504:VAL:HG13 | 1:B:521:ARG:CD   | 2.31                     | 0.60              |
| 1:E:154:GLU:O    | 1:E:158:ARG:HB2  | 2.02                     | 0.60              |
| 1:F:481:GLY:N    | 1:F:505:SER:OG   | 2.23                     | 0.60              |
| 1:G:154:GLU:O    | 1:G:158:ARG:HB2  | 2.02                     | 0.60              |
| 1:H:438:PRO:HG3  | 1:H:482:ILE:CG2  | 2.32                     | 0.60              |
| 1:L:184:VAL:HG13 | 1:L:187:LEU:HD12 | 1.82                     | 0.60              |
| 1:M:506:ASN:C    | 1:M:506:ASN:HD22 | 2.04                     | 0.60              |
| 1:N:226:LYS:HA   | 1:N:229:ILE:HD12 | 1.82                     | 0.60              |
| 1:N:504:VAL:HG13 | 1:N:521:ARG:CD   | 2.31                     | 0.60              |
| 1:B:184:VAL:HG13 | 1:B:187:LEU:HD12 | 1.82                     | 0.60              |
| 1:C:142:ILE:HD11 | 1:C:156:ILE:HD12 | 1.84                     | 0.60              |
| 1:H:260:LYS:O    | 1:H:263:SER:OG   | 2.17                     | 0.60              |
| 1:K:477:ARG:HH11 | 1:K:477:ARG:CG   | 2.14                     | 0.60              |
| 1:N:477:ARG:HG2  | 1:N:477:ARG:HH11 | 1.66                     | 0.60              |
| 1:N:506:ASN:C    | 1:N:506:ASN:HD22 | 2.04                     | 0.60              |
| 1:O:244:VAL:HG22 | 1:O:295:VAL:HG22 | 1.81                     | 0.60              |
| 1:C:154:GLU:O    | 1:C:158:ARG:HB2  | 2.02                     | 0.60              |
| 1:C:438:PRO:HG3  | 1:C:482:ILE:CG2  | 2.32                     | 0.60              |
| 1:E:142:ILE:HD11 | 1:E:156:ILE:HD12 | 1.84                     | 0.60              |
| 1:F:142:ILE:HD11 | 1:F:156:ILE:HD12 | 1.84                     | 0.60              |
| 1:G:226:LYS:HA   | 1:G:229:ILE:HD12 | 1.82                     | 0.60              |
| 1:H:154:GLU:O    | 1:H:158:ARG:HB2  | 2.02                     | 0.60              |
| 1:I:477:ARG:CG   | 1:I:477:ARG:HH11 | 2.14                     | 0.60              |
| 1:I:480:VAL:HA   | 1:I:505:SER:HB2  | 1.83                     | 0.60              |
| 1:J:260:LYS:O    | 1:J:263:SER:OG   | 2.17                     | 0.60              |
| 1:K:609:PHE:CG   | 1:L:639:ILE:HD12 | 2.34                     | 0.60              |
| 1:O:142:ILE:HD11 | 1:O:156:ILE:HD12 | 1.84                     | 0.60              |
| 1:A:452:VAL:O    | 1:A:481:GLY:HA3  | 2.01                     | 0.60              |
| 1:A:506:ASN:C    | 1:A:506:ASN:HD22 | 2.04                     | 0.60              |
| 1:B:508:LEU:N    | 1:B:508:LEU:HD12 | 2.16                     | 0.60              |
| 1:C:458:VAL:HB   | 1:C:476:ASP:O    | 2.01                     | 0.60              |
| 1:G:142:ILE:HD11 | 1:G:156:ILE:HD12 | 1.84                     | 0.60              |
| 1:H:508:LEU:HD12 | 1:H:508:LEU:N    | 2.16                     | 0.60              |
| 1:I:104:VAL:HG22 | 1:I:141:LEU:HD23 | 1.84                     | 0.60              |
| 1:M:458:VAL:HB   | 1:M:476:ASP:O    | 2.01                     | 0.60              |
| 1:M:609:PHE:CG   | 1:N:639:ILE:HD12 | 2.34                     | 0.60              |
| 1:O:508:LEU:N    | 1:O:508:LEU:HD12 | 2.16                     | 0.60              |
| 1:B:480:VAL:HA   | 1:B:505:SER:HB2  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:154:GLU:O    | 1:D:158:ARG:HB2  | 2.02                     | 0.60              |
| 1:D:438:PRO:HG3  | 1:D:482:ILE:CG2  | 2.32                     | 0.60              |
| 1:G:104:VAL:HG22 | 1:G:141:LEU:HD23 | 1.84                     | 0.60              |
| 1:I:121:GLN:O    | 1:I:125:ASN:N    | 2.33                     | 0.60              |
| 1:L:504:VAL:HG13 | 1:L:521:ARG:CD   | 2.31                     | 0.60              |
| 1:N:142:ILE:HD11 | 1:N:156:ILE:HD12 | 1.84                     | 0.60              |
| 1:O:459:ILE:HG23 | 1:O:474:THR:C    | 2.16                     | 0.60              |
| 1:B:166:GLU:HB2  | 1:B:222:ARG:HH21 | 1.67                     | 0.59              |
| 1:E:504:VAL:HG13 | 1:E:521:ARG:CD   | 2.31                     | 0.59              |
| 1:F:458:VAL:HB   | 1:F:476:ASP:O    | 2.01                     | 0.59              |
| 1:G:438:PRO:HG3  | 1:G:482:ILE:CG2  | 2.32                     | 0.59              |
| 1:H:477:ARG:HH11 | 1:H:477:ARG:HG2  | 1.66                     | 0.59              |
| 1:H:490:ILE:HG22 | 1:H:491:ASN:O    | 2.03                     | 0.59              |
| 1:G:609:PHE:CG   | 1:H:639:ILE:HD12 | 2.34                     | 0.59              |
| 1:I:166:GLU:HB2  | 1:I:222:ARG:HH21 | 1.67                     | 0.59              |
| 1:J:166:GLU:HB2  | 1:J:222:ARG:HH21 | 1.67                     | 0.59              |
| 1:K:506:ASN:C    | 1:K:506:ASN:HD22 | 2.04                     | 0.59              |
| 1:O:226:LYS:HA   | 1:O:229:ILE:HD12 | 1.82                     | 0.59              |
| 1:C:166:GLU:HB2  | 1:C:222:ARG:HH21 | 1.67                     | 0.59              |
| 1:E:438:PRO:HG3  | 1:E:482:ILE:CG2  | 2.32                     | 0.59              |
| 1:E:480:VAL:HA   | 1:E:505:SER:HB2  | 1.83                     | 0.59              |
| 1:J:480:VAL:HA   | 1:J:505:SER:HB2  | 1.83                     | 0.59              |
| 1:K:477:ARG:HG2  | 1:K:477:ARG:HH11 | 1.66                     | 0.59              |
| 1:L:490:ILE:HG22 | 1:L:491:ASN:O    | 2.02                     | 0.59              |
| 1:N:490:ILE:HG22 | 1:N:491:ASN:O    | 2.03                     | 0.59              |
| 1:A:490:ILE:HG22 | 1:A:491:ASN:O    | 2.03                     | 0.59              |
| 1:B:438:PRO:HG3  | 1:B:482:ILE:CG2  | 2.31                     | 0.59              |
| 1:C:480:VAL:HA   | 1:C:505:SER:HB2  | 1.83                     | 0.59              |
| 1:F:490:ILE:HG22 | 1:F:491:ASN:O    | 2.03                     | 0.59              |
| 1:I:154:GLU:O    | 1:I:158:ARG:HB2  | 2.02                     | 0.59              |
| 1:I:504:VAL:HG13 | 1:I:521:ARG:CD   | 2.31                     | 0.59              |
| 1:J:490:ILE:HG22 | 1:J:491:ASN:O    | 2.02                     | 0.59              |
| 1:K:260:LYS:O    | 1:K:263:SER:OG   | 2.17                     | 0.59              |
| 1:K:458:VAL:HB   | 1:K:476:ASP:O    | 2.01                     | 0.59              |
| 1:K:438:PRO:HG3  | 1:K:482:ILE:CG2  | 2.32                     | 0.59              |
| 1:M:458:VAL:CB   | 1:M:476:ASP:O    | 2.51                     | 0.59              |
| 1:M:452:VAL:O    | 1:M:481:GLY:HA3  | 2.01                     | 0.59              |
| 1:N:166:GLU:HB2  | 1:N:222:ARG:HH21 | 1.67                     | 0.59              |
| 1:N:438:PRO:HG3  | 1:N:482:ILE:CG2  | 2.32                     | 0.59              |
| 1:N:458:VAL:CB   | 1:N:476:ASP:O    | 2.51                     | 0.59              |
| 1:O:104:VAL:HG22 | 1:O:141:LEU:HD23 | 1.84                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:177:ALA:HB3  | 1:A:208:GLU:CG   | 2.33                     | 0.59              |
| 1:B:458:VAL:HB   | 1:B:476:ASP:O    | 2.01                     | 0.59              |
| 1:E:166:GLU:HB2  | 1:E:222:ARG:HH21 | 1.67                     | 0.59              |
| 1:F:166:GLU:HB2  | 1:F:222:ARG:HH21 | 1.67                     | 0.59              |
| 1:F:459:ILE:HG23 | 1:F:474:THR:C    | 2.16                     | 0.59              |
| 1:H:459:ILE:HD12 | 1:H:459:ILE:H    | 1.67                     | 0.59              |
| 1:J:104:VAL:HG22 | 1:J:141:LEU:HD23 | 1.84                     | 0.59              |
| 1:J:177:ALA:HB3  | 1:J:208:GLU:CG   | 2.33                     | 0.59              |
| 1:J:458:VAL:HB   | 1:J:476:ASP:O    | 2.01                     | 0.59              |
| 1:K:104:VAL:HG22 | 1:K:141:LEU:HD23 | 1.84                     | 0.59              |
| 1:L:438:PRO:HG3  | 1:L:482:ILE:CG2  | 2.32                     | 0.59              |
| 1:O:177:ALA:HB3  | 1:O:208:GLU:CG   | 2.33                     | 0.59              |
| 1:O:458:VAL:CB   | 1:O:476:ASP:O    | 2.51                     | 0.59              |
| 1:A:104:VAL:HG22 | 1:A:141:LEU:HD23 | 1.84                     | 0.59              |
| 1:B:154:GLU:O    | 1:B:158:ARG:HB2  | 2.02                     | 0.59              |
| 1:B:458:VAL:CB   | 1:B:476:ASP:O    | 2.51                     | 0.59              |
| 1:F:477:ARG:HG2  | 1:F:477:ARG:HH11 | 1.66                     | 0.59              |
| 1:G:166:GLU:HB2  | 1:G:222:ARG:HH21 | 1.67                     | 0.59              |
| 1:G:458:VAL:HB   | 1:G:476:ASP:O    | 2.01                     | 0.59              |
| 1:H:104:VAL:HG22 | 1:H:141:LEU:HD23 | 1.84                     | 0.59              |
| 1:K:177:ALA:HB3  | 1:K:208:GLU:CG   | 2.33                     | 0.59              |
| 1:L:260:LYS:O    | 1:L:263:SER:OG   | 2.17                     | 0.59              |
| 1:L:458:VAL:CB   | 1:L:476:ASP:O    | 2.51                     | 0.59              |
| 1:L:458:VAL:HB   | 1:L:476:ASP:O    | 2.01                     | 0.59              |
| 1:M:166:GLU:HB2  | 1:M:222:ARG:HH21 | 1.67                     | 0.59              |
| 1:M:177:ALA:HB3  | 1:M:208:GLU:CG   | 2.33                     | 0.59              |
| 1:A:458:VAL:CB   | 1:A:476:ASP:O    | 2.51                     | 0.59              |
| 1:B:104:VAL:HG22 | 1:B:141:LEU:HD23 | 1.84                     | 0.59              |
| 1:B:490:ILE:HG22 | 1:B:491:ASN:O    | 2.02                     | 0.59              |
| 1:C:104:VAL:HG22 | 1:C:141:LEU:HD23 | 1.84                     | 0.59              |
| 1:C:490:ILE:HG22 | 1:C:491:ASN:O    | 2.03                     | 0.59              |
| 1:H:166:GLU:HB2  | 1:H:222:ARG:HH21 | 1.67                     | 0.59              |
| 1:I:177:ALA:HB3  | 1:I:208:GLU:CG   | 2.33                     | 0.59              |
| 1:I:458:VAL:HB   | 1:I:476:ASP:O    | 2.01                     | 0.59              |
| 1:J:459:ILE:HD12 | 1:J:459:ILE:H    | 1.67                     | 0.59              |
| 1:K:458:VAL:CB   | 1:K:476:ASP:O    | 2.51                     | 0.59              |
| 1:K:504:VAL:HG13 | 1:K:521:ARG:CD   | 2.31                     | 0.59              |
| 1:K:609:PHE:CD2  | 1:L:639:ILE:CD1  | 2.75                     | 0.59              |
| 1:M:142:ILE:HD11 | 1:M:156:ILE:HD12 | 1.84                     | 0.59              |
| 1:M:477:ARG:HG2  | 1:M:477:ARG:HH11 | 1.66                     | 0.59              |
| 1:A:438:PRO:HG3  | 1:A:482:ILE:CG2  | 2.32                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:506:ASN:HD22 | 1:B:506:ASN:C    | 2.04                     | 0.59              |
| 1:E:459:ILE:HD12 | 1:E:459:ILE:H    | 1.67                     | 0.59              |
| 1:F:224:ARG:O    | 1:F:227:ARG:HB2  | 2.03                     | 0.59              |
| 1:F:459:ILE:HD12 | 1:F:459:ILE:H    | 1.68                     | 0.59              |
| 1:G:458:VAL:CB   | 1:G:476:ASP:O    | 2.51                     | 0.59              |
| 1:G:480:VAL:HA   | 1:G:505:SER:HB2  | 1.83                     | 0.59              |
| 1:H:121:GLN:O    | 1:H:125:ASN:N    | 2.33                     | 0.59              |
| 1:H:142:ILE:HD11 | 1:H:156:ILE:HD12 | 1.84                     | 0.59              |
| 1:H:458:VAL:CB   | 1:H:476:ASP:O    | 2.51                     | 0.59              |
| 1:I:458:VAL:CB   | 1:I:476:ASP:O    | 2.51                     | 0.59              |
| 1:H:609:PHE:CG   | 1:I:639:ILE:HD12 | 2.34                     | 0.59              |
| 1:K:118:LEU:O    | 1:K:121:GLN:HB3  | 2.03                     | 0.59              |
| 1:M:260:LYS:O    | 1:M:263:SER:OG   | 2.17                     | 0.59              |
| 1:N:104:VAL:HG22 | 1:N:141:LEU:HD23 | 1.84                     | 0.59              |
| 1:O:154:GLU:O    | 1:O:158:ARG:HB2  | 2.02                     | 0.59              |
| 1:B:177:ALA:HB3  | 1:B:208:GLU:CG   | 2.33                     | 0.59              |
| 1:C:459:ILE:HD12 | 1:C:459:ILE:H    | 1.68                     | 0.59              |
| 1:C:506:ASN:HD22 | 1:C:507:VAL:H    | 1.50                     | 0.59              |
| 1:D:166:GLU:HB2  | 1:D:222:ARG:HH21 | 1.67                     | 0.59              |
| 1:D:458:VAL:CB   | 1:D:476:ASP:O    | 2.51                     | 0.59              |
| 1:D:490:ILE:HG22 | 1:D:491:ASN:O    | 2.03                     | 0.59              |
| 1:F:118:LEU:O    | 1:F:121:GLN:HB3  | 2.03                     | 0.59              |
| 1:F:176:SER:OG   | 1:F:208:GLU:OE2  | 2.16                     | 0.59              |
| 1:F:480:VAL:HA   | 1:F:505:SER:HB2  | 1.83                     | 0.59              |
| 1:J:154:GLU:O    | 1:J:158:ARG:HB2  | 2.02                     | 0.59              |
| 1:J:458:VAL:CB   | 1:J:476:ASP:O    | 2.51                     | 0.59              |
| 1:K:166:GLU:HB2  | 1:K:222:ARG:HH21 | 1.67                     | 0.59              |
| 1:N:177:ALA:HB3  | 1:N:208:GLU:CG   | 2.33                     | 0.59              |
| 1:C:458:VAL:CB   | 1:C:476:ASP:O    | 2.51                     | 0.59              |
| 1:E:118:LEU:O    | 1:E:121:GLN:HB3  | 2.03                     | 0.59              |
| 1:E:104:VAL:HG22 | 1:E:141:LEU:HD23 | 1.84                     | 0.59              |
| 1:E:224:ARG:O    | 1:E:227:ARG:HB2  | 2.03                     | 0.59              |
| 1:E:458:VAL:CB   | 1:E:476:ASP:O    | 2.51                     | 0.59              |
| 1:F:458:VAL:CB   | 1:F:476:ASP:O    | 2.51                     | 0.59              |
| 1:H:444:ASP:OD1  | 1:H:445:ASN:N    | 2.36                     | 0.59              |
| 1:H:504:VAL:HG13 | 1:H:521:ARG:CD   | 2.31                     | 0.59              |
| 1:J:118:LEU:O    | 1:J:121:GLN:HB3  | 2.03                     | 0.59              |
| 1:J:438:PRO:HG3  | 1:J:482:ILE:CG2  | 2.32                     | 0.59              |
| 1:L:118:LEU:O    | 1:L:121:GLN:HB3  | 2.03                     | 0.59              |
| 1:M:480:VAL:HA   | 1:M:505:SER:HB2  | 1.83                     | 0.59              |
| 1:N:154:GLU:O    | 1:N:158:ARG:HB2  | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:438:PRO:HG3  | 1:O:482:ILE:CG2  | 2.32                     | 0.59              |
| 1:O:506:ASN:C    | 1:O:506:ASN:HD22 | 2.04                     | 0.59              |
| 1:A:166:GLU:HB2  | 1:A:222:ARG:HH21 | 1.67                     | 0.59              |
| 1:A:504:VAL:HG13 | 1:A:521:ARG:CD   | 2.31                     | 0.59              |
| 1:E:508:LEU:HD12 | 1:E:508:LEU:N    | 2.16                     | 0.59              |
| 1:F:104:VAL:HG22 | 1:F:141:LEU:HD23 | 1.84                     | 0.59              |
| 1:G:118:LEU:O    | 1:G:121:GLN:HB3  | 2.03                     | 0.59              |
| 1:G:444:ASP:OD1  | 1:G:445:ASN:N    | 2.36                     | 0.59              |
| 1:H:177:ALA:HB3  | 1:H:208:GLU:CG   | 2.33                     | 0.59              |
| 1:H:458:VAL:HB   | 1:H:476:ASP:O    | 2.01                     | 0.59              |
| 1:I:142:ILE:HD11 | 1:I:156:ILE:HD12 | 1.84                     | 0.59              |
| 1:I:444:ASP:OD1  | 1:I:445:ASN:N    | 2.36                     | 0.59              |
| 1:J:142:ILE:HD11 | 1:J:156:ILE:HD12 | 1.84                     | 0.59              |
| 1:J:444:ASP:OD1  | 1:J:445:ASN:N    | 2.36                     | 0.59              |
| 1:J:506:ASN:HD22 | 1:J:506:ASN:C    | 2.04                     | 0.59              |
| 1:K:154:GLU:O    | 1:K:158:ARG:HB2  | 2.02                     | 0.59              |
| 1:L:177:ALA:HB3  | 1:L:208:GLU:CG   | 2.33                     | 0.59              |
| 1:L:506:ASN:C    | 1:L:506:ASN:HD22 | 2.04                     | 0.59              |
| 1:M:154:GLU:O    | 1:M:158:ARG:HB2  | 2.02                     | 0.59              |
| 1:D:104:VAL:HG22 | 1:D:141:LEU:HD23 | 1.83                     | 0.58              |
| 1:G:459:ILE:H    | 1:G:459:ILE:HD12 | 1.68                     | 0.58              |
| 1:L:154:GLU:O    | 1:L:158:ARG:HB2  | 2.02                     | 0.58              |
| 1:N:459:ILE:H    | 1:N:459:ILE:HD12 | 1.67                     | 0.58              |
| 1:A:154:GLU:O    | 1:A:158:ARG:HB2  | 2.02                     | 0.58              |
| 1:C:444:ASP:OD1  | 1:C:445:ASN:N    | 2.36                     | 0.58              |
| 1:D:444:ASP:OD1  | 1:D:445:ASN:N    | 2.36                     | 0.58              |
| 1:F:177:ALA:HB3  | 1:F:208:GLU:CG   | 2.33                     | 0.58              |
| 1:F:444:ASP:OD1  | 1:F:445:ASN:N    | 2.36                     | 0.58              |
| 1:F:506:ASN:HD22 | 1:F:507:VAL:H    | 1.50                     | 0.58              |
| 1:G:177:ALA:HB3  | 1:G:208:GLU:CG   | 2.33                     | 0.58              |
| 1:J:504:VAL:HG13 | 1:J:521:ARG:CD   | 2.31                     | 0.58              |
| 1:K:142:ILE:HD11 | 1:K:156:ILE:HD12 | 1.84                     | 0.58              |
| 1:L:142:ILE:HD11 | 1:L:156:ILE:HD12 | 1.84                     | 0.58              |
| 1:N:206:ALA:HA   | 1:N:212:SER:O    | 2.04                     | 0.58              |
| 1:A:480:VAL:HA   | 1:A:505:SER:HB2  | 1.83                     | 0.58              |
| 1:D:118:LEU:O    | 1:D:121:GLN:HB3  | 2.03                     | 0.58              |
| 1:E:444:ASP:OD1  | 1:E:445:ASN:N    | 2.36                     | 0.58              |
| 1:E:490:ILE:HG22 | 1:E:491:ASN:O    | 2.02                     | 0.58              |
| 1:G:206:ALA:HA   | 1:G:212:SER:O    | 2.04                     | 0.58              |
| 1:G:504:VAL:HG13 | 1:G:521:ARG:CD   | 2.31                     | 0.58              |
| 1:J:224:ARG:O    | 1:J:227:ARG:HB2  | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:444:ASP:OD1  | 1:K:445:ASN:N    | 2.36                     | 0.58              |
| 1:M:104:VAL:HG22 | 1:M:141:LEU:HD23 | 1.84                     | 0.58              |
| 1:N:164:ASP:O    | 1:N:219:PRO:HD2  | 2.04                     | 0.58              |
| 1:A:206:ALA:HA   | 1:A:212:SER:O    | 2.04                     | 0.58              |
| 1:D:506:ASN:HD22 | 1:D:506:ASN:C    | 2.04                     | 0.58              |
| 1:E:164:ASP:O    | 1:E:219:PRO:HD2  | 2.04                     | 0.58              |
| 1:G:224:ARG:O    | 1:G:227:ARG:HB2  | 2.03                     | 0.58              |
| 1:G:477:ARG:HH11 | 1:G:477:ARG:HG2  | 1.66                     | 0.58              |
| 1:I:224:ARG:O    | 1:I:227:ARG:HB2  | 2.03                     | 0.58              |
| 1:I:490:ILE:HG22 | 1:I:491:ASN:O    | 2.02                     | 0.58              |
| 1:K:490:ILE:HG22 | 1:K:491:ASN:O    | 2.03                     | 0.58              |
| 1:L:104:VAL:HG22 | 1:L:141:LEU:HD23 | 1.84                     | 0.58              |
| 1:M:118:LEU:O    | 1:M:121:GLN:HB3  | 2.03                     | 0.58              |
| 1:M:504:VAL:HG13 | 1:M:521:ARG:CD   | 2.31                     | 0.58              |
| 1:N:260:LYS:O    | 1:N:263:SER:OG   | 2.17                     | 0.58              |
| 1:A:118:LEU:O    | 1:A:121:GLN:HB3  | 2.03                     | 0.58              |
| 1:B:206:ALA:HA   | 1:B:212:SER:O    | 2.04                     | 0.58              |
| 1:C:177:ALA:HB3  | 1:C:208:GLU:CG   | 2.33                     | 0.58              |
| 1:D:206:ALA:HA   | 1:D:212:SER:O    | 2.03                     | 0.58              |
| 1:E:107:VAL:HG22 | 1:E:160:ASP:HB2  | 1.86                     | 0.58              |
| 1:G:490:ILE:HG22 | 1:G:491:ASN:O    | 2.03                     | 0.58              |
| 1:H:206:ALA:HA   | 1:H:212:SER:O    | 2.04                     | 0.58              |
| 1:H:224:ARG:O    | 1:H:227:ARG:HB2  | 2.03                     | 0.58              |
| 1:L:477:ARG:HG2  | 1:L:477:ARG:HH11 | 1.66                     | 0.58              |
| 1:N:224:ARG:O    | 1:N:227:ARG:HB2  | 2.03                     | 0.58              |
| 1:O:224:ARG:O    | 1:O:227:ARG:HB2  | 2.03                     | 0.58              |
| 1:B:444:ASP:OD1  | 1:B:445:ASN:N    | 2.36                     | 0.58              |
| 1:D:164:ASP:O    | 1:D:219:PRO:HD2  | 2.04                     | 0.58              |
| 1:F:164:ASP:O    | 1:F:219:PRO:HD2  | 2.04                     | 0.58              |
| 1:F:206:ALA:HA   | 1:F:212:SER:O    | 2.03                     | 0.58              |
| 1:H:118:LEU:O    | 1:H:121:GLN:HB3  | 2.03                     | 0.58              |
| 1:H:506:ASN:C    | 1:H:506:ASN:HD22 | 2.04                     | 0.58              |
| 1:I:118:LEU:O    | 1:I:121:GLN:HB3  | 2.03                     | 0.58              |
| 1:I:506:ASN:C    | 1:I:506:ASN:HD22 | 2.04                     | 0.58              |
| 1:J:107:VAL:HG22 | 1:J:160:ASP:HB2  | 1.86                     | 0.58              |
| 1:L:107:VAL:HG22 | 1:L:160:ASP:HB2  | 1.86                     | 0.58              |
| 1:L:444:ASP:OD1  | 1:L:445:ASN:N    | 2.36                     | 0.58              |
| 1:M:164:ASP:O    | 1:M:219:PRO:HD2  | 2.04                     | 0.58              |
| 1:A:459:ILE:HG23 | 1:A:474:THR:C    | 2.16                     | 0.58              |
| 1:C:132:VAL:HG12 | 1:C:134:TYR:CE1  | 2.39                     | 0.58              |
| 1:C:256:VAL:O    | 1:C:260:LYS:HG2  | 2.04                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:459:ILE:HD12 | 1:D:459:ILE:H    | 1.67                     | 0.58              |
| 1:E:177:ALA:HB3  | 1:E:208:GLU:CG   | 2.33                     | 0.58              |
| 1:E:481:GLY:N    | 1:E:505:SER:OG   | 2.23                     | 0.58              |
| 1:G:121:GLN:O    | 1:G:125:ASN:N    | 2.33                     | 0.58              |
| 1:G:107:VAL:HG22 | 1:G:160:ASP:HB2  | 1.86                     | 0.58              |
| 1:M:107:VAL:HG22 | 1:M:160:ASP:HB2  | 1.86                     | 0.58              |
| 1:M:224:ARG:O    | 1:M:227:ARG:HB2  | 2.03                     | 0.58              |
| 1:M:438:PRO:HG3  | 1:M:482:ILE:CG2  | 2.32                     | 0.58              |
| 1:M:444:ASP:OD1  | 1:M:445:ASN:N    | 2.36                     | 0.58              |
| 1:M:459:ILE:H    | 1:M:459:ILE:HD12 | 1.68                     | 0.58              |
| 1:M:490:ILE:HG22 | 1:M:491:ASN:O    | 2.03                     | 0.58              |
| 1:N:444:ASP:OD1  | 1:N:445:ASN:N    | 2.36                     | 0.58              |
| 1:O:105:VAL:HG11 | 1:O:157:ARG:HE   | 1.69                     | 0.58              |
| 1:O:164:ASP:O    | 1:O:219:PRO:HD2  | 2.04                     | 0.58              |
| 1:O:490:ILE:HG22 | 1:O:491:ASN:O    | 2.02                     | 0.58              |
| 1:B:118:LEU:O    | 1:B:121:GLN:HB3  | 2.03                     | 0.58              |
| 1:D:132:VAL:HG12 | 1:D:134:TYR:CE1  | 2.39                     | 0.58              |
| 1:D:256:VAL:O    | 1:D:260:LYS:HG2  | 2.04                     | 0.58              |
| 1:E:256:VAL:O    | 1:E:260:LYS:HG2  | 2.04                     | 0.58              |
| 1:F:107:VAL:HG22 | 1:F:160:ASP:HB2  | 1.86                     | 0.58              |
| 1:G:164:ASP:O    | 1:G:219:PRO:HD2  | 2.04                     | 0.58              |
| 1:H:256:VAL:O    | 1:H:260:LYS:HG2  | 2.04                     | 0.58              |
| 1:K:206:ALA:HA   | 1:K:212:SER:O    | 2.04                     | 0.58              |
| 1:A:224:ARG:O    | 1:A:227:ARG:HB2  | 2.03                     | 0.58              |
| 1:A:459:ILE:HD12 | 1:A:459:ILE:H    | 1.67                     | 0.58              |
| 1:D:107:VAL:HG22 | 1:D:160:ASP:HB2  | 1.86                     | 0.58              |
| 1:D:224:ARG:O    | 1:D:227:ARG:HB2  | 2.03                     | 0.58              |
| 1:D:504:VAL:HG13 | 1:D:521:ARG:CD   | 2.31                     | 0.58              |
| 1:H:107:VAL:HG22 | 1:H:160:ASP:HB2  | 1.86                     | 0.58              |
| 1:I:132:VAL:HG12 | 1:I:134:TYR:CE1  | 2.39                     | 0.58              |
| 1:I:107:VAL:HG22 | 1:I:160:ASP:HB2  | 1.86                     | 0.58              |
| 1:K:107:VAL:HG22 | 1:K:160:ASP:HB2  | 1.86                     | 0.58              |
| 1:K:224:ARG:O    | 1:K:227:ARG:HB2  | 2.03                     | 0.58              |
| 1:L:164:ASP:O    | 1:L:219:PRO:HD2  | 2.04                     | 0.58              |
| 1:M:105:VAL:HG11 | 1:M:157:ARG:HE   | 1.69                     | 0.58              |
| 1:O:118:LEU:O    | 1:O:121:GLN:HB3  | 2.03                     | 0.58              |
| 1:O:132:VAL:HG12 | 1:O:134:TYR:CE1  | 2.39                     | 0.58              |
| 1:A:181:VAL:O    | 1:A:185:GLU:HG3  | 2.04                     | 0.58              |
| 1:A:444:ASP:OD1  | 1:A:445:ASN:N    | 2.36                     | 0.58              |
| 1:B:105:VAL:HG11 | 1:B:157:ARG:HE   | 1.69                     | 0.58              |
| 1:B:224:ARG:O    | 1:B:227:ARG:HB2  | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:256:VAL:O    | 1:B:260:LYS:HG2  | 2.04                     | 0.58              |
| 1:C:224:ARG:O    | 1:C:227:ARG:HB2  | 2.03                     | 0.58              |
| 1:C:459:ILE:HG23 | 1:C:474:THR:C    | 2.16                     | 0.58              |
| 1:D:459:ILE:HG23 | 1:D:474:THR:C    | 2.16                     | 0.58              |
| 1:H:164:ASP:O    | 1:H:219:PRO:HD2  | 2.04                     | 0.58              |
| 1:I:459:ILE:HD12 | 1:I:459:ILE:H    | 1.67                     | 0.58              |
| 1:L:459:ILE:HD12 | 1:L:459:ILE:H    | 1.67                     | 0.58              |
| 1:M:206:ALA:HA   | 1:M:212:SER:O    | 2.04                     | 0.58              |
| 1:O:444:ASP:OD1  | 1:O:445:ASN:N    | 2.36                     | 0.58              |
| 1:O:459:ILE:H    | 1:O:459:ILE:HD12 | 1.67                     | 0.58              |
| 1:A:107:VAL:HG22 | 1:A:160:ASP:HB2  | 1.86                     | 0.57              |
| 1:B:107:VAL:HG22 | 1:B:160:ASP:HB2  | 1.86                     | 0.57              |
| 1:B:459:ILE:HD12 | 1:B:459:ILE:H    | 1.67                     | 0.57              |
| 1:C:107:VAL:HG22 | 1:C:160:ASP:HB2  | 1.86                     | 0.57              |
| 1:C:164:ASP:O    | 1:C:219:PRO:HD2  | 2.04                     | 0.57              |
| 1:D:177:ALA:HB3  | 1:D:208:GLU:CG   | 2.33                     | 0.57              |
| 1:D:480:VAL:HA   | 1:D:505:SER:HB2  | 1.83                     | 0.57              |
| 1:F:506:ASN:HD22 | 1:F:506:ASN:C    | 2.04                     | 0.57              |
| 1:I:206:ALA:HA   | 1:I:212:SER:O    | 2.04                     | 0.57              |
| 1:I:256:VAL:O    | 1:I:260:LYS:HG2  | 2.04                     | 0.57              |
| 1:L:224:ARG:O    | 1:L:227:ARG:HB2  | 2.03                     | 0.57              |
| 1:O:181:VAL:O    | 1:O:185:GLU:HG3  | 2.04                     | 0.57              |
| 1:A:256:VAL:O    | 1:A:260:LYS:HG2  | 2.04                     | 0.57              |
| 1:B:132:VAL:HG12 | 1:B:134:TYR:CE1  | 2.39                     | 0.57              |
| 1:B:181:VAL:O    | 1:B:185:GLU:HG3  | 2.04                     | 0.57              |
| 1:B:459:ILE:HG23 | 1:B:474:THR:C    | 2.16                     | 0.57              |
| 1:C:118:LEU:O    | 1:C:121:GLN:HB3  | 2.03                     | 0.57              |
| 1:K:132:VAL:HG12 | 1:K:134:TYR:CE1  | 2.39                     | 0.57              |
| 1:L:132:VAL:HG12 | 1:L:134:TYR:CE1  | 2.39                     | 0.57              |
| 1:L:256:VAL:O    | 1:L:260:LYS:HG2  | 2.04                     | 0.57              |
| 1:N:107:VAL:HG22 | 1:N:160:ASP:HB2  | 1.86                     | 0.57              |
| 1:C:105:VAL:HG11 | 1:C:157:ARG:HE   | 1.69                     | 0.57              |
| 1:E:105:VAL:HG11 | 1:E:157:ARG:HE   | 1.69                     | 0.57              |
| 1:E:459:ILE:HG23 | 1:E:474:THR:C    | 2.16                     | 0.57              |
| 1:F:256:VAL:O    | 1:F:260:LYS:HG2  | 2.04                     | 0.57              |
| 1:H:507:VAL:CA   | 1:H:518:PHE:HB3  | 2.35                     | 0.57              |
| 1:I:164:ASP:O    | 1:I:219:PRO:HD2  | 2.04                     | 0.57              |
| 1:K:256:VAL:O    | 1:K:260:LYS:HG2  | 2.04                     | 0.57              |
| 1:L:506:ASN:HD22 | 1:L:507:VAL:H    | 1.51                     | 0.57              |
| 1:N:181:VAL:O    | 1:N:185:GLU:HG3  | 2.04                     | 0.57              |
| 1:O:107:VAL:HG22 | 1:O:160:ASP:HB2  | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:260:LYS:O    | 1:O:263:SER:OG   | 2.17                     | 0.57              |
| 1:A:164:ASP:O    | 1:A:219:PRO:HD2  | 2.04                     | 0.57              |
| 1:E:206:ALA:HA   | 1:E:212:SER:O    | 2.04                     | 0.57              |
| 1:E:507:VAL:CA   | 1:E:518:PHE:HB3  | 2.35                     | 0.57              |
| 1:I:181:VAL:O    | 1:I:185:GLU:HG3  | 2.04                     | 0.57              |
| 1:J:164:ASP:O    | 1:J:219:PRO:HD2  | 2.04                     | 0.57              |
| 1:M:256:VAL:O    | 1:M:260:LYS:HG2  | 2.04                     | 0.57              |
| 1:N:118:LEU:O    | 1:N:121:GLN:HB3  | 2.03                     | 0.57              |
| 1:N:132:VAL:HG12 | 1:N:134:TYR:CE1  | 2.39                     | 0.57              |
| 1:N:256:VAL:O    | 1:N:260:LYS:HG2  | 2.04                     | 0.57              |
| 1:O:256:VAL:O    | 1:O:260:LYS:HG2  | 2.04                     | 0.57              |
| 1:A:105:VAL:HG11 | 1:A:157:ARG:HE   | 1.69                     | 0.57              |
| 1:A:132:VAL:HG12 | 1:A:134:TYR:CE1  | 2.39                     | 0.57              |
| 1:B:112:VAL:HG21 | 1:B:140:ILE:HD11 | 1.87                     | 0.57              |
| 1:C:206:ALA:HA   | 1:C:212:SER:O    | 2.03                     | 0.57              |
| 1:G:181:VAL:O    | 1:G:185:GLU:HG3  | 2.04                     | 0.57              |
| 1:H:181:VAL:O    | 1:H:185:GLU:HG3  | 2.04                     | 0.57              |
| 1:J:105:VAL:HG11 | 1:J:157:ARG:HE   | 1.69                     | 0.57              |
| 1:K:164:ASP:O    | 1:K:219:PRO:HD2  | 2.04                     | 0.57              |
| 1:K:459:ILE:HD12 | 1:K:459:ILE:H    | 1.68                     | 0.57              |
| 1:L:206:ALA:HA   | 1:L:212:SER:O    | 2.04                     | 0.57              |
| 1:C:112:VAL:HG21 | 1:C:140:ILE:HD11 | 1.87                     | 0.57              |
| 1:F:181:VAL:O    | 1:F:185:GLU:HG3  | 2.04                     | 0.57              |
| 1:G:132:VAL:HG12 | 1:G:134:TYR:CE1  | 2.39                     | 0.57              |
| 1:J:181:VAL:O    | 1:J:185:GLU:HG3  | 2.04                     | 0.57              |
| 1:K:181:VAL:O    | 1:K:185:GLU:HG3  | 2.04                     | 0.57              |
| 1:A:112:VAL:HG21 | 1:A:140:ILE:HD11 | 1.87                     | 0.57              |
| 1:D:112:VAL:HG21 | 1:D:140:ILE:HD11 | 1.87                     | 0.57              |
| 1:F:132:VAL:HG12 | 1:F:134:TYR:CE1  | 2.39                     | 0.57              |
| 1:G:105:VAL:HG11 | 1:G:157:ARG:HE   | 1.69                     | 0.57              |
| 1:H:132:VAL:HG12 | 1:H:134:TYR:CE1  | 2.39                     | 0.57              |
| 1:J:206:ALA:HA   | 1:J:212:SER:O    | 2.04                     | 0.57              |
| 1:J:256:VAL:O    | 1:J:260:LYS:HG2  | 2.04                     | 0.57              |
| 1:L:105:VAL:HG11 | 1:L:157:ARG:HE   | 1.69                     | 0.57              |
| 1:O:206:ALA:HA   | 1:O:212:SER:O    | 2.04                     | 0.57              |
| 1:D:507:VAL:CA   | 1:D:518:PHE:HB3  | 2.35                     | 0.57              |
| 1:E:181:VAL:O    | 1:E:185:GLU:HG3  | 2.04                     | 0.57              |
| 1:E:259:LEU:HD11 | 1:E:310:ILE:HG13 | 1.87                     | 0.57              |
| 1:G:256:VAL:O    | 1:G:260:LYS:HG2  | 2.04                     | 0.57              |
| 1:H:259:LEU:HD11 | 1:H:310:ILE:HG13 | 1.86                     | 0.57              |
| 1:J:132:VAL:HG12 | 1:J:134:TYR:CE1  | 2.39                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:105:VAL:HG11 | 1:K:157:ARG:HE   | 1.69                     | 0.57              |
| 1:M:181:VAL:O    | 1:M:185:GLU:HG3  | 2.04                     | 0.57              |
| 1:N:105:VAL:HG11 | 1:N:157:ARG:HE   | 1.69                     | 0.57              |
| 1:O:112:VAL:HG21 | 1:O:140:ILE:HD11 | 1.87                     | 0.57              |
| 1:C:456:VAL:CG2  | 1:C:457:PRO:CD   | 2.83                     | 0.57              |
| 1:G:259:LEU:HD11 | 1:G:310:ILE:HG13 | 1.87                     | 0.57              |
| 1:G:507:VAL:CA   | 1:G:518:PHE:HB3  | 2.35                     | 0.57              |
| 1:I:506:ASN:HD22 | 1:I:507:VAL:H    | 1.50                     | 0.57              |
| 1:L:181:VAL:O    | 1:L:185:GLU:HG3  | 2.04                     | 0.57              |
| 1:M:112:VAL:HG21 | 1:M:140:ILE:HD11 | 1.87                     | 0.57              |
| 1:N:112:VAL:HG21 | 1:N:140:ILE:HD11 | 1.87                     | 0.57              |
| 1:B:164:ASP:O    | 1:B:219:PRO:HD2  | 2.04                     | 0.57              |
| 1:C:181:VAL:O    | 1:C:185:GLU:HG3  | 2.04                     | 0.57              |
| 1:D:105:VAL:HG11 | 1:D:157:ARG:HE   | 1.69                     | 0.57              |
| 1:G:506:ASN:C    | 1:G:506:ASN:HD22 | 2.04                     | 0.57              |
| 1:H:105:VAL:HG11 | 1:H:157:ARG:HE   | 1.69                     | 0.57              |
| 1:I:172:LEU:HG   | 1:I:212:SER:HA   | 1.87                     | 0.57              |
| 1:J:172:LEU:HG   | 1:J:212:SER:HA   | 1.87                     | 0.57              |
| 1:K:507:VAL:CA   | 1:K:518:PHE:HB3  | 2.35                     | 0.57              |
| 1:L:112:VAL:HG21 | 1:L:140:ILE:HD11 | 1.87                     | 0.57              |
| 1:A:121:GLN:O    | 1:A:125:ASN:N    | 2.33                     | 0.56              |
| 1:B:507:VAL:CA   | 1:B:518:PHE:HB3  | 2.35                     | 0.56              |
| 1:D:259:LEU:HD11 | 1:D:310:ILE:HG13 | 1.87                     | 0.56              |
| 1:D:456:VAL:CG2  | 1:D:457:PRO:CD   | 2.83                     | 0.56              |
| 1:E:112:VAL:HG21 | 1:E:140:ILE:HD11 | 1.87                     | 0.56              |
| 1:E:132:VAL:HG12 | 1:E:134:TYR:CE1  | 2.39                     | 0.56              |
| 1:F:259:LEU:HD11 | 1:F:310:ILE:HG13 | 1.87                     | 0.56              |
| 1:G:456:VAL:CG2  | 1:G:457:PRO:CD   | 2.83                     | 0.56              |
| 1:I:259:LEU:HD11 | 1:I:310:ILE:HG13 | 1.87                     | 0.56              |
| 1:J:180:MET:HE2  | 1:J:213:ILE:HD11 | 1.85                     | 0.56              |
| 1:K:172:LEU:HG   | 1:K:212:SER:HA   | 1.87                     | 0.56              |
| 1:L:172:LEU:HG   | 1:L:212:SER:HA   | 1.87                     | 0.56              |
| 1:M:121:GLN:O    | 1:M:125:ASN:N    | 2.33                     | 0.56              |
| 1:D:506:ASN:HD22 | 1:D:507:VAL:H    | 1.51                     | 0.56              |
| 1:F:121:GLN:O    | 1:F:125:ASN:N    | 2.33                     | 0.56              |
| 1:O:456:VAL:CG2  | 1:O:457:PRO:CD   | 2.83                     | 0.56              |
| 1:B:121:GLN:O    | 1:B:125:ASN:N    | 2.33                     | 0.56              |
| 1:C:506:ASN:C    | 1:C:506:ASN:HD22 | 2.04                     | 0.56              |
| 1:E:506:ASN:C    | 1:E:506:ASN:HD22 | 2.04                     | 0.56              |
| 1:F:456:VAL:CG2  | 1:F:457:PRO:CD   | 2.83                     | 0.56              |
| 1:H:172:LEU:HG   | 1:H:212:SER:HA   | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:172:LEU:HG   | 1:M:212:SER:HA   | 1.87                     | 0.56              |
| 1:N:172:LEU:HG   | 1:N:212:SER:HA   | 1.87                     | 0.56              |
| 1:A:504:VAL:CG1  | 1:A:521:ARG:CG   | 2.83                     | 0.56              |
| 1:C:259:LEU:HD11 | 1:C:310:ILE:HG13 | 1.87                     | 0.56              |
| 1:D:181:VAL:O    | 1:D:185:GLU:HG3  | 2.04                     | 0.56              |
| 1:F:481:GLY:H    | 1:F:505:SER:HB3  | 0.42                     | 0.56              |
| 1:K:112:VAL:HG21 | 1:K:140:ILE:HD11 | 1.87                     | 0.56              |
| 1:K:330:ALA:HB3  | 1:K:432:SER:HB3  | 1.88                     | 0.56              |
| 1:L:330:ALA:HB3  | 1:L:432:SER:HB3  | 1.88                     | 0.56              |
| 1:A:260:LYS:O    | 1:A:263:SER:OG   | 2.17                     | 0.56              |
| 1:D:504:VAL:CG1  | 1:D:521:ARG:CG   | 2.83                     | 0.56              |
| 1:F:112:VAL:HG21 | 1:F:140:ILE:HD11 | 1.87                     | 0.56              |
| 1:J:259:LEU:HD11 | 1:J:310:ILE:HG13 | 1.87                     | 0.56              |
| 1:J:507:VAL:CA   | 1:J:518:PHE:HB3  | 2.35                     | 0.56              |
| 1:M:132:VAL:HG12 | 1:M:134:TYR:CE1  | 2.39                     | 0.56              |
| 1:M:259:LEU:HD11 | 1:M:310:ILE:HG13 | 1.87                     | 0.56              |
| 1:O:172:LEU:HG   | 1:O:212:SER:HA   | 1.87                     | 0.56              |
| 1:A:456:VAL:CG2  | 1:A:457:PRO:CD   | 2.83                     | 0.56              |
| 1:B:456:VAL:CG2  | 1:B:457:PRO:CD   | 2.83                     | 0.56              |
| 1:J:112:VAL:HG21 | 1:J:140:ILE:HD11 | 1.87                     | 0.56              |
| 1:N:259:LEU:HD11 | 1:N:310:ILE:HG13 | 1.87                     | 0.56              |
| 1:N:507:VAL:CA   | 1:N:518:PHE:HB3  | 2.35                     | 0.56              |
| 1:O:259:LEU:HD11 | 1:O:310:ILE:HG13 | 1.87                     | 0.56              |
| 1:A:172:LEU:HG   | 1:A:212:SER:HA   | 1.87                     | 0.56              |
| 1:A:259:LEU:HD11 | 1:A:310:ILE:HG13 | 1.87                     | 0.56              |
| 1:A:507:VAL:CA   | 1:A:518:PHE:HB3  | 2.35                     | 0.56              |
| 1:C:330:ALA:HB3  | 1:C:432:SER:HB3  | 1.88                     | 0.56              |
| 1:C:504:VAL:CG1  | 1:C:521:ARG:CG   | 2.83                     | 0.56              |
| 1:D:215:ILE:HD11 | 1:D:225:LEU:HD13 | 1.88                     | 0.56              |
| 1:D:330:ALA:HB3  | 1:D:432:SER:HB3  | 1.88                     | 0.56              |
| 1:E:215:ILE:HD11 | 1:E:225:LEU:HD13 | 1.88                     | 0.56              |
| 1:F:105:VAL:HG11 | 1:F:157:ARG:HE   | 1.69                     | 0.56              |
| 1:H:456:VAL:CG2  | 1:H:457:PRO:CD   | 2.83                     | 0.56              |
| 1:I:207:ASP:OD1  | 1:I:209:ARG:N    | 2.33                     | 0.56              |
| 1:J:330:ALA:HB3  | 1:J:432:SER:HB3  | 1.88                     | 0.56              |
| 1:O:121:GLN:O    | 1:O:125:ASN:N    | 2.33                     | 0.56              |
| 1:A:506:ASN:HD22 | 1:A:507:VAL:H    | 1.50                     | 0.56              |
| 1:D:481:GLY:N    | 1:D:505:SER:OG   | 2.23                     | 0.56              |
| 1:J:207:ASP:OD1  | 1:J:209:ARG:N    | 2.33                     | 0.56              |
| 1:L:259:LEU:HD11 | 1:L:310:ILE:HG13 | 1.87                     | 0.56              |
| 1:M:330:ALA:HB3  | 1:M:432:SER:HB3  | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:456:VAL:CG2  | 1:N:457:PRO:CD   | 2.83                     | 0.56              |
| 1:C:215:ILE:HD11 | 1:C:225:LEU:HD13 | 1.88                     | 0.56              |
| 1:D:521:ARG:N    | 1:D:521:ARG:HD3  | 2.21                     | 0.56              |
| 1:E:330:ALA:HB3  | 1:E:432:SER:HB3  | 1.88                     | 0.56              |
| 1:E:456:VAL:CG2  | 1:E:457:PRO:CD   | 2.83                     | 0.56              |
| 1:F:215:ILE:HD11 | 1:F:225:LEU:HD13 | 1.88                     | 0.56              |
| 1:F:521:ARG:N    | 1:F:521:ARG:HD3  | 2.21                     | 0.56              |
| 1:G:172:LEU:HG   | 1:G:212:SER:HA   | 1.87                     | 0.56              |
| 1:G:506:ASN:HD22 | 1:G:507:VAL:H    | 1.50                     | 0.56              |
| 1:O:506:ASN:HD22 | 1:O:507:VAL:H    | 1.50                     | 0.56              |
| 1:O:504:VAL:CG1  | 1:O:521:ARG:CG   | 2.83                     | 0.56              |
| 1:H:521:ARG:HD3  | 1:H:521:ARG:N    | 2.21                     | 0.56              |
| 1:J:521:ARG:HD3  | 1:J:521:ARG:N    | 2.21                     | 0.56              |
| 1:L:521:ARG:N    | 1:L:521:ARG:HD3  | 2.21                     | 0.56              |
| 1:B:172:LEU:HG   | 1:B:212:SER:HA   | 1.87                     | 0.56              |
| 1:B:259:LEU:HD11 | 1:B:310:ILE:HG13 | 1.87                     | 0.56              |
| 1:B:330:ALA:HB3  | 1:B:432:SER:HB3  | 1.88                     | 0.56              |
| 1:B:504:VAL:CG1  | 1:B:521:ARG:CG   | 2.83                     | 0.56              |
| 1:B:521:ARG:N    | 1:B:521:ARG:HD3  | 2.21                     | 0.56              |
| 1:C:207:ASP:O    | 1:C:211:ASN:CA   | 2.55                     | 0.56              |
| 1:C:481:GLY:H    | 1:C:505:SER:HB3  | 0.42                     | 0.56              |
| 1:G:112:VAL:HG21 | 1:G:140:ILE:HD11 | 1.87                     | 0.56              |
| 1:I:112:VAL:HG21 | 1:I:140:ILE:HD11 | 1.87                     | 0.56              |
| 1:I:330:ALA:HB3  | 1:I:432:SER:HB3  | 1.88                     | 0.56              |
| 1:C:121:GLN:O    | 1:C:125:ASN:N    | 2.33                     | 0.55              |
| 1:G:215:ILE:HD11 | 1:G:225:LEU:HD13 | 1.88                     | 0.55              |
| 1:J:207:ASP:O    | 1:J:211:ASN:CA   | 2.54                     | 0.55              |
| 1:K:207:ASP:OD1  | 1:K:209:ARG:N    | 2.33                     | 0.55              |
| 1:K:259:LEU:HD11 | 1:K:310:ILE:HG13 | 1.87                     | 0.55              |
| 1:L:207:ASP:O    | 1:L:211:ASN:CA   | 2.54                     | 0.55              |
| 1:L:507:VAL:CA   | 1:L:518:PHE:HB3  | 2.35                     | 0.55              |
| 1:B:609:PHE:CE2  | 1:C:639:ILE:HD11 | 2.42                     | 0.55              |
| 1:C:172:LEU:HG   | 1:C:212:SER:HA   | 1.87                     | 0.55              |
| 1:E:207:ASP:O    | 1:E:211:ASN:CA   | 2.54                     | 0.55              |
| 1:E:177:ALA:HB3  | 1:E:208:GLU:HG2  | 1.89                     | 0.55              |
| 1:I:504:VAL:CG1  | 1:I:521:ARG:CG   | 2.83                     | 0.55              |
| 1:J:456:VAL:CG2  | 1:J:457:PRO:CD   | 2.83                     | 0.55              |
| 1:K:456:VAL:CG2  | 1:K:457:PRO:CD   | 2.83                     | 0.55              |
| 1:L:481:GLY:H    | 1:L:505:SER:HB3  | 0.41                     | 0.55              |
| 1:M:207:ASP:O    | 1:M:211:ASN:CA   | 2.54                     | 0.55              |
| 1:M:507:VAL:CA   | 1:M:518:PHE:HB3  | 2.35                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:207:ASP:O    | 1:N:211:ASN:CA   | 2.54                     | 0.55              |
| 1:N:521:ARG:HD3  | 1:N:521:ARG:N    | 2.21                     | 0.55              |
| 1:B:215:ILE:HD11 | 1:B:225:LEU:HD13 | 1.88                     | 0.55              |
| 1:E:521:ARG:N    | 1:E:521:ARG:HD3  | 2.21                     | 0.55              |
| 1:F:609:PHE:CE2  | 1:G:639:ILE:HD11 | 2.42                     | 0.55              |
| 1:H:112:VAL:HG21 | 1:H:140:ILE:HD11 | 1.87                     | 0.55              |
| 1:I:105:VAL:HG11 | 1:I:157:ARG:HE   | 1.69                     | 0.55              |
| 1:I:481:GLY:N    | 1:I:505:SER:OG   | 2.23                     | 0.55              |
| 1:K:207:ASP:O    | 1:K:211:ASN:CA   | 2.55                     | 0.55              |
| 1:K:521:ARG:N    | 1:K:521:ARG:HD3  | 2.21                     | 0.55              |
| 1:O:207:ASP:O    | 1:O:211:ASN:CA   | 2.55                     | 0.55              |
| 1:A:207:ASP:O    | 1:A:211:ASN:CA   | 2.54                     | 0.55              |
| 1:A:521:ARG:N    | 1:A:521:ARG:HD3  | 2.21                     | 0.55              |
| 1:C:507:VAL:CA   | 1:C:518:PHE:HB3  | 2.35                     | 0.55              |
| 1:D:121:GLN:O    | 1:D:125:ASN:N    | 2.33                     | 0.55              |
| 1:C:609:PHE:CE2  | 1:D:639:ILE:HD11 | 2.42                     | 0.55              |
| 1:F:172:LEU:HG   | 1:F:212:SER:HA   | 1.87                     | 0.55              |
| 1:F:507:VAL:CA   | 1:F:518:PHE:HB3  | 2.35                     | 0.55              |
| 1:G:207:ASP:O    | 1:G:211:ASN:CA   | 2.54                     | 0.55              |
| 1:H:207:ASP:O    | 1:H:211:ASN:CA   | 2.54                     | 0.55              |
| 1:E:121:GLN:O    | 1:E:125:ASN:N    | 2.33                     | 0.55              |
| 1:E:609:PHE:CE2  | 1:F:639:ILE:HD11 | 2.42                     | 0.55              |
| 1:F:330:ALA:HB3  | 1:F:432:SER:HB3  | 1.88                     | 0.55              |
| 1:H:330:ALA:HB3  | 1:H:432:SER:HB3  | 1.88                     | 0.55              |
| 1:I:456:VAL:CG2  | 1:I:457:PRO:CD   | 2.83                     | 0.55              |
| 1:I:521:ARG:N    | 1:I:521:ARG:HD3  | 2.21                     | 0.55              |
| 1:L:456:VAL:CG2  | 1:L:457:PRO:CD   | 2.83                     | 0.55              |
| 1:N:330:ALA:HB3  | 1:N:432:SER:HB3  | 1.88                     | 0.55              |
| 1:A:330:ALA:HB3  | 1:A:432:SER:HB3  | 1.88                     | 0.55              |
| 1:B:207:ASP:O    | 1:B:211:ASN:CA   | 2.54                     | 0.55              |
| 1:C:521:ARG:N    | 1:C:521:ARG:HD3  | 2.21                     | 0.55              |
| 1:D:172:LEU:HG   | 1:D:212:SER:HA   | 1.87                     | 0.55              |
| 1:E:207:ASP:OD1  | 1:E:209:ARG:N    | 2.33                     | 0.55              |
| 1:E:504:VAL:CG1  | 1:E:521:ARG:CG   | 2.83                     | 0.55              |
| 1:G:521:ARG:HD3  | 1:G:521:ARG:N    | 2.21                     | 0.55              |
| 1:H:215:ILE:HD11 | 1:H:225:LEU:HD13 | 1.88                     | 0.55              |
| 1:I:207:ASP:O    | 1:I:211:ASN:CA   | 2.55                     | 0.55              |
| 1:I:215:ILE:HD11 | 1:I:225:LEU:HD13 | 1.88                     | 0.55              |
| 1:I:481:GLY:H    | 1:I:505:SER:HB3  | 0.42                     | 0.55              |
| 1:A:215:ILE:HD11 | 1:A:225:LEU:HD13 | 1.88                     | 0.55              |
| 1:D:177:ALA:HB3  | 1:D:208:GLU:HG2  | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:172:LEU:HG   | 1:E:212:SER:HA   | 1.87                     | 0.55              |
| 1:M:504:VAL:CG1  | 1:M:521:ARG:CG   | 2.83                     | 0.55              |
| 1:A:609:PHE:CE2  | 1:B:639:ILE:HD11 | 2.42                     | 0.55              |
| 1:H:177:ALA:HB3  | 1:H:208:GLU:HG2  | 1.89                     | 0.55              |
| 1:M:456:VAL:CG2  | 1:M:457:PRO:CD   | 2.83                     | 0.55              |
| 1:O:481:GLY:H    | 1:O:505:SER:HB3  | 0.42                     | 0.55              |
| 1:O:521:ARG:N    | 1:O:521:ARG:HD3  | 2.21                     | 0.55              |
| 1:C:207:ASP:OD1  | 1:C:209:ARG:N    | 2.33                     | 0.55              |
| 1:F:207:ASP:O    | 1:F:211:ASN:CA   | 2.55                     | 0.55              |
| 1:F:504:VAL:CG1  | 1:F:521:ARG:CG   | 2.83                     | 0.55              |
| 1:G:330:ALA:HB3  | 1:G:432:SER:HB3  | 1.88                     | 0.55              |
| 1:J:506:ASN:HD22 | 1:J:507:VAL:H    | 1.51                     | 0.55              |
| 1:M:506:ASN:HD22 | 1:M:507:VAL:H    | 1.50                     | 0.55              |
| 1:F:177:ALA:HB3  | 1:F:208:GLU:HG2  | 1.89                     | 0.55              |
| 1:J:215:ILE:HD11 | 1:J:225:LEU:HD13 | 1.88                     | 0.55              |
| 1:M:215:ILE:HD11 | 1:M:225:LEU:HD13 | 1.88                     | 0.55              |
| 1:N:504:VAL:CG1  | 1:N:521:ARG:CG   | 2.83                     | 0.55              |
| 1:O:215:ILE:HD11 | 1:O:225:LEU:HD13 | 1.88                     | 0.55              |
| 1:O:507:VAL:CA   | 1:O:518:PHE:HB3  | 2.35                     | 0.55              |
| 1:A:177:ALA:HB3  | 1:A:208:GLU:HG2  | 1.89                     | 0.54              |
| 1:B:177:ALA:HB3  | 1:B:208:GLU:HG2  | 1.89                     | 0.54              |
| 1:D:207:ASP:O    | 1:D:211:ASN:CA   | 2.54                     | 0.54              |
| 1:F:183:ILE:HD12 | 1:F:232:LEU:HD13 | 1.89                     | 0.54              |
| 1:N:121:GLN:O    | 1:N:125:ASN:N    | 2.33                     | 0.54              |
| 1:G:183:ILE:HD12 | 1:G:232:LEU:HD13 | 1.89                     | 0.54              |
| 1:G:504:VAL:CG1  | 1:G:521:ARG:CG   | 2.83                     | 0.54              |
| 1:I:177:ALA:HB3  | 1:I:208:GLU:HG2  | 1.89                     | 0.54              |
| 1:L:121:GLN:O    | 1:L:125:ASN:N    | 2.33                     | 0.54              |
| 1:N:215:ILE:HD11 | 1:N:225:LEU:HD13 | 1.88                     | 0.54              |
| 1:A:504:VAL:CG1  | 1:A:521:ARG:CD   | 2.86                     | 0.54              |
| 1:B:504:VAL:CG1  | 1:B:521:ARG:CD   | 2.86                     | 0.54              |
| 1:D:259:LEU:HD11 | 1:D:310:ILE:CG1  | 2.38                     | 0.54              |
| 1:E:259:LEU:HD11 | 1:E:310:ILE:CG1  | 2.38                     | 0.54              |
| 1:H:183:ILE:HD12 | 1:H:232:LEU:HD13 | 1.89                     | 0.54              |
| 1:O:183:ILE:HD12 | 1:O:232:LEU:HD13 | 1.89                     | 0.54              |
| 1:A:639:ILE:HD11 | 1:O:609:PHE:CE2  | 2.42                     | 0.54              |
| 1:C:259:LEU:HD11 | 1:C:310:ILE:CG1  | 2.38                     | 0.54              |
| 1:G:177:ALA:HB3  | 1:G:208:GLU:HG2  | 1.89                     | 0.54              |
| 1:I:507:VAL:CA   | 1:I:518:PHE:HB3  | 2.35                     | 0.54              |
| 1:K:215:ILE:HD11 | 1:K:225:LEU:HD13 | 1.88                     | 0.54              |
| 1:L:215:ILE:HD11 | 1:L:225:LEU:HD13 | 1.88                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:183:ILE:HD12 | 1:A:232:LEU:HD13 | 1.89                     | 0.54              |
| 1:E:183:ILE:HD12 | 1:E:232:LEU:HD13 | 1.89                     | 0.54              |
| 1:D:609:PHE:CE2  | 1:E:639:ILE:HD11 | 2.42                     | 0.54              |
| 1:G:132:VAL:HA   | 1:G:141:LEU:O    | 2.08                     | 0.54              |
| 1:H:132:VAL:HA   | 1:H:141:LEU:O    | 2.08                     | 0.54              |
| 1:K:259:LEU:HD11 | 1:K:310:ILE:CG1  | 2.38                     | 0.54              |
| 1:L:259:LEU:HD11 | 1:L:310:ILE:CG1  | 2.38                     | 0.54              |
| 1:O:330:ALA:HB3  | 1:O:432:SER:HB3  | 1.88                     | 0.54              |
| 1:C:504:VAL:CG1  | 1:C:521:ARG:CD   | 2.86                     | 0.54              |
| 1:I:504:VAL:CG1  | 1:I:521:ARG:CD   | 2.86                     | 0.54              |
| 1:K:481:GLY:H    | 1:K:505:SER:HB3  | 0.42                     | 0.54              |
| 1:N:132:VAL:HA   | 1:N:141:LEU:O    | 2.08                     | 0.54              |
| 1:F:132:VAL:HA   | 1:F:141:LEU:O    | 2.08                     | 0.54              |
| 1:F:259:LEU:HD11 | 1:F:310:ILE:CG1  | 2.38                     | 0.54              |
| 1:H:259:LEU:HD11 | 1:H:310:ILE:CG1  | 2.38                     | 0.54              |
| 1:I:132:VAL:HA   | 1:I:141:LEU:O    | 2.08                     | 0.54              |
| 1:M:132:VAL:HA   | 1:M:141:LEU:O    | 2.08                     | 0.54              |
| 1:M:259:LEU:HD11 | 1:M:310:ILE:CG1  | 2.38                     | 0.54              |
| 1:M:521:ARG:N    | 1:M:521:ARG:HD3  | 2.21                     | 0.54              |
| 1:N:183:ILE:HD12 | 1:N:232:LEU:HD13 | 1.89                     | 0.54              |
| 1:N:259:LEU:HD11 | 1:N:310:ILE:CG1  | 2.38                     | 0.54              |
| 1:O:259:LEU:HD11 | 1:O:310:ILE:CG1  | 2.38                     | 0.54              |
| 1:C:132:VAL:HA   | 1:C:141:LEU:O    | 2.08                     | 0.54              |
| 1:J:259:LEU:HD11 | 1:J:310:ILE:CG1  | 2.38                     | 0.54              |
| 1:J:459:ILE:CA   | 1:J:474:THR:O    | 2.55                     | 0.54              |
| 1:L:504:VAL:CG1  | 1:L:521:ARG:CG   | 2.83                     | 0.54              |
| 1:L:609:PHE:CE2  | 1:M:639:ILE:HD11 | 2.42                     | 0.54              |
| 1:N:481:GLY:H    | 1:N:505:SER:HB3  | 0.42                     | 0.54              |
| 1:O:504:VAL:CG1  | 1:O:521:ARG:CD   | 2.86                     | 0.54              |
| 1:B:183:ILE:HD12 | 1:B:232:LEU:HD13 | 1.89                     | 0.54              |
| 1:B:259:LEU:HD11 | 1:B:310:ILE:CG1  | 2.38                     | 0.54              |
| 1:D:183:ILE:HD12 | 1:D:232:LEU:HD13 | 1.89                     | 0.54              |
| 1:J:609:PHE:CE2  | 1:K:639:ILE:HD11 | 2.42                     | 0.54              |
| 1:O:177:ALA:HB3  | 1:O:208:GLU:HG2  | 1.89                     | 0.54              |
| 1:F:207:ASP:OD1  | 1:F:209:ARG:N    | 2.33                     | 0.54              |
| 1:G:259:LEU:HD11 | 1:G:310:ILE:CG1  | 2.38                     | 0.54              |
| 1:J:177:ALA:HB3  | 1:J:208:GLU:HG2  | 1.89                     | 0.54              |
| 1:L:177:ALA:HB3  | 1:L:208:GLU:HG2  | 1.89                     | 0.54              |
| 1:B:132:VAL:HA   | 1:B:141:LEU:O    | 2.08                     | 0.53              |
| 1:C:177:ALA:HB3  | 1:C:208:GLU:HG2  | 1.89                     | 0.53              |
| 1:I:183:ILE:HD12 | 1:I:232:LEU:HD13 | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:504:VAL:CG1  | 1:J:521:ARG:CD   | 2.86                     | 0.53              |
| 1:J:504:VAL:CG1  | 1:J:521:ARG:CG   | 2.83                     | 0.53              |
| 1:M:183:ILE:HD12 | 1:M:232:LEU:HD13 | 1.89                     | 0.53              |
| 1:N:177:ALA:HB3  | 1:N:208:GLU:HG2  | 1.89                     | 0.53              |
| 1:C:481:GLY:N    | 1:C:505:SER:OG   | 2.23                     | 0.53              |
| 1:G:504:VAL:CG1  | 1:G:521:ARG:CD   | 2.86                     | 0.53              |
| 1:H:481:GLY:H    | 1:H:505:SER:HB3  | 0.42                     | 0.53              |
| 1:H:609:PHE:CE2  | 1:I:639:ILE:HD11 | 2.42                     | 0.53              |
| 1:K:177:ALA:HB3  | 1:K:208:GLU:HG2  | 1.89                     | 0.53              |
| 1:B:508:LEU:N    | 1:B:508:LEU:CD1  | 2.72                     | 0.53              |
| 1:E:508:LEU:CD1  | 1:E:508:LEU:N    | 2.72                     | 0.53              |
| 1:H:504:VAL:CG1  | 1:H:521:ARG:CD   | 2.86                     | 0.53              |
| 1:I:259:LEU:HD11 | 1:I:310:ILE:CG1  | 2.38                     | 0.53              |
| 1:J:132:VAL:HA   | 1:J:141:LEU:O    | 2.08                     | 0.53              |
| 1:M:504:VAL:CG1  | 1:M:521:ARG:CD   | 2.86                     | 0.53              |
| 1:N:180:MET:HE2  | 1:N:213:ILE:HD11 | 1.89                     | 0.53              |
| 1:O:132:VAL:HA   | 1:O:141:LEU:O    | 2.08                     | 0.53              |
| 1:C:183:ILE:HD12 | 1:C:232:LEU:HD13 | 1.89                     | 0.53              |
| 1:D:504:VAL:CG1  | 1:D:521:ARG:CD   | 2.86                     | 0.53              |
| 1:F:504:VAL:CG1  | 1:F:521:ARG:CD   | 2.86                     | 0.53              |
| 1:L:132:VAL:HA   | 1:L:141:LEU:O    | 2.08                     | 0.53              |
| 1:L:504:VAL:CG1  | 1:L:521:ARG:CD   | 2.86                     | 0.53              |
| 1:C:508:LEU:N    | 1:C:508:LEU:CD1  | 2.72                     | 0.53              |
| 1:D:132:VAL:HA   | 1:D:141:LEU:O    | 2.08                     | 0.53              |
| 1:K:504:VAL:CG1  | 1:K:521:ARG:CD   | 2.86                     | 0.53              |
| 1:M:177:ALA:HB3  | 1:M:208:GLU:HG2  | 1.89                     | 0.53              |
| 1:M:459:ILE:CA   | 1:M:474:THR:O    | 2.55                     | 0.53              |
| 1:B:481:GLY:H    | 1:B:505:SER:HB3  | 0.42                     | 0.53              |
| 1:C:155:ILE:HG12 | 1:C:158:ARG:NH2  | 2.24                     | 0.53              |
| 1:D:142:ILE:HG22 | 1:D:149:VAL:HG22 | 1.91                     | 0.53              |
| 1:E:504:VAL:CG1  | 1:E:521:ARG:CD   | 2.86                     | 0.53              |
| 1:G:508:LEU:CD1  | 1:G:508:LEU:N    | 2.72                     | 0.53              |
| 1:J:155:ILE:HG12 | 1:J:158:ARG:NH2  | 2.24                     | 0.53              |
| 1:L:142:ILE:HG22 | 1:L:149:VAL:HG22 | 1.91                     | 0.53              |
| 1:N:504:VAL:CG1  | 1:N:521:ARG:CD   | 2.86                     | 0.53              |
| 1:O:508:LEU:N    | 1:O:508:LEU:CD1  | 2.72                     | 0.53              |
| 1:A:259:LEU:HD11 | 1:A:310:ILE:CG1  | 2.38                     | 0.53              |
| 1:A:508:LEU:N    | 1:A:508:LEU:CD1  | 2.72                     | 0.53              |
| 1:C:174:ASN:HB2  | 1:C:233:ASP:O    | 2.09                     | 0.53              |
| 1:E:132:VAL:HA   | 1:E:141:LEU:O    | 2.08                     | 0.53              |
| 1:E:142:ILE:HG22 | 1:E:149:VAL:HG22 | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:504:VAL:CG1  | 1:H:521:ARG:CG   | 2.83                     | 0.53              |
| 1:I:609:PHE:CE2  | 1:J:639:ILE:HD11 | 2.42                     | 0.53              |
| 1:B:142:ILE:HG22 | 1:B:149:VAL:HG22 | 1.91                     | 0.53              |
| 1:F:155:ILE:HG12 | 1:F:158:ARG:NH2  | 2.24                     | 0.53              |
| 1:G:174:ASN:HB2  | 1:G:233:ASP:O    | 2.09                     | 0.53              |
| 1:H:142:ILE:HG22 | 1:H:149:VAL:HG22 | 1.91                     | 0.53              |
| 1:I:142:ILE:HG22 | 1:I:149:VAL:HG22 | 1.91                     | 0.53              |
| 1:I:155:ILE:HG12 | 1:I:158:ARG:NH2  | 2.24                     | 0.53              |
| 1:J:183:ILE:HD12 | 1:J:232:LEU:HD13 | 1.89                     | 0.53              |
| 1:K:142:ILE:HG22 | 1:K:149:VAL:HG22 | 1.91                     | 0.53              |
| 1:K:155:ILE:HG12 | 1:K:158:ARG:NH2  | 2.24                     | 0.53              |
| 1:L:609:PHE:CD2  | 1:M:639:ILE:CD1  | 2.75                     | 0.53              |
| 1:D:174:ASN:HB2  | 1:D:233:ASP:O    | 2.09                     | 0.53              |
| 1:G:345:GLU:OE2  | 1:G:418:ASP:OD2  | 2.27                     | 0.53              |
| 1:H:174:ASN:HB2  | 1:H:233:ASP:O    | 2.09                     | 0.53              |
| 1:I:459:ILE:CA   | 1:I:474:THR:O    | 2.55                     | 0.53              |
| 1:K:183:ILE:HD12 | 1:K:232:LEU:HD13 | 1.89                     | 0.53              |
| 1:K:609:PHE:CE2  | 1:L:639:ILE:HD11 | 2.42                     | 0.53              |
| 1:N:609:PHE:CE2  | 1:O:639:ILE:HD11 | 2.42                     | 0.53              |
| 1:D:508:LEU:N    | 1:D:508:LEU:CD1  | 2.72                     | 0.53              |
| 1:E:155:ILE:HG12 | 1:E:158:ARG:NH2  | 2.24                     | 0.53              |
| 1:F:142:ILE:HG22 | 1:F:149:VAL:HG22 | 1.91                     | 0.53              |
| 1:F:345:GLU:OE2  | 1:F:418:ASP:OD2  | 2.27                     | 0.53              |
| 1:H:155:ILE:HG12 | 1:H:158:ARG:NH2  | 2.24                     | 0.53              |
| 1:H:345:GLU:OE2  | 1:H:418:ASP:OD2  | 2.27                     | 0.53              |
| 1:K:132:VAL:HA   | 1:K:141:LEU:O    | 2.08                     | 0.53              |
| 1:K:504:VAL:CG1  | 1:K:521:ARG:CG   | 2.83                     | 0.53              |
| 1:L:155:ILE:HG12 | 1:L:158:ARG:NH2  | 2.24                     | 0.53              |
| 1:M:142:ILE:HG22 | 1:M:149:VAL:HG22 | 1.91                     | 0.53              |
| 1:N:142:ILE:HG22 | 1:N:149:VAL:HG22 | 1.91                     | 0.53              |
| 1:E:481:GLY:H    | 1:E:505:SER:HB3  | 0.42                     | 0.52              |
| 1:G:142:ILE:HG22 | 1:G:149:VAL:HG22 | 1.91                     | 0.52              |
| 1:H:223:GLU:O    | 1:H:227:ARG:HG3  | 2.10                     | 0.52              |
| 1:G:609:PHE:CE2  | 1:H:639:ILE:HD11 | 2.42                     | 0.52              |
| 1:J:142:ILE:HG22 | 1:J:149:VAL:HG22 | 1.91                     | 0.52              |
| 1:N:174:ASN:HB2  | 1:N:233:ASP:O    | 2.09                     | 0.52              |
| 1:O:142:ILE:HG22 | 1:O:149:VAL:HG22 | 1.91                     | 0.52              |
| 1:A:132:VAL:HA   | 1:A:141:LEU:O    | 2.08                     | 0.52              |
| 1:A:142:ILE:HG22 | 1:A:149:VAL:HG22 | 1.91                     | 0.52              |
| 1:A:626:LEU:HD23 | 1:O:435:LEU:HD21 | 1.91                     | 0.52              |
| 1:C:142:ILE:HG22 | 1:C:149:VAL:HG22 | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:345:GLU:OE2  | 1:E:418:ASP:OD2  | 2.27                     | 0.52              |
| 1:G:108:LYS:HA   | 1:G:138:ASN:HD21 | 1.75                     | 0.52              |
| 1:I:223:GLU:O    | 1:I:227:ARG:HG3  | 2.09                     | 0.52              |
| 1:K:174:ASN:HB2  | 1:K:233:ASP:O    | 2.09                     | 0.52              |
| 1:L:183:ILE:HD12 | 1:L:232:LEU:HD13 | 1.89                     | 0.52              |
| 1:M:174:ASN:HB2  | 1:M:233:ASP:O    | 2.09                     | 0.52              |
| 1:A:223:GLU:O    | 1:A:227:ARG:HG3  | 2.10                     | 0.52              |
| 1:B:174:ASN:HB2  | 1:B:233:ASP:O    | 2.09                     | 0.52              |
| 1:D:155:ILE:HG12 | 1:D:158:ARG:NH2  | 2.24                     | 0.52              |
| 1:G:155:ILE:HG12 | 1:G:158:ARG:NH2  | 2.24                     | 0.52              |
| 1:H:163:GLY:O    | 1:H:165:LYS:HG3  | 2.10                     | 0.52              |
| 1:I:345:GLU:OE2  | 1:I:418:ASP:OD2  | 2.27                     | 0.52              |
| 1:L:180:MET:HE2  | 1:L:213:ILE:HD11 | 1.90                     | 0.52              |
| 1:M:508:LEU:N    | 1:M:508:LEU:CD1  | 2.72                     | 0.52              |
| 1:N:223:GLU:O    | 1:N:227:ARG:HG3  | 2.10                     | 0.52              |
| 1:O:174:ASN:HB2  | 1:O:233:ASP:O    | 2.09                     | 0.52              |
| 1:A:104:VAL:HA   | 1:A:140:ILE:O    | 2.10                     | 0.52              |
| 1:A:155:ILE:HG12 | 1:A:158:ARG:NH2  | 2.24                     | 0.52              |
| 1:A:109:ASN:ND2  | 1:A:160:ASP:O    | 2.43                     | 0.52              |
| 1:A:163:GLY:O    | 1:A:165:LYS:HG3  | 2.10                     | 0.52              |
| 1:A:174:ASN:HB2  | 1:A:233:ASP:O    | 2.09                     | 0.52              |
| 1:A:459:ILE:CA   | 1:A:474:THR:O    | 2.55                     | 0.52              |
| 1:B:109:ASN:ND2  | 1:B:160:ASP:O    | 2.43                     | 0.52              |
| 1:A:435:LEU:HD21 | 1:B:626:LEU:HD23 | 1.91                     | 0.52              |
| 1:C:104:VAL:HA   | 1:C:140:ILE:O    | 2.10                     | 0.52              |
| 1:D:108:LYS:HA   | 1:D:138:ASN:HD21 | 1.75                     | 0.52              |
| 1:D:207:ASP:OD1  | 1:D:209:ARG:N    | 2.33                     | 0.52              |
| 1:F:508:LEU:N    | 1:F:508:LEU:CD1  | 2.72                     | 0.52              |
| 1:H:105:VAL:O    | 1:H:140:ILE:CB   | 2.49                     | 0.52              |
| 1:I:508:LEU:N    | 1:I:508:LEU:CD1  | 2.72                     | 0.52              |
| 1:J:345:GLU:OE2  | 1:J:418:ASP:OD2  | 2.27                     | 0.52              |
| 1:J:521:ARG:CD   | 1:J:521:ARG:N    | 2.73                     | 0.52              |
| 1:I:435:LEU:HD21 | 1:J:626:LEU:HD23 | 1.91                     | 0.52              |
| 1:L:174:ASN:HB2  | 1:L:233:ASP:O    | 2.09                     | 0.52              |
| 1:M:140:ILE:HD13 | 1:M:156:ILE:CG2  | 2.40                     | 0.52              |
| 1:M:155:ILE:HG12 | 1:M:158:ARG:NH2  | 2.24                     | 0.52              |
| 1:M:481:GLY:H    | 1:M:505:SER:HB3  | 0.41                     | 0.52              |
| 1:O:207:ASP:OD1  | 1:O:209:ARG:N    | 2.33                     | 0.52              |
| 1:N:435:LEU:HD21 | 1:O:626:LEU:HD23 | 1.91                     | 0.52              |
| 1:A:140:ILE:HD13 | 1:A:156:ILE:CG2  | 2.40                     | 0.52              |
| 1:B:104:VAL:HA   | 1:B:140:ILE:O    | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:223:GLU:O    | 1:B:227:ARG:HG3  | 2.10                     | 0.52              |
| 1:C:109:ASN:ND2  | 1:C:160:ASP:O    | 2.43                     | 0.52              |
| 1:D:104:VAL:HA   | 1:D:140:ILE:O    | 2.10                     | 0.52              |
| 1:E:506:ASN:HD22 | 1:E:507:VAL:H    | 1.51                     | 0.52              |
| 1:G:223:GLU:O    | 1:G:227:ARG:HG3  | 2.10                     | 0.52              |
| 1:G:640:GLN:NE2  | 1:G:643:ILE:CG2  | 2.73                     | 0.52              |
| 1:H:109:ASN:ND2  | 1:H:160:ASP:O    | 2.43                     | 0.52              |
| 1:I:109:ASN:ND2  | 1:I:160:ASP:O    | 2.43                     | 0.52              |
| 1:J:109:ASN:ND2  | 1:J:160:ASP:O    | 2.43                     | 0.52              |
| 1:J:163:GLY:O    | 1:J:165:LYS:HG3  | 2.10                     | 0.52              |
| 1:K:108:LYS:HA   | 1:K:138:ASN:HD21 | 1.75                     | 0.52              |
| 1:K:121:GLN:O    | 1:K:125:ASN:N    | 2.33                     | 0.52              |
| 1:K:109:ASN:ND2  | 1:K:160:ASP:O    | 2.43                     | 0.52              |
| 1:J:435:LEU:HD21 | 1:K:626:LEU:HD23 | 1.91                     | 0.52              |
| 1:M:223:GLU:O    | 1:M:227:ARG:HG3  | 2.10                     | 0.52              |
| 1:N:104:VAL:HA   | 1:N:140:ILE:O    | 2.10                     | 0.52              |
| 1:N:122:LEU:HD23 | 1:N:125:ASN:ND2  | 2.19                     | 0.52              |
| 1:N:508:LEU:N    | 1:N:508:LEU:CD1  | 2.72                     | 0.52              |
| 1:O:163:GLY:O    | 1:O:165:LYS:HG3  | 2.10                     | 0.52              |
| 1:O:223:GLU:O    | 1:O:227:ARG:HG3  | 2.10                     | 0.52              |
| 1:B:163:GLY:O    | 1:B:165:LYS:HG3  | 2.10                     | 0.52              |
| 1:C:223:GLU:O    | 1:C:227:ARG:HG3  | 2.10                     | 0.52              |
| 1:C:221:VAL:HG22 | 1:C:224:ARG:HH21 | 1.75                     | 0.52              |
| 1:D:223:GLU:O    | 1:D:227:ARG:HG3  | 2.10                     | 0.52              |
| 1:D:521:ARG:CD   | 1:D:521:ARG:N    | 2.73                     | 0.52              |
| 1:E:163:GLY:O    | 1:E:165:LYS:HG3  | 2.10                     | 0.52              |
| 1:E:521:ARG:CD   | 1:E:521:ARG:N    | 2.73                     | 0.52              |
| 1:F:174:ASN:HB2  | 1:F:233:ASP:O    | 2.09                     | 0.52              |
| 1:G:109:ASN:ND2  | 1:G:160:ASP:O    | 2.43                     | 0.52              |
| 1:G:207:ASP:OD1  | 1:G:209:ARG:N    | 2.33                     | 0.52              |
| 1:H:108:LYS:HA   | 1:H:138:ASN:HD21 | 1.75                     | 0.52              |
| 1:I:521:ARG:N    | 1:I:521:ARG:CD   | 2.73                     | 0.52              |
| 1:I:640:GLN:NE2  | 1:I:643:ILE:CG2  | 2.73                     | 0.52              |
| 1:J:108:LYS:HA   | 1:J:138:ASN:HD21 | 1.75                     | 0.52              |
| 1:J:174:ASN:HB2  | 1:J:233:ASP:O    | 2.09                     | 0.52              |
| 1:J:481:GLY:H    | 1:J:505:SER:HB3  | 0.42                     | 0.52              |
| 1:K:345:GLU:OE2  | 1:K:418:ASP:OD2  | 2.27                     | 0.52              |
| 1:K:521:ARG:N    | 1:K:521:ARG:CD   | 2.73                     | 0.52              |
| 1:L:508:LEU:N    | 1:L:508:LEU:CD1  | 2.72                     | 0.52              |
| 1:N:155:ILE:HG12 | 1:N:158:ARG:NH2  | 2.24                     | 0.52              |
| 1:O:104:VAL:HA   | 1:O:140:ILE:O    | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:477:ARG:CG   | 1:A:477:ARG:NH1  | 2.73                     | 0.52              |
| 1:A:640:GLN:NE2  | 1:A:643:ILE:CG2  | 2.73                     | 0.52              |
| 1:B:506:ASN:HD22 | 1:B:507:VAL:H    | 1.51                     | 0.52              |
| 1:B:640:GLN:NE2  | 1:B:643:ILE:CG2  | 2.73                     | 0.52              |
| 1:D:345:GLU:OE2  | 1:D:418:ASP:OD2  | 2.27                     | 0.52              |
| 1:F:163:GLY:O    | 1:F:165:LYS:HG3  | 2.10                     | 0.52              |
| 1:G:122:LEU:HD23 | 1:G:125:ASN:ND2  | 2.19                     | 0.52              |
| 1:K:508:LEU:CD1  | 1:K:508:LEU:N    | 2.72                     | 0.52              |
| 1:K:640:GLN:NE2  | 1:K:643:ILE:CG2  | 2.73                     | 0.52              |
| 1:M:224:ARG:HA   | 1:M:227:ARG:HD2  | 1.92                     | 0.52              |
| 1:N:640:GLN:NE2  | 1:N:643:ILE:CG2  | 2.73                     | 0.52              |
| 1:O:109:ASN:ND2  | 1:O:160:ASP:O    | 2.43                     | 0.52              |
| 1:D:109:ASN:ND2  | 1:D:160:ASP:O    | 2.43                     | 0.52              |
| 1:D:640:GLN:NE2  | 1:D:643:ILE:CG2  | 2.73                     | 0.52              |
| 1:F:223:GLU:O    | 1:F:227:ARG:HG3  | 2.10                     | 0.52              |
| 1:F:640:GLN:NE2  | 1:F:643:ILE:CG2  | 2.73                     | 0.52              |
| 1:G:163:GLY:O    | 1:G:165:LYS:HG3  | 2.10                     | 0.52              |
| 1:J:508:LEU:N    | 1:J:508:LEU:CD1  | 2.72                     | 0.52              |
| 1:K:163:GLY:O    | 1:K:165:LYS:HG3  | 2.10                     | 0.52              |
| 1:L:109:ASN:ND2  | 1:L:160:ASP:O    | 2.43                     | 0.52              |
| 1:L:163:GLY:O    | 1:L:165:LYS:HG3  | 2.10                     | 0.52              |
| 1:N:224:ARG:HA   | 1:N:227:ARG:HD2  | 1.92                     | 0.52              |
| 1:O:221:VAL:HG22 | 1:O:224:ARG:HH21 | 1.75                     | 0.52              |
| 1:A:481:GLY:H    | 1:A:505:SER:HB3  | 0.42                     | 0.52              |
| 1:B:140:ILE:HD13 | 1:B:156:ILE:CG2  | 2.40                     | 0.52              |
| 1:C:345:GLU:OE2  | 1:C:418:ASP:OD2  | 2.27                     | 0.52              |
| 1:C:521:ARG:N    | 1:C:521:ARG:CD   | 2.73                     | 0.52              |
| 1:E:104:VAL:HA   | 1:E:140:ILE:O    | 2.10                     | 0.52              |
| 1:E:640:GLN:NE2  | 1:E:643:ILE:CG2  | 2.73                     | 0.52              |
| 1:F:104:VAL:HA   | 1:F:140:ILE:O    | 2.10                     | 0.52              |
| 1:F:109:ASN:ND2  | 1:F:160:ASP:O    | 2.43                     | 0.52              |
| 1:H:508:LEU:CD1  | 1:H:508:LEU:N    | 2.72                     | 0.52              |
| 1:H:640:GLN:NE2  | 1:H:643:ILE:CG2  | 2.73                     | 0.52              |
| 1:I:174:ASN:HB2  | 1:I:233:ASP:O    | 2.09                     | 0.52              |
| 1:J:140:ILE:HD13 | 1:J:156:ILE:CG2  | 2.40                     | 0.52              |
| 1:J:223:GLU:O    | 1:J:227:ARG:HG3  | 2.10                     | 0.52              |
| 1:L:140:ILE:HD13 | 1:L:156:ILE:CG2  | 2.40                     | 0.52              |
| 1:L:224:ARG:HA   | 1:L:227:ARG:HD2  | 1.92                     | 0.52              |
| 1:L:345:GLU:OE2  | 1:L:418:ASP:OD2  | 2.27                     | 0.52              |
| 1:K:435:LEU:HD21 | 1:L:626:LEU:HD23 | 1.91                     | 0.52              |
| 1:M:435:LEU:HD21 | 1:N:626:LEU:HD23 | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:640:GLN:NE2  | 1:M:643:ILE:CG2  | 2.73                     | 0.52              |
| 1:D:140:ILE:HD13 | 1:D:156:ILE:CG2  | 2.40                     | 0.52              |
| 1:D:163:GLY:O    | 1:D:165:LYS:HG3  | 2.10                     | 0.52              |
| 1:E:122:LEU:HD23 | 1:E:125:ASN:ND2  | 2.19                     | 0.52              |
| 1:E:174:ASN:HB2  | 1:E:233:ASP:O    | 2.09                     | 0.52              |
| 1:E:456:VAL:HG22 | 1:E:457:PRO:N    | 2.25                     | 0.52              |
| 1:F:221:VAL:HG22 | 1:F:224:ARG:HH21 | 1.75                     | 0.52              |
| 1:F:521:ARG:N    | 1:F:521:ARG:CD   | 2.73                     | 0.52              |
| 1:H:521:ARG:N    | 1:H:521:ARG:CD   | 2.73                     | 0.52              |
| 1:L:521:ARG:N    | 1:L:521:ARG:CD   | 2.73                     | 0.52              |
| 1:O:224:ARG:HA   | 1:O:227:ARG:HD2  | 1.92                     | 0.52              |
| 1:B:155:ILE:HG12 | 1:B:158:ARG:NH2  | 2.24                     | 0.51              |
| 1:E:223:GLU:O    | 1:E:227:ARG:HG3  | 2.09                     | 0.51              |
| 1:J:640:GLN:NE2  | 1:J:643:ILE:CG2  | 2.73                     | 0.51              |
| 1:L:223:GLU:O    | 1:L:227:ARG:HG3  | 2.10                     | 0.51              |
| 1:O:155:ILE:HG12 | 1:O:158:ARG:NH2  | 2.24                     | 0.51              |
| 1:B:221:VAL:HG22 | 1:B:224:ARG:HH21 | 1.75                     | 0.51              |
| 1:B:345:GLU:OE2  | 1:B:418:ASP:OD2  | 2.27                     | 0.51              |
| 1:B:456:VAL:HG22 | 1:B:457:PRO:N    | 2.26                     | 0.51              |
| 1:C:163:GLY:O    | 1:C:165:LYS:HG3  | 2.10                     | 0.51              |
| 1:D:224:ARG:HA   | 1:D:227:ARG:HD2  | 1.92                     | 0.51              |
| 1:E:108:LYS:HA   | 1:E:138:ASN:HD21 | 1.75                     | 0.51              |
| 1:G:521:ARG:CD   | 1:G:521:ARG:N    | 2.73                     | 0.51              |
| 1:H:435:LEU:HD21 | 1:I:626:LEU:HD23 | 1.91                     | 0.51              |
| 1:K:456:VAL:HG22 | 1:K:457:PRO:N    | 2.26                     | 0.51              |
| 1:M:104:VAL:HA   | 1:M:140:ILE:O    | 2.10                     | 0.51              |
| 1:M:109:ASN:ND2  | 1:M:160:ASP:O    | 2.43                     | 0.51              |
| 1:M:521:ARG:N    | 1:M:521:ARG:CD   | 2.73                     | 0.51              |
| 1:N:109:ASN:ND2  | 1:N:160:ASP:O    | 2.43                     | 0.51              |
| 1:N:345:GLU:OE2  | 1:N:418:ASP:OD2  | 2.27                     | 0.51              |
| 1:C:640:GLN:NE2  | 1:C:643:ILE:CG2  | 2.73                     | 0.51              |
| 1:D:459:ILE:CA   | 1:D:474:THR:O    | 2.55                     | 0.51              |
| 1:E:224:ARG:HA   | 1:E:227:ARG:HD2  | 1.92                     | 0.51              |
| 1:E:221:VAL:HG22 | 1:E:224:ARG:HH21 | 1.75                     | 0.51              |
| 1:G:104:VAL:HA   | 1:G:140:ILE:O    | 2.10                     | 0.51              |
| 1:I:163:GLY:O    | 1:I:165:LYS:HG3  | 2.10                     | 0.51              |
| 1:J:224:ARG:HA   | 1:J:227:ARG:HD2  | 1.92                     | 0.51              |
| 1:K:224:ARG:HA   | 1:K:227:ARG:HD2  | 1.92                     | 0.51              |
| 1:L:640:GLN:NE2  | 1:L:643:ILE:CG2  | 2.73                     | 0.51              |
| 1:N:521:ARG:N    | 1:N:521:ARG:CD   | 2.73                     | 0.51              |
| 1:O:108:LYS:HA   | 1:O:138:ASN:HD21 | 1.75                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:140:ILE:HD13 | 1:O:156:ILE:CG2  | 2.40                     | 0.51              |
| 1:O:345:GLU:OE2  | 1:O:418:ASP:OD2  | 2.27                     | 0.51              |
| 1:A:456:VAL:HG22 | 1:A:457:PRO:N    | 2.26                     | 0.51              |
| 1:B:108:LYS:HA   | 1:B:138:ASN:HD21 | 1.75                     | 0.51              |
| 1:B:435:LEU:HD21 | 1:C:626:LEU:HD23 | 1.91                     | 0.51              |
| 1:D:477:ARG:CG   | 1:D:477:ARG:NH1  | 2.73                     | 0.51              |
| 1:E:109:ASN:ND2  | 1:E:160:ASP:O    | 2.43                     | 0.51              |
| 1:G:140:ILE:HD13 | 1:G:156:ILE:CG2  | 2.40                     | 0.51              |
| 1:G:481:GLY:H    | 1:G:505:SER:HB3  | 0.42                     | 0.51              |
| 1:I:105:VAL:O    | 1:I:140:ILE:CB   | 2.49                     | 0.51              |
| 1:J:456:VAL:HG22 | 1:J:457:PRO:N    | 2.26                     | 0.51              |
| 1:K:223:GLU:O    | 1:K:227:ARG:HG3  | 2.10                     | 0.51              |
| 1:N:108:LYS:HA   | 1:N:138:ASN:HD21 | 1.75                     | 0.51              |
| 1:N:163:GLY:O    | 1:N:165:LYS:HG3  | 2.10                     | 0.51              |
| 1:M:609:PHE:CE2  | 1:N:639:ILE:HD11 | 2.42                     | 0.51              |
| 1:O:521:ARG:CD   | 1:O:521:ARG:N    | 2.73                     | 0.51              |
| 1:O:640:GLN:NE2  | 1:O:643:ILE:CG2  | 2.73                     | 0.51              |
| 1:A:108:LYS:HA   | 1:A:138:ASN:HD21 | 1.75                     | 0.51              |
| 1:A:224:ARG:HA   | 1:A:227:ARG:HD2  | 1.92                     | 0.51              |
| 1:A:345:GLU:OE2  | 1:A:418:ASP:OD2  | 2.27                     | 0.51              |
| 1:B:521:ARG:CD   | 1:B:521:ARG:N    | 2.73                     | 0.51              |
| 1:D:456:VAL:HG22 | 1:D:457:PRO:N    | 2.26                     | 0.51              |
| 1:E:140:ILE:HD13 | 1:E:156:ILE:CG2  | 2.40                     | 0.51              |
| 1:H:506:ASN:HD22 | 1:H:507:VAL:H    | 1.50                     | 0.51              |
| 1:I:140:ILE:HD13 | 1:I:156:ILE:CG2  | 2.40                     | 0.51              |
| 1:I:224:ARG:HA   | 1:I:227:ARG:HD2  | 1.92                     | 0.51              |
| 1:J:121:GLN:O    | 1:J:125:ASN:N    | 2.33                     | 0.51              |
| 1:L:459:ILE:CA   | 1:L:474:THR:O    | 2.55                     | 0.51              |
| 1:M:108:LYS:HA   | 1:M:138:ASN:HD21 | 1.75                     | 0.51              |
| 1:M:163:GLY:O    | 1:M:165:LYS:HG3  | 2.10                     | 0.51              |
| 1:M:345:GLU:OE2  | 1:M:418:ASP:OD2  | 2.27                     | 0.51              |
| 1:A:221:VAL:HG22 | 1:A:224:ARG:HH21 | 1.75                     | 0.51              |
| 1:A:521:ARG:N    | 1:A:521:ARG:CD   | 2.73                     | 0.51              |
| 1:H:481:GLY:N    | 1:H:505:SER:OG   | 2.23                     | 0.51              |
| 1:L:108:LYS:HA   | 1:L:138:ASN:HD21 | 1.74                     | 0.51              |
| 1:N:333:ASP:OD1  | 1:N:334:GLY:N    | 2.44                     | 0.51              |
| 1:O:477:ARG:NH1  | 1:O:477:ARG:CG   | 2.73                     | 0.51              |
| 1:C:224:ARG:HA   | 1:C:227:ARG:HD2  | 1.92                     | 0.51              |
| 1:D:481:GLY:H    | 1:D:505:SER:HB3  | 0.42                     | 0.51              |
| 1:F:108:LYS:HA   | 1:F:138:ASN:HD21 | 1.75                     | 0.51              |
| 1:F:224:ARG:HA   | 1:F:227:ARG:HD2  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:435:LEU:HD21 | 1:F:626:LEU:HD23 | 1.91                     | 0.51              |
| 1:J:104:VAL:HA   | 1:J:140:ILE:O    | 2.10                     | 0.51              |
| 1:K:104:VAL:HA   | 1:K:140:ILE:O    | 2.10                     | 0.51              |
| 1:L:221:VAL:HG22 | 1:L:224:ARG:HH21 | 1.75                     | 0.51              |
| 1:L:435:LEU:HD21 | 1:M:626:LEU:HD23 | 1.91                     | 0.51              |
| 1:N:221:VAL:HG22 | 1:N:224:ARG:HH21 | 1.75                     | 0.51              |
| 1:C:140:ILE:HD13 | 1:C:156:ILE:CG2  | 2.40                     | 0.51              |
| 1:C:459:ILE:CA   | 1:C:474:THR:O    | 2.55                     | 0.51              |
| 1:K:478:LYS:HD2  | 1:K:518:PHE:CZ   | 2.46                     | 0.51              |
| 1:M:478:LYS:HD2  | 1:M:518:PHE:CZ   | 2.46                     | 0.51              |
| 1:D:221:VAL:HG22 | 1:D:224:ARG:HH21 | 1.75                     | 0.51              |
| 1:D:435:LEU:HD21 | 1:E:626:LEU:HD23 | 1.91                     | 0.51              |
| 1:H:456:VAL:HG22 | 1:H:457:PRO:N    | 2.26                     | 0.51              |
| 1:H:459:ILE:CA   | 1:H:474:THR:O    | 2.55                     | 0.51              |
| 1:I:221:VAL:HG22 | 1:I:224:ARG:HH21 | 1.75                     | 0.51              |
| 1:K:506:ASN:HD22 | 1:K:507:VAL:H    | 1.50                     | 0.51              |
| 1:L:104:VAL:HA   | 1:L:140:ILE:O    | 2.10                     | 0.51              |
| 1:A:207:ASP:OD1  | 1:A:209:ARG:N    | 2.33                     | 0.51              |
| 1:B:477:ARG:NH1  | 1:B:477:ARG:CG   | 2.73                     | 0.51              |
| 1:C:108:LYS:HA   | 1:C:138:ASN:HD21 | 1.75                     | 0.51              |
| 1:E:459:ILE:CA   | 1:E:474:THR:O    | 2.56                     | 0.51              |
| 1:F:456:VAL:HG22 | 1:F:457:PRO:N    | 2.26                     | 0.51              |
| 1:H:224:ARG:HA   | 1:H:227:ARG:HD2  | 1.92                     | 0.51              |
| 1:L:333:ASP:OD1  | 1:L:334:GLY:N    | 2.44                     | 0.51              |
| 1:M:333:ASP:OD1  | 1:M:334:GLY:N    | 2.44                     | 0.51              |
| 1:N:506:ASN:HD22 | 1:N:507:VAL:H    | 1.50                     | 0.51              |
| 1:O:333:ASP:OD1  | 1:O:334:GLY:N    | 2.44                     | 0.51              |
| 1:C:477:ARG:CG   | 1:C:477:ARG:NH1  | 2.73                     | 0.50              |
| 1:D:478:LYS:HD2  | 1:D:518:PHE:CZ   | 2.46                     | 0.50              |
| 1:E:333:ASP:OD1  | 1:E:334:GLY:N    | 2.44                     | 0.50              |
| 1:F:140:ILE:HD13 | 1:F:156:ILE:CG2  | 2.40                     | 0.50              |
| 1:H:221:VAL:HG22 | 1:H:224:ARG:HH21 | 1.75                     | 0.50              |
| 1:I:235:GLU:H    | 1:I:235:GLU:CD   | 2.11                     | 0.50              |
| 1:I:456:VAL:HG22 | 1:I:457:PRO:N    | 2.26                     | 0.50              |
| 1:J:105:VAL:O    | 1:J:140:ILE:CB   | 2.49                     | 0.50              |
| 1:O:122:LEU:HD23 | 1:O:125:ASN:ND2  | 2.19                     | 0.50              |
| 1:B:224:ARG:HA   | 1:B:227:ARG:HD2  | 1.92                     | 0.50              |
| 1:C:435:LEU:HD21 | 1:D:626:LEU:HD23 | 1.91                     | 0.50              |
| 1:C:478:LYS:HD2  | 1:C:518:PHE:CZ   | 2.46                     | 0.50              |
| 1:F:177:ALA:HB1  | 1:F:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:F:321:LEU:CD1  | 1:F:441:THR:OG1  | 2.60                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:435:LEU:HD21 | 1:G:626:LEU:HD23 | 1.91                     | 0.50              |
| 1:J:122:LEU:HD23 | 1:J:125:ASN:ND2  | 2.19                     | 0.50              |
| 1:J:221:VAL:HG22 | 1:J:224:ARG:HH21 | 1.75                     | 0.50              |
| 1:J:478:LYS:HD2  | 1:J:518:PHE:CZ   | 2.46                     | 0.50              |
| 1:K:333:ASP:OD1  | 1:K:334:GLY:N    | 2.44                     | 0.50              |
| 1:M:456:VAL:HG22 | 1:M:457:PRO:N    | 2.26                     | 0.50              |
| 1:A:177:ALA:HB1  | 1:A:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:C:456:VAL:HG22 | 1:C:457:PRO:N    | 2.26                     | 0.50              |
| 1:G:177:ALA:HB1  | 1:G:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:F:519:ALA:CB   | 1:G:454:GLU:HG3  | 2.41                     | 0.50              |
| 1:G:519:ALA:CB   | 1:H:454:GLU:HG3  | 2.41                     | 0.50              |
| 1:H:333:ASP:OD1  | 1:H:334:GLY:N    | 2.44                     | 0.50              |
| 1:I:108:LYS:HA   | 1:I:138:ASN:HD21 | 1.75                     | 0.50              |
| 1:I:180:MET:SD   | 1:I:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:J:333:ASP:OD1  | 1:J:334:GLY:N    | 2.44                     | 0.50              |
| 1:L:177:ALA:HB1  | 1:L:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:L:478:LYS:HD2  | 1:L:518:PHE:CZ   | 2.46                     | 0.50              |
| 1:M:177:ALA:HB1  | 1:M:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:M:221:VAL:HG22 | 1:M:224:ARG:HH21 | 1.75                     | 0.50              |
| 1:E:321:LEU:CD1  | 1:E:441:THR:OG1  | 2.60                     | 0.50              |
| 1:E:459:ILE:N    | 1:E:459:ILE:HD12 | 2.27                     | 0.50              |
| 1:F:333:ASP:OD1  | 1:F:334:GLY:N    | 2.44                     | 0.50              |
| 1:E:519:ALA:CB   | 1:F:454:GLU:HG3  | 2.41                     | 0.50              |
| 1:G:224:ARG:HA   | 1:G:227:ARG:HD2  | 1.92                     | 0.50              |
| 1:G:321:LEU:CD1  | 1:G:441:THR:OG1  | 2.60                     | 0.50              |
| 1:G:456:VAL:HG22 | 1:G:457:PRO:N    | 2.26                     | 0.50              |
| 1:H:478:LYS:HD2  | 1:H:518:PHE:CZ   | 2.46                     | 0.50              |
| 1:I:104:VAL:HA   | 1:I:140:ILE:O    | 2.10                     | 0.50              |
| 1:J:180:MET:SD   | 1:J:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:N:177:ALA:HB1  | 1:N:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:N:456:VAL:HG22 | 1:N:457:PRO:N    | 2.26                     | 0.50              |
| 1:O:177:ALA:HB1  | 1:O:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:A:454:GLU:HG3  | 1:O:519:ALA:CB   | 2.41                     | 0.50              |
| 1:A:519:ALA:CB   | 1:B:454:GLU:HG3  | 2.41                     | 0.50              |
| 1:B:333:ASP:OD1  | 1:B:334:GLY:N    | 2.44                     | 0.50              |
| 1:C:122:LEU:HD23 | 1:C:125:ASN:ND2  | 2.19                     | 0.50              |
| 1:C:205:VAL:HG12 | 1:C:206:ALA:N    | 2.27                     | 0.50              |
| 1:D:459:ILE:HD12 | 1:D:459:ILE:N    | 2.27                     | 0.50              |
| 1:F:459:ILE:N    | 1:F:459:ILE:HD12 | 2.27                     | 0.50              |
| 1:G:333:ASP:OD1  | 1:G:334:GLY:N    | 2.44                     | 0.50              |
| 1:G:435:LEU:HD21 | 1:H:626:LEU:HD23 | 1.91                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:552:VAL:HG23 | 1:G:553:PRO:C    | 2.32                     | 0.50              |
| 1:H:104:VAL:HA   | 1:H:140:ILE:O    | 2.10                     | 0.50              |
| 1:H:180:MET:SD   | 1:H:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:H:207:ASP:OD1  | 1:H:209:ARG:N    | 2.33                     | 0.50              |
| 1:H:552:VAL:HG23 | 1:H:553:PRO:C    | 2.32                     | 0.50              |
| 1:I:177:ALA:HB1  | 1:I:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:K:177:ALA:HB1  | 1:K:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:K:221:VAL:HG22 | 1:K:224:ARG:HH21 | 1.75                     | 0.50              |
| 1:M:552:VAL:HG23 | 1:M:553:PRO:C    | 2.32                     | 0.50              |
| 1:N:180:MET:SD   | 1:N:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:N:478:LYS:HD2  | 1:N:518:PHE:CZ   | 2.46                     | 0.50              |
| 1:C:333:ASP:OD1  | 1:C:334:GLY:N    | 2.44                     | 0.50              |
| 1:C:458:VAL:O    | 1:C:475:VAL:C    | 2.49                     | 0.50              |
| 1:D:177:ALA:HB1  | 1:D:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:D:321:LEU:CD1  | 1:D:441:THR:OG1  | 2.60                     | 0.50              |
| 1:E:180:MET:SD   | 1:E:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:F:102:THR:OG1  | 1:F:142:ILE:O    | 2.25                     | 0.50              |
| 1:F:180:MET:SD   | 1:F:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:G:478:LYS:HD2  | 1:G:518:PHE:CZ   | 2.46                     | 0.50              |
| 1:H:177:ALA:HB1  | 1:H:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:H:519:ALA:CB   | 1:I:454:GLU:HG3  | 2.41                     | 0.50              |
| 1:J:177:ALA:HB1  | 1:J:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:K:140:ILE:HD13 | 1:K:156:ILE:CG2  | 2.40                     | 0.50              |
| 1:K:180:MET:SD   | 1:K:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:K:552:VAL:HG23 | 1:K:553:PRO:C    | 2.32                     | 0.50              |
| 1:L:552:VAL:HG23 | 1:L:553:PRO:C    | 2.32                     | 0.50              |
| 1:O:180:MET:SD   | 1:O:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:O:459:ILE:CA   | 1:O:474:THR:O    | 2.55                     | 0.50              |
| 1:A:333:ASP:OD1  | 1:A:334:GLY:N    | 2.44                     | 0.50              |
| 1:B:177:ALA:HB1  | 1:B:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:B:205:VAL:HG12 | 1:B:206:ALA:N    | 2.27                     | 0.50              |
| 1:C:180:MET:SD   | 1:C:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:D:180:MET:SD   | 1:D:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:D:205:VAL:HG12 | 1:D:206:ALA:N    | 2.27                     | 0.50              |
| 1:E:177:ALA:HB1  | 1:E:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:F:478:LYS:HD2  | 1:F:518:PHE:CZ   | 2.46                     | 0.50              |
| 1:F:552:VAL:HG23 | 1:F:553:PRO:C    | 2.32                     | 0.50              |
| 1:G:180:MET:SD   | 1:G:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:G:221:VAL:HG22 | 1:G:224:ARG:HH21 | 1.75                     | 0.50              |
| 1:H:140:ILE:HD13 | 1:H:156:ILE:CG2  | 2.40                     | 0.50              |
| 1:H:321:LEU:CD1  | 1:H:441:THR:OG1  | 2.60                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:105:VAL:O    | 1:K:140:ILE:CB   | 2.49                     | 0.50              |
| 1:K:519:ALA:CB   | 1:L:454:GLU:HG3  | 2.41                     | 0.50              |
| 1:M:180:MET:SD   | 1:M:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:M:205:VAL:HG12 | 1:M:206:ALA:N    | 2.27                     | 0.50              |
| 1:N:519:ALA:CB   | 1:O:454:GLU:HG3  | 2.41                     | 0.50              |
| 1:A:180:MET:SD   | 1:A:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:A:205:VAL:HG12 | 1:A:206:ALA:N    | 2.27                     | 0.50              |
| 1:C:177:ALA:HB1  | 1:C:206:ALA:HB1  | 1.94                     | 0.50              |
| 1:B:519:ALA:CB   | 1:C:454:GLU:HG3  | 2.41                     | 0.50              |
| 1:E:478:LYS:HD2  | 1:E:518:PHE:CZ   | 2.46                     | 0.50              |
| 1:F:477:ARG:N    | 1:F:477:ARG:HD2  | 2.27                     | 0.50              |
| 1:G:459:ILE:CA   | 1:G:474:THR:O    | 2.55                     | 0.50              |
| 1:K:477:ARG:N    | 1:K:477:ARG:HD2  | 2.27                     | 0.50              |
| 1:L:459:ILE:N    | 1:L:459:ILE:HD12 | 2.27                     | 0.50              |
| 1:K:435:LEU:HD11 | 1:L:607:GLN:HE22 | 1.77                     | 0.50              |
| 1:L:519:ALA:CB   | 1:M:454:GLU:HG3  | 2.41                     | 0.50              |
| 1:N:552:VAL:HG23 | 1:N:553:PRO:C    | 2.32                     | 0.50              |
| 1:A:478:LYS:HD2  | 1:A:518:PHE:CZ   | 2.46                     | 0.50              |
| 1:B:180:MET:SD   | 1:B:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:B:218:ASP:N    | 1:B:221:VAL:HB   | 2.27                     | 0.50              |
| 1:C:218:ASP:N    | 1:C:221:VAL:HB   | 2.27                     | 0.50              |
| 1:D:333:ASP:OD1  | 1:D:334:GLY:N    | 2.44                     | 0.50              |
| 1:E:205:VAL:HG12 | 1:E:206:ALA:N    | 2.27                     | 0.50              |
| 1:F:459:ILE:CA   | 1:F:474:THR:O    | 2.55                     | 0.50              |
| 1:I:478:LYS:HD2  | 1:I:518:PHE:CZ   | 2.46                     | 0.50              |
| 1:J:205:VAL:HG12 | 1:J:206:ALA:N    | 2.27                     | 0.50              |
| 1:I:519:ALA:CB   | 1:J:454:GLU:HG3  | 2.41                     | 0.50              |
| 1:J:552:VAL:HG23 | 1:J:553:PRO:C    | 2.32                     | 0.50              |
| 1:K:205:VAL:HG12 | 1:K:206:ALA:N    | 2.27                     | 0.50              |
| 1:J:519:ALA:CB   | 1:K:454:GLU:HG3  | 2.41                     | 0.50              |
| 1:K:458:VAL:O    | 1:K:475:VAL:C    | 2.49                     | 0.50              |
| 1:L:180:MET:SD   | 1:L:183:ILE:HD11 | 2.51                     | 0.50              |
| 1:M:459:ILE:HD12 | 1:M:459:ILE:N    | 2.27                     | 0.50              |
| 1:O:456:VAL:HG22 | 1:O:457:PRO:N    | 2.26                     | 0.50              |
| 1:O:552:VAL:HG23 | 1:O:553:PRO:C    | 2.32                     | 0.50              |
| 1:F:442:VAL:HG12 | 1:F:448:ALA:HB2  | 1.94                     | 0.49              |
| 1:G:218:ASP:N    | 1:G:221:VAL:HB   | 2.27                     | 0.49              |
| 1:H:205:VAL:HG12 | 1:H:206:ALA:N    | 2.27                     | 0.49              |
| 1:H:218:ASP:N    | 1:H:221:VAL:HB   | 2.27                     | 0.49              |
| 1:I:552:VAL:HG23 | 1:I:553:PRO:C    | 2.32                     | 0.49              |
| 1:L:456:VAL:HG22 | 1:L:457:PRO:N    | 2.26                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:435:LEU:HD11 | 1:M:607:GLN:HE22 | 1.77                     | 0.49              |
| 1:N:459:ILE:N    | 1:N:459:ILE:HD12 | 2.27                     | 0.49              |
| 1:O:321:LEU:CD1  | 1:O:441:THR:OG1  | 2.60                     | 0.49              |
| 1:A:218:ASP:N    | 1:A:221:VAL:HB   | 2.27                     | 0.49              |
| 1:A:506:ASN:O    | 1:A:519:ALA:N    | 2.46                     | 0.49              |
| 1:C:321:LEU:CD1  | 1:C:441:THR:OG1  | 2.60                     | 0.49              |
| 1:C:506:ASN:O    | 1:C:519:ALA:N    | 2.46                     | 0.49              |
| 1:D:477:ARG:N    | 1:D:477:ARG:HD2  | 2.27                     | 0.49              |
| 1:G:442:VAL:HG12 | 1:G:448:ALA:HB2  | 1.94                     | 0.49              |
| 1:G:459:ILE:N    | 1:G:459:ILE:HD12 | 2.27                     | 0.49              |
| 1:H:235:GLU:CD   | 1:H:235:GLU:H    | 2.12                     | 0.49              |
| 1:I:218:ASP:N    | 1:I:221:VAL:HB   | 2.27                     | 0.49              |
| 1:K:459:ILE:N    | 1:K:459:ILE:HD12 | 2.27                     | 0.49              |
| 1:J:435:LEU:HD11 | 1:K:607:GLN:HE22 | 1.77                     | 0.49              |
| 1:M:477:ARG:N    | 1:M:477:ARG:HD2  | 2.27                     | 0.49              |
| 1:N:140:ILE:HD13 | 1:N:156:ILE:CG2  | 2.40                     | 0.49              |
| 1:N:442:VAL:HG12 | 1:N:448:ALA:HB2  | 1.94                     | 0.49              |
| 1:N:477:ARG:CG   | 1:N:477:ARG:NH1  | 2.73                     | 0.49              |
| 1:O:506:ASN:O    | 1:O:519:ALA:N    | 2.46                     | 0.49              |
| 1:O:478:LYS:HD2  | 1:O:518:PHE:CZ   | 2.46                     | 0.49              |
| 1:C:459:ILE:HD12 | 1:C:459:ILE:N    | 2.27                     | 0.49              |
| 1:D:218:ASP:N    | 1:D:221:VAL:HB   | 2.27                     | 0.49              |
| 1:D:506:ASN:O    | 1:D:519:ALA:N    | 2.45                     | 0.49              |
| 1:E:105:VAL:O    | 1:E:140:ILE:CB   | 2.49                     | 0.49              |
| 1:E:218:ASP:N    | 1:E:221:VAL:HB   | 2.27                     | 0.49              |
| 1:E:442:VAL:HG12 | 1:E:448:ALA:HB2  | 1.94                     | 0.49              |
| 1:E:552:VAL:HG23 | 1:E:553:PRO:C    | 2.32                     | 0.49              |
| 1:H:477:ARG:HD2  | 1:H:477:ARG:N    | 2.27                     | 0.49              |
| 1:I:205:VAL:HG12 | 1:I:206:ALA:N    | 2.27                     | 0.49              |
| 1:I:321:LEU:CD1  | 1:I:441:THR:OG1  | 2.60                     | 0.49              |
| 1:I:477:ARG:N    | 1:I:477:ARG:HD2  | 2.27                     | 0.49              |
| 1:I:435:LEU:HD11 | 1:J:607:GLN:HE22 | 1.77                     | 0.49              |
| 1:N:506:ASN:O    | 1:N:519:ALA:N    | 2.45                     | 0.49              |
| 1:O:442:VAL:HG12 | 1:O:448:ALA:HB2  | 1.94                     | 0.49              |
| 1:O:459:ILE:N    | 1:O:459:ILE:HD12 | 2.27                     | 0.49              |
| 1:A:442:VAL:HG12 | 1:A:448:ALA:HB2  | 1.94                     | 0.49              |
| 1:B:459:ILE:CA   | 1:B:474:THR:O    | 2.55                     | 0.49              |
| 1:D:552:VAL:HG23 | 1:D:553:PRO:C    | 2.32                     | 0.49              |
| 1:F:205:VAL:HG12 | 1:F:206:ALA:N    | 2.27                     | 0.49              |
| 1:F:472:PHE:CD1  | 1:F:472:PHE:C    | 2.86                     | 0.49              |
| 1:I:167:ILE:CA   | 1:I:215:ILE:O    | 2.42                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:333:ASP:OD1  | 1:I:334:GLY:N    | 2.44                     | 0.49              |
| 1:J:218:ASP:N    | 1:J:221:VAL:HB   | 2.27                     | 0.49              |
| 1:J:459:ILE:HD12 | 1:J:459:ILE:N    | 2.27                     | 0.49              |
| 1:K:122:LEU:HD23 | 1:K:125:ASN:ND2  | 2.19                     | 0.49              |
| 1:L:218:ASP:N    | 1:L:221:VAL:HB   | 2.27                     | 0.49              |
| 1:L:458:VAL:O    | 1:L:475:VAL:C    | 2.49                     | 0.49              |
| 1:N:205:VAL:HG12 | 1:N:206:ALA:N    | 2.27                     | 0.49              |
| 1:N:218:ASP:N    | 1:N:221:VAL:HB   | 2.27                     | 0.49              |
| 1:O:205:VAL:HG12 | 1:O:206:ALA:N    | 2.27                     | 0.49              |
| 1:B:552:VAL:HG23 | 1:B:553:PRO:C    | 2.32                     | 0.49              |
| 1:F:218:ASP:N    | 1:F:221:VAL:HB   | 2.27                     | 0.49              |
| 1:L:205:VAL:HG12 | 1:L:206:ALA:N    | 2.27                     | 0.49              |
| 1:L:321:LEU:CD1  | 1:L:441:THR:OG1  | 2.60                     | 0.49              |
| 1:N:321:LEU:CD1  | 1:N:441:THR:OG1  | 2.60                     | 0.49              |
| 1:M:519:ALA:CB   | 1:N:454:GLU:HG3  | 2.41                     | 0.49              |
| 1:B:478:LYS:HD2  | 1:B:518:PHE:CZ   | 2.46                     | 0.49              |
| 1:B:586:ILE:HG21 | 1:B:592:ALA:HB2  | 1.95                     | 0.49              |
| 1:C:472:PHE:C    | 1:C:472:PHE:CD1  | 2.86                     | 0.49              |
| 1:C:519:ALA:CB   | 1:D:454:GLU:HG3  | 2.41                     | 0.49              |
| 1:G:177:ALA:N    | 1:G:211:ASN:OD1  | 2.41                     | 0.49              |
| 1:H:122:LEU:HD23 | 1:H:125:ASN:ND2  | 2.19                     | 0.49              |
| 1:H:442:VAL:HG12 | 1:H:448:ALA:HB2  | 1.94                     | 0.49              |
| 1:J:321:LEU:CD1  | 1:J:441:THR:OG1  | 2.60                     | 0.49              |
| 1:J:458:VAL:O    | 1:J:475:VAL:C    | 2.49                     | 0.49              |
| 1:L:177:ALA:N    | 1:L:211:ASN:OD1  | 2.41                     | 0.49              |
| 1:L:442:VAL:HG12 | 1:L:448:ALA:HB2  | 1.94                     | 0.49              |
| 1:M:177:ALA:N    | 1:M:211:ASN:OD1  | 2.41                     | 0.49              |
| 1:M:321:LEU:CD1  | 1:M:441:THR:OG1  | 2.60                     | 0.49              |
| 1:M:442:VAL:HG12 | 1:M:448:ALA:HB2  | 1.95                     | 0.49              |
| 1:B:477:ARG:HD2  | 1:B:477:ARG:N    | 2.27                     | 0.49              |
| 1:H:435:LEU:HD11 | 1:I:607:GLN:HE22 | 1.77                     | 0.49              |
| 1:L:105:VAL:O    | 1:L:140:ILE:CB   | 2.49                     | 0.49              |
| 1:O:218:ASP:N    | 1:O:221:VAL:HB   | 2.27                     | 0.49              |
| 1:B:321:LEU:CD1  | 1:B:441:THR:OG1  | 2.60                     | 0.49              |
| 1:C:586:ILE:HG21 | 1:C:592:ALA:HB2  | 1.95                     | 0.49              |
| 1:I:459:ILE:HD12 | 1:I:459:ILE:N    | 2.27                     | 0.49              |
| 1:K:177:ALA:O    | 1:K:180:MET:N    | 2.46                     | 0.49              |
| 1:K:321:LEU:CD1  | 1:K:441:THR:OG1  | 2.60                     | 0.49              |
| 1:M:177:ALA:O    | 1:M:180:MET:N    | 2.46                     | 0.49              |
| 1:M:435:LEU:HD11 | 1:N:607:GLN:HE22 | 1.77                     | 0.49              |
| 1:O:472:PHE:CD1  | 1:O:472:PHE:C    | 2.86                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:477:ARG:N    | 1:O:477:ARG:HD2  | 2.27                     | 0.49              |
| 1:A:586:ILE:HG21 | 1:A:592:ALA:HB2  | 1.95                     | 0.49              |
| 1:B:442:VAL:HG12 | 1:B:448:ALA:HB2  | 1.94                     | 0.49              |
| 1:B:506:ASN:O    | 1:B:519:ALA:N    | 2.45                     | 0.49              |
| 1:D:442:VAL:HG12 | 1:D:448:ALA:HB2  | 1.94                     | 0.49              |
| 1:E:506:ASN:O    | 1:E:519:ALA:N    | 2.45                     | 0.49              |
| 1:K:374:GLN:HG3  | 1:L:392:THR:O    | 2.13                     | 0.49              |
| 1:K:442:VAL:HG12 | 1:K:448:ALA:HB2  | 1.94                     | 0.49              |
| 1:A:459:ILE:HD12 | 1:A:459:ILE:N    | 2.27                     | 0.49              |
| 1:G:205:VAL:HG12 | 1:G:206:ALA:N    | 2.27                     | 0.49              |
| 1:G:477:ARG:N    | 1:G:477:ARG:HD2  | 2.27                     | 0.49              |
| 1:G:374:GLN:HG3  | 1:H:392:THR:O    | 2.13                     | 0.49              |
| 1:H:477:ARG:CG   | 1:H:477:ARG:NH1  | 2.73                     | 0.49              |
| 1:I:177:ALA:O    | 1:I:180:MET:N    | 2.46                     | 0.49              |
| 1:H:374:GLN:HG3  | 1:I:392:THR:O    | 2.13                     | 0.49              |
| 1:I:506:ASN:O    | 1:I:519:ALA:N    | 2.46                     | 0.49              |
| 1:K:218:ASP:N    | 1:K:221:VAL:HB   | 2.27                     | 0.49              |
| 1:L:374:GLN:HG3  | 1:M:392:THR:O    | 2.13                     | 0.49              |
| 1:L:477:ARG:HD2  | 1:L:477:ARG:N    | 2.27                     | 0.49              |
| 1:O:177:ALA:O    | 1:O:180:MET:N    | 2.46                     | 0.49              |
| 1:A:552:VAL:HG23 | 1:A:553:PRO:C    | 2.32                     | 0.48              |
| 1:C:552:VAL:HG23 | 1:C:553:PRO:C    | 2.32                     | 0.48              |
| 1:E:472:PHE:C    | 1:E:472:PHE:CD1  | 2.86                     | 0.48              |
| 1:G:506:ASN:O    | 1:G:519:ALA:N    | 2.46                     | 0.48              |
| 1:K:177:ALA:N    | 1:K:211:ASN:OD1  | 2.41                     | 0.48              |
| 1:K:459:ILE:CA   | 1:K:474:THR:O    | 2.55                     | 0.48              |
| 1:K:506:ASN:O    | 1:K:519:ALA:N    | 2.46                     | 0.48              |
| 1:L:177:ALA:O    | 1:L:180:MET:N    | 2.46                     | 0.48              |
| 1:M:218:ASP:N    | 1:M:221:VAL:HB   | 2.27                     | 0.48              |
| 1:M:374:GLN:HG3  | 1:N:392:THR:O    | 2.13                     | 0.48              |
| 1:N:374:GLN:HG3  | 1:O:392:THR:O    | 2.13                     | 0.48              |
| 1:N:374:GLN:O    | 1:N:391:THR:HG22 | 2.13                     | 0.48              |
| 1:B:472:PHE:C    | 1:B:472:PHE:CD1  | 2.86                     | 0.48              |
| 1:D:458:VAL:O    | 1:D:475:VAL:C    | 2.49                     | 0.48              |
| 1:F:113:ARG:HD2  | 1:F:134:TYR:HD2  | 1.79                     | 0.48              |
| 1:F:374:GLN:O    | 1:F:391:THR:HG22 | 2.14                     | 0.48              |
| 1:G:479:GLU:CD   | 1:G:479:GLU:H    | 2.07                     | 0.48              |
| 1:H:458:VAL:O    | 1:H:475:VAL:C    | 2.49                     | 0.48              |
| 1:I:442:VAL:HG12 | 1:I:448:ALA:HB2  | 1.94                     | 0.48              |
| 1:L:506:ASN:O    | 1:L:519:ALA:N    | 2.45                     | 0.48              |
| 1:M:113:ARG:HD2  | 1:M:134:TYR:HD2  | 1.79                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:177:ALA:O    | 1:N:180:MET:N    | 2.46                     | 0.48              |
| 1:N:177:ALA:N    | 1:N:211:ASN:OD1  | 2.41                     | 0.48              |
| 1:B:207:ASP:OD1  | 1:B:209:ARG:N    | 2.33                     | 0.48              |
| 1:C:374:GLN:O    | 1:C:391:THR:HG22 | 2.13                     | 0.48              |
| 1:D:435:LEU:HD11 | 1:E:607:GLN:HE22 | 1.77                     | 0.48              |
| 1:F:506:ASN:O    | 1:F:519:ALA:N    | 2.45                     | 0.48              |
| 1:H:459:ILE:N    | 1:H:459:ILE:HD12 | 2.27                     | 0.48              |
| 1:J:374:GLN:HG3  | 1:K:392:THR:O    | 2.13                     | 0.48              |
| 1:M:472:PHE:C    | 1:M:472:PHE:CD1  | 2.86                     | 0.48              |
| 1:A:321:LEU:CD1  | 1:A:441:THR:OG1  | 2.60                     | 0.48              |
| 1:C:113:ARG:HD2  | 1:C:134:TYR:HD2  | 1.79                     | 0.48              |
| 1:D:586:ILE:HG21 | 1:D:592:ALA:HB2  | 1.95                     | 0.48              |
| 1:G:113:ARG:HD2  | 1:G:134:TYR:HD2  | 1.79                     | 0.48              |
| 1:H:113:ARG:HD2  | 1:H:134:TYR:HD2  | 1.79                     | 0.48              |
| 1:I:458:VAL:O    | 1:I:475:VAL:C    | 2.49                     | 0.48              |
| 1:J:177:ALA:O    | 1:J:180:MET:N    | 2.46                     | 0.48              |
| 1:J:442:VAL:HG12 | 1:J:448:ALA:HB2  | 1.94                     | 0.48              |
| 1:J:477:ARG:HD2  | 1:J:477:ARG:N    | 2.27                     | 0.48              |
| 1:L:113:ARG:HD2  | 1:L:134:TYR:HD2  | 1.79                     | 0.48              |
| 1:M:506:ASN:O    | 1:M:519:ALA:N    | 2.46                     | 0.48              |
| 1:N:477:ARG:HD2  | 1:N:477:ARG:N    | 2.27                     | 0.48              |
| 1:O:586:ILE:HG21 | 1:O:592:ALA:HB2  | 1.95                     | 0.48              |
| 1:A:472:PHE:C    | 1:A:472:PHE:CD1  | 2.86                     | 0.48              |
| 1:A:435:LEU:HD11 | 1:B:607:GLN:HE22 | 1.77                     | 0.48              |
| 1:D:519:ALA:CB   | 1:E:454:GLU:HG3  | 2.41                     | 0.48              |
| 1:H:177:ALA:O    | 1:H:180:MET:N    | 2.46                     | 0.48              |
| 1:I:374:GLN:HG3  | 1:J:392:THR:O    | 2.13                     | 0.48              |
| 1:K:504:VAL:HG12 | 1:K:521:ARG:HG2  | 1.94                     | 0.48              |
| 1:O:113:ARG:HD2  | 1:O:134:TYR:HD2  | 1.79                     | 0.48              |
| 1:O:180:MET:HE2  | 1:O:213:ILE:HD11 | 1.94                     | 0.48              |
| 1:A:392:THR:O    | 1:O:374:GLN:HG3  | 2.13                     | 0.48              |
| 1:O:374:GLN:O    | 1:O:391:THR:HG22 | 2.14                     | 0.48              |
| 1:B:374:GLN:O    | 1:B:391:THR:HG22 | 2.14                     | 0.48              |
| 1:C:435:LEU:HD11 | 1:D:607:GLN:HE22 | 1.77                     | 0.48              |
| 1:E:374:GLN:O    | 1:E:391:THR:HG22 | 2.13                     | 0.48              |
| 1:E:477:ARG:N    | 1:E:477:ARG:HD2  | 2.27                     | 0.48              |
| 1:G:119:LEU:HD12 | 1:G:134:TYR:OH   | 2.14                     | 0.48              |
| 1:G:235:GLU:H    | 1:G:235:GLU:CD   | 2.11                     | 0.48              |
| 1:G:477:ARG:CG   | 1:G:477:ARG:NH1  | 2.73                     | 0.48              |
| 1:H:119:LEU:HD12 | 1:H:134:TYR:OH   | 2.14                     | 0.48              |
| 1:H:506:ASN:O    | 1:H:519:ALA:N    | 2.45                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:374:GLN:O    | 1:I:391:THR:HG22 | 2.14                     | 0.48              |
| 1:K:374:GLN:O    | 1:K:391:THR:HG22 | 2.14                     | 0.48              |
| 1:M:458:VAL:O    | 1:M:475:VAL:C    | 2.49                     | 0.48              |
| 1:M:477:ARG:NH1  | 1:M:477:ARG:CG   | 2.73                     | 0.48              |
| 1:A:113:ARG:HD2  | 1:A:134:TYR:HD2  | 1.79                     | 0.48              |
| 1:A:177:ALA:O    | 1:A:180:MET:N    | 2.46                     | 0.48              |
| 1:F:235:GLU:CD   | 1:F:235:GLU:H    | 2.11                     | 0.48              |
| 1:F:479:GLU:H    | 1:F:479:GLU:CD   | 2.07                     | 0.48              |
| 1:G:177:ALA:O    | 1:G:180:MET:N    | 2.46                     | 0.48              |
| 1:H:374:GLN:O    | 1:H:391:THR:HG22 | 2.13                     | 0.48              |
| 1:J:113:ARG:HD2  | 1:J:134:TYR:HD2  | 1.79                     | 0.48              |
| 1:J:506:ASN:O    | 1:J:519:ALA:N    | 2.46                     | 0.48              |
| 1:K:113:ARG:HD2  | 1:K:134:TYR:HD2  | 1.79                     | 0.48              |
| 1:L:374:GLN:O    | 1:L:391:THR:HG22 | 2.14                     | 0.48              |
| 1:A:225:LEU:HD23 | 1:A:225:LEU:HA   | 1.74                     | 0.48              |
| 1:A:247:LEU:HD11 | 1:A:294:LEU:HD23 | 1.96                     | 0.48              |
| 1:B:177:ALA:O    | 1:B:180:MET:N    | 2.46                     | 0.48              |
| 1:C:442:VAL:HG12 | 1:C:448:ALA:HB2  | 1.94                     | 0.48              |
| 1:E:113:ARG:HD2  | 1:E:134:TYR:HD2  | 1.79                     | 0.48              |
| 1:F:119:LEU:HD12 | 1:F:134:TYR:OH   | 2.14                     | 0.48              |
| 1:G:458:VAL:O    | 1:G:475:VAL:C    | 2.49                     | 0.48              |
| 1:L:122:LEU:HD23 | 1:L:125:ASN:ND2  | 2.19                     | 0.48              |
| 1:J:335:ILE:HG22 | 1:L:617:LEU:HD13 | 1.96                     | 0.48              |
| 1:M:586:ILE:HG21 | 1:M:592:ALA:HB2  | 1.95                     | 0.48              |
| 1:K:335:ILE:HG22 | 1:M:617:LEU:HD13 | 1.96                     | 0.48              |
| 1:N:108:LYS:HA   | 1:N:138:ASN:ND2  | 2.29                     | 0.48              |
| 1:N:435:LEU:HD11 | 1:O:607:GLN:HE22 | 1.77                     | 0.48              |
| 1:N:458:VAL:O    | 1:N:475:VAL:C    | 2.49                     | 0.48              |
| 1:A:108:LYS:HA   | 1:A:138:ASN:ND2  | 2.29                     | 0.48              |
| 1:A:374:GLN:HG3  | 1:B:392:THR:O    | 2.13                     | 0.48              |
| 1:A:261:GLY:HA3  | 1:B:284:MET:HG2  | 1.96                     | 0.48              |
| 1:B:459:ILE:HD12 | 1:B:459:ILE:N    | 2.27                     | 0.48              |
| 1:C:247:LEU:HD11 | 1:C:294:LEU:HD23 | 1.96                     | 0.48              |
| 1:B:435:LEU:HD11 | 1:C:607:GLN:HE22 | 1.77                     | 0.48              |
| 1:E:435:LEU:HD11 | 1:F:607:GLN:HE22 | 1.77                     | 0.48              |
| 1:H:108:LYS:HA   | 1:H:138:ASN:ND2  | 2.29                     | 0.48              |
| 1:I:108:LYS:HA   | 1:I:138:ASN:ND2  | 2.29                     | 0.48              |
| 1:I:119:LEU:HD12 | 1:I:134:TYR:OH   | 2.14                     | 0.48              |
| 1:I:247:LEU:HD11 | 1:I:294:LEU:HD23 | 1.96                     | 0.48              |
| 1:I:335:ILE:HG22 | 1:K:617:LEU:HD13 | 1.96                     | 0.48              |
| 1:J:108:LYS:HA   | 1:J:138:ASN:ND2  | 2.29                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:472:PHE:CD1  | 1:J:472:PHE:C    | 2.86                     | 0.48              |
| 1:K:247:LEU:HD11 | 1:K:294:LEU:HD23 | 1.96                     | 0.48              |
| 1:L:586:ILE:HG21 | 1:L:592:ALA:HB2  | 1.95                     | 0.48              |
| 1:M:180:MET:HE2  | 1:M:213:ILE:HD11 | 1.95                     | 0.48              |
| 1:N:247:LEU:HD11 | 1:N:294:LEU:HD23 | 1.96                     | 0.48              |
| 1:O:108:LYS:HA   | 1:O:138:ASN:ND2  | 2.29                     | 0.48              |
| 1:B:108:LYS:HA   | 1:B:138:ASN:ND2  | 2.29                     | 0.48              |
| 1:B:226:LYS:HA   | 1:B:229:ILE:HB   | 1.96                     | 0.48              |
| 1:B:374:GLN:HG3  | 1:C:392:THR:O    | 2.13                     | 0.48              |
| 1:D:113:ARG:HD2  | 1:D:134:TYR:HD2  | 1.78                     | 0.48              |
| 1:D:374:GLN:HG3  | 1:E:392:THR:O    | 2.13                     | 0.48              |
| 1:E:255:LEU:HA   | 1:E:255:LEU:HD23 | 1.73                     | 0.48              |
| 1:F:283:VAL:HA   | 1:F:297:THR:O    | 2.14                     | 0.48              |
| 1:G:108:LYS:HA   | 1:G:138:ASN:ND2  | 2.29                     | 0.48              |
| 1:G:261:GLY:HA3  | 1:H:284:MET:HG2  | 1.96                     | 0.48              |
| 1:F:435:LEU:HD11 | 1:G:607:GLN:HE22 | 1.77                     | 0.48              |
| 1:I:472:PHE:C    | 1:I:472:PHE:CD1  | 2.86                     | 0.48              |
| 1:G:335:ILE:HG22 | 1:I:617:LEU:HD13 | 1.96                     | 0.48              |
| 1:J:478:LYS:HD2  | 1:J:518:PHE:HZ   | 1.79                     | 0.48              |
| 1:H:335:ILE:HG22 | 1:J:617:LEU:HD13 | 1.96                     | 0.48              |
| 1:K:586:ILE:HG21 | 1:K:592:ALA:HB2  | 1.95                     | 0.48              |
| 1:L:119:LEU:HD12 | 1:L:134:TYR:OH   | 2.14                     | 0.48              |
| 1:L:335:ILE:HG22 | 1:N:617:LEU:HD13 | 1.96                     | 0.48              |
| 1:L:478:LYS:HD2  | 1:L:518:PHE:HZ   | 1.79                     | 0.48              |
| 1:N:235:GLU:H    | 1:N:235:GLU:CD   | 2.11                     | 0.48              |
| 1:A:284:MET:HG2  | 1:O:261:GLY:HA3  | 1.96                     | 0.48              |
| 1:C:177:ALA:O    | 1:C:180:MET:N    | 2.46                     | 0.47              |
| 1:C:374:GLN:HG3  | 1:D:392:THR:O    | 2.13                     | 0.47              |
| 1:D:226:LYS:HA   | 1:D:229:ILE:HB   | 1.96                     | 0.47              |
| 1:D:472:PHE:C    | 1:D:472:PHE:CD1  | 2.86                     | 0.47              |
| 1:E:235:GLU:H    | 1:E:235:GLU:CD   | 2.11                     | 0.47              |
| 1:E:374:GLN:HG3  | 1:F:392:THR:O    | 2.13                     | 0.47              |
| 1:G:283:VAL:HA   | 1:G:297:THR:O    | 2.14                     | 0.47              |
| 1:H:261:GLY:HA3  | 1:I:284:MET:HG2  | 1.96                     | 0.47              |
| 1:M:119:LEU:HD12 | 1:M:134:TYR:OH   | 2.14                     | 0.47              |
| 1:M:235:GLU:CD   | 1:M:235:GLU:H    | 2.11                     | 0.47              |
| 1:M:374:GLN:O    | 1:M:391:THR:HG22 | 2.13                     | 0.47              |
| 1:O:328:GLU:HG2  | 1:O:577:LEU:HG   | 1.96                     | 0.47              |
| 1:O:458:VAL:O    | 1:O:475:VAL:C    | 2.49                     | 0.47              |
| 1:A:607:GLN:HE22 | 1:O:435:LEU:HD11 | 1.77                     | 0.47              |
| 1:B:261:GLY:HA3  | 1:C:284:MET:HG2  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:477:ARG:N    | 1:C:477:ARG:HD2  | 2.27                     | 0.47              |
| 1:D:177:ALA:O    | 1:D:180:MET:N    | 2.46                     | 0.47              |
| 1:E:283:VAL:HA   | 1:E:297:THR:O    | 2.14                     | 0.47              |
| 1:C:335:ILE:HG22 | 1:E:617:LEU:HD13 | 1.95                     | 0.47              |
| 1:F:122:LEU:HD23 | 1:F:125:ASN:ND2  | 2.19                     | 0.47              |
| 1:F:261:GLY:HA3  | 1:G:284:MET:HG2  | 1.96                     | 0.47              |
| 1:F:374:GLN:HG3  | 1:G:392:THR:O    | 2.13                     | 0.47              |
| 1:G:374:GLN:O    | 1:G:391:THR:HG22 | 2.14                     | 0.47              |
| 1:H:586:ILE:HG21 | 1:H:592:ALA:HB2  | 1.95                     | 0.47              |
| 1:I:261:GLY:HA3  | 1:J:284:MET:HG2  | 1.96                     | 0.47              |
| 1:I:239:LYS:HE3  | 1:I:300:GLN:HB2  | 1.97                     | 0.47              |
| 1:I:586:ILE:HG21 | 1:I:592:ALA:HB2  | 1.95                     | 0.47              |
| 1:J:177:ALA:N    | 1:J:211:ASN:OD1  | 2.41                     | 0.47              |
| 1:M:207:ASP:OD1  | 1:M:209:ARG:N    | 2.33                     | 0.47              |
| 1:M:457:PRO:HA   | 1:M:477:ARG:HE   | 1.79                     | 0.47              |
| 1:N:113:ARG:HD2  | 1:N:134:TYR:HD2  | 1.79                     | 0.47              |
| 1:N:283:VAL:HA   | 1:N:297:THR:O    | 2.14                     | 0.47              |
| 1:N:457:PRO:HA   | 1:N:477:ARG:HE   | 1.80                     | 0.47              |
| 1:A:328:GLU:HG2  | 1:A:577:LEU:HG   | 1.96                     | 0.47              |
| 1:A:477:ARG:N    | 1:A:477:ARG:HD2  | 2.27                     | 0.47              |
| 1:D:374:GLN:O    | 1:D:391:THR:HG22 | 2.13                     | 0.47              |
| 1:E:119:LEU:HD12 | 1:E:134:TYR:OH   | 2.14                     | 0.47              |
| 1:E:247:LEU:HD11 | 1:E:294:LEU:HD23 | 1.96                     | 0.47              |
| 1:G:435:LEU:HD11 | 1:H:607:GLN:HE22 | 1.77                     | 0.47              |
| 1:F:335:ILE:HG22 | 1:H:617:LEU:HD13 | 1.96                     | 0.47              |
| 1:J:119:LEU:HD12 | 1:J:134:TYR:OH   | 2.14                     | 0.47              |
| 1:J:239:LYS:HE3  | 1:J:300:GLN:HB2  | 1.97                     | 0.47              |
| 1:J:374:GLN:O    | 1:J:391:THR:HG22 | 2.14                     | 0.47              |
| 1:J:586:ILE:HG21 | 1:J:592:ALA:HB2  | 1.95                     | 0.47              |
| 1:K:108:LYS:HA   | 1:K:138:ASN:ND2  | 2.29                     | 0.47              |
| 1:K:477:ARG:CG   | 1:K:477:ARG:NH1  | 2.73                     | 0.47              |
| 1:K:634:ARG:HG3  | 1:K:635:HIS:O    | 2.15                     | 0.47              |
| 1:M:167:ILE:CA   | 1:M:215:ILE:O    | 2.42                     | 0.47              |
| 1:M:283:VAL:HA   | 1:M:297:THR:O    | 2.14                     | 0.47              |
| 1:M:247:LEU:HD11 | 1:M:294:LEU:HD23 | 1.96                     | 0.47              |
| 1:C:283:VAL:HA   | 1:C:297:THR:O    | 2.14                     | 0.47              |
| 1:C:457:PRO:HA   | 1:C:477:ARG:HE   | 1.80                     | 0.47              |
| 1:D:457:PRO:HA   | 1:D:477:ARG:HE   | 1.80                     | 0.47              |
| 1:D:507:VAL:HG22 | 1:D:508:LEU:N    | 2.29                     | 0.47              |
| 1:B:335:ILE:HG22 | 1:D:617:LEU:HD13 | 1.96                     | 0.47              |
| 1:E:177:ALA:O    | 1:E:180:MET:N    | 2.46                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:586:ILE:HG21 | 1:E:592:ALA:HB2  | 1.95                     | 0.47              |
| 1:F:108:LYS:HA   | 1:F:138:ASN:ND2  | 2.29                     | 0.47              |
| 1:F:226:LYS:HA   | 1:F:229:ILE:HB   | 1.96                     | 0.47              |
| 1:F:239:LYS:HE3  | 1:F:300:GLN:HB2  | 1.97                     | 0.47              |
| 1:F:457:PRO:HA   | 1:F:477:ARG:HE   | 1.80                     | 0.47              |
| 1:F:507:VAL:HG22 | 1:F:508:LEU:N    | 2.29                     | 0.47              |
| 1:G:247:LEU:HD11 | 1:G:294:LEU:HD23 | 1.96                     | 0.47              |
| 1:G:239:LYS:HE3  | 1:G:300:GLN:HB2  | 1.97                     | 0.47              |
| 1:G:457:PRO:HA   | 1:G:477:ARG:HE   | 1.79                     | 0.47              |
| 1:I:113:ARG:HD2  | 1:I:134:TYR:HD2  | 1.78                     | 0.47              |
| 1:J:167:ILE:CA   | 1:J:215:ILE:O    | 2.42                     | 0.47              |
| 1:L:108:LYS:HA   | 1:L:138:ASN:ND2  | 2.29                     | 0.47              |
| 1:L:457:PRO:HA   | 1:L:477:ARG:HE   | 1.80                     | 0.47              |
| 1:O:235:GLU:H    | 1:O:235:GLU:CD   | 2.11                     | 0.47              |
| 1:N:261:GLY:HA3  | 1:O:284:MET:HG2  | 1.96                     | 0.47              |
| 1:A:120:ARG:HG2  | 1:A:123:ILE:HD12 | 1.96                     | 0.47              |
| 1:A:122:LEU:HD23 | 1:A:125:ASN:ND2  | 2.19                     | 0.47              |
| 1:A:226:LYS:HA   | 1:A:229:ILE:HB   | 1.96                     | 0.47              |
| 1:A:457:PRO:HA   | 1:A:477:ARG:HE   | 1.79                     | 0.47              |
| 1:B:119:LEU:HD12 | 1:B:134:TYR:OH   | 2.14                     | 0.47              |
| 1:C:108:LYS:HA   | 1:C:138:ASN:ND2  | 2.29                     | 0.47              |
| 1:D:235:GLU:CD   | 1:D:235:GLU:H    | 2.12                     | 0.47              |
| 1:D:283:VAL:HA   | 1:D:297:THR:O    | 2.14                     | 0.47              |
| 1:D:634:ARG:HG3  | 1:D:635:HIS:O    | 2.15                     | 0.47              |
| 1:F:177:ALA:N    | 1:F:211:ASN:OD1  | 2.41                     | 0.47              |
| 1:D:335:ILE:HG22 | 1:F:617:LEU:HD13 | 1.95                     | 0.47              |
| 1:G:158:ARG:O    | 1:G:162:ALA:HB2  | 2.15                     | 0.47              |
| 1:G:586:ILE:HG21 | 1:G:592:ALA:HB2  | 1.95                     | 0.47              |
| 1:H:283:VAL:HA   | 1:H:297:THR:O    | 2.14                     | 0.47              |
| 1:I:328:GLU:HG2  | 1:I:577:LEU:HG   | 1.96                     | 0.47              |
| 1:J:261:GLY:HA3  | 1:K:284:MET:HG2  | 1.96                     | 0.47              |
| 1:L:235:GLU:H    | 1:L:235:GLU:CD   | 2.11                     | 0.47              |
| 1:L:239:LYS:HE3  | 1:L:300:GLN:HB2  | 1.97                     | 0.47              |
| 1:L:472:PHE:CD1  | 1:L:472:PHE:C    | 2.86                     | 0.47              |
| 1:L:634:ARG:HG3  | 1:L:635:HIS:O    | 2.15                     | 0.47              |
| 1:M:239:LYS:HE3  | 1:M:300:GLN:HB2  | 1.97                     | 0.47              |
| 1:M:335:ILE:HG22 | 1:O:617:LEU:HD13 | 1.96                     | 0.47              |
| 1:N:119:LEU:HD12 | 1:N:134:TYR:OH   | 2.14                     | 0.47              |
| 1:N:158:ARG:O    | 1:N:162:ALA:HB2  | 2.15                     | 0.47              |
| 1:N:459:ILE:CA   | 1:N:474:THR:O    | 2.55                     | 0.47              |
| 1:N:586:ILE:HG21 | 1:N:592:ALA:HB2  | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:283:VAL:HA   | 1:O:297:THR:O    | 2.14                     | 0.47              |
| 1:O:457:PRO:HA   | 1:O:477:ARG:HE   | 1.80                     | 0.47              |
| 1:A:235:GLU:CD   | 1:A:235:GLU:H    | 2.11                     | 0.47              |
| 1:A:374:GLN:O    | 1:A:391:THR:HG22 | 2.14                     | 0.47              |
| 1:B:120:ARG:HG2  | 1:B:123:ILE:HD12 | 1.96                     | 0.47              |
| 1:B:507:VAL:HG22 | 1:B:508:LEU:N    | 2.29                     | 0.47              |
| 1:C:226:LYS:HA   | 1:C:229:ILE:HB   | 1.96                     | 0.47              |
| 1:C:235:GLU:CD   | 1:C:235:GLU:H    | 2.11                     | 0.47              |
| 1:C:261:GLY:HA3  | 1:D:284:MET:HG2  | 1.96                     | 0.47              |
| 1:E:479:GLU:H    | 1:E:479:GLU:CD   | 2.07                     | 0.47              |
| 1:F:477:ARG:NH1  | 1:F:477:ARG:CG   | 2.73                     | 0.47              |
| 1:F:634:ARG:HG3  | 1:F:635:HIS:O    | 2.15                     | 0.47              |
| 1:H:158:ARG:O    | 1:H:162:ALA:HB2  | 2.15                     | 0.47              |
| 1:H:239:LYS:HE3  | 1:H:300:GLN:HB2  | 1.97                     | 0.47              |
| 1:J:504:VAL:HG12 | 1:J:521:ARG:HG2  | 1.94                     | 0.47              |
| 1:J:634:ARG:HG3  | 1:J:635:HIS:O    | 2.15                     | 0.47              |
| 1:K:119:LEU:HD12 | 1:K:134:TYR:OH   | 2.14                     | 0.47              |
| 1:K:239:LYS:HE3  | 1:K:300:GLN:HB2  | 1.97                     | 0.47              |
| 1:L:247:LEU:HD11 | 1:L:294:LEU:HD23 | 1.96                     | 0.47              |
| 1:N:226:LYS:HA   | 1:N:229:ILE:HB   | 1.96                     | 0.47              |
| 1:N:328:GLU:HG2  | 1:N:577:LEU:HG   | 1.96                     | 0.47              |
| 1:O:158:ARG:O    | 1:O:162:ALA:HB2  | 2.15                     | 0.47              |
| 1:A:105:VAL:O    | 1:A:140:ILE:CB   | 2.49                     | 0.47              |
| 1:A:119:LEU:HD12 | 1:A:134:TYR:OH   | 2.14                     | 0.47              |
| 1:A:335:ILE:HG22 | 1:C:617:LEU:HD13 | 1.96                     | 0.47              |
| 1:B:113:ARG:HD2  | 1:B:134:TYR:HD2  | 1.79                     | 0.47              |
| 1:D:478:LYS:HD2  | 1:D:518:PHE:HZ   | 1.79                     | 0.47              |
| 1:E:108:LYS:HA   | 1:E:138:ASN:ND2  | 2.29                     | 0.47              |
| 1:E:335:ILE:HG22 | 1:G:617:LEU:HD13 | 1.95                     | 0.47              |
| 1:E:478:LYS:HD2  | 1:E:518:PHE:HZ   | 1.79                     | 0.47              |
| 1:F:177:ALA:O    | 1:F:180:MET:N    | 2.46                     | 0.47              |
| 1:G:478:LYS:HD2  | 1:G:518:PHE:HZ   | 1.79                     | 0.47              |
| 1:I:283:VAL:HA   | 1:I:297:THR:O    | 2.14                     | 0.47              |
| 1:I:457:PRO:HA   | 1:I:477:ARG:HE   | 1.80                     | 0.47              |
| 1:J:120:ARG:HG2  | 1:J:123:ILE:HD12 | 1.96                     | 0.47              |
| 1:K:457:PRO:HA   | 1:K:477:ARG:HE   | 1.80                     | 0.47              |
| 1:M:108:LYS:HA   | 1:M:138:ASN:ND2  | 2.29                     | 0.47              |
| 1:N:207:ASP:OD1  | 1:N:209:ARG:N    | 2.33                     | 0.47              |
| 1:O:120:ARG:HG2  | 1:O:123:ILE:HD12 | 1.96                     | 0.47              |
| 1:B:617:LEU:HD13 | 1:O:335:ILE:HG22 | 1.96                     | 0.47              |
| 1:O:478:LYS:HD2  | 1:O:518:PHE:HZ   | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:105:VAL:O    | 1:B:140:ILE:CB   | 2.49                     | 0.47              |
| 1:B:235:GLU:CD   | 1:B:235:GLU:H    | 2.11                     | 0.47              |
| 1:B:283:VAL:HA   | 1:B:297:THR:O    | 2.14                     | 0.47              |
| 1:B:478:LYS:HD2  | 1:B:518:PHE:HZ   | 1.79                     | 0.47              |
| 1:B:634:ARG:HG3  | 1:B:635:HIS:O    | 2.15                     | 0.47              |
| 1:C:119:LEU:HD12 | 1:C:134:TYR:OH   | 2.14                     | 0.47              |
| 1:J:226:LYS:HA   | 1:J:229:ILE:HB   | 1.96                     | 0.47              |
| 1:J:457:PRO:HA   | 1:J:477:ARG:HE   | 1.79                     | 0.47              |
| 1:K:120:ARG:HG2  | 1:K:123:ILE:HD12 | 1.96                     | 0.47              |
| 1:K:261:GLY:HA3  | 1:L:284:MET:HG2  | 1.96                     | 0.47              |
| 1:L:207:ASP:OD1  | 1:L:209:ARG:N    | 2.33                     | 0.47              |
| 1:L:283:VAL:HA   | 1:L:297:THR:O    | 2.14                     | 0.47              |
| 1:A:617:LEU:HD13 | 1:N:335:ILE:HG22 | 1.95                     | 0.47              |
| 1:O:167:ILE:CA   | 1:O:215:ILE:O    | 2.42                     | 0.47              |
| 1:A:634:ARG:HG3  | 1:A:635:HIS:O    | 2.15                     | 0.47              |
| 1:B:328:GLU:HG2  | 1:B:577:LEU:HG   | 1.96                     | 0.47              |
| 1:B:457:PRO:HA   | 1:B:477:ARG:HE   | 1.79                     | 0.47              |
| 1:C:120:ARG:HG2  | 1:C:123:ILE:HD12 | 1.96                     | 0.47              |
| 1:C:180:MET:HE2  | 1:C:213:ILE:HD11 | 1.97                     | 0.47              |
| 1:D:180:MET:HE2  | 1:D:213:ILE:HD11 | 1.97                     | 0.47              |
| 1:E:239:LYS:HE3  | 1:E:300:GLN:HB2  | 1.97                     | 0.47              |
| 1:E:261:GLY:HA3  | 1:F:284:MET:HG2  | 1.96                     | 0.47              |
| 1:F:586:ILE:HG21 | 1:F:592:ALA:HB2  | 1.95                     | 0.47              |
| 1:H:472:PHE:CD1  | 1:H:472:PHE:C    | 2.86                     | 0.47              |
| 1:H:328:GLU:HG2  | 1:H:577:LEU:HG   | 1.96                     | 0.47              |
| 1:I:120:ARG:HG2  | 1:I:123:ILE:HD12 | 1.96                     | 0.47              |
| 1:I:478:LYS:HD2  | 1:I:518:PHE:HZ   | 1.79                     | 0.47              |
| 1:K:328:GLU:HG2  | 1:K:577:LEU:HG   | 1.96                     | 0.47              |
| 1:M:158:ARG:O    | 1:M:162:ALA:HB2  | 2.15                     | 0.47              |
| 1:N:478:LYS:HD2  | 1:N:518:PHE:HZ   | 1.79                     | 0.47              |
| 1:A:478:LYS:HD2  | 1:A:518:PHE:HZ   | 1.79                     | 0.47              |
| 1:B:182:ARG:HA   | 1:B:185:GLU:CD   | 2.36                     | 0.47              |
| 1:B:450:PHE:O    | 1:B:483:LYS:HA   | 2.15                     | 0.47              |
| 1:B:504:VAL:HG12 | 1:B:521:ARG:HG2  | 1.94                     | 0.47              |
| 1:C:158:ARG:O    | 1:C:162:ALA:HB2  | 2.15                     | 0.47              |
| 1:D:119:LEU:HD12 | 1:D:134:TYR:OH   | 2.14                     | 0.47              |
| 1:E:328:GLU:HG2  | 1:E:577:LEU:HG   | 1.96                     | 0.47              |
| 1:G:481:GLY:N    | 1:G:505:SER:OG   | 2.23                     | 0.47              |
| 1:I:438:PRO:HB3  | 1:I:450:PHE:CE2  | 2.50                     | 0.47              |
| 1:J:438:PRO:HB3  | 1:J:450:PHE:CE2  | 2.50                     | 0.47              |
| 1:J:328:GLU:HG2  | 1:J:577:LEU:HG   | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:283:VAL:HA   | 1:K:297:THR:O    | 2.14                     | 0.47              |
| 1:K:438:PRO:HB3  | 1:K:450:PHE:CE2  | 2.50                     | 0.47              |
| 1:K:476:ASP:OD1  | 1:K:476:ASP:N    | 2.48                     | 0.47              |
| 1:L:158:ARG:O    | 1:L:162:ALA:HB2  | 2.15                     | 0.47              |
| 1:M:122:LEU:HD23 | 1:M:125:ASN:ND2  | 2.19                     | 0.47              |
| 1:N:239:LYS:HE3  | 1:N:300:GLN:HB2  | 1.97                     | 0.47              |
| 1:O:119:LEU:HD12 | 1:O:134:TYR:OH   | 2.14                     | 0.47              |
| 1:A:102:THR:OG1  | 1:A:142:ILE:O    | 2.25                     | 0.47              |
| 1:A:182:ARG:HA   | 1:A:185:GLU:CD   | 2.36                     | 0.47              |
| 1:B:247:LEU:HD11 | 1:B:294:LEU:HD23 | 1.96                     | 0.47              |
| 1:C:634:ARG:HG3  | 1:C:635:HIS:O    | 2.15                     | 0.47              |
| 1:D:108:LYS:HA   | 1:D:138:ASN:ND2  | 2.29                     | 0.47              |
| 1:D:158:ARG:O    | 1:D:162:ALA:HB2  | 2.15                     | 0.47              |
| 1:D:247:LEU:HD11 | 1:D:294:LEU:HD23 | 1.96                     | 0.47              |
| 1:D:328:GLU:HG2  | 1:D:577:LEU:HG   | 1.96                     | 0.47              |
| 1:E:458:VAL:O    | 1:E:475:VAL:C    | 2.49                     | 0.47              |
| 1:F:450:PHE:O    | 1:F:483:LYS:HA   | 2.15                     | 0.47              |
| 1:G:328:GLU:HG2  | 1:G:577:LEU:HG   | 1.96                     | 0.47              |
| 1:H:207:ASP:O    | 1:H:211:ASN:HA   | 2.16                     | 0.47              |
| 1:I:226:LYS:HA   | 1:I:229:ILE:HB   | 1.96                     | 0.47              |
| 1:J:283:VAL:HA   | 1:J:297:THR:O    | 2.14                     | 0.47              |
| 1:J:450:PHE:O    | 1:J:483:LYS:HA   | 2.15                     | 0.47              |
| 1:K:158:ARG:O    | 1:K:162:ALA:HB2  | 2.15                     | 0.47              |
| 1:K:450:PHE:O    | 1:K:483:LYS:HA   | 2.15                     | 0.47              |
| 1:L:261:GLY:HA3  | 1:M:284:MET:HG2  | 1.96                     | 0.47              |
| 1:M:261:GLY:HA3  | 1:N:284:MET:HG2  | 1.96                     | 0.47              |
| 1:M:506:ASN:O    | 1:M:518:PHE:CB   | 2.63                     | 0.47              |
| 1:O:105:VAL:O    | 1:O:140:ILE:CB   | 2.49                     | 0.47              |
| 1:O:226:LYS:HA   | 1:O:229:ILE:HB   | 1.96                     | 0.47              |
| 1:O:247:LEU:HD11 | 1:O:294:LEU:HD23 | 1.96                     | 0.47              |
| 1:O:450:PHE:O    | 1:O:483:LYS:HA   | 2.15                     | 0.47              |
| 1:O:634:ARG:HG3  | 1:O:635:HIS:O    | 2.15                     | 0.47              |
| 1:A:458:VAL:O    | 1:A:475:VAL:C    | 2.49                     | 0.46              |
| 1:C:182:ARG:HA   | 1:C:185:GLU:CD   | 2.36                     | 0.46              |
| 1:D:177:ALA:N    | 1:D:211:ASN:OD1  | 2.41                     | 0.46              |
| 1:D:476:ASP:OD1  | 1:D:476:ASP:N    | 2.48                     | 0.46              |
| 1:D:450:PHE:O    | 1:D:483:LYS:HA   | 2.15                     | 0.46              |
| 1:F:105:VAL:O    | 1:F:140:ILE:CB   | 2.49                     | 0.46              |
| 1:F:158:ARG:O    | 1:F:162:ALA:HB2  | 2.15                     | 0.46              |
| 1:G:450:PHE:O    | 1:G:483:LYS:HA   | 2.15                     | 0.46              |
| 1:H:120:ARG:HG2  | 1:H:123:ILE:HD12 | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:438:PRO:HB3  | 1:H:450:PHE:CE2  | 2.50                     | 0.46              |
| 1:I:158:ARG:O    | 1:I:162:ALA:HB2  | 2.15                     | 0.46              |
| 1:J:247:LEU:HD11 | 1:J:294:LEU:HD23 | 1.96                     | 0.46              |
| 1:L:438:PRO:HB3  | 1:L:450:PHE:CE2  | 2.50                     | 0.46              |
| 1:L:506:ASN:O    | 1:L:518:PHE:CB   | 2.63                     | 0.46              |
| 1:N:102:THR:OG1  | 1:N:142:ILE:O    | 2.25                     | 0.46              |
| 1:A:283:VAL:HA   | 1:A:297:THR:O    | 2.14                     | 0.46              |
| 1:C:239:LYS:HE3  | 1:C:300:GLN:HB2  | 1.97                     | 0.46              |
| 1:D:239:LYS:HE3  | 1:D:300:GLN:HB2  | 1.97                     | 0.46              |
| 1:F:458:VAL:O    | 1:F:475:VAL:C    | 2.49                     | 0.46              |
| 1:G:207:ASP:O    | 1:G:211:ASN:HA   | 2.16                     | 0.46              |
| 1:H:182:ARG:HA   | 1:H:185:GLU:CD   | 2.36                     | 0.46              |
| 1:J:476:ASP:N    | 1:J:476:ASP:OD1  | 2.48                     | 0.46              |
| 1:L:120:ARG:HG2  | 1:L:123:ILE:HD12 | 1.96                     | 0.46              |
| 1:L:328:GLU:HG2  | 1:L:577:LEU:HG   | 1.96                     | 0.46              |
| 1:L:477:ARG:CG   | 1:L:477:ARG:NH1  | 2.73                     | 0.46              |
| 1:M:634:ARG:HG3  | 1:M:635:HIS:O    | 2.15                     | 0.46              |
| 1:N:120:ARG:HG2  | 1:N:123:ILE:HD12 | 1.96                     | 0.46              |
| 1:O:507:VAL:HG22 | 1:O:508:LEU:N    | 2.29                     | 0.46              |
| 1:A:158:ARG:O    | 1:A:162:ALA:HB2  | 2.15                     | 0.46              |
| 1:A:227:ARG:O    | 1:A:231:GLN:HG3  | 2.16                     | 0.46              |
| 1:A:239:LYS:HE3  | 1:A:300:GLN:HB2  | 1.97                     | 0.46              |
| 1:D:120:ARG:HG2  | 1:D:123:ILE:HD12 | 1.96                     | 0.46              |
| 1:D:438:PRO:HB3  | 1:D:450:PHE:CE2  | 2.50                     | 0.46              |
| 1:D:261:GLY:HA3  | 1:E:284:MET:HG2  | 1.96                     | 0.46              |
| 1:F:328:GLU:HG2  | 1:F:577:LEU:HG   | 1.96                     | 0.46              |
| 1:G:438:PRO:HB3  | 1:G:450:PHE:CE2  | 2.50                     | 0.46              |
| 1:H:634:ARG:HG3  | 1:H:635:HIS:O    | 2.15                     | 0.46              |
| 1:I:207:ASP:O    | 1:I:211:ASN:HA   | 2.16                     | 0.46              |
| 1:I:634:ARG:HG3  | 1:I:635:HIS:O    | 2.15                     | 0.46              |
| 1:J:158:ARG:O    | 1:J:162:ALA:HB2  | 2.15                     | 0.46              |
| 1:N:450:PHE:O    | 1:N:483:LYS:HA   | 2.15                     | 0.46              |
| 1:O:239:LYS:HE3  | 1:O:300:GLN:HB2  | 1.97                     | 0.46              |
| 1:B:180:MET:HE2  | 1:B:213:ILE:HD11 | 1.97                     | 0.46              |
| 1:C:340:GLN:HE21 | 1:C:352:TYR:HB2  | 1.81                     | 0.46              |
| 1:C:476:ASP:OD1  | 1:C:476:ASP:N    | 2.48                     | 0.46              |
| 1:D:340:GLN:HE21 | 1:D:352:TYR:HB2  | 1.81                     | 0.46              |
| 1:E:227:ARG:O    | 1:E:231:GLN:HG3  | 2.16                     | 0.46              |
| 1:G:182:ARG:HA   | 1:G:185:GLU:CD   | 2.36                     | 0.46              |
| 1:H:457:PRO:HA   | 1:H:477:ARG:HE   | 1.80                     | 0.46              |
| 1:I:182:ARG:HA   | 1:I:185:GLU:CD   | 2.36                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:203:LYS:N    | 1:I:216:SER:HG   | 2.14                     | 0.46              |
| 1:I:476:ASP:OD1  | 1:I:476:ASP:N    | 2.48                     | 0.46              |
| 1:K:225:LEU:HA   | 1:K:225:LEU:HD23 | 1.74                     | 0.46              |
| 1:M:328:GLU:HG2  | 1:M:577:LEU:HG   | 1.96                     | 0.46              |
| 1:M:438:PRO:HB3  | 1:M:450:PHE:CE2  | 2.50                     | 0.46              |
| 1:N:203:LYS:N    | 1:N:216:SER:HG   | 2.14                     | 0.46              |
| 1:O:182:ARG:HA   | 1:O:185:GLU:CD   | 2.36                     | 0.46              |
| 1:A:506:ASN:O    | 1:A:518:PHE:CB   | 2.63                     | 0.46              |
| 1:B:340:GLN:HE21 | 1:B:352:TYR:HB2  | 1.81                     | 0.46              |
| 1:B:476:ASP:N    | 1:B:476:ASP:OD1  | 2.48                     | 0.46              |
| 1:B:506:ASN:O    | 1:B:518:PHE:CB   | 2.63                     | 0.46              |
| 1:C:105:VAL:O    | 1:C:140:ILE:CB   | 2.49                     | 0.46              |
| 1:C:438:PRO:HB3  | 1:C:450:PHE:CE2  | 2.50                     | 0.46              |
| 1:C:504:VAL:HG12 | 1:C:521:ARG:HG2  | 1.94                     | 0.46              |
| 1:D:207:ASP:O    | 1:D:211:ASN:HA   | 2.16                     | 0.46              |
| 1:E:205:VAL:HG12 | 1:E:206:ALA:H    | 1.81                     | 0.46              |
| 1:E:340:GLN:HE21 | 1:E:352:TYR:HB2  | 1.81                     | 0.46              |
| 1:E:476:ASP:OD1  | 1:E:476:ASP:N    | 2.48                     | 0.46              |
| 1:E:457:PRO:HA   | 1:E:477:ARG:HE   | 1.79                     | 0.46              |
| 1:E:634:ARG:HG3  | 1:E:635:HIS:O    | 2.15                     | 0.46              |
| 1:F:227:ARG:O    | 1:F:231:GLN:HG3  | 2.16                     | 0.46              |
| 1:F:247:LEU:HD11 | 1:F:294:LEU:HD23 | 1.96                     | 0.46              |
| 1:H:247:LEU:HD11 | 1:H:294:LEU:HD23 | 1.96                     | 0.46              |
| 1:H:476:ASP:N    | 1:H:476:ASP:OD1  | 2.48                     | 0.46              |
| 1:H:478:LYS:HD2  | 1:H:518:PHE:HZ   | 1.79                     | 0.46              |
| 1:J:207:ASP:O    | 1:J:211:ASN:HA   | 2.16                     | 0.46              |
| 1:J:340:GLN:HE21 | 1:J:352:TYR:HB2  | 1.81                     | 0.46              |
| 1:K:226:LYS:HA   | 1:K:229:ILE:HB   | 1.96                     | 0.46              |
| 1:K:501:GLU:HG2  | 1:K:524:ASN:HB2  | 1.98                     | 0.46              |
| 1:L:203:LYS:N    | 1:L:216:SER:HG   | 2.14                     | 0.46              |
| 1:L:507:VAL:HG22 | 1:L:508:LEU:N    | 2.29                     | 0.46              |
| 1:L:501:GLU:HG2  | 1:L:524:ASN:HB2  | 1.98                     | 0.46              |
| 1:M:205:VAL:HG12 | 1:M:206:ALA:H    | 1.81                     | 0.46              |
| 1:O:177:ALA:N    | 1:O:211:ASN:OD1  | 2.41                     | 0.46              |
| 1:A:340:GLN:HE21 | 1:A:352:TYR:HB2  | 1.81                     | 0.46              |
| 1:C:177:ALA:N    | 1:C:211:ASN:OD1  | 2.41                     | 0.46              |
| 1:C:328:GLU:HG2  | 1:C:577:LEU:HG   | 1.96                     | 0.46              |
| 1:D:140:ILE:HG21 | 1:D:156:ILE:HD13 | 1.98                     | 0.46              |
| 1:D:203:LYS:N    | 1:D:216:SER:HG   | 2.14                     | 0.46              |
| 1:D:255:LEU:HA   | 1:D:255:LEU:HD23 | 1.73                     | 0.46              |
| 1:E:140:ILE:HG21 | 1:E:156:ILE:HD13 | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:226:LYS:HA   | 1:E:229:ILE:HB   | 1.96                     | 0.46              |
| 1:F:207:ASP:O    | 1:F:211:ASN:HA   | 2.16                     | 0.46              |
| 1:F:504:VAL:HG12 | 1:F:521:ARG:O    | 2.16                     | 0.46              |
| 1:G:227:ARG:O    | 1:G:231:GLN:HG3  | 2.16                     | 0.46              |
| 1:G:634:ARG:HG3  | 1:G:635:HIS:O    | 2.15                     | 0.46              |
| 1:H:227:ARG:O    | 1:H:231:GLN:HG3  | 2.16                     | 0.46              |
| 1:J:140:ILE:HG21 | 1:J:156:ILE:HD13 | 1.98                     | 0.46              |
| 1:J:205:VAL:HG12 | 1:J:206:ALA:H    | 1.81                     | 0.46              |
| 1:J:501:GLU:HG2  | 1:J:524:ASN:HB2  | 1.98                     | 0.46              |
| 1:K:203:LYS:N    | 1:K:216:SER:HG   | 2.14                     | 0.46              |
| 1:K:235:GLU:H    | 1:K:235:GLU:CD   | 2.11                     | 0.46              |
| 1:K:340:GLN:HE21 | 1:K:352:TYR:HB2  | 1.81                     | 0.46              |
| 1:K:478:LYS:HD2  | 1:K:518:PHE:HZ   | 1.79                     | 0.46              |
| 1:L:182:ARG:HA   | 1:L:185:GLU:CD   | 2.36                     | 0.46              |
| 1:L:476:ASP:OD1  | 1:L:476:ASP:N    | 2.48                     | 0.46              |
| 1:M:226:LYS:HA   | 1:M:229:ILE:HB   | 1.96                     | 0.46              |
| 1:M:450:PHE:O    | 1:M:483:LYS:HA   | 2.15                     | 0.46              |
| 1:N:438:PRO:HB3  | 1:N:450:PHE:CE2  | 2.50                     | 0.46              |
| 1:N:506:ASN:O    | 1:N:518:PHE:CB   | 2.63                     | 0.46              |
| 1:N:634:ARG:HG3  | 1:N:635:HIS:O    | 2.15                     | 0.46              |
| 1:B:227:ARG:O    | 1:B:231:GLN:HG3  | 2.16                     | 0.46              |
| 1:C:140:ILE:HG21 | 1:C:156:ILE:HD13 | 1.98                     | 0.46              |
| 1:D:182:ARG:HA   | 1:D:185:GLU:CD   | 2.36                     | 0.46              |
| 1:E:182:ARG:HA   | 1:E:185:GLU:CD   | 2.36                     | 0.46              |
| 1:E:450:PHE:O    | 1:E:483:LYS:HA   | 2.15                     | 0.46              |
| 1:F:182:ARG:HA   | 1:F:185:GLU:CD   | 2.36                     | 0.46              |
| 1:F:438:PRO:HB3  | 1:F:450:PHE:CE2  | 2.50                     | 0.46              |
| 1:G:476:ASP:OD1  | 1:G:476:ASP:N    | 2.48                     | 0.46              |
| 1:I:122:LEU:HD23 | 1:I:125:ASN:ND2  | 2.19                     | 0.46              |
| 1:J:182:ARG:HA   | 1:J:185:GLU:CD   | 2.36                     | 0.46              |
| 1:J:339:VAL:HG22 | 1:J:423:ILE:HG12 | 1.98                     | 0.46              |
| 1:J:507:VAL:HG22 | 1:J:508:LEU:N    | 2.30                     | 0.46              |
| 1:K:506:ASN:O    | 1:K:518:PHE:CB   | 2.63                     | 0.46              |
| 1:L:226:LYS:HA   | 1:L:229:ILE:HB   | 1.96                     | 0.46              |
| 1:L:504:VAL:HG12 | 1:L:521:ARG:O    | 2.16                     | 0.46              |
| 1:M:120:ARG:HG2  | 1:M:123:ILE:HD12 | 1.96                     | 0.46              |
| 1:M:203:LYS:N    | 1:M:216:SER:HG   | 2.14                     | 0.46              |
| 1:M:501:GLU:HG2  | 1:M:524:ASN:HB2  | 1.98                     | 0.46              |
| 1:N:472:PHE:C    | 1:N:472:PHE:CD1  | 2.86                     | 0.46              |
| 1:N:476:ASP:N    | 1:N:476:ASP:OD1  | 2.48                     | 0.46              |
| 1:N:322:ILE:HG23 | 1:N:581:ILE:HD11 | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:450:PHE:O    | 1:A:483:LYS:HA   | 2.15                     | 0.46              |
| 1:A:476:ASP:N    | 1:A:476:ASP:OD1  | 2.48                     | 0.46              |
| 1:A:504:VAL:HG12 | 1:A:521:ARG:O    | 2.16                     | 0.46              |
| 1:B:158:ARG:O    | 1:B:162:ALA:HB2  | 2.15                     | 0.46              |
| 1:D:227:ARG:O    | 1:D:231:GLN:HG3  | 2.16                     | 0.46              |
| 1:E:120:ARG:HG2  | 1:E:123:ILE:HD12 | 1.96                     | 0.46              |
| 1:E:207:ASP:O    | 1:E:211:ASN:HA   | 2.16                     | 0.46              |
| 1:F:140:ILE:HG21 | 1:F:156:ILE:HD13 | 1.98                     | 0.46              |
| 1:F:171:GLU:HA   | 1:F:212:SER:OG   | 2.16                     | 0.46              |
| 1:F:203:LYS:N    | 1:F:216:SER:HG   | 2.14                     | 0.46              |
| 1:G:339:VAL:HG22 | 1:G:423:ILE:HG12 | 1.98                     | 0.46              |
| 1:H:205:VAL:HG12 | 1:H:206:ALA:H    | 1.81                     | 0.46              |
| 1:H:450:PHE:O    | 1:H:483:LYS:HA   | 2.15                     | 0.46              |
| 1:H:504:VAL:HG12 | 1:H:521:ARG:O    | 2.16                     | 0.46              |
| 1:H:501:GLU:HG2  | 1:H:524:ASN:HB2  | 1.98                     | 0.46              |
| 1:I:140:ILE:HG21 | 1:I:156:ILE:HD13 | 1.98                     | 0.46              |
| 1:I:450:PHE:O    | 1:I:483:LYS:HA   | 2.15                     | 0.46              |
| 1:I:501:GLU:HG2  | 1:I:524:ASN:HB2  | 1.98                     | 0.46              |
| 1:J:504:VAL:HG12 | 1:J:521:ARG:O    | 2.16                     | 0.46              |
| 1:L:339:VAL:HG22 | 1:L:423:ILE:HG12 | 1.98                     | 0.46              |
| 1:M:227:ARG:O    | 1:M:231:GLN:HG3  | 2.16                     | 0.46              |
| 1:M:476:ASP:OD1  | 1:M:476:ASP:N    | 2.48                     | 0.46              |
| 1:N:182:ARG:HA   | 1:N:185:GLU:CD   | 2.36                     | 0.46              |
| 1:N:504:VAL:HG12 | 1:N:521:ARG:O    | 2.16                     | 0.46              |
| 1:O:205:VAL:HG12 | 1:O:206:ALA:H    | 1.81                     | 0.46              |
| 1:O:215:ILE:HA   | 1:O:215:ILE:HD12 | 1.82                     | 0.46              |
| 1:O:340:GLN:HE21 | 1:O:352:TYR:HB2  | 1.81                     | 0.46              |
| 1:A:322:ILE:HG23 | 1:A:581:ILE:HD11 | 1.98                     | 0.46              |
| 1:B:239:LYS:HE3  | 1:B:300:GLN:HB2  | 1.97                     | 0.46              |
| 1:D:157:ARG:HA   | 1:D:160:ASP:HB3  | 1.98                     | 0.46              |
| 1:D:171:GLU:HA   | 1:D:212:SER:OG   | 2.16                     | 0.46              |
| 1:D:479:GLU:CD   | 1:D:479:GLU:H    | 2.07                     | 0.46              |
| 1:E:158:ARG:O    | 1:E:162:ALA:HB2  | 2.15                     | 0.46              |
| 1:E:171:GLU:HA   | 1:E:212:SER:OG   | 2.16                     | 0.46              |
| 1:E:504:VAL:HG12 | 1:E:521:ARG:HG2  | 1.94                     | 0.46              |
| 1:E:322:ILE:HG23 | 1:E:581:ILE:HD11 | 1.98                     | 0.46              |
| 1:F:340:GLN:HE21 | 1:F:352:TYR:HB2  | 1.81                     | 0.46              |
| 1:F:476:ASP:N    | 1:F:476:ASP:OD1  | 2.48                     | 0.46              |
| 1:G:140:ILE:HG21 | 1:G:156:ILE:HD13 | 1.98                     | 0.46              |
| 1:G:203:LYS:N    | 1:G:216:SER:HG   | 2.14                     | 0.46              |
| 1:G:226:LYS:HA   | 1:G:229:ILE:HB   | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:501:GLU:HG2  | 1:G:524:ASN:HB2  | 1.98                     | 0.46              |
| 1:H:339:VAL:HG22 | 1:H:423:ILE:HG12 | 1.98                     | 0.46              |
| 1:I:227:ARG:O    | 1:I:231:GLN:HG3  | 2.16                     | 0.46              |
| 1:I:339:VAL:HG22 | 1:I:423:ILE:HG12 | 1.98                     | 0.46              |
| 1:I:340:GLN:HE21 | 1:I:352:TYR:HB2  | 1.81                     | 0.46              |
| 1:K:205:VAL:HG12 | 1:K:206:ALA:H    | 1.81                     | 0.46              |
| 1:L:450:PHE:O    | 1:L:483:LYS:HA   | 2.15                     | 0.46              |
| 1:M:322:ILE:HG23 | 1:M:581:ILE:HD11 | 1.98                     | 0.46              |
| 1:O:227:ARG:O    | 1:O:231:GLN:HG3  | 2.16                     | 0.46              |
| 1:O:322:ILE:HG23 | 1:O:581:ILE:HD11 | 1.98                     | 0.46              |
| 1:B:157:ARG:HA   | 1:B:160:ASP:HB3  | 1.99                     | 0.46              |
| 1:B:322:ILE:HG23 | 1:B:581:ILE:HD11 | 1.98                     | 0.46              |
| 1:C:450:PHE:O    | 1:C:483:LYS:HA   | 2.15                     | 0.46              |
| 1:C:506:ASN:O    | 1:C:518:PHE:CB   | 2.63                     | 0.46              |
| 1:C:478:LYS:HD2  | 1:C:518:PHE:HZ   | 1.79                     | 0.46              |
| 1:D:504:VAL:HG12 | 1:D:521:ARG:O    | 2.16                     | 0.46              |
| 1:E:438:PRO:HB3  | 1:E:450:PHE:CE2  | 2.50                     | 0.46              |
| 1:F:120:ARG:HG2  | 1:F:123:ILE:HD12 | 1.96                     | 0.46              |
| 1:G:171:GLU:HA   | 1:G:212:SER:OG   | 2.16                     | 0.46              |
| 1:H:140:ILE:HG21 | 1:H:156:ILE:HD13 | 1.98                     | 0.46              |
| 1:I:177:ALA:N    | 1:I:211:ASN:OD1  | 2.41                     | 0.46              |
| 1:I:504:VAL:HG12 | 1:I:521:ARG:HG2  | 1.94                     | 0.46              |
| 1:L:205:VAL:HG12 | 1:L:206:ALA:H    | 1.81                     | 0.46              |
| 1:L:340:GLN:HE21 | 1:L:352:TYR:HB2  | 1.81                     | 0.46              |
| 1:M:182:ARG:HA   | 1:M:185:GLU:CD   | 2.36                     | 0.46              |
| 1:M:339:VAL:HG22 | 1:M:423:ILE:HG12 | 1.98                     | 0.46              |
| 1:M:478:LYS:HD2  | 1:M:518:PHE:HZ   | 1.79                     | 0.46              |
| 1:O:476:ASP:OD1  | 1:O:476:ASP:N    | 2.48                     | 0.46              |
| 1:A:140:ILE:HG21 | 1:A:156:ILE:HD13 | 1.98                     | 0.45              |
| 1:A:504:VAL:HG12 | 1:A:521:ARG:HG2  | 1.94                     | 0.45              |
| 1:B:140:ILE:HG21 | 1:B:156:ILE:HD13 | 1.98                     | 0.45              |
| 1:B:205:VAL:HG12 | 1:B:206:ALA:H    | 1.81                     | 0.45              |
| 1:B:167:ILE:CA   | 1:B:215:ILE:O    | 2.42                     | 0.45              |
| 1:B:203:LYS:N    | 1:B:216:SER:HG   | 2.14                     | 0.45              |
| 1:C:171:GLU:HA   | 1:C:212:SER:OG   | 2.16                     | 0.45              |
| 1:F:322:ILE:HG23 | 1:F:581:ILE:HD11 | 1.98                     | 0.45              |
| 1:G:120:ARG:HG2  | 1:G:123:ILE:HD12 | 1.96                     | 0.45              |
| 1:H:171:GLU:HA   | 1:H:212:SER:OG   | 2.16                     | 0.45              |
| 1:H:226:LYS:HA   | 1:H:229:ILE:HB   | 1.96                     | 0.45              |
| 1:I:171:GLU:HA   | 1:I:212:SER:OG   | 2.16                     | 0.45              |
| 1:I:506:ASN:O    | 1:I:518:PHE:CB   | 2.63                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:203:LYS:N    | 1:J:216:SER:HG   | 2.14                     | 0.45              |
| 1:J:227:ARG:O    | 1:J:231:GLN:HG3  | 2.16                     | 0.45              |
| 1:K:140:ILE:HG21 | 1:K:156:ILE:HD13 | 1.98                     | 0.45              |
| 1:K:207:ASP:O    | 1:K:211:ASN:HA   | 2.16                     | 0.45              |
| 1:K:339:VAL:HG22 | 1:K:423:ILE:HG12 | 1.98                     | 0.45              |
| 1:L:227:ARG:O    | 1:L:231:GLN:HG3  | 2.16                     | 0.45              |
| 1:N:105:VAL:O    | 1:N:140:ILE:CB   | 2.49                     | 0.45              |
| 1:O:157:ARG:HA   | 1:O:160:ASP:HB3  | 1.98                     | 0.45              |
| 1:O:203:LYS:N    | 1:O:216:SER:HG   | 2.14                     | 0.45              |
| 1:O:438:PRO:HB3  | 1:O:450:PHE:CE2  | 2.50                     | 0.45              |
| 1:O:506:ASN:O    | 1:O:518:PHE:CB   | 2.63                     | 0.45              |
| 1:A:180:MET:HE2  | 1:A:213:ILE:HD11 | 1.97                     | 0.45              |
| 1:A:207:ASP:O    | 1:A:211:ASN:HA   | 2.16                     | 0.45              |
| 1:A:177:ALA:N    | 1:A:211:ASN:OD1  | 2.41                     | 0.45              |
| 1:B:225:LEU:HA   | 1:B:225:LEU:HD23 | 1.74                     | 0.45              |
| 1:B:504:VAL:HG12 | 1:B:521:ARG:O    | 2.16                     | 0.45              |
| 1:C:227:ARG:O    | 1:C:231:GLN:HG3  | 2.16                     | 0.45              |
| 1:C:522:GLN:H    | 1:D:451:ILE:HG23 | 1.82                     | 0.45              |
| 1:C:322:ILE:HG23 | 1:C:581:ILE:HD11 | 1.98                     | 0.45              |
| 1:D:322:ILE:HG23 | 1:D:581:ILE:HD11 | 1.98                     | 0.45              |
| 1:F:339:VAL:HG22 | 1:F:423:ILE:HG12 | 1.98                     | 0.45              |
| 1:H:340:GLN:HE21 | 1:H:352:TYR:HB2  | 1.81                     | 0.45              |
| 1:H:506:ASN:O    | 1:H:518:PHE:CB   | 2.63                     | 0.45              |
| 1:K:227:ARG:O    | 1:K:231:GLN:HG3  | 2.16                     | 0.45              |
| 1:K:472:PHE:C    | 1:K:472:PHE:CD1  | 2.86                     | 0.45              |
| 1:L:207:ASP:O    | 1:L:211:ASN:HA   | 2.16                     | 0.45              |
| 1:N:501:GLU:HG2  | 1:N:524:ASN:HB2  | 1.98                     | 0.45              |
| 1:O:140:ILE:HG21 | 1:O:156:ILE:HD13 | 1.98                     | 0.45              |
| 1:O:207:ASP:O    | 1:O:211:ASN:HA   | 2.16                     | 0.45              |
| 1:A:203:LYS:N    | 1:A:216:SER:HG   | 2.14                     | 0.45              |
| 1:A:218:ASP:O    | 1:A:222:ARG:N    | 2.50                     | 0.45              |
| 1:A:451:ILE:HG23 | 1:O:522:GLN:H    | 1.82                     | 0.45              |
| 1:B:207:ASP:O    | 1:B:211:ASN:HA   | 2.16                     | 0.45              |
| 1:B:218:ASP:O    | 1:B:222:ARG:N    | 2.50                     | 0.45              |
| 1:C:491:ASN:ND2  | 1:D:249:TYR:OH   | 2.50                     | 0.45              |
| 1:D:122:LEU:HD23 | 1:D:125:ASN:ND2  | 2.19                     | 0.45              |
| 1:D:504:VAL:HG12 | 1:D:521:ARG:HG2  | 1.94                     | 0.45              |
| 1:E:477:ARG:NH1  | 1:E:477:ARG:CG   | 2.73                     | 0.45              |
| 1:G:322:ILE:HG23 | 1:G:581:ILE:HD11 | 1.98                     | 0.45              |
| 1:H:203:LYS:N    | 1:H:216:SER:HG   | 2.14                     | 0.45              |
| 1:I:218:ASP:O    | 1:I:222:ARG:N    | 2.50                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:504:VAL:HG12 | 1:K:521:ARG:O    | 2.16                     | 0.45              |
| 1:L:218:ASP:O    | 1:L:222:ARG:N    | 2.50                     | 0.45              |
| 1:L:322:ILE:HG23 | 1:L:581:ILE:HD11 | 1.98                     | 0.45              |
| 1:M:218:ASP:O    | 1:M:222:ARG:N    | 2.50                     | 0.45              |
| 1:M:340:GLN:HE21 | 1:M:352:TYR:HB2  | 1.81                     | 0.45              |
| 1:M:507:VAL:HG22 | 1:M:508:LEU:N    | 2.29                     | 0.45              |
| 1:N:207:ASP:O    | 1:N:211:ASN:HA   | 2.16                     | 0.45              |
| 1:N:227:ARG:O    | 1:N:231:GLN:HG3  | 2.16                     | 0.45              |
| 1:N:340:GLN:HE21 | 1:N:352:TYR:HB2  | 1.81                     | 0.45              |
| 1:B:171:GLU:HA   | 1:B:212:SER:OG   | 2.16                     | 0.45              |
| 1:B:438:PRO:HB3  | 1:B:450:PHE:CE2  | 2.50                     | 0.45              |
| 1:C:504:VAL:HG12 | 1:C:521:ARG:O    | 2.16                     | 0.45              |
| 1:D:205:VAL:HG12 | 1:D:206:ALA:H    | 1.81                     | 0.45              |
| 1:D:219:PRO:HA   | 1:D:222:ARG:CB   | 2.45                     | 0.45              |
| 1:E:339:VAL:HG22 | 1:E:423:ILE:HG12 | 1.98                     | 0.45              |
| 1:F:157:ARG:HA   | 1:F:160:ASP:HB3  | 1.98                     | 0.45              |
| 1:F:501:GLU:HG2  | 1:F:524:ASN:HB2  | 1.98                     | 0.45              |
| 1:H:218:ASP:O    | 1:H:222:ARG:N    | 2.50                     | 0.45              |
| 1:I:491:ASN:ND2  | 1:J:249:TYR:OH   | 2.50                     | 0.45              |
| 1:K:182:ARG:HA   | 1:K:185:GLU:CD   | 2.36                     | 0.45              |
| 1:L:140:ILE:HG21 | 1:L:156:ILE:HD13 | 1.98                     | 0.45              |
| 1:M:140:ILE:HG21 | 1:M:156:ILE:HD13 | 1.98                     | 0.45              |
| 1:M:207:ASP:O    | 1:M:211:ASN:HA   | 2.16                     | 0.45              |
| 1:O:504:VAL:HG12 | 1:O:521:ARG:O    | 2.16                     | 0.45              |
| 1:A:438:PRO:HB3  | 1:A:450:PHE:CE2  | 2.50                     | 0.45              |
| 1:A:504:VAL:HG11 | 1:A:521:ARG:CG   | 2.47                     | 0.45              |
| 1:B:177:ALA:N    | 1:B:211:ASN:OD1  | 2.41                     | 0.45              |
| 1:F:478:LYS:HD2  | 1:F:518:PHE:HZ   | 1.79                     | 0.45              |
| 1:G:220:LYS:O    | 1:G:224:ARG:HG2  | 2.17                     | 0.45              |
| 1:G:340:GLN:HE21 | 1:G:352:TYR:HB2  | 1.81                     | 0.45              |
| 1:H:322:ILE:HG23 | 1:H:581:ILE:HD11 | 1.98                     | 0.45              |
| 1:J:506:ASN:O    | 1:J:518:PHE:CB   | 2.63                     | 0.45              |
| 1:J:491:ASN:ND2  | 1:K:249:TYR:OH   | 2.50                     | 0.45              |
| 1:L:522:GLN:H    | 1:M:451:ILE:HG23 | 1.82                     | 0.45              |
| 1:A:220:LYS:O    | 1:A:224:ARG:HG2  | 2.17                     | 0.45              |
| 1:A:522:GLN:H    | 1:B:451:ILE:HG23 | 1.82                     | 0.45              |
| 1:B:491:ASN:ND2  | 1:C:249:TYR:OH   | 2.50                     | 0.45              |
| 1:B:504:VAL:HG11 | 1:B:521:ARG:CG   | 2.47                     | 0.45              |
| 1:C:167:ILE:CA   | 1:C:215:ILE:O    | 2.42                     | 0.45              |
| 1:C:504:VAL:HG11 | 1:C:521:ARG:CG   | 2.47                     | 0.45              |
| 1:D:220:LYS:O    | 1:D:224:ARG:HG2  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:339:VAL:HG22 | 1:D:423:ILE:HG12 | 1.98                     | 0.45              |
| 1:D:491:ASN:ND2  | 1:E:249:TYR:OH   | 2.50                     | 0.45              |
| 1:E:504:VAL:HG12 | 1:E:521:ARG:O    | 2.16                     | 0.45              |
| 1:F:220:LYS:O    | 1:F:224:ARG:HG2  | 2.17                     | 0.45              |
| 1:G:157:ARG:HA   | 1:G:160:ASP:HB3  | 1.98                     | 0.45              |
| 1:G:472:PHE:CD1  | 1:G:472:PHE:C    | 2.86                     | 0.45              |
| 1:G:506:ASN:O    | 1:G:518:PHE:CB   | 2.63                     | 0.45              |
| 1:I:504:VAL:HG12 | 1:I:521:ARG:O    | 2.16                     | 0.45              |
| 1:J:171:GLU:HA   | 1:J:212:SER:OG   | 2.16                     | 0.45              |
| 1:K:322:ILE:HG23 | 1:K:581:ILE:HD11 | 1.98                     | 0.45              |
| 1:M:504:VAL:HG12 | 1:M:521:ARG:O    | 2.16                     | 0.45              |
| 1:M:522:GLN:H    | 1:N:451:ILE:HG23 | 1.82                     | 0.45              |
| 1:N:339:VAL:HG22 | 1:N:423:ILE:HG12 | 1.98                     | 0.45              |
| 1:N:507:VAL:HG22 | 1:N:508:LEU:N    | 2.29                     | 0.45              |
| 1:O:504:VAL:HG11 | 1:O:521:ARG:CG   | 2.47                     | 0.45              |
| 1:A:347:GLY:H    | 1:B:366:LEU:HD21 | 1.82                     | 0.45              |
| 1:A:456:VAL:CG2  | 1:A:457:PRO:N    | 2.80                     | 0.45              |
| 1:C:218:ASP:O    | 1:C:222:ARG:N    | 2.50                     | 0.45              |
| 1:C:347:GLY:H    | 1:D:366:LEU:HD21 | 1.82                     | 0.45              |
| 1:D:522:GLN:H    | 1:E:451:ILE:HG23 | 1.82                     | 0.45              |
| 1:E:609:PHE:CB   | 1:F:639:ILE:HD12 | 2.47                     | 0.45              |
| 1:F:180:MET:HE2  | 1:F:213:ILE:HD11 | 1.98                     | 0.45              |
| 1:F:205:VAL:HG12 | 1:F:206:ALA:H    | 1.81                     | 0.45              |
| 1:F:347:GLY:H    | 1:G:366:LEU:HD21 | 1.82                     | 0.45              |
| 1:G:504:VAL:HG12 | 1:G:521:ARG:O    | 2.16                     | 0.45              |
| 1:H:220:LYS:O    | 1:H:224:ARG:HG2  | 2.17                     | 0.45              |
| 1:H:347:GLY:H    | 1:I:366:LEU:HD21 | 1.82                     | 0.45              |
| 1:H:456:VAL:CG2  | 1:H:457:PRO:N    | 2.80                     | 0.45              |
| 1:H:507:VAL:HG22 | 1:H:508:LEU:N    | 2.29                     | 0.45              |
| 1:I:347:GLY:H    | 1:J:366:LEU:HD21 | 1.82                     | 0.45              |
| 1:L:102:THR:OG1  | 1:L:142:ILE:O    | 2.25                     | 0.45              |
| 1:O:481:GLY:O    | 1:O:505:SER:HB3  | 2.17                     | 0.45              |
| 1:N:609:PHE:CB   | 1:O:639:ILE:HD12 | 2.47                     | 0.45              |
| 1:A:205:VAL:HG12 | 1:A:206:ALA:H    | 1.81                     | 0.45              |
| 1:A:366:LEU:HD21 | 1:O:347:GLY:H    | 1.82                     | 0.45              |
| 1:B:458:VAL:O    | 1:B:475:VAL:C    | 2.49                     | 0.45              |
| 1:C:203:LYS:N    | 1:C:216:SER:HG   | 2.14                     | 0.45              |
| 1:C:205:VAL:HG12 | 1:C:206:ALA:H    | 1.81                     | 0.45              |
| 1:C:207:ASP:O    | 1:C:211:ASN:HA   | 2.16                     | 0.45              |
| 1:D:105:VAL:O    | 1:D:140:ILE:CB   | 2.49                     | 0.45              |
| 1:E:220:LYS:O    | 1:E:224:ARG:HG2  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:218:ASP:O    | 1:G:222:ARG:N    | 2.50                     | 0.45              |
| 1:H:255:LEU:HA   | 1:H:255:LEU:HD23 | 1.73                     | 0.45              |
| 1:I:220:LYS:O    | 1:I:224:ARG:HG2  | 2.17                     | 0.45              |
| 1:I:255:LEU:HD23 | 1:I:255:LEU:HA   | 1.73                     | 0.45              |
| 1:I:322:ILE:HG23 | 1:I:581:ILE:HD11 | 1.98                     | 0.45              |
| 1:J:218:ASP:O    | 1:J:222:ARG:N    | 2.50                     | 0.45              |
| 1:J:322:ILE:HG23 | 1:J:581:ILE:HD11 | 1.98                     | 0.45              |
| 1:L:220:LYS:O    | 1:L:224:ARG:HG2  | 2.17                     | 0.45              |
| 1:M:220:LYS:O    | 1:M:224:ARG:HG2  | 2.17                     | 0.45              |
| 1:N:140:ILE:HG21 | 1:N:156:ILE:HD13 | 1.98                     | 0.45              |
| 1:C:219:PRO:HA   | 1:C:222:ARG:CB   | 2.45                     | 0.45              |
| 1:B:347:GLY:H    | 1:C:366:LEU:HD21 | 1.82                     | 0.45              |
| 1:C:339:VAL:HG22 | 1:C:423:ILE:HG12 | 1.98                     | 0.45              |
| 1:B:609:PHE:CB   | 1:C:639:ILE:HD12 | 2.47                     | 0.45              |
| 1:D:501:GLU:HG2  | 1:D:524:ASN:HB2  | 1.98                     | 0.45              |
| 1:E:157:ARG:HA   | 1:E:160:ASP:HB3  | 1.98                     | 0.45              |
| 1:E:456:VAL:CG2  | 1:E:457:PRO:N    | 2.80                     | 0.45              |
| 1:E:501:GLU:HG2  | 1:E:524:ASN:HB2  | 1.98                     | 0.45              |
| 1:F:491:ASN:ND2  | 1:G:249:TYR:OH   | 2.50                     | 0.45              |
| 1:F:522:GLN:H    | 1:G:451:ILE:HG23 | 1.82                     | 0.45              |
| 1:G:491:ASN:ND2  | 1:H:249:TYR:OH   | 2.50                     | 0.45              |
| 1:G:507:VAL:HG22 | 1:G:508:LEU:N    | 2.29                     | 0.45              |
| 1:J:220:LYS:O    | 1:J:224:ARG:HG2  | 2.17                     | 0.45              |
| 1:J:255:LEU:HA   | 1:J:255:LEU:HD23 | 1.73                     | 0.45              |
| 1:K:220:LYS:O    | 1:K:224:ARG:HG2  | 2.17                     | 0.45              |
| 1:L:157:ARG:HA   | 1:L:160:ASP:HB3  | 1.98                     | 0.45              |
| 1:M:491:ASN:ND2  | 1:N:249:TYR:OH   | 2.50                     | 0.45              |
| 1:N:218:ASP:O    | 1:N:222:ARG:N    | 2.50                     | 0.45              |
| 1:N:220:LYS:O    | 1:N:224:ARG:HG2  | 2.17                     | 0.45              |
| 1:N:491:ASN:ND2  | 1:O:249:TYR:OH   | 2.50                     | 0.45              |
| 1:N:504:VAL:HG11 | 1:N:521:ARG:CG   | 2.47                     | 0.45              |
| 1:B:339:VAL:HG22 | 1:B:423:ILE:HG12 | 1.98                     | 0.45              |
| 1:B:456:VAL:CG2  | 1:B:457:PRO:N    | 2.80                     | 0.45              |
| 1:D:456:VAL:CG2  | 1:D:457:PRO:N    | 2.80                     | 0.45              |
| 1:D:506:ASN:O    | 1:D:518:PHE:CB   | 2.63                     | 0.45              |
| 1:E:203:LYS:N    | 1:E:216:SER:HG   | 2.14                     | 0.45              |
| 1:E:177:ALA:N    | 1:E:211:ASN:OD1  | 2.41                     | 0.45              |
| 1:F:506:ASN:O    | 1:F:518:PHE:CB   | 2.63                     | 0.45              |
| 1:J:522:GLN:H    | 1:K:451:ILE:HG23 | 1.82                     | 0.45              |
| 1:K:218:ASP:O    | 1:K:222:ARG:N    | 2.50                     | 0.45              |
| 1:M:171:GLU:HA   | 1:M:212:SER:OG   | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:491:ASN:ND2  | 1:M:249:TYR:OH   | 2.50                     | 0.45              |
| 1:N:205:VAL:HG12 | 1:N:206:ALA:H    | 1.81                     | 0.45              |
| 1:N:481:GLY:O    | 1:N:505:SER:HB3  | 2.17                     | 0.45              |
| 1:O:218:ASP:O    | 1:O:222:ARG:N    | 2.50                     | 0.45              |
| 1:O:352:TYR:CD2  | 1:O:567:SER:HB2  | 2.52                     | 0.45              |
| 1:A:639:ILE:HD12 | 1:O:609:PHE:CB   | 2.47                     | 0.45              |
| 1:A:352:TYR:CD2  | 1:A:567:SER:HB2  | 2.52                     | 0.44              |
| 1:A:339:VAL:HG22 | 1:A:423:ILE:HG12 | 1.98                     | 0.44              |
| 1:A:491:ASN:ND2  | 1:B:249:TYR:OH   | 2.50                     | 0.44              |
| 1:A:481:GLY:O    | 1:A:505:SER:HB3  | 2.17                     | 0.44              |
| 1:C:157:ARG:HA   | 1:C:160:ASP:HB3  | 1.98                     | 0.44              |
| 1:C:501:GLU:HG2  | 1:C:524:ASN:HB2  | 1.98                     | 0.44              |
| 1:D:167:ILE:CA   | 1:D:215:ILE:O    | 2.42                     | 0.44              |
| 1:E:347:GLY:H    | 1:F:366:LEU:HD21 | 1.82                     | 0.44              |
| 1:F:504:VAL:HG12 | 1:F:521:ARG:HG2  | 1.94                     | 0.44              |
| 1:G:347:GLY:H    | 1:H:366:LEU:HD21 | 1.82                     | 0.44              |
| 1:G:456:VAL:CG2  | 1:G:457:PRO:N    | 2.80                     | 0.44              |
| 1:I:157:ARG:HA   | 1:I:160:ASP:HB3  | 1.99                     | 0.44              |
| 1:I:507:VAL:HG22 | 1:I:508:LEU:N    | 2.29                     | 0.44              |
| 1:I:522:GLN:H    | 1:J:451:ILE:HG23 | 1.82                     | 0.44              |
| 1:J:347:GLY:H    | 1:K:366:LEU:HD21 | 1.82                     | 0.44              |
| 1:M:389:GLU:OE2  | 1:M:391:THR:HB   | 2.18                     | 0.44              |
| 1:M:504:VAL:HG11 | 1:M:521:ARG:CG   | 2.47                     | 0.44              |
| 1:N:504:VAL:HG12 | 1:N:521:ARG:HG2  | 1.94                     | 0.44              |
| 1:O:504:VAL:HG12 | 1:O:521:ARG:HG2  | 1.94                     | 0.44              |
| 1:O:501:GLU:HG2  | 1:O:524:ASN:HB2  | 1.98                     | 0.44              |
| 1:A:171:GLU:HA   | 1:A:212:SER:OG   | 2.16                     | 0.44              |
| 1:B:220:LYS:O    | 1:B:224:ARG:HG2  | 2.17                     | 0.44              |
| 1:E:522:GLN:H    | 1:F:451:ILE:HG23 | 1.82                     | 0.44              |
| 1:F:215:ILE:HA   | 1:F:215:ILE:HD12 | 1.82                     | 0.44              |
| 1:I:219:PRO:HA   | 1:I:222:ARG:CB   | 2.45                     | 0.44              |
| 1:I:456:VAL:CG2  | 1:I:457:PRO:N    | 2.80                     | 0.44              |
| 1:J:481:GLY:O    | 1:J:505:SER:HB3  | 2.17                     | 0.44              |
| 1:K:481:GLY:O    | 1:K:505:SER:HB3  | 2.17                     | 0.44              |
| 1:K:507:VAL:HG22 | 1:K:508:LEU:N    | 2.30                     | 0.44              |
| 1:K:522:GLN:H    | 1:L:451:ILE:HG23 | 1.82                     | 0.44              |
| 1:L:352:TYR:CD2  | 1:L:567:SER:HB2  | 2.53                     | 0.44              |
| 1:N:215:ILE:HA   | 1:N:215:ILE:HD12 | 1.82                     | 0.44              |
| 1:O:220:LYS:O    | 1:O:224:ARG:HG2  | 2.17                     | 0.44              |
| 1:O:339:VAL:HG22 | 1:O:423:ILE:HG12 | 1.98                     | 0.44              |
| 1:N:347:GLY:H    | 1:O:366:LEU:HD21 | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:249:TYR:OH   | 1:O:491:ASN:ND2  | 2.50                     | 0.44              |
| 1:A:427:SER:HB2  | 1:O:553:PRO:HB3  | 2.00                     | 0.44              |
| 1:C:389:GLU:OE2  | 1:C:391:THR:HB   | 2.18                     | 0.44              |
| 1:E:491:ASN:ND2  | 1:F:249:TYR:OH   | 2.50                     | 0.44              |
| 1:E:507:VAL:HG22 | 1:E:508:LEU:N    | 2.30                     | 0.44              |
| 1:F:218:ASP:O    | 1:F:222:ARG:N    | 2.50                     | 0.44              |
| 1:F:389:GLU:OE2  | 1:F:391:THR:HB   | 2.17                     | 0.44              |
| 1:G:205:VAL:HG12 | 1:G:206:ALA:H    | 1.81                     | 0.44              |
| 1:G:522:GLN:H    | 1:H:451:ILE:HG23 | 1.82                     | 0.44              |
| 1:I:205:VAL:HG12 | 1:I:206:ALA:H    | 1.81                     | 0.44              |
| 1:H:609:PHE:CB   | 1:I:639:ILE:HD12 | 2.47                     | 0.44              |
| 1:J:225:LEU:HA   | 1:J:225:LEU:HD23 | 1.74                     | 0.44              |
| 1:J:235:GLU:CD   | 1:J:235:GLU:H    | 2.11                     | 0.44              |
| 1:I:609:PHE:CE1  | 1:J:639:ILE:HD13 | 2.52                     | 0.44              |
| 1:K:167:ILE:CA   | 1:K:215:ILE:O    | 2.42                     | 0.44              |
| 1:K:352:TYR:CD2  | 1:K:567:SER:HB2  | 2.52                     | 0.44              |
| 1:K:491:ASN:ND2  | 1:L:249:TYR:OH   | 2.50                     | 0.44              |
| 1:L:389:GLU:OE2  | 1:L:391:THR:HB   | 2.17                     | 0.44              |
| 1:L:456:VAL:CG2  | 1:L:457:PRO:N    | 2.80                     | 0.44              |
| 1:L:491:ASN:O    | 1:L:493:GLY:N    | 2.51                     | 0.44              |
| 1:M:456:VAL:CG2  | 1:M:457:PRO:N    | 2.80                     | 0.44              |
| 1:N:157:ARG:HA   | 1:N:160:ASP:HB3  | 1.98                     | 0.44              |
| 1:N:352:TYR:CD2  | 1:N:567:SER:HB2  | 2.52                     | 0.44              |
| 1:N:389:GLU:OE2  | 1:N:391:THR:HB   | 2.18                     | 0.44              |
| 1:O:456:VAL:CG2  | 1:O:457:PRO:N    | 2.80                     | 0.44              |
| 1:A:501:GLU:HG2  | 1:A:524:ASN:HB2  | 1.98                     | 0.44              |
| 1:B:522:GLN:H    | 1:C:451:ILE:HG23 | 1.82                     | 0.44              |
| 1:C:255:LEU:HD23 | 1:C:255:LEU:HA   | 1.73                     | 0.44              |
| 1:D:218:ASP:O    | 1:D:222:ARG:N    | 2.50                     | 0.44              |
| 1:G:255:LEU:HD23 | 1:G:255:LEU:HA   | 1.73                     | 0.44              |
| 1:F:553:PRO:HB3  | 1:G:427:SER:HB2  | 2.00                     | 0.44              |
| 1:F:609:PHE:CB   | 1:G:639:ILE:HD12 | 2.47                     | 0.44              |
| 1:H:553:PRO:HB3  | 1:I:427:SER:HB2  | 2.00                     | 0.44              |
| 1:I:218:ASP:O    | 1:I:222:ARG:HG3  | 2.18                     | 0.44              |
| 1:H:491:ASN:ND2  | 1:I:249:TYR:OH   | 2.50                     | 0.44              |
| 1:I:481:GLY:O    | 1:I:505:SER:HB3  | 2.17                     | 0.44              |
| 1:H:609:PHE:CE1  | 1:I:639:ILE:HD13 | 2.52                     | 0.44              |
| 1:J:609:PHE:CE1  | 1:K:639:ILE:HD13 | 2.52                     | 0.44              |
| 1:M:609:PHE:CB   | 1:N:639:ILE:HD12 | 2.47                     | 0.44              |
| 1:N:171:GLU:HA   | 1:N:212:SER:OG   | 2.16                     | 0.44              |
| 1:N:218:ASP:O    | 1:N:222:ARG:HG3  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:219:PRO:HA   | 1:B:222:ARG:CB   | 2.45                     | 0.44              |
| 1:B:389:GLU:OE2  | 1:B:391:THR:HB   | 2.18                     | 0.44              |
| 1:C:220:LYS:O    | 1:C:224:ARG:HG2  | 2.17                     | 0.44              |
| 1:D:389:GLU:OE2  | 1:D:391:THR:HB   | 2.18                     | 0.44              |
| 1:F:218:ASP:O    | 1:F:222:ARG:HG3  | 2.18                     | 0.44              |
| 1:F:352:TYR:CD2  | 1:F:567:SER:HB2  | 2.52                     | 0.44              |
| 1:G:218:ASP:O    | 1:G:222:ARG:HG3  | 2.18                     | 0.44              |
| 1:G:609:PHE:CB   | 1:H:639:ILE:HD12 | 2.47                     | 0.44              |
| 1:I:389:GLU:OE2  | 1:I:391:THR:HB   | 2.17                     | 0.44              |
| 1:I:609:PHE:CB   | 1:J:639:ILE:HD12 | 2.47                     | 0.44              |
| 1:J:139:ILE:HG22 | 1:J:140:ILE:N    | 2.27                     | 0.44              |
| 1:K:180:MET:HE3  | 1:K:180:MET:HB3  | 1.88                     | 0.44              |
| 1:K:491:ASN:O    | 1:K:493:GLY:N    | 2.51                     | 0.44              |
| 1:L:219:PRO:HA   | 1:L:222:ARG:CB   | 2.45                     | 0.44              |
| 1:L:609:PHE:CB   | 1:M:639:ILE:HD12 | 2.47                     | 0.44              |
| 1:M:157:ARG:HA   | 1:M:160:ASP:HB3  | 1.98                     | 0.44              |
| 1:M:553:PRO:HB3  | 1:N:427:SER:HB2  | 2.00                     | 0.44              |
| 1:A:177:ALA:HB3  | 1:A:208:GLU:HG3  | 2.00                     | 0.44              |
| 1:A:167:ILE:CA   | 1:A:215:ILE:O    | 2.42                     | 0.44              |
| 1:B:218:ASP:O    | 1:B:222:ARG:HG3  | 2.18                     | 0.44              |
| 1:B:553:PRO:HB3  | 1:C:427:SER:HB2  | 2.00                     | 0.44              |
| 1:C:479:GLU:H    | 1:C:479:GLU:CD   | 2.07                     | 0.44              |
| 1:D:347:GLY:H    | 1:E:366:LEU:HD21 | 1.82                     | 0.44              |
| 1:C:609:PHE:CB   | 1:D:639:ILE:HD12 | 2.47                     | 0.44              |
| 1:E:506:ASN:O    | 1:E:518:PHE:CB   | 2.63                     | 0.44              |
| 1:G:389:GLU:OE2  | 1:G:391:THR:HB   | 2.18                     | 0.44              |
| 1:H:389:GLU:OE2  | 1:H:391:THR:HB   | 2.18                     | 0.44              |
| 1:I:491:ASN:O    | 1:I:493:GLY:N    | 2.51                     | 0.44              |
| 1:I:518:PHE:HD1  | 1:I:518:PHE:O    | 2.01                     | 0.44              |
| 1:J:491:ASN:O    | 1:J:493:GLY:N    | 2.51                     | 0.44              |
| 1:J:553:PRO:HB3  | 1:K:427:SER:HB2  | 2.00                     | 0.44              |
| 1:K:218:ASP:O    | 1:K:222:ARG:HG3  | 2.18                     | 0.44              |
| 1:K:456:VAL:CG2  | 1:K:457:PRO:N    | 2.80                     | 0.44              |
| 1:L:218:ASP:O    | 1:L:222:ARG:HG3  | 2.18                     | 0.44              |
| 1:M:352:TYR:CD2  | 1:M:567:SER:HB2  | 2.52                     | 0.44              |
| 1:M:491:ASN:O    | 1:M:493:GLY:N    | 2.51                     | 0.44              |
| 1:M:518:PHE:HD1  | 1:M:518:PHE:O    | 2.01                     | 0.44              |
| 1:N:225:LEU:HD23 | 1:N:225:LEU:HA   | 1.74                     | 0.44              |
| 1:O:518:PHE:HD1  | 1:O:518:PHE:O    | 2.01                     | 0.44              |
| 1:A:157:ARG:HA   | 1:A:160:ASP:HB3  | 1.98                     | 0.44              |
| 1:A:218:ASP:O    | 1:A:222:ARG:HG3  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:285:ILE:HD12 | 1:B:296:LEU:CD2  | 2.48                     | 0.44              |
| 1:B:501:GLU:HG2  | 1:B:524:ASN:HB2  | 1.98                     | 0.44              |
| 1:B:609:PHE:CE1  | 1:C:639:ILE:HD13 | 2.52                     | 0.44              |
| 1:A:609:PHE:CB   | 1:B:639:ILE:HD12 | 2.47                     | 0.44              |
| 1:C:507:VAL:HG22 | 1:C:508:LEU:N    | 2.29                     | 0.44              |
| 1:D:218:ASP:O    | 1:D:222:ARG:HG3  | 2.18                     | 0.44              |
| 1:D:553:PRO:HB3  | 1:E:427:SER:HB2  | 2.00                     | 0.44              |
| 1:C:609:PHE:CE1  | 1:D:639:ILE:HD13 | 2.52                     | 0.44              |
| 1:E:167:ILE:CA   | 1:E:215:ILE:O    | 2.42                     | 0.44              |
| 1:D:609:PHE:CB   | 1:E:639:ILE:HD12 | 2.47                     | 0.44              |
| 1:G:105:VAL:O    | 1:G:140:ILE:CB   | 2.49                     | 0.44              |
| 1:G:518:PHE:HD1  | 1:G:518:PHE:O    | 2.01                     | 0.44              |
| 1:K:553:PRO:HB3  | 1:L:427:SER:HB2  | 2.00                     | 0.44              |
| 1:L:177:ALA:HB3  | 1:L:208:GLU:HG3  | 2.00                     | 0.44              |
| 1:M:105:VAL:O    | 1:M:140:ILE:CB   | 2.49                     | 0.44              |
| 1:N:522:GLN:H    | 1:O:451:ILE:HG23 | 1.82                     | 0.44              |
| 1:O:171:GLU:HA   | 1:O:212:SER:OG   | 2.16                     | 0.44              |
| 1:O:479:GLU:H    | 1:O:479:GLU:CD   | 2.07                     | 0.44              |
| 1:A:100:VAL:HG13 | 1:A:144:GLY:HA2  | 2.00                     | 0.44              |
| 1:B:491:ASN:O    | 1:B:493:GLY:N    | 2.51                     | 0.44              |
| 1:B:481:GLY:O    | 1:B:505:SER:HB3  | 2.17                     | 0.44              |
| 1:A:609:PHE:CE1  | 1:B:639:ILE:HD13 | 2.52                     | 0.44              |
| 1:C:518:PHE:O    | 1:C:518:PHE:HD1  | 2.01                     | 0.44              |
| 1:E:218:ASP:O    | 1:E:222:ARG:HG3  | 2.18                     | 0.44              |
| 1:E:285:ILE:HD12 | 1:E:296:LEU:CD2  | 2.48                     | 0.44              |
| 1:F:456:VAL:CG2  | 1:F:457:PRO:N    | 2.80                     | 0.44              |
| 1:G:139:ILE:HG22 | 1:G:140:ILE:N    | 2.27                     | 0.44              |
| 1:H:491:ASN:O    | 1:H:493:GLY:N    | 2.51                     | 0.44              |
| 1:H:352:TYR:CD2  | 1:H:567:SER:HB2  | 2.53                     | 0.44              |
| 1:J:157:ARG:HA   | 1:J:160:ASP:HB3  | 1.99                     | 0.44              |
| 1:L:171:GLU:HA   | 1:L:212:SER:OG   | 2.16                     | 0.44              |
| 1:L:285:ILE:HD12 | 1:L:296:LEU:CD2  | 2.48                     | 0.44              |
| 1:L:504:VAL:HG11 | 1:L:521:ARG:CG   | 2.47                     | 0.44              |
| 1:M:481:GLY:O    | 1:M:505:SER:HB3  | 2.17                     | 0.44              |
| 1:M:347:GLY:H    | 1:N:366:LEU:HD21 | 1.82                     | 0.44              |
| 1:O:285:ILE:HD12 | 1:O:296:LEU:CD2  | 2.48                     | 0.44              |
| 1:A:518:PHE:O    | 1:A:518:PHE:HD1  | 2.01                     | 0.44              |
| 1:B:100:VAL:HG13 | 1:B:144:GLY:HA2  | 2.00                     | 0.44              |
| 1:B:352:TYR:CD2  | 1:B:567:SER:HB2  | 2.52                     | 0.44              |
| 1:C:218:ASP:O    | 1:C:222:ARG:HG3  | 2.18                     | 0.44              |
| 1:D:285:ILE:HD12 | 1:D:296:LEU:CD2  | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:491:ASN:O    | 1:D:493:GLY:N    | 2.51                     | 0.44              |
| 1:D:518:PHE:O    | 1:D:518:PHE:HD1  | 2.01                     | 0.44              |
| 1:E:105:VAL:CG1  | 1:E:157:ARG:HE   | 2.31                     | 0.44              |
| 1:E:218:ASP:O    | 1:E:222:ARG:N    | 2.50                     | 0.44              |
| 1:E:389:GLU:OE2  | 1:E:391:THR:HB   | 2.18                     | 0.44              |
| 1:E:491:ASN:O    | 1:E:493:GLY:N    | 2.51                     | 0.44              |
| 1:F:285:ILE:HD12 | 1:F:296:LEU:CD2  | 2.48                     | 0.44              |
| 1:F:491:ASN:O    | 1:F:493:GLY:N    | 2.51                     | 0.44              |
| 1:F:518:PHE:O    | 1:F:518:PHE:HD1  | 2.01                     | 0.44              |
| 1:G:491:ASN:O    | 1:G:493:GLY:N    | 2.51                     | 0.44              |
| 1:H:481:GLY:O    | 1:H:505:SER:HB3  | 2.17                     | 0.44              |
| 1:I:352:TYR:CD2  | 1:I:567:SER:HB2  | 2.52                     | 0.44              |
| 1:J:518:PHE:HD1  | 1:J:518:PHE:O    | 2.01                     | 0.44              |
| 1:L:481:GLY:O    | 1:L:505:SER:HB3  | 2.17                     | 0.44              |
| 1:K:609:PHE:CB   | 1:L:639:ILE:HD12 | 2.47                     | 0.44              |
| 1:M:177:ALA:HB3  | 1:M:208:GLU:HG3  | 2.00                     | 0.44              |
| 1:M:218:ASP:O    | 1:M:222:ARG:HG3  | 2.18                     | 0.44              |
| 1:O:100:VAL:HG13 | 1:O:144:GLY:HA2  | 2.00                     | 0.44              |
| 1:O:177:ALA:HB3  | 1:O:208:GLU:HG3  | 2.00                     | 0.44              |
| 1:O:389:GLU:OE2  | 1:O:391:THR:HB   | 2.17                     | 0.44              |
| 1:A:553:PRO:HB3  | 1:B:427:SER:HB2  | 2.00                     | 0.43              |
| 1:A:639:ILE:HD13 | 1:O:609:PHE:CE1  | 2.52                     | 0.43              |
| 1:C:100:VAL:HG13 | 1:C:144:GLY:HA2  | 2.00                     | 0.43              |
| 1:C:285:ILE:HD12 | 1:C:296:LEU:CD2  | 2.48                     | 0.43              |
| 1:C:456:VAL:CG2  | 1:C:457:PRO:N    | 2.80                     | 0.43              |
| 1:C:491:ASN:O    | 1:C:493:GLY:N    | 2.51                     | 0.43              |
| 1:E:100:VAL:HG13 | 1:E:144:GLY:HA2  | 2.00                     | 0.43              |
| 1:G:609:PHE:CE1  | 1:H:639:ILE:HD13 | 2.52                     | 0.43              |
| 1:H:105:VAL:CG1  | 1:H:157:ARG:HE   | 2.32                     | 0.43              |
| 1:H:522:GLN:H    | 1:I:451:ILE:HG23 | 1.82                     | 0.43              |
| 1:H:643:ILE:HA   | 1:H:643:ILE:HD12 | 1.86                     | 0.43              |
| 1:J:389:GLU:OE2  | 1:J:391:THR:HB   | 2.17                     | 0.43              |
| 1:K:347:GLY:H    | 1:L:366:LEU:HD21 | 1.82                     | 0.43              |
| 1:K:389:GLU:OE2  | 1:K:391:THR:HB   | 2.17                     | 0.43              |
| 1:J:609:PHE:CB   | 1:K:639:ILE:HD12 | 2.47                     | 0.43              |
| 1:L:225:LEU:HA   | 1:L:225:LEU:HD23 | 1.74                     | 0.43              |
| 1:L:518:PHE:HD1  | 1:L:518:PHE:O    | 2.01                     | 0.43              |
| 1:K:609:PHE:CE1  | 1:L:639:ILE:HD13 | 2.52                     | 0.43              |
| 1:N:285:ILE:HD12 | 1:N:296:LEU:CD2  | 2.48                     | 0.43              |
| 1:N:456:VAL:CG2  | 1:N:457:PRO:N    | 2.80                     | 0.43              |
| 1:N:491:ASN:O    | 1:N:493:GLY:N    | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:491:ASN:O    | 1:A:493:GLY:N    | 2.51                     | 0.43              |
| 1:D:177:ALA:HB3  | 1:D:208:GLU:HG3  | 2.00                     | 0.43              |
| 1:C:553:PRO:HB3  | 1:D:427:SER:HB2  | 2.00                     | 0.43              |
| 1:E:481:GLY:O    | 1:E:505:SER:HB3  | 2.17                     | 0.43              |
| 1:F:100:VAL:HG13 | 1:F:144:GLY:HA2  | 2.00                     | 0.43              |
| 1:G:100:VAL:HG13 | 1:G:144:GLY:HA2  | 2.00                     | 0.43              |
| 1:H:218:ASP:O    | 1:H:222:ARG:HG3  | 2.18                     | 0.43              |
| 1:I:553:PRO:HB3  | 1:J:427:SER:HB2  | 2.00                     | 0.43              |
| 1:J:477:ARG:CG   | 1:J:477:ARG:NH1  | 2.73                     | 0.43              |
| 1:K:171:GLU:HA   | 1:K:212:SER:OG   | 2.16                     | 0.43              |
| 1:A:219:PRO:HA   | 1:A:222:ARG:CB   | 2.45                     | 0.43              |
| 1:A:255:LEU:HA   | 1:A:255:LEU:HD23 | 1.73                     | 0.43              |
| 1:A:389:GLU:OE2  | 1:A:391:THR:HB   | 2.18                     | 0.43              |
| 1:B:255:LEU:HA   | 1:B:255:LEU:HD23 | 1.73                     | 0.43              |
| 1:B:518:PHE:HD1  | 1:B:518:PHE:O    | 2.01                     | 0.43              |
| 1:C:352:TYR:CD2  | 1:C:567:SER:HB2  | 2.52                     | 0.43              |
| 1:G:285:ILE:HD12 | 1:G:296:LEU:CD2  | 2.48                     | 0.43              |
| 1:G:481:GLY:O    | 1:G:505:SER:HB3  | 2.17                     | 0.43              |
| 1:I:177:ALA:HB3  | 1:I:208:GLU:HG3  | 2.00                     | 0.43              |
| 1:J:177:ALA:HB3  | 1:J:208:GLU:HG3  | 2.00                     | 0.43              |
| 1:J:456:VAL:CG2  | 1:J:457:PRO:N    | 2.80                     | 0.43              |
| 1:K:105:VAL:CG1  | 1:K:157:ARG:HE   | 2.32                     | 0.43              |
| 1:K:285:ILE:HD12 | 1:K:296:LEU:CD2  | 2.48                     | 0.43              |
| 1:N:167:ILE:CA   | 1:N:215:ILE:O    | 2.42                     | 0.43              |
| 1:N:518:PHE:HD1  | 1:N:518:PHE:O    | 2.01                     | 0.43              |
| 1:O:218:ASP:O    | 1:O:222:ARG:HG3  | 2.18                     | 0.43              |
| 1:D:100:VAL:HG13 | 1:D:144:GLY:HA2  | 2.00                     | 0.43              |
| 1:D:352:TYR:CD2  | 1:D:567:SER:HB2  | 2.52                     | 0.43              |
| 1:E:352:TYR:CD2  | 1:E:567:SER:HB2  | 2.52                     | 0.43              |
| 1:H:518:PHE:HD1  | 1:H:518:PHE:O    | 2.01                     | 0.43              |
| 1:N:139:ILE:HG22 | 1:N:140:ILE:N    | 2.27                     | 0.43              |
| 1:B:516:VAL:O    | 1:B:516:VAL:HG23 | 2.19                     | 0.43              |
| 1:F:255:LEU:HD23 | 1:F:255:LEU:HA   | 1.73                     | 0.43              |
| 1:G:352:TYR:CD2  | 1:G:567:SER:HB2  | 2.52                     | 0.43              |
| 1:H:177:ALA:N    | 1:H:211:ASN:OD1  | 2.41                     | 0.43              |
| 1:G:553:PRO:HB3  | 1:H:427:SER:HB2  | 2.00                     | 0.43              |
| 1:J:219:PRO:HA   | 1:J:222:ARG:CB   | 2.45                     | 0.43              |
| 1:J:285:ILE:HD12 | 1:J:296:LEU:CD2  | 2.48                     | 0.43              |
| 1:K:157:ARG:HA   | 1:K:160:ASP:HB3  | 1.98                     | 0.43              |
| 1:K:504:VAL:HG11 | 1:K:521:ARG:CG   | 2.47                     | 0.43              |
| 1:N:100:VAL:HG13 | 1:N:144:GLY:HA2  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:507:VAL:HG22 | 1:A:508:LEU:N    | 2.30                     | 0.43              |
| 1:B:435:LEU:CD2  | 1:C:626:LEU:HD23 | 2.49                     | 0.43              |
| 1:C:177:ALA:HB3  | 1:C:208:GLU:HG3  | 2.00                     | 0.43              |
| 1:C:225:LEU:HA   | 1:C:225:LEU:HD23 | 1.74                     | 0.43              |
| 1:E:102:THR:HA   | 1:E:143:THR:HA   | 2.01                     | 0.43              |
| 1:E:518:PHE:HD1  | 1:E:518:PHE:O    | 2.01                     | 0.43              |
| 1:D:435:LEU:CD2  | 1:E:626:LEU:HD23 | 2.49                     | 0.43              |
| 1:F:167:ILE:CA   | 1:F:215:ILE:O    | 2.42                     | 0.43              |
| 1:E:553:PRO:HB3  | 1:F:427:SER:HB2  | 2.00                     | 0.43              |
| 1:G:105:VAL:CG1  | 1:G:157:ARG:HE   | 2.32                     | 0.43              |
| 1:H:102:THR:HA   | 1:H:143:THR:HA   | 2.01                     | 0.43              |
| 1:H:157:ARG:HA   | 1:H:160:ASP:HB3  | 1.99                     | 0.43              |
| 1:I:225:LEU:HD23 | 1:I:225:LEU:HA   | 1.74                     | 0.43              |
| 1:J:102:THR:HA   | 1:J:143:THR:HA   | 2.01                     | 0.43              |
| 1:J:218:ASP:O    | 1:J:222:ARG:HG3  | 2.18                     | 0.43              |
| 1:J:352:TYR:CD2  | 1:J:567:SER:HB2  | 2.53                     | 0.43              |
| 1:N:609:PHE:CE1  | 1:O:639:ILE:HD13 | 2.52                     | 0.43              |
| 1:H:100:VAL:HG13 | 1:H:144:GLY:HA2  | 2.00                     | 0.43              |
| 1:H:504:VAL:HG12 | 1:H:521:ARG:HG2  | 1.94                     | 0.43              |
| 1:I:285:ILE:HD12 | 1:I:296:LEU:CD2  | 2.48                     | 0.43              |
| 1:I:357:ALA:HB3  | 1:I:407:ILE:HD11 | 2.01                     | 0.43              |
| 1:K:102:THR:HA   | 1:K:143:THR:HA   | 2.01                     | 0.43              |
| 1:K:458:VAL:CG2  | 1:K:478:LYS:HG2  | 2.48                     | 0.43              |
| 1:L:553:PRO:HB3  | 1:M:427:SER:HB2  | 2.00                     | 0.43              |
| 1:M:102:THR:HA   | 1:M:143:THR:HA   | 2.01                     | 0.43              |
| 1:M:100:VAL:HG13 | 1:M:144:GLY:HA2  | 2.00                     | 0.43              |
| 1:M:435:LEU:CD2  | 1:N:626:LEU:HD23 | 2.49                     | 0.43              |
| 1:M:504:VAL:HG12 | 1:M:521:ARG:HG2  | 1.94                     | 0.43              |
| 1:B:177:ALA:HB3  | 1:B:208:GLU:HG3  | 2.00                     | 0.43              |
| 1:D:102:THR:HA   | 1:D:143:THR:HA   | 2.01                     | 0.43              |
| 1:D:609:PHE:CE1  | 1:E:639:ILE:HD13 | 2.52                     | 0.43              |
| 1:G:102:THR:HA   | 1:G:143:THR:HA   | 2.01                     | 0.43              |
| 1:G:435:LEU:CD2  | 1:H:626:LEU:HD23 | 2.49                     | 0.43              |
| 1:H:285:ILE:HD12 | 1:H:296:LEU:CD2  | 2.48                     | 0.43              |
| 1:H:357:ALA:HB3  | 1:H:407:ILE:HD11 | 2.01                     | 0.43              |
| 1:I:102:THR:HA   | 1:I:143:THR:HA   | 2.01                     | 0.43              |
| 1:I:105:VAL:CG1  | 1:I:157:ARG:HE   | 2.31                     | 0.43              |
| 1:I:180:MET:HE3  | 1:I:180:MET:HB3  | 1.87                     | 0.43              |
| 1:N:521:ARG:HA   | 1:O:451:ILE:O    | 2.19                     | 0.43              |
| 1:N:553:PRO:HB3  | 1:O:427:SER:HB2  | 2.00                     | 0.43              |
| 1:O:491:ASN:O    | 1:O:493:GLY:N    | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:435:LEU:CD2  | 1:O:626:LEU:HD23 | 2.49                     | 0.43              |
| 1:A:458:VAL:CG2  | 1:A:478:LYS:HG2  | 2.48                     | 0.43              |
| 1:B:458:VAL:CG2  | 1:B:478:LYS:HG2  | 2.48                     | 0.43              |
| 1:C:481:GLY:O    | 1:C:505:SER:HB3  | 2.17                     | 0.43              |
| 1:C:516:VAL:O    | 1:C:516:VAL:HG23 | 2.19                     | 0.43              |
| 1:E:215:ILE:HD12 | 1:E:215:ILE:HA   | 1.82                     | 0.43              |
| 1:D:521:ARG:HA   | 1:E:451:ILE:O    | 2.19                     | 0.43              |
| 1:F:102:THR:HA   | 1:F:143:THR:HA   | 2.01                     | 0.43              |
| 1:F:435:LEU:CD2  | 1:G:626:LEU:HD23 | 2.49                     | 0.43              |
| 1:F:481:GLY:O    | 1:F:505:SER:HB3  | 2.17                     | 0.43              |
| 1:G:357:ALA:HB3  | 1:G:407:ILE:HD11 | 2.01                     | 0.43              |
| 1:H:166:GLU:HB3  | 1:H:167:ILE:H    | 1.67                     | 0.43              |
| 1:I:100:VAL:HG13 | 1:I:144:GLY:HA2  | 2.00                     | 0.43              |
| 1:J:225:LEU:O    | 1:J:229:ILE:HG13 | 2.19                     | 0.43              |
| 1:J:521:ARG:HA   | 1:K:451:ILE:O    | 2.19                     | 0.43              |
| 1:I:435:LEU:CD2  | 1:J:626:LEU:HD23 | 2.49                     | 0.43              |
| 1:K:166:GLU:HB3  | 1:K:167:ILE:H    | 1.67                     | 0.43              |
| 1:K:225:LEU:O    | 1:K:229:ILE:HG13 | 2.19                     | 0.43              |
| 1:M:285:ILE:HD12 | 1:M:296:LEU:CD2  | 2.48                     | 0.43              |
| 1:L:435:LEU:CD2  | 1:M:626:LEU:HD23 | 2.49                     | 0.43              |
| 1:N:102:THR:HA   | 1:N:143:THR:HA   | 2.01                     | 0.43              |
| 1:N:479:GLU:H    | 1:N:479:GLU:CD   | 2.07                     | 0.43              |
| 1:N:516:VAL:HG23 | 1:N:516:VAL:O    | 2.19                     | 0.43              |
| 1:O:219:PRO:HA   | 1:O:222:ARG:CB   | 2.45                     | 0.43              |
| 1:A:516:VAL:HG23 | 1:A:516:VAL:O    | 2.19                     | 0.43              |
| 1:C:521:ARG:HA   | 1:D:451:ILE:O    | 2.19                     | 0.43              |
| 1:F:105:VAL:CG1  | 1:F:157:ARG:HE   | 2.32                     | 0.43              |
| 1:E:609:PHE:CE1  | 1:F:639:ILE:HD13 | 2.52                     | 0.43              |
| 1:G:115:LEU:HB3  | 1:G:119:LEU:HG   | 2.01                     | 0.43              |
| 1:H:521:ARG:HA   | 1:I:451:ILE:O    | 2.19                     | 0.43              |
| 1:J:301:ASP:OD1  | 1:J:302:ILE:N    | 2.52                     | 0.43              |
| 1:J:504:VAL:HG11 | 1:J:521:ARG:CG   | 2.47                     | 0.43              |
| 1:L:102:THR:HA   | 1:L:143:THR:HA   | 2.01                     | 0.43              |
| 1:L:115:LEU:HB3  | 1:L:119:LEU:HG   | 2.01                     | 0.43              |
| 1:K:435:LEU:CD2  | 1:L:626:LEU:HD23 | 2.49                     | 0.43              |
| 1:M:115:LEU:HB3  | 1:M:119:LEU:HG   | 2.01                     | 0.43              |
| 1:M:166:GLU:HB3  | 1:M:167:ILE:H    | 1.67                     | 0.43              |
| 1:O:102:THR:HA   | 1:O:143:THR:HA   | 2.01                     | 0.43              |
| 1:A:626:LEU:HD23 | 1:O:435:LEU:CD2  | 2.49                     | 0.43              |
| 1:A:451:ILE:O    | 1:O:521:ARG:HA   | 2.19                     | 0.43              |
| 1:C:105:VAL:CG1  | 1:C:157:ARG:HE   | 2.32                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:516:VAL:O    | 1:E:516:VAL:HG23 | 2.19                     | 0.42              |
| 1:G:504:VAL:HG12 | 1:G:521:ARG:HG2  | 1.94                     | 0.42              |
| 1:H:115:LEU:HB3  | 1:H:119:LEU:HG   | 2.01                     | 0.42              |
| 1:K:115:LEU:HB3  | 1:K:119:LEU:HG   | 2.01                     | 0.42              |
| 1:K:99:GLU:O     | 1:K:145:ARG:HA   | 2.19                     | 0.42              |
| 1:K:219:PRO:HA   | 1:K:222:ARG:CB   | 2.45                     | 0.42              |
| 1:L:225:LEU:O    | 1:L:229:ILE:HG13 | 2.19                     | 0.42              |
| 1:L:551:LYS:HB3  | 1:L:566:ARG:HG2  | 2.01                     | 0.42              |
| 1:M:215:ILE:HA   | 1:M:215:ILE:HD12 | 1.82                     | 0.42              |
| 1:L:521:ARG:HA   | 1:M:451:ILE:O    | 2.19                     | 0.42              |
| 1:M:551:LYS:HB3  | 1:M:566:ARG:HG2  | 2.01                     | 0.42              |
| 1:O:301:ASP:OD1  | 1:O:302:ILE:N    | 2.52                     | 0.42              |
| 1:A:435:LEU:CD2  | 1:B:626:LEU:HD23 | 2.49                     | 0.42              |
| 1:C:102:THR:HA   | 1:C:143:THR:HA   | 2.01                     | 0.42              |
| 1:C:458:VAL:CG2  | 1:C:478:LYS:HG2  | 2.48                     | 0.42              |
| 1:D:357:ALA:HB3  | 1:D:407:ILE:HD11 | 2.01                     | 0.42              |
| 1:D:481:GLY:O    | 1:D:505:SER:HB3  | 2.17                     | 0.42              |
| 1:E:180:MET:HE2  | 1:E:213:ILE:HD11 | 2.01                     | 0.42              |
| 1:E:225:LEU:HA   | 1:E:225:LEU:HD23 | 1.74                     | 0.42              |
| 1:E:357:ALA:HB3  | 1:E:407:ILE:HD11 | 2.01                     | 0.42              |
| 1:F:115:LEU:HB3  | 1:F:119:LEU:HG   | 2.01                     | 0.42              |
| 1:F:177:ALA:HB3  | 1:F:208:GLU:HG3  | 2.00                     | 0.42              |
| 1:F:219:PRO:HA   | 1:F:222:ARG:CB   | 2.45                     | 0.42              |
| 1:F:225:LEU:HD23 | 1:F:225:LEU:HA   | 1.74                     | 0.42              |
| 1:F:357:ALA:HB3  | 1:F:407:ILE:HD11 | 2.01                     | 0.42              |
| 1:F:609:PHE:CE1  | 1:G:639:ILE:HD13 | 2.52                     | 0.42              |
| 1:H:539:GLY:CA   | 1:H:577:LEU:O    | 2.68                     | 0.42              |
| 1:I:170:VAL:HG11 | 1:I:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:J:357:ALA:HB3  | 1:J:407:ILE:HD11 | 2.01                     | 0.42              |
| 1:J:609:PHE:CD2  | 1:K:639:ILE:CD1  | 2.75                     | 0.42              |
| 1:K:177:ALA:HB3  | 1:K:208:GLU:HG3  | 2.00                     | 0.42              |
| 1:L:99:GLU:O     | 1:L:145:ARG:HA   | 2.19                     | 0.42              |
| 1:L:105:VAL:CG1  | 1:L:157:ARG:HE   | 2.31                     | 0.42              |
| 1:L:347:GLY:H    | 1:M:366:LEU:HD21 | 1.82                     | 0.42              |
| 1:L:609:PHE:CE1  | 1:M:639:ILE:HD13 | 2.52                     | 0.42              |
| 1:M:170:VAL:HG11 | 1:M:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:N:170:VAL:HG11 | 1:N:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:N:551:LYS:HB3  | 1:N:566:ARG:HG2  | 2.01                     | 0.42              |
| 1:M:609:PHE:CE1  | 1:N:639:ILE:HD13 | 2.53                     | 0.42              |
| 1:O:170:VAL:HG11 | 1:O:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:O:643:ILE:HD12 | 1:O:643:ILE:HA   | 1.86                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:102:THR:HA   | 1:A:143:THR:HA   | 2.01                     | 0.42              |
| 1:A:285:ILE:HD12 | 1:A:296:LEU:CD2  | 2.48                     | 0.42              |
| 1:A:551:LYS:HB3  | 1:A:566:ARG:HG2  | 2.01                     | 0.42              |
| 1:B:225:LEU:O    | 1:B:229:ILE:HG13 | 2.19                     | 0.42              |
| 1:B:551:LYS:HB3  | 1:B:566:ARG:HG2  | 2.01                     | 0.42              |
| 1:C:181:VAL:HG12 | 1:C:185:GLU:OE2  | 2.20                     | 0.42              |
| 1:E:170:VAL:HG11 | 1:E:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:E:435:LEU:CD2  | 1:F:626:LEU:HD23 | 2.49                     | 0.42              |
| 1:G:99:GLU:O     | 1:G:145:ARG:HA   | 2.19                     | 0.42              |
| 1:G:521:ARG:HA   | 1:H:451:ILE:O    | 2.19                     | 0.42              |
| 1:I:115:LEU:HB3  | 1:I:119:LEU:HG   | 2.01                     | 0.42              |
| 1:J:115:LEU:HB3  | 1:J:119:LEU:HG   | 2.01                     | 0.42              |
| 1:L:100:VAL:HG13 | 1:L:144:GLY:HA2  | 2.00                     | 0.42              |
| 1:M:516:VAL:HG23 | 1:M:516:VAL:O    | 2.19                     | 0.42              |
| 1:N:115:LEU:HB3  | 1:N:119:LEU:HG   | 2.01                     | 0.42              |
| 1:N:177:ALA:HB3  | 1:N:208:GLU:HG3  | 2.00                     | 0.42              |
| 1:O:181:VAL:HG12 | 1:O:185:GLU:OE2  | 2.20                     | 0.42              |
| 1:A:181:VAL:HG12 | 1:A:185:GLU:OE2  | 2.20                     | 0.42              |
| 1:A:225:LEU:O    | 1:A:229:ILE:HG13 | 2.19                     | 0.42              |
| 1:C:551:LYS:HB3  | 1:C:566:ARG:HG2  | 2.01                     | 0.42              |
| 1:D:170:VAL:HG11 | 1:D:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:F:170:VAL:HG11 | 1:F:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:F:516:VAL:O    | 1:F:516:VAL:HG23 | 2.19                     | 0.42              |
| 1:G:454:GLU:N    | 1:G:454:GLU:CD   | 2.73                     | 0.42              |
| 1:H:435:LEU:CD2  | 1:I:626:LEU:HD23 | 2.49                     | 0.42              |
| 1:J:100:VAL:HG13 | 1:J:144:GLY:HA2  | 2.00                     | 0.42              |
| 1:J:170:VAL:HG11 | 1:J:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:J:458:VAL:CG2  | 1:J:478:LYS:HG2  | 2.48                     | 0.42              |
| 1:K:247:LEU:CD1  | 1:K:255:LEU:HD12 | 2.50                     | 0.42              |
| 1:K:551:LYS:HB3  | 1:K:566:ARG:HG2  | 2.01                     | 0.42              |
| 1:J:435:LEU:CD2  | 1:K:626:LEU:HD23 | 2.49                     | 0.42              |
| 1:M:225:LEU:O    | 1:M:229:ILE:HG13 | 2.19                     | 0.42              |
| 1:N:181:VAL:HG12 | 1:N:185:GLU:OE2  | 2.20                     | 0.42              |
| 1:N:219:PRO:HA   | 1:N:222:ARG:CB   | 2.45                     | 0.42              |
| 1:O:458:VAL:CG2  | 1:O:478:LYS:HG2  | 2.48                     | 0.42              |
| 1:O:551:LYS:HB3  | 1:O:566:ARG:HG2  | 2.01                     | 0.42              |
| 1:B:102:THR:HA   | 1:B:143:THR:HA   | 2.01                     | 0.42              |
| 1:B:122:LEU:HD23 | 1:B:125:ASN:ND2  | 2.19                     | 0.42              |
| 1:B:181:VAL:HG12 | 1:B:185:GLU:OE2  | 2.20                     | 0.42              |
| 1:B:454:GLU:CD   | 1:B:454:GLU:N    | 2.73                     | 0.42              |
| 1:C:170:VAL:HG11 | 1:C:229:ILE:HG21 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:357:ALA:HB3  | 1:C:407:ILE:HD11 | 2.01                     | 0.42              |
| 1:E:539:GLY:CA   | 1:E:577:LEU:O    | 2.68                     | 0.42              |
| 1:F:454:GLU:CD   | 1:F:454:GLU:N    | 2.73                     | 0.42              |
| 1:H:99:GLU:O     | 1:H:145:ARG:HA   | 2.19                     | 0.42              |
| 1:H:170:VAL:HG11 | 1:H:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:I:225:LEU:O    | 1:I:229:ILE:HG13 | 2.19                     | 0.42              |
| 1:I:504:VAL:HG11 | 1:I:521:ARG:CG   | 2.47                     | 0.42              |
| 1:I:521:ARG:HA   | 1:J:451:ILE:O    | 2.19                     | 0.42              |
| 1:K:100:VAL:HG13 | 1:K:144:GLY:HA2  | 2.00                     | 0.42              |
| 1:M:181:VAL:HG12 | 1:M:185:GLU:OE2  | 2.20                     | 0.42              |
| 1:M:521:ARG:HA   | 1:N:451:ILE:O    | 2.19                     | 0.42              |
| 1:O:105:VAL:CG1  | 1:O:157:ARG:HE   | 2.31                     | 0.42              |
| 1:A:454:GLU:CD   | 1:A:454:GLU:N    | 2.73                     | 0.42              |
| 1:B:170:VAL:HG11 | 1:B:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:C:207:ASP:OD2  | 1:C:209:ARG:HB3  | 2.20                     | 0.42              |
| 1:D:352:TYR:OH   | 1:D:565:PHE:O    | 2.33                     | 0.42              |
| 1:C:435:LEU:CD2  | 1:D:626:LEU:HD23 | 2.49                     | 0.42              |
| 1:E:225:LEU:O    | 1:E:229:ILE:HG13 | 2.19                     | 0.42              |
| 1:E:521:ARG:HA   | 1:F:451:ILE:O    | 2.19                     | 0.42              |
| 1:F:521:ARG:HA   | 1:G:451:ILE:O    | 2.19                     | 0.42              |
| 1:H:247:LEU:CD1  | 1:H:255:LEU:HD12 | 2.50                     | 0.42              |
| 1:H:454:GLU:CD   | 1:H:454:GLU:N    | 2.73                     | 0.42              |
| 1:K:518:PHE:O    | 1:K:518:PHE:HD1  | 2.01                     | 0.42              |
| 1:M:219:PRO:HA   | 1:M:222:ARG:CB   | 2.45                     | 0.42              |
| 1:N:207:ASP:OD2  | 1:N:209:ARG:HB3  | 2.20                     | 0.42              |
| 1:N:357:ALA:HB3  | 1:N:407:ILE:HD11 | 2.01                     | 0.42              |
| 1:O:225:LEU:HA   | 1:O:225:LEU:HD23 | 1.74                     | 0.42              |
| 1:A:170:VAL:HG11 | 1:A:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:A:521:ARG:HA   | 1:B:451:ILE:O    | 2.19                     | 0.42              |
| 1:C:247:LEU:CD1  | 1:C:255:LEU:HD12 | 2.50                     | 0.42              |
| 1:E:339:VAL:HB   | 1:E:564:LEU:O    | 2.20                     | 0.42              |
| 1:F:225:LEU:O    | 1:F:229:ILE:HG13 | 2.19                     | 0.42              |
| 1:J:99:GLU:O     | 1:J:145:ARG:HA   | 2.19                     | 0.42              |
| 1:K:357:ALA:HB3  | 1:K:407:ILE:HD11 | 2.01                     | 0.42              |
| 1:L:170:VAL:HG11 | 1:L:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:O:115:LEU:HB3  | 1:O:119:LEU:HG   | 2.01                     | 0.42              |
| 1:A:115:LEU:HB3  | 1:A:119:LEU:HG   | 2.01                     | 0.42              |
| 1:A:642:PHE:CE2  | 1:O:612:GLU:CG   | 2.81                     | 0.42              |
| 1:B:207:ASP:OD2  | 1:B:209:ARG:HB3  | 2.20                     | 0.42              |
| 1:C:454:GLU:CD   | 1:C:454:GLU:N    | 2.73                     | 0.42              |
| 1:D:115:LEU:HB3  | 1:D:119:LEU:HG   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:225:LEU:O    | 1:D:229:ILE:HG13 | 2.19                     | 0.42              |
| 1:D:458:VAL:CG2  | 1:D:478:LYS:HG2  | 2.48                     | 0.42              |
| 1:E:115:LEU:HB3  | 1:E:119:LEU:HG   | 2.01                     | 0.42              |
| 1:E:247:LEU:CD1  | 1:E:255:LEU:HD12 | 2.50                     | 0.42              |
| 1:F:99:GLU:O     | 1:F:145:ARG:HA   | 2.19                     | 0.42              |
| 1:G:170:VAL:HG11 | 1:G:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:H:225:LEU:HA   | 1:H:225:LEU:HD23 | 1.74                     | 0.42              |
| 1:H:504:VAL:HG11 | 1:H:521:ARG:CG   | 2.47                     | 0.42              |
| 1:I:539:GLY:CA   | 1:I:577:LEU:O    | 2.68                     | 0.42              |
| 1:J:247:LEU:CD1  | 1:J:255:LEU:HD12 | 2.50                     | 0.42              |
| 1:J:481:GLY:N    | 1:J:505:SER:OG   | 2.23                     | 0.42              |
| 1:J:516:VAL:O    | 1:J:516:VAL:HG23 | 2.19                     | 0.42              |
| 1:J:551:LYS:HB3  | 1:J:566:ARG:HG2  | 2.01                     | 0.42              |
| 1:L:181:VAL:HG12 | 1:L:185:GLU:OE2  | 2.20                     | 0.42              |
| 1:M:479:GLU:H    | 1:M:479:GLU:CD   | 2.07                     | 0.42              |
| 1:O:207:ASP:OD2  | 1:O:209:ARG:HB3  | 2.20                     | 0.42              |
| 1:O:357:ALA:HB3  | 1:O:407:ILE:HD11 | 2.01                     | 0.42              |
| 1:O:454:GLU:N    | 1:O:454:GLU:CD   | 2.73                     | 0.42              |
| 1:B:247:LEU:CD1  | 1:B:255:LEU:HD12 | 2.50                     | 0.42              |
| 1:B:301:ASP:OD1  | 1:B:302:ILE:N    | 2.52                     | 0.42              |
| 1:B:479:GLU:H    | 1:B:479:GLU:CD   | 2.07                     | 0.42              |
| 1:C:301:ASP:OD1  | 1:C:302:ILE:N    | 2.52                     | 0.42              |
| 1:D:551:LYS:HB3  | 1:D:566:ARG:HG2  | 2.01                     | 0.42              |
| 1:E:454:GLU:N    | 1:E:454:GLU:CD   | 2.73                     | 0.42              |
| 1:G:225:LEU:O    | 1:G:229:ILE:HG13 | 2.19                     | 0.42              |
| 1:G:301:ASP:OD1  | 1:G:302:ILE:N    | 2.52                     | 0.42              |
| 1:G:504:VAL:HG11 | 1:G:521:ARG:CG   | 2.47                     | 0.42              |
| 1:H:219:PRO:HA   | 1:H:222:ARG:CB   | 2.45                     | 0.42              |
| 1:H:301:ASP:OD1  | 1:H:302:ILE:N    | 2.52                     | 0.42              |
| 1:I:247:LEU:CD1  | 1:I:255:LEU:HD12 | 2.50                     | 0.42              |
| 1:I:516:VAL:O    | 1:I:516:VAL:HG23 | 2.19                     | 0.42              |
| 1:K:170:VAL:HG11 | 1:K:229:ILE:HG21 | 2.01                     | 0.42              |
| 1:L:247:LEU:CD1  | 1:L:255:LEU:HD12 | 2.50                     | 0.42              |
| 1:L:339:VAL:HB   | 1:L:564:LEU:O    | 2.20                     | 0.42              |
| 1:M:339:VAL:HB   | 1:M:564:LEU:O    | 2.20                     | 0.42              |
| 1:M:539:GLY:CA   | 1:M:577:LEU:O    | 2.68                     | 0.42              |
| 1:N:247:LEU:CD1  | 1:N:255:LEU:HD12 | 2.50                     | 0.42              |
| 1:O:516:VAL:HG23 | 1:O:516:VAL:O    | 2.19                     | 0.42              |
| 1:A:142:ILE:CG2  | 1:A:149:VAL:HG22 | 2.50                     | 0.42              |
| 1:A:301:ASP:OD1  | 1:A:302:ILE:N    | 2.52                     | 0.42              |
| 1:B:123:ILE:HG23 | 1:B:130:ASN:HB2  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:521:ARG:HA   | 1:C:451:ILE:O    | 2.19                     | 0.42              |
| 1:C:115:LEU:HB3  | 1:C:119:LEU:HG   | 2.01                     | 0.42              |
| 1:D:181:VAL:HG12 | 1:D:185:GLU:OE2  | 2.20                     | 0.42              |
| 1:D:454:GLU:CD   | 1:D:454:GLU:N    | 2.73                     | 0.42              |
| 1:F:181:VAL:HG12 | 1:F:185:GLU:OE2  | 2.20                     | 0.42              |
| 1:F:301:ASP:OD1  | 1:F:302:ILE:N    | 2.52                     | 0.42              |
| 1:F:506:ASN:ND2  | 1:F:506:ASN:C    | 2.73                     | 0.42              |
| 1:F:339:VAL:HB   | 1:F:564:LEU:O    | 2.20                     | 0.42              |
| 1:G:167:ILE:CA   | 1:G:215:ILE:O    | 2.42                     | 0.42              |
| 1:G:247:LEU:CD1  | 1:G:255:LEU:HD12 | 2.50                     | 0.42              |
| 1:G:339:VAL:HB   | 1:G:564:LEU:O    | 2.20                     | 0.42              |
| 1:H:207:ASP:OD2  | 1:H:209:ARG:HB3  | 2.20                     | 0.42              |
| 1:I:207:ASP:OD2  | 1:I:209:ARG:HB3  | 2.20                     | 0.42              |
| 1:I:301:ASP:OD1  | 1:I:302:ILE:N    | 2.52                     | 0.42              |
| 1:L:504:VAL:HG12 | 1:L:521:ARG:HG2  | 1.94                     | 0.42              |
| 1:M:99:GLU:O     | 1:M:145:ARG:HA   | 2.20                     | 0.42              |
| 1:M:357:ALA:HB3  | 1:M:407:ILE:HD11 | 2.01                     | 0.42              |
| 1:M:454:GLU:CD   | 1:M:454:GLU:N    | 2.73                     | 0.42              |
| 1:N:225:LEU:O    | 1:N:229:ILE:HG13 | 2.19                     | 0.42              |
| 1:N:454:GLU:CD   | 1:N:454:GLU:N    | 2.73                     | 0.42              |
| 1:O:225:LEU:O    | 1:O:229:ILE:HG13 | 2.19                     | 0.42              |
| 1:A:339:VAL:HB   | 1:A:564:LEU:O    | 2.20                     | 0.41              |
| 1:B:139:ILE:HG22 | 1:B:140:ILE:N    | 2.27                     | 0.41              |
| 1:B:357:ALA:HB3  | 1:B:407:ILE:HD11 | 2.01                     | 0.41              |
| 1:C:123:ILE:HG23 | 1:C:130:ASN:HB2  | 2.02                     | 0.41              |
| 1:C:225:LEU:O    | 1:C:229:ILE:HG13 | 2.19                     | 0.41              |
| 1:D:215:ILE:HA   | 1:D:215:ILE:HD12 | 1.82                     | 0.41              |
| 1:D:301:ASP:OD1  | 1:D:302:ILE:N    | 2.52                     | 0.41              |
| 1:H:339:VAL:HB   | 1:H:564:LEU:O    | 2.20                     | 0.41              |
| 1:J:643:ILE:HD12 | 1:J:643:ILE:HA   | 1.86                     | 0.41              |
| 1:K:181:VAL:HG12 | 1:K:185:GLU:OE2  | 2.20                     | 0.41              |
| 1:K:246:TYR:HD1  | 1:K:293:SER:HB3  | 1.85                     | 0.41              |
| 1:K:454:GLU:N    | 1:K:454:GLU:CD   | 2.73                     | 0.41              |
| 1:K:521:ARG:HA   | 1:L:451:ILE:O    | 2.19                     | 0.41              |
| 1:L:454:GLU:N    | 1:L:454:GLU:CD   | 2.73                     | 0.41              |
| 1:A:247:LEU:CD1  | 1:A:255:LEU:HD12 | 2.50                     | 0.41              |
| 1:C:139:ILE:HG22 | 1:C:140:ILE:N    | 2.27                     | 0.41              |
| 1:C:288:HIS:HD2  | 1:C:291:THR:HB   | 1.86                     | 0.41              |
| 1:D:166:GLU:HB3  | 1:D:167:ILE:H    | 1.67                     | 0.41              |
| 1:D:339:VAL:HB   | 1:D:564:LEU:O    | 2.20                     | 0.41              |
| 1:D:516:VAL:HG23 | 1:D:516:VAL:O    | 2.19                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:640:GLN:NE2  | 1:D:643:ILE:HG21 | 2.35                     | 0.41              |
| 1:E:181:VAL:HG12 | 1:E:185:GLU:OE2  | 2.20                     | 0.41              |
| 1:E:246:TYR:HD1  | 1:E:293:SER:HB3  | 1.85                     | 0.41              |
| 1:E:301:ASP:OD1  | 1:E:302:ILE:N    | 2.52                     | 0.41              |
| 1:F:504:VAL:HG11 | 1:F:521:ARG:CG   | 2.47                     | 0.41              |
| 1:G:207:ASP:OD2  | 1:G:209:ARG:HB3  | 2.20                     | 0.41              |
| 1:H:516:VAL:O    | 1:H:516:VAL:HG23 | 2.19                     | 0.41              |
| 1:I:454:GLU:CD   | 1:I:454:GLU:N    | 2.73                     | 0.41              |
| 1:I:339:VAL:HB   | 1:I:564:LEU:O    | 2.20                     | 0.41              |
| 1:L:139:ILE:C    | 1:L:140:ILE:HG13 | 2.41                     | 0.41              |
| 1:M:140:ILE:HG21 | 1:M:156:ILE:HG21 | 2.02                     | 0.41              |
| 1:M:288:HIS:HD2  | 1:M:291:THR:HB   | 1.86                     | 0.41              |
| 1:N:113:ARG:HD2  | 1:N:134:TYR:CD2  | 2.55                     | 0.41              |
| 1:N:140:ILE:HG21 | 1:N:156:ILE:HG21 | 2.02                     | 0.41              |
| 1:N:288:HIS:HD2  | 1:N:291:THR:HB   | 1.85                     | 0.41              |
| 1:O:247:LEU:CD1  | 1:O:255:LEU:HD12 | 2.50                     | 0.41              |
| 1:A:246:TYR:HD1  | 1:A:293:SER:HB3  | 1.86                     | 0.41              |
| 1:A:256:VAL:HG23 | 1:A:285:ILE:HG22 | 2.03                     | 0.41              |
| 1:A:357:ALA:HB3  | 1:A:407:ILE:HD11 | 2.01                     | 0.41              |
| 1:A:99:GLU:O     | 1:A:145:ARG:HA   | 2.19                     | 0.41              |
| 1:B:115:LEU:HB3  | 1:B:119:LEU:HG   | 2.01                     | 0.41              |
| 1:B:440:ILE:HA   | 1:B:440:ILE:HD12 | 1.91                     | 0.41              |
| 1:C:142:ILE:CG2  | 1:C:149:VAL:HG22 | 2.50                     | 0.41              |
| 1:D:247:LEU:CD1  | 1:D:255:LEU:HD12 | 2.50                     | 0.41              |
| 1:D:246:TYR:HD1  | 1:D:293:SER:HB3  | 1.86                     | 0.41              |
| 1:E:140:ILE:HG21 | 1:E:156:ILE:HG21 | 2.02                     | 0.41              |
| 1:E:458:VAL:CG2  | 1:E:478:LYS:HG2  | 2.48                     | 0.41              |
| 1:E:352:TYR:OH   | 1:E:565:PHE:O    | 2.33                     | 0.41              |
| 1:E:551:LYS:HB3  | 1:E:566:ARG:HG2  | 2.01                     | 0.41              |
| 1:F:246:TYR:HD1  | 1:F:293:SER:HB3  | 1.85                     | 0.41              |
| 1:G:516:VAL:O    | 1:G:516:VAL:HG23 | 2.19                     | 0.41              |
| 1:H:288:HIS:HD2  | 1:H:291:THR:HB   | 1.86                     | 0.41              |
| 1:I:99:GLU:O     | 1:I:145:ARG:HA   | 2.19                     | 0.41              |
| 1:I:551:LYS:HB3  | 1:I:566:ARG:HG2  | 2.01                     | 0.41              |
| 1:I:643:ILE:HD12 | 1:I:643:ILE:HA   | 1.86                     | 0.41              |
| 1:J:207:ASP:OD2  | 1:J:209:ARG:HB3  | 2.20                     | 0.41              |
| 1:J:339:VAL:HB   | 1:J:564:LEU:O    | 2.20                     | 0.41              |
| 1:K:139:ILE:HG22 | 1:K:140:ILE:N    | 2.27                     | 0.41              |
| 1:L:357:ALA:HB3  | 1:L:407:ILE:HD11 | 2.01                     | 0.41              |
| 1:M:113:ARG:HD2  | 1:M:134:TYR:CD2  | 2.55                     | 0.41              |
| 1:M:139:ILE:C    | 1:M:140:ILE:HG13 | 2.41                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:178:ALA:O    | 1:M:181:VAL:HB   | 2.21                     | 0.41              |
| 1:N:142:ILE:CG2  | 1:N:149:VAL:HG22 | 2.50                     | 0.41              |
| 1:O:140:ILE:HG21 | 1:O:156:ILE:HG21 | 2.02                     | 0.41              |
| 1:O:99:GLU:O     | 1:O:145:ARG:HA   | 2.19                     | 0.41              |
| 1:A:123:ILE:HG23 | 1:A:130:ASN:HB2  | 2.02                     | 0.41              |
| 1:B:178:ALA:O    | 1:B:181:VAL:HB   | 2.21                     | 0.41              |
| 1:B:313:LEU:HD11 | 1:C:295:VAL:HG21 | 2.03                     | 0.41              |
| 1:B:643:ILE:HD12 | 1:B:643:ILE:HA   | 1.86                     | 0.41              |
| 1:E:178:ALA:O    | 1:E:181:VAL:HB   | 2.21                     | 0.41              |
| 1:F:640:GLN:NE2  | 1:F:643:ILE:HG21 | 2.35                     | 0.41              |
| 1:G:181:VAL:HG12 | 1:G:185:GLU:OE2  | 2.20                     | 0.41              |
| 1:G:577:LEU:O    | 1:G:578:MET:HE2  | 2.21                     | 0.41              |
| 1:I:123:ILE:HG23 | 1:I:130:ASN:HB2  | 2.02                     | 0.41              |
| 1:I:458:VAL:CG2  | 1:I:478:LYS:HG2  | 2.48                     | 0.41              |
| 1:J:139:ILE:C    | 1:J:140:ILE:HG13 | 2.41                     | 0.41              |
| 1:J:246:TYR:HD1  | 1:J:293:SER:HB3  | 1.86                     | 0.41              |
| 1:J:454:GLU:CD   | 1:J:454:GLU:N    | 2.73                     | 0.41              |
| 1:K:123:ILE:HG23 | 1:K:130:ASN:HB2  | 2.02                     | 0.41              |
| 1:K:139:ILE:C    | 1:K:140:ILE:HG13 | 2.41                     | 0.41              |
| 1:K:339:VAL:HB   | 1:K:564:LEU:O    | 2.20                     | 0.41              |
| 1:L:178:ALA:O    | 1:L:181:VAL:HB   | 2.21                     | 0.41              |
| 1:L:479:GLU:CD   | 1:L:479:GLU:H    | 2.07                     | 0.41              |
| 1:M:142:ILE:CG2  | 1:M:149:VAL:HG22 | 2.50                     | 0.41              |
| 1:M:247:LEU:CD1  | 1:M:255:LEU:HD12 | 2.50                     | 0.41              |
| 1:N:256:VAL:HG23 | 1:N:285:ILE:HG22 | 2.03                     | 0.41              |
| 1:N:458:VAL:CG2  | 1:N:478:LYS:HG2  | 2.48                     | 0.41              |
| 1:N:539:GLY:CA   | 1:N:577:LEU:O    | 2.68                     | 0.41              |
| 1:O:113:ARG:HD2  | 1:O:134:TYR:CD2  | 2.55                     | 0.41              |
| 1:A:178:ALA:O    | 1:A:181:VAL:HB   | 2.21                     | 0.41              |
| 1:A:215:ILE:HA   | 1:A:215:ILE:HD12 | 1.82                     | 0.41              |
| 1:B:99:GLU:O     | 1:B:145:ARG:HA   | 2.19                     | 0.41              |
| 1:B:339:VAL:HB   | 1:B:564:LEU:O    | 2.20                     | 0.41              |
| 1:B:640:GLN:NE2  | 1:B:643:ILE:HG21 | 2.35                     | 0.41              |
| 1:C:577:LEU:O    | 1:C:578:MET:HE2  | 2.20                     | 0.41              |
| 1:D:140:ILE:HG21 | 1:D:156:ILE:HG21 | 2.02                     | 0.41              |
| 1:C:313:LEU:HD11 | 1:D:295:VAL:HG21 | 2.03                     | 0.41              |
| 1:E:207:ASP:OD2  | 1:E:209:ARG:HB3  | 2.20                     | 0.41              |
| 1:E:504:VAL:HG11 | 1:E:521:ARG:CG   | 2.47                     | 0.41              |
| 1:F:140:ILE:HG21 | 1:F:156:ILE:HG21 | 2.02                     | 0.41              |
| 1:F:178:ALA:O    | 1:F:181:VAL:HB   | 2.21                     | 0.41              |
| 1:F:539:GLY:CA   | 1:F:577:LEU:O    | 2.68                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:345:GLU:HG3  | 1:G:346:SER:H    | 1.86                     | 0.41              |
| 1:H:345:GLU:HG3  | 1:H:346:SER:H    | 1.86                     | 0.41              |
| 1:J:577:LEU:O    | 1:J:578:MET:HE2  | 2.20                     | 0.41              |
| 1:K:178:ALA:O    | 1:K:181:VAL:HB   | 2.21                     | 0.41              |
| 1:K:288:HIS:HD2  | 1:K:291:THR:HB   | 1.86                     | 0.41              |
| 1:L:123:ILE:HG23 | 1:L:130:ASN:HB2  | 2.02                     | 0.41              |
| 1:L:140:ILE:HG21 | 1:L:156:ILE:HG21 | 2.02                     | 0.41              |
| 1:L:207:ASP:OD2  | 1:L:209:ARG:HB3  | 2.20                     | 0.41              |
| 1:L:256:VAL:HG23 | 1:L:285:ILE:HG22 | 2.03                     | 0.41              |
| 1:L:288:HIS:HD2  | 1:L:291:THR:HB   | 1.86                     | 0.41              |
| 1:M:246:TYR:HD1  | 1:M:293:SER:HB3  | 1.86                     | 0.41              |
| 1:N:178:ALA:O    | 1:N:181:VAL:HB   | 2.21                     | 0.41              |
| 1:N:246:TYR:HD1  | 1:N:293:SER:HB3  | 1.85                     | 0.41              |
| 1:N:99:GLU:O     | 1:N:145:ARG:HA   | 2.19                     | 0.41              |
| 1:O:288:HIS:HD2  | 1:O:291:THR:HB   | 1.86                     | 0.41              |
| 1:O:339:VAL:HB   | 1:O:564:LEU:O    | 2.20                     | 0.41              |
| 1:A:166:GLU:HB3  | 1:A:167:ILE:H    | 1.67                     | 0.41              |
| 1:B:132:VAL:HG22 | 1:B:142:ILE:HG23 | 2.03                     | 0.41              |
| 1:A:313:LEU:HD11 | 1:B:295:VAL:HG21 | 2.03                     | 0.41              |
| 1:C:99:GLU:O     | 1:C:145:ARG:HA   | 2.20                     | 0.41              |
| 1:C:339:VAL:HB   | 1:C:564:LEU:O    | 2.20                     | 0.41              |
| 1:D:207:ASP:OD2  | 1:D:209:ARG:HB3  | 2.20                     | 0.41              |
| 1:D:225:LEU:HA   | 1:D:225:LEU:HD23 | 1.74                     | 0.41              |
| 1:E:99:GLU:O     | 1:E:145:ARG:HA   | 2.19                     | 0.41              |
| 1:E:288:HIS:HD2  | 1:E:291:THR:HB   | 1.86                     | 0.41              |
| 1:F:288:HIS:HD2  | 1:F:291:THR:HB   | 1.86                     | 0.41              |
| 1:F:458:VAL:CG2  | 1:F:478:LYS:HG2  | 2.48                     | 0.41              |
| 1:F:577:LEU:O    | 1:F:578:MET:HE2  | 2.21                     | 0.41              |
| 1:G:256:VAL:HG13 | 1:G:257:GLU:N    | 2.36                     | 0.41              |
| 1:H:246:TYR:HD1  | 1:H:293:SER:HB3  | 1.85                     | 0.41              |
| 1:I:246:TYR:HD1  | 1:I:293:SER:HB3  | 1.86                     | 0.41              |
| 1:J:123:ILE:HG23 | 1:J:130:ASN:HB2  | 2.02                     | 0.41              |
| 1:J:178:ALA:O    | 1:J:181:VAL:HB   | 2.21                     | 0.41              |
| 1:J:181:VAL:HG12 | 1:J:185:GLU:OE2  | 2.20                     | 0.41              |
| 1:L:516:VAL:O    | 1:L:516:VAL:HG23 | 2.19                     | 0.41              |
| 1:M:207:ASP:OD2  | 1:M:209:ARG:HB3  | 2.20                     | 0.41              |
| 1:O:139:ILE:C    | 1:O:140:ILE:HG13 | 2.41                     | 0.41              |
| 1:A:113:ARG:HD2  | 1:A:134:TYR:CD2  | 2.55                     | 0.41              |
| 1:A:132:VAL:HG22 | 1:A:142:ILE:HG23 | 2.03                     | 0.41              |
| 1:A:207:ASP:OD2  | 1:A:209:ARG:HB3  | 2.20                     | 0.41              |
| 1:A:288:HIS:HD2  | 1:A:291:THR:HB   | 1.86                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:256:VAL:HG13 | 1:B:257:GLU:N    | 2.36                     | 0.41              |
| 1:B:345:GLU:HG3  | 1:B:346:SER:H    | 1.86                     | 0.41              |
| 1:C:215:ILE:HA   | 1:C:215:ILE:HD12 | 1.82                     | 0.41              |
| 1:C:256:VAL:HG23 | 1:C:285:ILE:HG22 | 2.03                     | 0.41              |
| 1:C:640:GLN:NE2  | 1:C:643:ILE:HG21 | 2.35                     | 0.41              |
| 1:D:123:ILE:HG23 | 1:D:130:ASN:HB2  | 2.02                     | 0.41              |
| 1:D:256:VAL:HG13 | 1:D:257:GLU:N    | 2.36                     | 0.41              |
| 1:E:142:ILE:CG2  | 1:E:149:VAL:HG22 | 2.50                     | 0.41              |
| 1:F:207:ASP:OD2  | 1:F:209:ARG:HB3  | 2.20                     | 0.41              |
| 1:F:551:LYS:HB3  | 1:F:566:ARG:HG2  | 2.01                     | 0.41              |
| 1:H:225:LEU:O    | 1:H:229:ILE:HG13 | 2.19                     | 0.41              |
| 1:H:577:LEU:O    | 1:H:578:MET:HE2  | 2.21                     | 0.41              |
| 1:K:207:ASP:OD2  | 1:K:209:ARG:HB3  | 2.20                     | 0.41              |
| 1:K:516:VAL:HG23 | 1:K:516:VAL:O    | 2.19                     | 0.41              |
| 1:K:613:LYS:HG3  | 1:K:613:LYS:O    | 2.21                     | 0.41              |
| 1:L:215:ILE:HA   | 1:L:215:ILE:HD12 | 1.82                     | 0.41              |
| 1:N:139:ILE:C    | 1:N:140:ILE:HG13 | 2.41                     | 0.41              |
| 1:N:313:LEU:HD11 | 1:O:295:VAL:HG21 | 2.03                     | 0.41              |
| 1:A:139:ILE:HG22 | 1:A:140:ILE:N    | 2.27                     | 0.41              |
| 1:A:295:VAL:HG21 | 1:O:313:LEU:HD11 | 2.03                     | 0.41              |
| 1:A:345:GLU:HG3  | 1:A:346:SER:H    | 1.86                     | 0.41              |
| 1:B:246:TYR:HD1  | 1:B:293:SER:HB3  | 1.85                     | 0.41              |
| 1:B:577:LEU:O    | 1:B:578:MET:HE2  | 2.21                     | 0.41              |
| 1:C:132:VAL:HG22 | 1:C:142:ILE:HG23 | 2.03                     | 0.41              |
| 1:C:140:ILE:HG21 | 1:C:156:ILE:HG21 | 2.02                     | 0.41              |
| 1:C:155:ILE:O    | 1:C:158:ARG:HB3  | 2.21                     | 0.41              |
| 1:C:246:TYR:HD1  | 1:C:293:SER:HB3  | 1.86                     | 0.41              |
| 1:D:504:VAL:HG11 | 1:D:521:ARG:CG   | 2.47                     | 0.41              |
| 1:E:177:ALA:HB3  | 1:E:208:GLU:HG3  | 2.00                     | 0.41              |
| 1:E:506:ASN:C    | 1:E:506:ASN:ND2  | 2.73                     | 0.41              |
| 1:F:113:ARG:HD2  | 1:F:134:TYR:CD2  | 2.55                     | 0.41              |
| 1:F:345:GLU:HG3  | 1:F:346:SER:H    | 1.86                     | 0.41              |
| 1:G:215:ILE:HA   | 1:G:215:ILE:HD12 | 1.82                     | 0.41              |
| 1:G:225:LEU:HA   | 1:G:225:LEU:HD23 | 1.74                     | 0.41              |
| 1:G:551:LYS:HB3  | 1:G:566:ARG:HG2  | 2.01                     | 0.41              |
| 1:H:142:ILE:CG2  | 1:H:149:VAL:HG22 | 2.50                     | 0.41              |
| 1:H:256:VAL:HG13 | 1:H:257:GLU:N    | 2.36                     | 0.41              |
| 1:I:345:GLU:HG3  | 1:I:346:SER:H    | 1.86                     | 0.41              |
| 1:J:613:LYS:HG3  | 1:J:613:LYS:O    | 2.21                     | 0.41              |
| 1:K:215:ILE:HD12 | 1:K:215:ILE:HA   | 1.82                     | 0.41              |
| 1:K:459:ILE:HG13 | 1:K:475:VAL:HG12 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:643:ILE:HD12 | 1:K:643:ILE:HA   | 1.86                     | 0.41              |
| 1:L:179:GLU:O    | 1:L:183:ILE:HG23 | 2.21                     | 0.41              |
| 1:L:342:GLY:HA3  | 1:L:363:MET:HE1  | 2.03                     | 0.41              |
| 1:N:105:VAL:CG1  | 1:N:157:ARG:HE   | 2.32                     | 0.41              |
| 1:O:166:GLU:HB3  | 1:O:167:ILE:H    | 1.67                     | 0.41              |
| 1:O:178:ALA:O    | 1:O:181:VAL:HB   | 2.21                     | 0.41              |
| 1:F:256:VAL:HG13 | 1:F:257:GLU:N    | 2.36                     | 0.41              |
| 1:F:552:VAL:HG22 | 1:F:552:VAL:H    | 1.59                     | 0.41              |
| 1:G:155:ILE:O    | 1:G:158:ARG:HB3  | 2.21                     | 0.41              |
| 1:G:180:MET:HE2  | 1:G:213:ILE:HD11 | 2.01                     | 0.41              |
| 1:H:551:LYS:HB3  | 1:H:566:ARG:HG2  | 2.02                     | 0.41              |
| 1:I:178:ALA:O    | 1:I:181:VAL:HB   | 2.21                     | 0.41              |
| 1:I:181:VAL:HG12 | 1:I:185:GLU:OE2  | 2.20                     | 0.41              |
| 1:I:256:VAL:HG13 | 1:I:257:GLU:N    | 2.36                     | 0.41              |
| 1:I:288:HIS:HD2  | 1:I:291:THR:HB   | 1.86                     | 0.41              |
| 1:H:524:ASN:OD1  | 1:I:449:SER:HB2  | 2.21                     | 0.41              |
| 1:J:142:ILE:CG2  | 1:J:149:VAL:HG22 | 2.50                     | 0.41              |
| 1:J:288:HIS:HD2  | 1:J:291:THR:HB   | 1.86                     | 0.41              |
| 1:I:524:ASN:OD1  | 1:J:449:SER:HB2  | 2.21                     | 0.41              |
| 1:J:459:ILE:HG13 | 1:J:475:VAL:HG12 | 2.03                     | 0.41              |
| 1:K:440:ILE:HA   | 1:K:440:ILE:HD12 | 1.91                     | 0.41              |
| 1:K:479:GLU:CD   | 1:K:479:GLU:H    | 2.07                     | 0.41              |
| 1:L:142:ILE:CG2  | 1:L:149:VAL:HG22 | 2.50                     | 0.41              |
| 1:L:506:ASN:C    | 1:L:506:ASN:ND2  | 2.73                     | 0.41              |
| 1:M:313:LEU:HD11 | 1:N:295:VAL:HG21 | 2.03                     | 0.41              |
| 1:N:339:VAL:HB   | 1:N:564:LEU:O    | 2.20                     | 0.41              |
| 1:O:359:ILE:HD13 | 1:O:422:LEU:HB2  | 2.03                     | 0.41              |
| 1:A:140:ILE:HG21 | 1:A:156:ILE:HG21 | 2.02                     | 0.41              |
| 1:C:178:ALA:O    | 1:C:181:VAL:HB   | 2.21                     | 0.41              |
| 1:E:139:ILE:HG22 | 1:E:140:ILE:N    | 2.27                     | 0.41              |
| 1:E:640:GLN:NE2  | 1:E:643:ILE:HG21 | 2.35                     | 0.41              |
| 1:F:247:LEU:CD1  | 1:F:255:LEU:HD12 | 2.50                     | 0.41              |
| 1:G:140:ILE:HG21 | 1:G:156:ILE:HG21 | 2.02                     | 0.41              |
| 1:H:123:ILE:HG23 | 1:H:130:ASN:HB2  | 2.02                     | 0.41              |
| 1:H:113:ARG:HD2  | 1:H:134:TYR:CD2  | 2.55                     | 0.41              |
| 1:J:102:THR:OG1  | 1:J:142:ILE:O    | 2.25                     | 0.41              |
| 1:J:105:VAL:CG1  | 1:J:157:ARG:HE   | 2.32                     | 0.41              |
| 1:J:539:GLY:CA   | 1:J:577:LEU:O    | 2.68                     | 0.41              |
| 1:K:140:ILE:HG21 | 1:K:156:ILE:HG21 | 2.02                     | 0.41              |
| 1:K:179:GLU:O    | 1:K:183:ILE:HG23 | 2.21                     | 0.41              |
| 1:J:524:ASN:OD1  | 1:K:449:SER:HB2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:640:GLN:NE2  | 1:K:643:ILE:HG21 | 2.35                     | 0.41              |
| 1:L:246:TYR:HD1  | 1:L:293:SER:HB3  | 1.86                     | 0.41              |
| 1:L:459:ILE:HG13 | 1:L:475:VAL:HG12 | 2.03                     | 0.41              |
| 1:L:613:LYS:HG3  | 1:L:613:LYS:O    | 2.21                     | 0.41              |
| 1:L:640:GLN:NE2  | 1:L:643:ILE:HG21 | 2.36                     | 0.41              |
| 1:M:123:ILE:HG23 | 1:M:130:ASN:HB2  | 2.02                     | 0.41              |
| 1:M:179:GLU:O    | 1:M:183:ILE:HG23 | 2.21                     | 0.41              |
| 1:M:613:LYS:HG3  | 1:M:613:LYS:O    | 2.21                     | 0.41              |
| 1:M:640:GLN:NE2  | 1:M:643:ILE:HG21 | 2.36                     | 0.41              |
| 1:N:643:ILE:HD12 | 1:N:643:ILE:HA   | 1.86                     | 0.41              |
| 1:O:123:ILE:HG23 | 1:O:130:ASN:HB2  | 2.02                     | 0.41              |
| 1:O:539:GLY:CA   | 1:O:577:LEU:O    | 2.68                     | 0.41              |
| 1:A:359:ILE:HD13 | 1:A:422:LEU:HB2  | 2.04                     | 0.41              |
| 1:B:139:ILE:C    | 1:B:140:ILE:HG13 | 2.41                     | 0.41              |
| 1:B:215:ILE:HD12 | 1:B:215:ILE:HA   | 1.82                     | 0.41              |
| 1:B:359:ILE:HD13 | 1:B:422:LEU:HB2  | 2.03                     | 0.41              |
| 1:D:139:ILE:HG22 | 1:D:140:ILE:N    | 2.27                     | 0.41              |
| 1:D:139:ILE:C    | 1:D:140:ILE:HG13 | 2.41                     | 0.41              |
| 1:D:105:VAL:CG1  | 1:D:157:ARG:HE   | 2.31                     | 0.41              |
| 1:D:313:LEU:HD11 | 1:E:295:VAL:HG21 | 2.03                     | 0.41              |
| 1:F:123:ILE:HG23 | 1:F:130:ASN:HB2  | 2.02                     | 0.41              |
| 1:G:640:GLN:NE2  | 1:G:643:ILE:HG21 | 2.35                     | 0.41              |
| 1:H:139:ILE:C    | 1:H:140:ILE:HG13 | 2.41                     | 0.41              |
| 1:H:181:VAL:HG12 | 1:H:185:GLU:OE2  | 2.20                     | 0.41              |
| 1:G:524:ASN:OD1  | 1:H:449:SER:HB2  | 2.21                     | 0.41              |
| 1:I:139:ILE:C    | 1:I:140:ILE:HG13 | 2.41                     | 0.41              |
| 1:J:155:ILE:O    | 1:J:158:ARG:HB3  | 2.21                     | 0.41              |
| 1:L:345:GLU:HG3  | 1:L:346:SER:H    | 1.86                     | 0.41              |
| 1:N:640:GLN:NE2  | 1:N:643:ILE:HG21 | 2.35                     | 0.41              |
| 1:B:113:ARG:HD2  | 1:B:134:TYR:CD2  | 2.55                     | 0.40              |
| 1:B:288:HIS:HD2  | 1:B:291:THR:HB   | 1.86                     | 0.40              |
| 1:C:139:ILE:C    | 1:C:140:ILE:HG13 | 2.41                     | 0.40              |
| 1:C:345:GLU:HG3  | 1:C:346:SER:H    | 1.86                     | 0.40              |
| 1:D:132:VAL:HG22 | 1:D:142:ILE:HG23 | 2.03                     | 0.40              |
| 1:D:99:GLU:O     | 1:D:145:ARG:HA   | 2.19                     | 0.40              |
| 1:D:155:ILE:O    | 1:D:158:ARG:HB3  | 2.21                     | 0.40              |
| 1:D:178:ALA:O    | 1:D:181:VAL:HB   | 2.21                     | 0.40              |
| 1:E:139:ILE:C    | 1:E:140:ILE:HG13 | 2.41                     | 0.40              |
| 1:E:313:LEU:HD11 | 1:F:295:VAL:HG21 | 2.03                     | 0.40              |
| 1:E:577:LEU:O    | 1:E:578:MET:HE2  | 2.21                     | 0.40              |
| 1:E:643:ILE:HD12 | 1:E:643:ILE:HA   | 1.86                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:113:ARG:HD2  | 1:G:134:TYR:CD2  | 2.55                     | 0.40              |
| 1:G:123:ILE:HG23 | 1:G:130:ASN:HB2  | 2.02                     | 0.40              |
| 1:G:285:ILE:HD12 | 1:G:296:LEU:HD23 | 2.03                     | 0.40              |
| 1:G:613:LYS:O    | 1:G:613:LYS:HG3  | 2.21                     | 0.40              |
| 1:H:132:VAL:HG22 | 1:H:142:ILE:HG23 | 2.03                     | 0.40              |
| 1:I:459:ILE:HG13 | 1:I:475:VAL:HG12 | 2.03                     | 0.40              |
| 1:J:479:GLU:CD   | 1:J:479:GLU:H    | 2.07                     | 0.40              |
| 1:K:155:ILE:O    | 1:K:158:ARG:HB3  | 2.21                     | 0.40              |
| 1:N:613:LYS:HG3  | 1:N:613:LYS:O    | 2.21                     | 0.40              |
| 1:O:506:ASN:C    | 1:O:506:ASN:ND2  | 2.73                     | 0.40              |
| 1:A:139:ILE:C    | 1:A:140:ILE:HG13 | 2.41                     | 0.40              |
| 1:A:522:GLN:HG2  | 1:B:451:ILE:HG21 | 2.04                     | 0.40              |
| 1:B:140:ILE:HG21 | 1:B:156:ILE:HG21 | 2.02                     | 0.40              |
| 1:E:552:VAL:HG22 | 1:E:552:VAL:H    | 1.59                     | 0.40              |
| 1:F:155:ILE:O    | 1:F:158:ARG:HB3  | 2.21                     | 0.40              |
| 1:G:177:ALA:HB3  | 1:G:208:GLU:HG3  | 2.00                     | 0.40              |
| 1:G:178:ALA:O    | 1:G:181:VAL:HB   | 2.21                     | 0.40              |
| 1:G:246:TYR:HD1  | 1:G:293:SER:HB3  | 1.86                     | 0.40              |
| 1:H:640:GLN:NE2  | 1:H:643:ILE:HG21 | 2.35                     | 0.40              |
| 1:I:132:VAL:HG22 | 1:I:142:ILE:HG23 | 2.03                     | 0.40              |
| 1:I:155:ILE:O    | 1:I:158:ARG:HB3  | 2.21                     | 0.40              |
| 1:I:285:ILE:HD12 | 1:I:296:LEU:HD23 | 2.04                     | 0.40              |
| 1:J:113:ARG:HD2  | 1:J:134:TYR:CD2  | 2.55                     | 0.40              |
| 1:J:179:GLU:O    | 1:J:183:ILE:HG23 | 2.21                     | 0.40              |
| 1:K:142:ILE:CG2  | 1:K:149:VAL:HG22 | 2.50                     | 0.40              |
| 1:M:345:GLU:HG3  | 1:M:346:SER:H    | 1.86                     | 0.40              |
| 1:M:359:ILE:HD13 | 1:M:422:LEU:HB2  | 2.03                     | 0.40              |
| 1:N:179:GLU:O    | 1:N:183:ILE:HG23 | 2.21                     | 0.40              |
| 1:N:359:ILE:HD13 | 1:N:422:LEU:HB2  | 2.04                     | 0.40              |
| 1:O:132:VAL:HG22 | 1:O:142:ILE:HG23 | 2.03                     | 0.40              |
| 1:O:142:ILE:CG2  | 1:O:149:VAL:HG22 | 2.50                     | 0.40              |
| 1:A:451:ILE:HG21 | 1:O:522:GLN:HG2  | 2.04                     | 0.40              |
| 1:A:105:VAL:CG1  | 1:A:157:ARG:HE   | 2.32                     | 0.40              |
| 1:A:155:ILE:O    | 1:A:158:ARG:HB3  | 2.21                     | 0.40              |
| 1:B:142:ILE:CG2  | 1:B:149:VAL:HG22 | 2.50                     | 0.40              |
| 1:B:105:VAL:CG1  | 1:B:157:ARG:HE   | 2.31                     | 0.40              |
| 1:B:256:VAL:HG23 | 1:B:285:ILE:HG22 | 2.03                     | 0.40              |
| 1:A:612:GLU:CG   | 1:B:642:PHE:CE2  | 2.81                     | 0.40              |
| 1:C:359:ILE:HD13 | 1:C:422:LEU:HB2  | 2.03                     | 0.40              |
| 1:E:166:GLU:HB3  | 1:E:167:ILE:H    | 1.67                     | 0.40              |
| 1:E:256:VAL:HG23 | 1:E:285:ILE:HG22 | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:345:GLU:HG3  | 1:E:346:SER:H    | 1.86                     | 0.40              |
| 1:G:132:VAL:HG22 | 1:G:142:ILE:HG23 | 2.03                     | 0.40              |
| 1:G:142:ILE:CG2  | 1:G:149:VAL:HG22 | 2.50                     | 0.40              |
| 1:G:288:HIS:HD2  | 1:G:291:THR:HB   | 1.86                     | 0.40              |
| 1:F:524:ASN:OD1  | 1:G:449:SER:HB2  | 2.21                     | 0.40              |
| 1:H:155:ILE:O    | 1:H:158:ARG:HB3  | 2.21                     | 0.40              |
| 1:H:179:GLU:O    | 1:H:183:ILE:HG23 | 2.21                     | 0.40              |
| 1:H:458:VAL:CG2  | 1:H:478:LYS:HG2  | 2.48                     | 0.40              |
| 1:I:113:ARG:HD2  | 1:I:134:TYR:CD2  | 2.55                     | 0.40              |
| 1:I:479:GLU:CD   | 1:I:479:GLU:H    | 2.07                     | 0.40              |
| 1:J:256:VAL:HG13 | 1:J:257:GLU:N    | 2.36                     | 0.40              |
| 1:J:256:VAL:HG23 | 1:J:285:ILE:HG22 | 2.03                     | 0.40              |
| 1:I:313:LEU:HD11 | 1:J:295:VAL:HG21 | 2.03                     | 0.40              |
| 1:K:113:ARG:HD2  | 1:K:134:TYR:CD2  | 2.55                     | 0.40              |
| 1:L:360:GLY:O    | 1:L:364:ILE:HG12 | 2.22                     | 0.40              |
| 1:K:524:ASN:OD1  | 1:L:449:SER:HB2  | 2.21                     | 0.40              |
| 1:L:524:ASN:N    | 1:L:524:ASN:OD1  | 2.55                     | 0.40              |
| 1:M:360:GLY:O    | 1:M:364:ILE:HG12 | 2.22                     | 0.40              |
| 1:M:459:ILE:HG13 | 1:M:475:VAL:HG12 | 2.03                     | 0.40              |
| 1:M:552:VAL:HG22 | 1:M:552:VAL:H    | 1.59                     | 0.40              |
| 1:O:155:ILE:O    | 1:O:158:ARG:HB3  | 2.21                     | 0.40              |
| 1:O:256:VAL:HG13 | 1:O:257:GLU:N    | 2.36                     | 0.40              |
| 1:O:524:ASN:N    | 1:O:524:ASN:OD1  | 2.55                     | 0.40              |
| 1:B:155:ILE:O    | 1:B:158:ARG:HB3  | 2.21                     | 0.40              |
| 1:B:539:GLY:CA   | 1:B:577:LEU:O    | 2.68                     | 0.40              |
| 1:D:288:HIS:HD2  | 1:D:291:THR:HB   | 1.86                     | 0.40              |
| 1:E:256:VAL:HG13 | 1:E:257:GLU:N    | 2.36                     | 0.40              |
| 1:F:139:ILE:C    | 1:F:140:ILE:HG13 | 2.41                     | 0.40              |
| 1:H:459:ILE:HG13 | 1:H:475:VAL:HG12 | 2.03                     | 0.40              |
| 1:H:613:LYS:O    | 1:H:613:LYS:HG3  | 2.21                     | 0.40              |
| 1:J:285:ILE:HD12 | 1:J:296:LEU:HD23 | 2.03                     | 0.40              |
| 1:K:256:VAL:HG13 | 1:K:257:GLU:N    | 2.36                     | 0.40              |
| 1:L:155:ILE:O    | 1:L:158:ARG:HB3  | 2.21                     | 0.40              |
| 1:L:167:ILE:CA   | 1:L:215:ILE:O    | 2.42                     | 0.40              |
| 1:M:105:VAL:CG1  | 1:M:157:ARG:HE   | 2.32                     | 0.40              |
| 1:N:123:ILE:HG23 | 1:N:130:ASN:HB2  | 2.02                     | 0.40              |
| 1:N:155:ILE:O    | 1:N:158:ARG:HB3  | 2.21                     | 0.40              |
| 1:N:506:ASN:ND2  | 1:N:506:ASN:C    | 2.73                     | 0.40              |
| 1:O:256:VAL:HG23 | 1:O:285:ILE:HG22 | 2.03                     | 0.40              |
| 1:O:613:LYS:O    | 1:O:613:LYS:HG3  | 2.21                     | 0.40              |
| 1:O:640:GLN:NE2  | 1:O:643:ILE:HG21 | 2.35                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:539:GLY:CA   | 1:A:577:LEU:O    | 2.68                     | 0.40              |
| 1:B:459:ILE:HG13 | 1:B:475:VAL:HG12 | 2.03                     | 0.40              |
| 1:B:522:GLN:HG2  | 1:C:451:ILE:HG21 | 2.04                     | 0.40              |
| 1:C:459:ILE:HG13 | 1:C:475:VAL:HG12 | 2.03                     | 0.40              |
| 1:D:459:ILE:HG13 | 1:D:475:VAL:HG12 | 2.03                     | 0.40              |
| 1:F:285:ILE:HD12 | 1:F:296:LEU:HD23 | 2.04                     | 0.40              |
| 1:G:360:GLY:O    | 1:G:364:ILE:HG12 | 2.22                     | 0.40              |
| 1:H:178:ALA:O    | 1:H:181:VAL:HB   | 2.21                     | 0.40              |
| 1:H:285:ILE:HD12 | 1:H:296:LEU:HD23 | 2.04                     | 0.40              |
| 1:H:479:GLU:H    | 1:H:479:GLU:CD   | 2.07                     | 0.40              |
| 1:I:140:ILE:HG21 | 1:I:156:ILE:HG21 | 2.02                     | 0.40              |
| 1:I:179:GLU:O    | 1:I:183:ILE:HG23 | 2.21                     | 0.40              |
| 1:J:140:ILE:HG21 | 1:J:156:ILE:HG21 | 2.02                     | 0.40              |
| 1:J:640:GLN:NE2  | 1:J:643:ILE:HG21 | 2.35                     | 0.40              |
| 1:K:119:LEU:HD13 | 1:K:132:VAL:HG11 | 2.04                     | 0.40              |
| 1:K:132:VAL:HG22 | 1:K:142:ILE:HG23 | 2.03                     | 0.40              |
| 1:K:506:ASN:C    | 1:K:506:ASN:ND2  | 2.73                     | 0.40              |
| 1:L:119:LEU:HD13 | 1:L:132:VAL:HG11 | 2.04                     | 0.40              |
| 1:L:256:VAL:HG13 | 1:L:257:GLU:N    | 2.36                     | 0.40              |
| 1:M:155:ILE:O    | 1:M:158:ARG:HB3  | 2.21                     | 0.40              |
| 1:N:360:GLY:O    | 1:N:364:ILE:HG12 | 2.22                     | 0.40              |
| 1:O:523:LEU:HD22 | 1:O:538:GLY:HA3  | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | A     | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%)   | 52          | 86 |
| 1   | B     | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%)   | 52          | 86 |
| 1   | C     | 481/650 (74%) | 459 (95%) | 21 (4%) | 1 (0%)   | 52          | 86 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | D     | 481/650 (74%)   | 459 (95%)  | 21 (4%)  | 1 (0%)   | 52          | 86 |
| 1   | E     | 481/650 (74%)   | 459 (95%)  | 21 (4%)  | 1 (0%)   | 52          | 86 |
| 1   | F     | 481/650 (74%)   | 459 (95%)  | 21 (4%)  | 1 (0%)   | 52          | 86 |
| 1   | G     | 481/650 (74%)   | 458 (95%)  | 22 (5%)  | 1 (0%)   | 52          | 86 |
| 1   | H     | 481/650 (74%)   | 459 (95%)  | 21 (4%)  | 1 (0%)   | 52          | 86 |
| 1   | I     | 481/650 (74%)   | 459 (95%)  | 21 (4%)  | 1 (0%)   | 52          | 86 |
| 1   | J     | 481/650 (74%)   | 459 (95%)  | 21 (4%)  | 1 (0%)   | 52          | 86 |
| 1   | K     | 481/650 (74%)   | 459 (95%)  | 21 (4%)  | 1 (0%)   | 52          | 86 |
| 1   | L     | 481/650 (74%)   | 459 (95%)  | 21 (4%)  | 1 (0%)   | 52          | 86 |
| 1   | M     | 481/650 (74%)   | 459 (95%)  | 21 (4%)  | 1 (0%)   | 52          | 86 |
| 1   | N     | 481/650 (74%)   | 459 (95%)  | 21 (4%)  | 1 (0%)   | 52          | 86 |
| 1   | O     | 481/650 (74%)   | 459 (95%)  | 21 (4%)  | 1 (0%)   | 52          | 86 |
| All | All   | 7215/9750 (74%) | 6884 (95%) | 316 (4%) | 15 (0%)  | 56          | 86 |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 181 | VAL  |
| 1   | B     | 181 | VAL  |
| 1   | C     | 181 | VAL  |
| 1   | E     | 181 | VAL  |
| 1   | F     | 181 | VAL  |
| 1   | G     | 181 | VAL  |
| 1   | H     | 181 | VAL  |
| 1   | I     | 181 | VAL  |
| 1   | J     | 181 | VAL  |
| 1   | K     | 181 | VAL  |
| 1   | L     | 181 | VAL  |
| 1   | M     | 181 | VAL  |
| 1   | N     | 181 | VAL  |
| 1   | O     | 181 | VAL  |
| 1   | D     | 181 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | B     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | C     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | D     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | E     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | F     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | G     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | H     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | I     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | J     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | K     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | L     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | M     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | N     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| 1   | O     | 415/550 (76%)   | 403 (97%)  | 12 (3%)  | 50          | 79 |
| All | All   | 6225/8250 (76%) | 6045 (97%) | 180 (3%) | 54          | 79 |

All (180) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 455 | GLU  |
| 1   | A     | 459 | ILE  |
| 1   | A     | 473 | GLN  |
| 1   | A     | 474 | THR  |
| 1   | A     | 476 | ASP  |
| 1   | A     | 477 | ARG  |
| 1   | A     | 478 | LYS  |
| 1   | A     | 506 | ASN  |
| 1   | A     | 517 | ARG  |
| 1   | A     | 518 | PHE  |
| 1   | A     | 520 | LYS  |
| 1   | A     | 521 | ARG  |
| 1   | B     | 455 | GLU  |
| 1   | B     | 459 | ILE  |
| 1   | B     | 473 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 474 | THR  |
| 1   | B     | 476 | ASP  |
| 1   | B     | 477 | ARG  |
| 1   | B     | 478 | LYS  |
| 1   | B     | 506 | ASN  |
| 1   | B     | 517 | ARG  |
| 1   | B     | 518 | PHE  |
| 1   | B     | 520 | LYS  |
| 1   | B     | 521 | ARG  |
| 1   | C     | 455 | GLU  |
| 1   | C     | 459 | ILE  |
| 1   | C     | 473 | GLN  |
| 1   | C     | 474 | THR  |
| 1   | C     | 476 | ASP  |
| 1   | C     | 477 | ARG  |
| 1   | C     | 478 | LYS  |
| 1   | C     | 506 | ASN  |
| 1   | C     | 517 | ARG  |
| 1   | C     | 518 | PHE  |
| 1   | C     | 520 | LYS  |
| 1   | C     | 521 | ARG  |
| 1   | D     | 455 | GLU  |
| 1   | D     | 459 | ILE  |
| 1   | D     | 473 | GLN  |
| 1   | D     | 474 | THR  |
| 1   | D     | 476 | ASP  |
| 1   | D     | 477 | ARG  |
| 1   | D     | 478 | LYS  |
| 1   | D     | 506 | ASN  |
| 1   | D     | 517 | ARG  |
| 1   | D     | 518 | PHE  |
| 1   | D     | 520 | LYS  |
| 1   | D     | 521 | ARG  |
| 1   | E     | 455 | GLU  |
| 1   | E     | 459 | ILE  |
| 1   | E     | 473 | GLN  |
| 1   | E     | 474 | THR  |
| 1   | E     | 476 | ASP  |
| 1   | E     | 477 | ARG  |
| 1   | E     | 478 | LYS  |
| 1   | E     | 506 | ASN  |
| 1   | E     | 517 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 518 | PHE  |
| 1   | E     | 520 | LYS  |
| 1   | E     | 521 | ARG  |
| 1   | F     | 455 | GLU  |
| 1   | F     | 459 | ILE  |
| 1   | F     | 473 | GLN  |
| 1   | F     | 474 | THR  |
| 1   | F     | 476 | ASP  |
| 1   | F     | 477 | ARG  |
| 1   | F     | 478 | LYS  |
| 1   | F     | 506 | ASN  |
| 1   | F     | 517 | ARG  |
| 1   | F     | 518 | PHE  |
| 1   | F     | 520 | LYS  |
| 1   | F     | 521 | ARG  |
| 1   | G     | 455 | GLU  |
| 1   | G     | 459 | ILE  |
| 1   | G     | 473 | GLN  |
| 1   | G     | 474 | THR  |
| 1   | G     | 476 | ASP  |
| 1   | G     | 477 | ARG  |
| 1   | G     | 478 | LYS  |
| 1   | G     | 506 | ASN  |
| 1   | G     | 517 | ARG  |
| 1   | G     | 518 | PHE  |
| 1   | G     | 520 | LYS  |
| 1   | G     | 521 | ARG  |
| 1   | H     | 455 | GLU  |
| 1   | H     | 459 | ILE  |
| 1   | H     | 473 | GLN  |
| 1   | H     | 474 | THR  |
| 1   | H     | 476 | ASP  |
| 1   | H     | 477 | ARG  |
| 1   | H     | 478 | LYS  |
| 1   | H     | 506 | ASN  |
| 1   | H     | 517 | ARG  |
| 1   | H     | 518 | PHE  |
| 1   | H     | 520 | LYS  |
| 1   | H     | 521 | ARG  |
| 1   | I     | 455 | GLU  |
| 1   | I     | 459 | ILE  |
| 1   | I     | 473 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 474 | THR  |
| 1   | I     | 476 | ASP  |
| 1   | I     | 477 | ARG  |
| 1   | I     | 478 | LYS  |
| 1   | I     | 506 | ASN  |
| 1   | I     | 517 | ARG  |
| 1   | I     | 518 | PHE  |
| 1   | I     | 520 | LYS  |
| 1   | I     | 521 | ARG  |
| 1   | J     | 455 | GLU  |
| 1   | J     | 459 | ILE  |
| 1   | J     | 473 | GLN  |
| 1   | J     | 474 | THR  |
| 1   | J     | 476 | ASP  |
| 1   | J     | 477 | ARG  |
| 1   | J     | 478 | LYS  |
| 1   | J     | 506 | ASN  |
| 1   | J     | 517 | ARG  |
| 1   | J     | 518 | PHE  |
| 1   | J     | 520 | LYS  |
| 1   | J     | 521 | ARG  |
| 1   | K     | 455 | GLU  |
| 1   | K     | 459 | ILE  |
| 1   | K     | 473 | GLN  |
| 1   | K     | 474 | THR  |
| 1   | K     | 476 | ASP  |
| 1   | K     | 477 | ARG  |
| 1   | K     | 478 | LYS  |
| 1   | K     | 506 | ASN  |
| 1   | K     | 517 | ARG  |
| 1   | K     | 518 | PHE  |
| 1   | K     | 520 | LYS  |
| 1   | K     | 521 | ARG  |
| 1   | L     | 455 | GLU  |
| 1   | L     | 459 | ILE  |
| 1   | L     | 473 | GLN  |
| 1   | L     | 474 | THR  |
| 1   | L     | 476 | ASP  |
| 1   | L     | 477 | ARG  |
| 1   | L     | 478 | LYS  |
| 1   | L     | 506 | ASN  |
| 1   | L     | 517 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 518 | PHE  |
| 1   | L     | 520 | LYS  |
| 1   | L     | 521 | ARG  |
| 1   | M     | 455 | GLU  |
| 1   | M     | 459 | ILE  |
| 1   | M     | 473 | GLN  |
| 1   | M     | 474 | THR  |
| 1   | M     | 476 | ASP  |
| 1   | M     | 477 | ARG  |
| 1   | M     | 478 | LYS  |
| 1   | M     | 506 | ASN  |
| 1   | M     | 517 | ARG  |
| 1   | M     | 518 | PHE  |
| 1   | M     | 520 | LYS  |
| 1   | M     | 521 | ARG  |
| 1   | N     | 455 | GLU  |
| 1   | N     | 459 | ILE  |
| 1   | N     | 473 | GLN  |
| 1   | N     | 474 | THR  |
| 1   | N     | 476 | ASP  |
| 1   | N     | 477 | ARG  |
| 1   | N     | 478 | LYS  |
| 1   | N     | 506 | ASN  |
| 1   | N     | 517 | ARG  |
| 1   | N     | 518 | PHE  |
| 1   | N     | 520 | LYS  |
| 1   | N     | 521 | ARG  |
| 1   | O     | 455 | GLU  |
| 1   | O     | 459 | ILE  |
| 1   | O     | 473 | GLN  |
| 1   | O     | 474 | THR  |
| 1   | O     | 476 | ASP  |
| 1   | O     | 477 | ARG  |
| 1   | O     | 478 | LYS  |
| 1   | O     | 506 | ASN  |
| 1   | O     | 517 | ARG  |
| 1   | O     | 518 | PHE  |
| 1   | O     | 520 | LYS  |
| 1   | O     | 521 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 125 | ASN  |
| 1   | A     | 138 | ASN  |
| 1   | A     | 288 | HIS  |
| 1   | A     | 300 | GLN  |
| 1   | A     | 340 | GLN  |
| 1   | A     | 354 | ASN  |
| 1   | A     | 424 | ASN  |
| 1   | A     | 428 | ASN  |
| 1   | A     | 502 | GLN  |
| 1   | A     | 506 | ASN  |
| 1   | A     | 640 | GLN  |
| 1   | B     | 125 | ASN  |
| 1   | B     | 138 | ASN  |
| 1   | B     | 288 | HIS  |
| 1   | B     | 300 | GLN  |
| 1   | B     | 340 | GLN  |
| 1   | B     | 354 | ASN  |
| 1   | B     | 424 | ASN  |
| 1   | B     | 428 | ASN  |
| 1   | B     | 502 | GLN  |
| 1   | B     | 506 | ASN  |
| 1   | B     | 640 | GLN  |
| 1   | C     | 125 | ASN  |
| 1   | C     | 138 | ASN  |
| 1   | C     | 288 | HIS  |
| 1   | C     | 300 | GLN  |
| 1   | C     | 340 | GLN  |
| 1   | C     | 354 | ASN  |
| 1   | C     | 424 | ASN  |
| 1   | C     | 428 | ASN  |
| 1   | C     | 502 | GLN  |
| 1   | C     | 506 | ASN  |
| 1   | C     | 640 | GLN  |
| 1   | D     | 125 | ASN  |
| 1   | D     | 138 | ASN  |
| 1   | D     | 288 | HIS  |
| 1   | D     | 300 | GLN  |
| 1   | D     | 340 | GLN  |
| 1   | D     | 354 | ASN  |
| 1   | D     | 424 | ASN  |
| 1   | D     | 428 | ASN  |
| 1   | D     | 502 | GLN  |
| 1   | D     | 506 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 640 | GLN  |
| 1   | E     | 125 | ASN  |
| 1   | E     | 138 | ASN  |
| 1   | E     | 288 | HIS  |
| 1   | E     | 300 | GLN  |
| 1   | E     | 340 | GLN  |
| 1   | E     | 354 | ASN  |
| 1   | E     | 424 | ASN  |
| 1   | E     | 428 | ASN  |
| 1   | E     | 502 | GLN  |
| 1   | E     | 506 | ASN  |
| 1   | E     | 640 | GLN  |
| 1   | F     | 125 | ASN  |
| 1   | F     | 138 | ASN  |
| 1   | F     | 288 | HIS  |
| 1   | F     | 300 | GLN  |
| 1   | F     | 340 | GLN  |
| 1   | F     | 354 | ASN  |
| 1   | F     | 424 | ASN  |
| 1   | F     | 428 | ASN  |
| 1   | F     | 502 | GLN  |
| 1   | F     | 506 | ASN  |
| 1   | F     | 640 | GLN  |
| 1   | G     | 125 | ASN  |
| 1   | G     | 138 | ASN  |
| 1   | G     | 288 | HIS  |
| 1   | G     | 300 | GLN  |
| 1   | G     | 340 | GLN  |
| 1   | G     | 354 | ASN  |
| 1   | G     | 424 | ASN  |
| 1   | G     | 428 | ASN  |
| 1   | G     | 502 | GLN  |
| 1   | G     | 506 | ASN  |
| 1   | G     | 640 | GLN  |
| 1   | H     | 125 | ASN  |
| 1   | H     | 138 | ASN  |
| 1   | H     | 288 | HIS  |
| 1   | H     | 300 | GLN  |
| 1   | H     | 340 | GLN  |
| 1   | H     | 354 | ASN  |
| 1   | H     | 424 | ASN  |
| 1   | H     | 428 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 502 | GLN  |
| 1   | H     | 506 | ASN  |
| 1   | H     | 640 | GLN  |
| 1   | I     | 125 | ASN  |
| 1   | I     | 138 | ASN  |
| 1   | I     | 288 | HIS  |
| 1   | I     | 300 | GLN  |
| 1   | I     | 340 | GLN  |
| 1   | I     | 354 | ASN  |
| 1   | I     | 424 | ASN  |
| 1   | I     | 428 | ASN  |
| 1   | I     | 502 | GLN  |
| 1   | I     | 506 | ASN  |
| 1   | I     | 640 | GLN  |
| 1   | J     | 125 | ASN  |
| 1   | J     | 138 | ASN  |
| 1   | J     | 288 | HIS  |
| 1   | J     | 300 | GLN  |
| 1   | J     | 340 | GLN  |
| 1   | J     | 354 | ASN  |
| 1   | J     | 424 | ASN  |
| 1   | J     | 428 | ASN  |
| 1   | J     | 502 | GLN  |
| 1   | J     | 506 | ASN  |
| 1   | J     | 640 | GLN  |
| 1   | K     | 125 | ASN  |
| 1   | K     | 138 | ASN  |
| 1   | K     | 288 | HIS  |
| 1   | K     | 300 | GLN  |
| 1   | K     | 340 | GLN  |
| 1   | K     | 354 | ASN  |
| 1   | K     | 424 | ASN  |
| 1   | K     | 428 | ASN  |
| 1   | K     | 502 | GLN  |
| 1   | K     | 506 | ASN  |
| 1   | K     | 640 | GLN  |
| 1   | L     | 125 | ASN  |
| 1   | L     | 138 | ASN  |
| 1   | L     | 288 | HIS  |
| 1   | L     | 300 | GLN  |
| 1   | L     | 340 | GLN  |
| 1   | L     | 354 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 424 | ASN  |
| 1   | L     | 428 | ASN  |
| 1   | L     | 502 | GLN  |
| 1   | L     | 506 | ASN  |
| 1   | L     | 640 | GLN  |
| 1   | M     | 125 | ASN  |
| 1   | M     | 138 | ASN  |
| 1   | M     | 288 | HIS  |
| 1   | M     | 300 | GLN  |
| 1   | M     | 340 | GLN  |
| 1   | M     | 354 | ASN  |
| 1   | M     | 424 | ASN  |
| 1   | M     | 428 | ASN  |
| 1   | M     | 502 | GLN  |
| 1   | M     | 506 | ASN  |
| 1   | M     | 640 | GLN  |
| 1   | N     | 125 | ASN  |
| 1   | N     | 138 | ASN  |
| 1   | N     | 288 | HIS  |
| 1   | N     | 300 | GLN  |
| 1   | N     | 340 | GLN  |
| 1   | N     | 354 | ASN  |
| 1   | N     | 424 | ASN  |
| 1   | N     | 428 | ASN  |
| 1   | N     | 502 | GLN  |
| 1   | N     | 506 | ASN  |
| 1   | N     | 640 | GLN  |
| 1   | O     | 125 | ASN  |
| 1   | O     | 138 | ASN  |
| 1   | O     | 288 | HIS  |
| 1   | O     | 300 | GLN  |
| 1   | O     | 340 | GLN  |
| 1   | O     | 354 | ASN  |
| 1   | O     | 424 | ASN  |
| 1   | O     | 428 | ASN  |
| 1   | O     | 502 | GLN  |
| 1   | O     | 506 | ASN  |
| 1   | O     | 640 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.