



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

Feb 16, 2018 – 06:36 am GMT

PDB ID : 4AB3  
EMDB ID: : EMD-2003  
Title : ATP-triggered molecular mechanics of the chaperonin GroEL  
Authors : Clare, D.K.; Vasishtan, D.; Stagg, S.; Quispe, J.; Farr, G.W.; Topf, M.; Horwich, A.L.; Saibil, H.R.  
Deposited on : 2011-12-06  
Resolution : 8.50 Å(reported)  
Based on PDB ID : 1OEL

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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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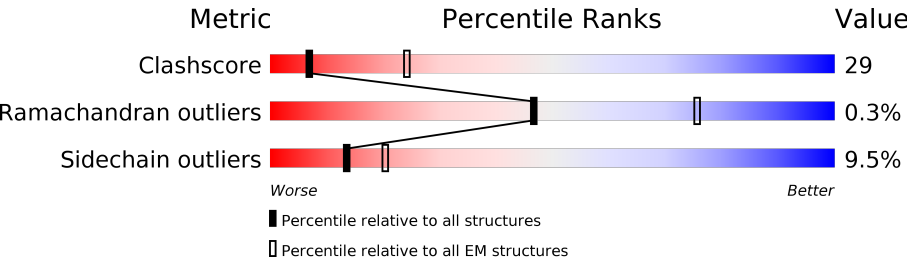
MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.50 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 136279                      | 1886                        |
| Ramachandran outliers | 132675                      | 1663                        |
| Sidechain outliers    | 132484                      | 1531                        |

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     | 548    | 57% 29% 7% . .   |
| 1   | B     | 548    | 56% 30% 7% . .   |
| 1   | C     | 548    | 56% 29% 7% . .   |
| 1   | D     | 548    | 56% 30% 7% . .   |
| 1   | E     | 548    | 57% 29% 7% . .   |
| 1   | F     | 548    | 57% 29% 7% . .   |
| 1   | G     | 548    | 57% 29% 7% . .   |
| 1   | H     | 548    | 52% 34% 9% . .   |
| 1   | I     | 548    | 52% 34% 8% . .   |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | J     | 548    |  |
| 1   | K     | 548    |  |
| 1   | L     | 548    |  |
| 1   | M     | 548    |  |
| 1   | N     | 548    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2   | PO4  | A     | 1525 | -         | -        | X       | -                |
| 2   | PO4  | B     | 1525 | -         | -        | X       | -                |
| 2   | PO4  | C     | 1525 | -         | -        | X       | -                |
| 2   | PO4  | D     | 1525 | -         | -        | X       | -                |
| 2   | PO4  | E     | 1525 | -         | -        | X       | -                |
| 2   | PO4  | F     | 1525 | -         | -        | X       | -                |
| 2   | PO4  | G     | 1525 | -         | -        | X       | -                |
| 2   | PO4  | H     | 1525 | -         | -        | X       | -                |
| 2   | PO4  | I     | 1525 | -         | -        | X       | -                |
| 2   | PO4  | J     | 1525 | -         | -        | X       | -                |
| 2   | PO4  | K     | 1525 | -         | -        | X       | -                |
| 2   | PO4  | L     | 1525 | -         | -        | X       | -                |
| 2   | PO4  | M     | 1525 | -         | -        | X       | -                |
| 2   | PO4  | N     | 1525 | -         | -        | X       | -                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 54293 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 60 KDA CHAPERONIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3846  | 2391 | 665 | 770 | 20 |         |       |
| 1   | B     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3845  | 2391 | 664 | 770 | 20 |         |       |
| 1   | C     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3845  | 2391 | 664 | 770 | 20 |         |       |
| 1   | D     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3845  | 2391 | 664 | 770 | 20 |         |       |
| 1   | E     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3845  | 2391 | 664 | 770 | 20 |         |       |
| 1   | F     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3845  | 2391 | 664 | 770 | 20 |         |       |
| 1   | G     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3845  | 2391 | 664 | 770 | 20 |         |       |
| 1   | H     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3845  | 2391 | 664 | 770 | 20 |         |       |
| 1   | I     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3845  | 2391 | 664 | 770 | 20 |         |       |
| 1   | J     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3845  | 2391 | 664 | 770 | 20 |         |       |
| 1   | K     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3845  | 2391 | 664 | 770 | 20 |         |       |
| 1   | L     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3845  | 2391 | 664 | 770 | 20 |         |       |
| 1   | M     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3845  | 2391 | 664 | 770 | 20 |         |       |
| 1   | N     | 524      | Total | C    | N   | O   | S  | 0       | 1     |
|     |       |          | 3845  | 2391 | 664 | 770 | 20 |         |       |

There are 14 discrepancies between the modelled and reference sequences:

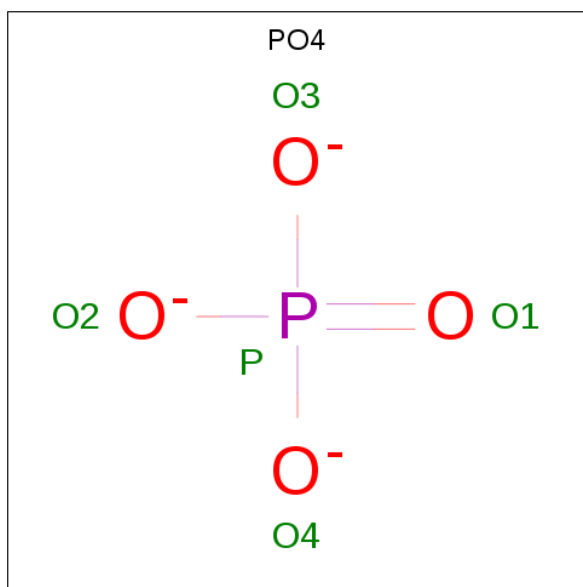
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| B     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| C     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| D     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| E     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| F     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| G     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| H     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| I     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| J     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| K     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| L     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| M     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |
| N     | 398     | ALA      | ASP    | engineered mutation | UNP P0A6F5 |

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms          | AltConf |
|-----|-------|----------|----------------|---------|
| 2   | A     | 1        | Total P<br>1 1 | 0       |
| 2   | B     | 1        | Total P<br>1 1 | 0       |
| 2   | C     | 1        | Total P<br>1 1 | 0       |
| 2   | D     | 1        | Total P<br>1 1 | 0       |
| 2   | E     | 1        | Total P<br>1 1 | 0       |

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| Mol | Chain | Residues | Atoms          | AltConf |
|-----|-------|----------|----------------|---------|
| 2   | F     | 1        | Total P<br>1 1 | 0       |
| 2   | G     | 1        | Total P<br>1 1 | 0       |
| 2   | H     | 1        | Total P<br>1 1 | 0       |
| 2   | I     | 1        | Total P<br>1 1 | 0       |
| 2   | J     | 1        | Total P<br>1 1 | 0       |
| 2   | K     | 1        | Total P<br>1 1 | 0       |
| 2   | L     | 1        | Total P<br>1 1 | 0       |
| 2   | M     | 1        | Total P<br>1 1 | 0       |
| 2   | N     | 1        | Total P<br>1 1 | 0       |

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

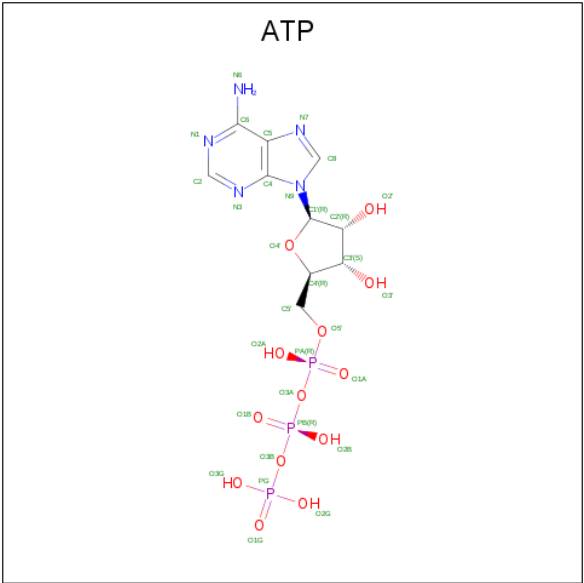
| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 3   | G     | 1        | Total Mg<br>1 1 | 0       |
| 3   | J     | 1        | Total Mg<br>1 1 | 0       |
| 3   | D     | 1        | Total Mg<br>1 1 | 0       |
| 3   | K     | 1        | Total Mg<br>1 1 | 0       |
| 3   | E     | 1        | Total Mg<br>1 1 | 0       |
| 3   | H     | 1        | Total Mg<br>1 1 | 0       |
| 3   | B     | 1        | Total Mg<br>1 1 | 0       |
| 3   | I     | 1        | Total Mg<br>1 1 | 0       |
| 3   | C     | 1        | Total Mg<br>1 1 | 0       |
| 3   | A     | 1        | Total Mg<br>1 1 | 0       |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 3   | N     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 3   | L     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 3   | F     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 3   | M     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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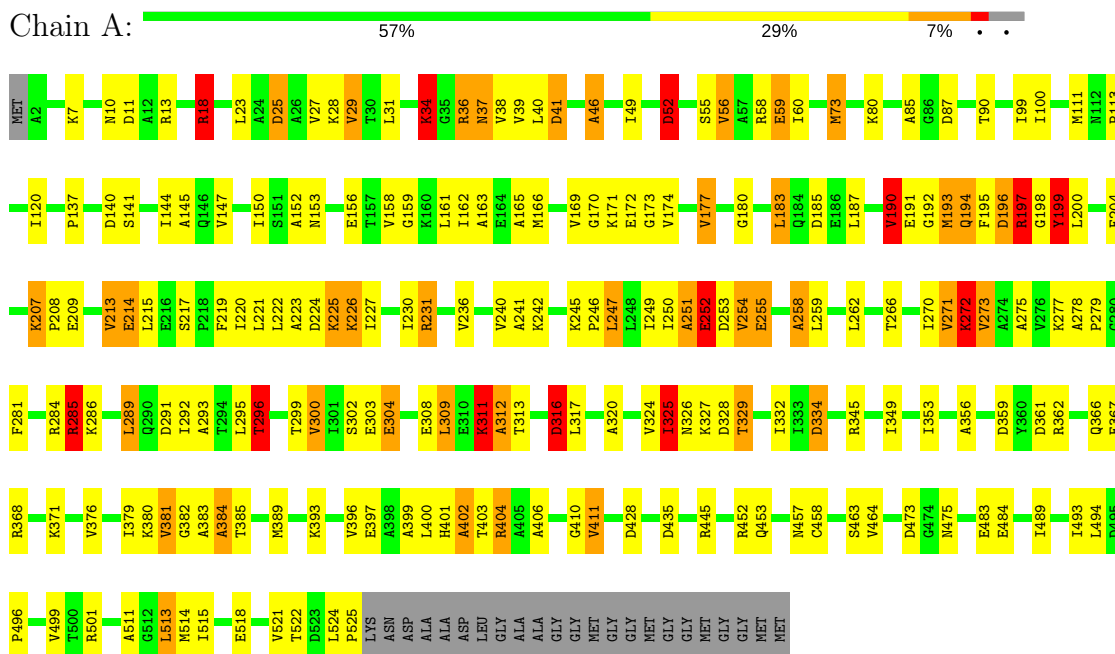
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 4   | H     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 4   | I     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 4   | J     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 4   | K     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 4   | L     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 4   | M     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 4   | N     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |



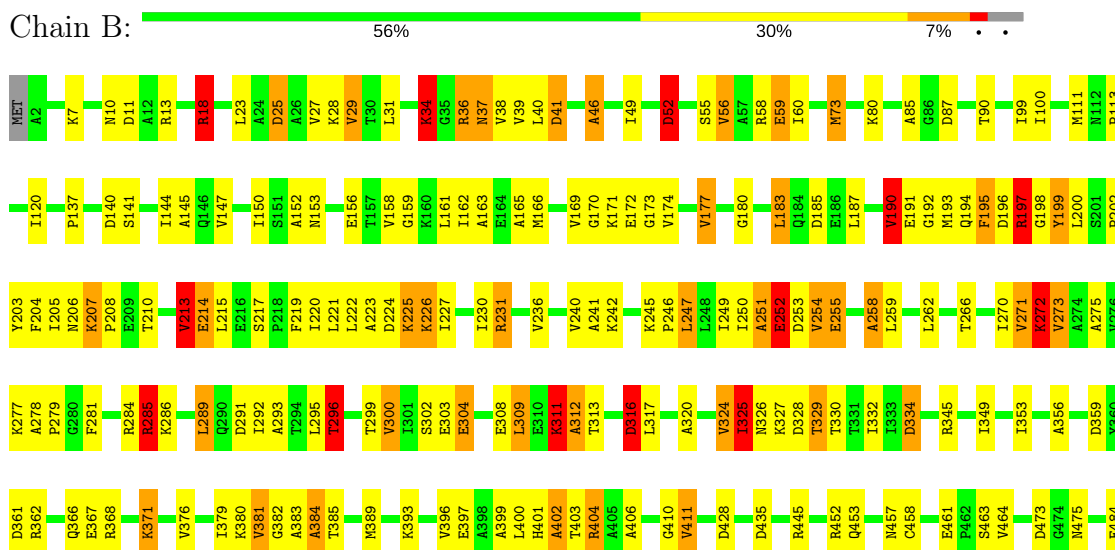
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: 60 KDA CHAPERONIN

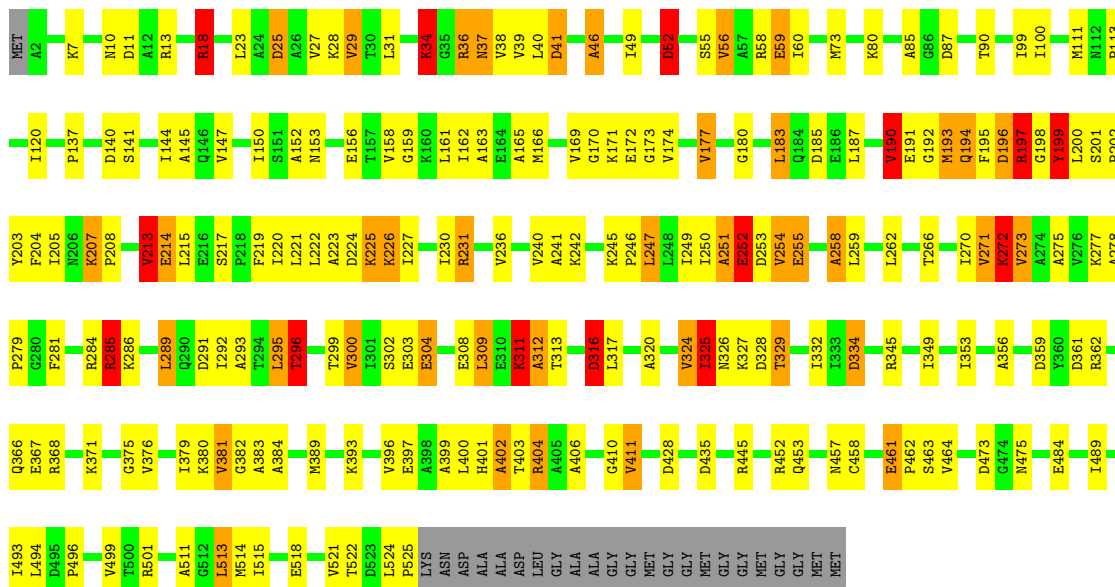


#### • Molecule 1: 60 KDA CHAPERONIN



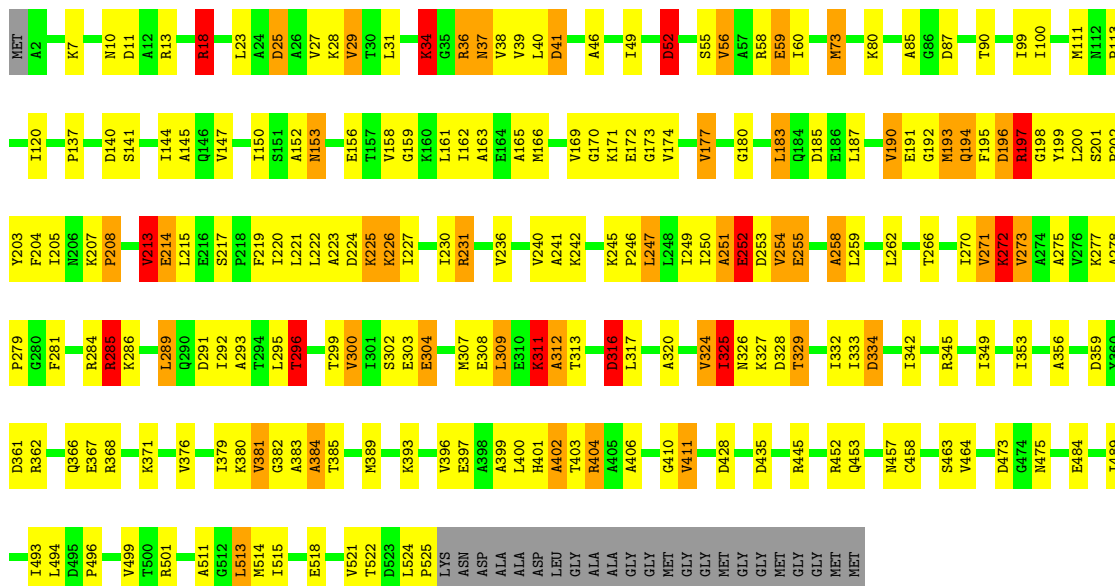
● Molecule 1: 60 KDA CHAPERONIN

Chain C:  56% 29% 7% . .



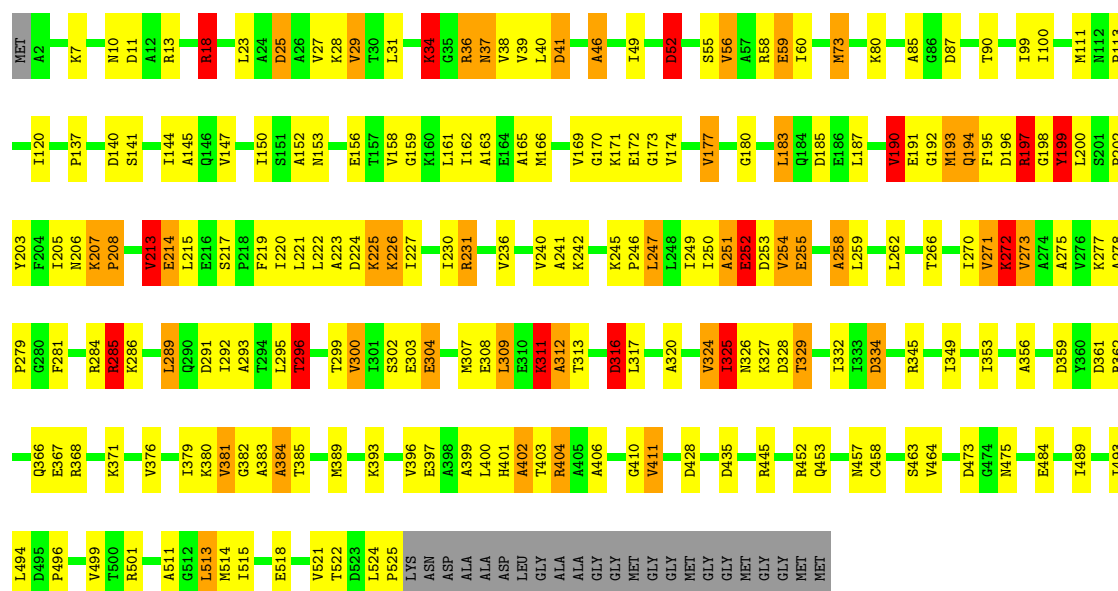
- Molecule 1: 60 KDA CHAPERONIN

Chain D:  56% 30% 7% . .



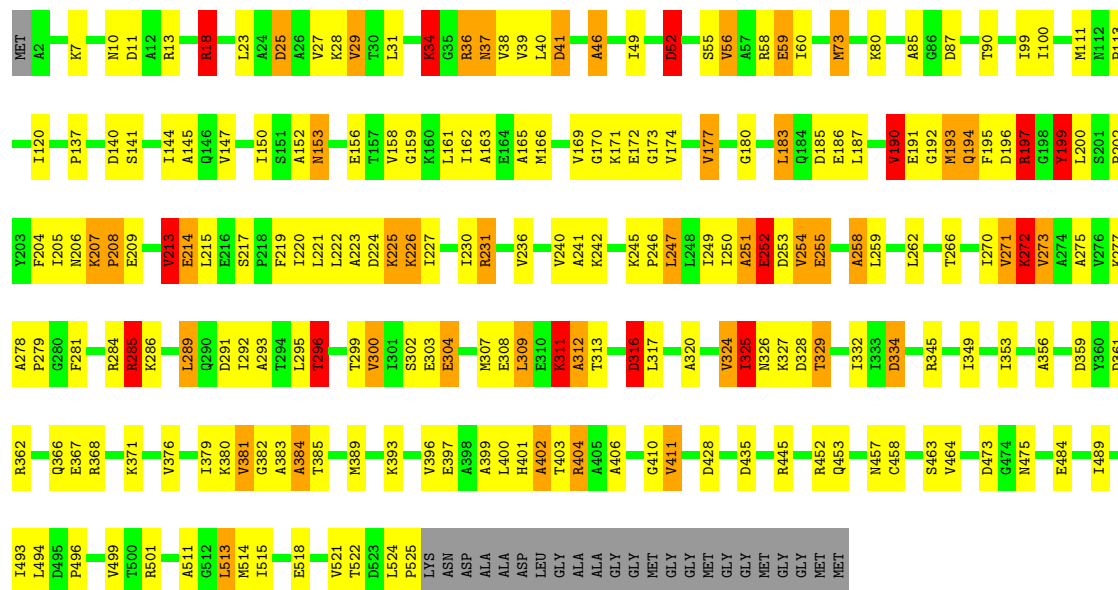
● Molecule 1: 60 KDA CHAPERONIN

Chain E:  57% 29% 7% . .



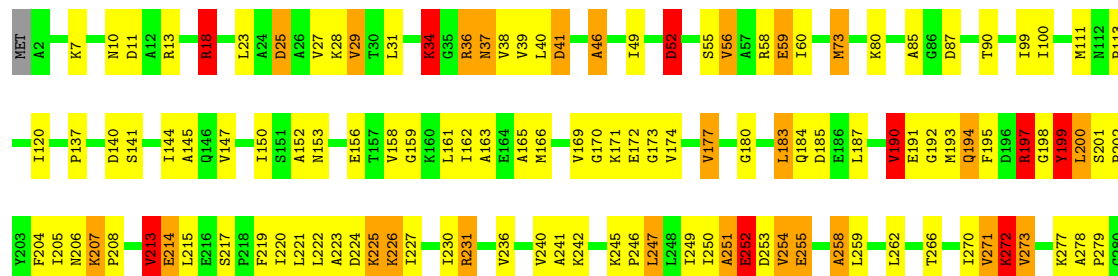
• Molecule 1: 60 KDA CHAPERONIN

Chain F: 57% 29% 7%



• Molecule 1: 60 KDA CHAPERONIN

Chain G: 57% 29% 7%

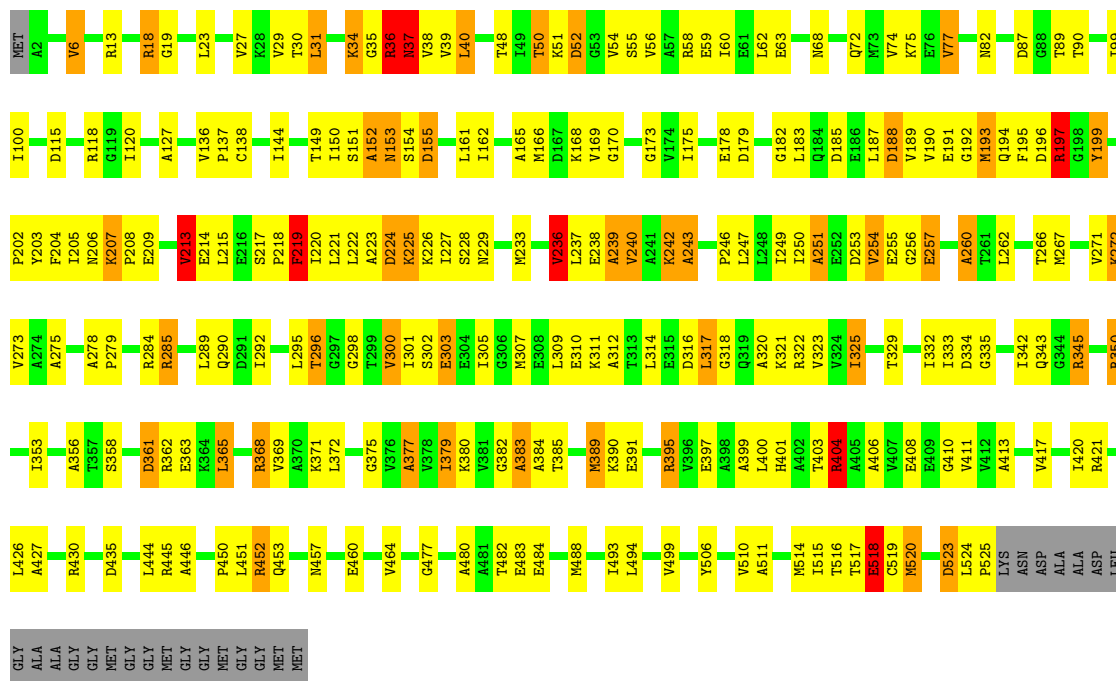






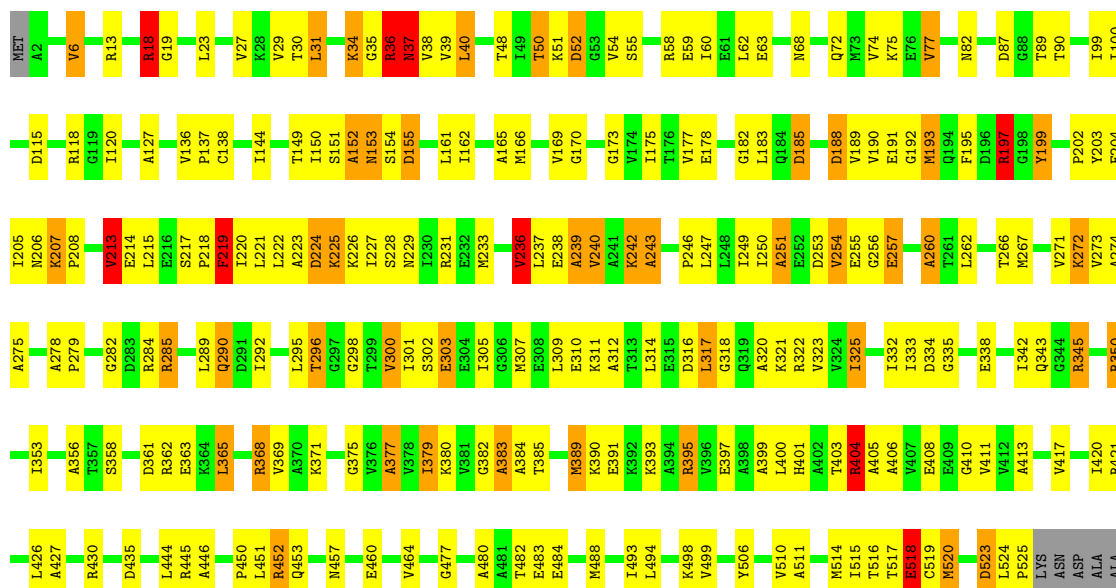
• Molecule 1: 60 KDA CHAPERONIN

Chain J: 52% 34% 8% . .



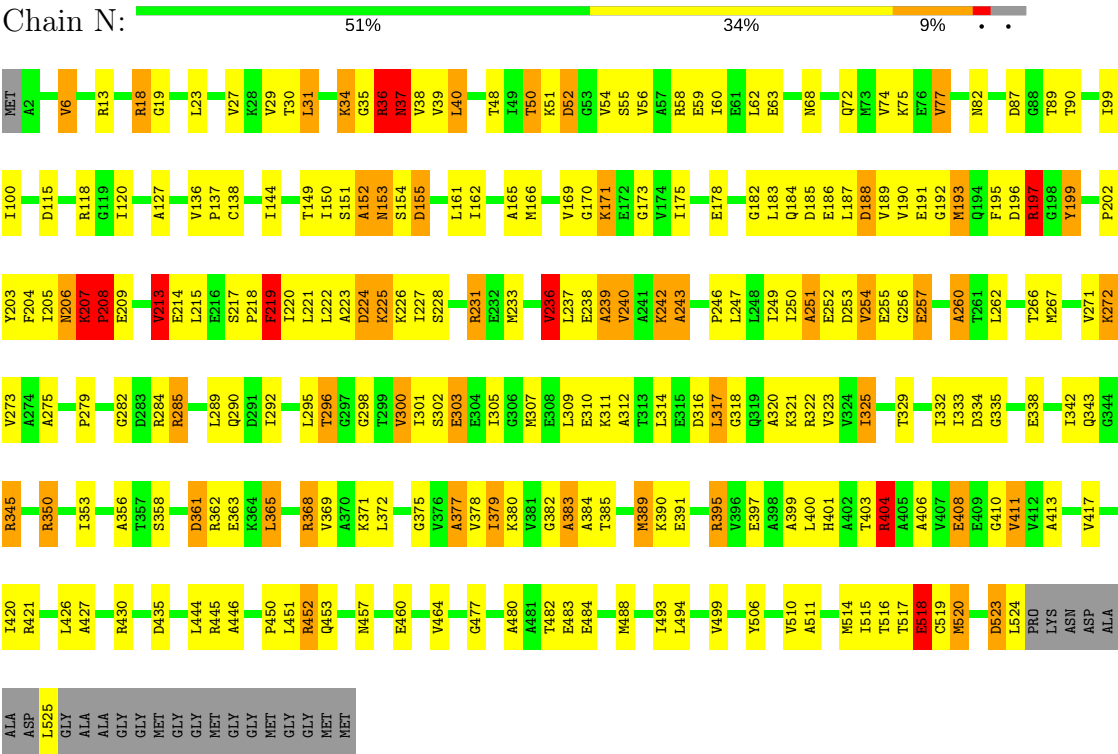
• Molecule 1: 60 KDA CHAPERONIN

Chain K: 52% 34% 8% . .





● Molecule 1: 60 KDA CHAPERONIN



## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, D7                       | Depositor |
| Number of particles used             | 15000                           | Depositor |
| Resolution determination method      | Not provided                    | Depositor |
| CTF correction method                | EACH PARTICLE WAS PHASE FLIPPED | Depositor |
| Microscope                           | FEI TECNAI F20                  | Depositor |
| Voltage (kV)                         | 120                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 15                              | Depositor |
| Minimum defocus (nm)                 | 700                             | Depositor |
| Maximum defocus (nm)                 | 3500                            | Depositor |
| Magnification                        | 148500                          | Depositor |
| Image detector                       | GATAN ULTRASCAN 4000 (4k x 4k)  | Depositor |



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ATP

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     | 0.84         | 6/3873 (0.2%)   | 1.48        | 78/5229 (1.5%)    |
| 1   | B     | 0.86         | 7/3872 (0.2%)   | 1.49        | 81/5227 (1.5%)    |
| 1   | C     | 0.86         | 7/3872 (0.2%)   | 1.49        | 82/5227 (1.6%)    |
| 1   | D     | 0.86         | 7/3872 (0.2%)   | 1.49        | 81/5227 (1.5%)    |
| 1   | E     | 0.86         | 7/3872 (0.2%)   | 1.49        | 81/5227 (1.5%)    |
| 1   | F     | 0.86         | 7/3872 (0.2%)   | 1.50        | 81/5227 (1.5%)    |
| 1   | G     | 0.86         | 7/3872 (0.2%)   | 1.50        | 85/5227 (1.6%)    |
| 1   | H     | 1.01         | 3/3872 (0.1%)   | 1.62        | 80/5227 (1.5%)    |
| 1   | I     | 1.01         | 2/3872 (0.1%)   | 1.61        | 82/5227 (1.6%)    |
| 1   | J     | 1.01         | 2/3872 (0.1%)   | 1.61        | 80/5227 (1.5%)    |
| 1   | K     | 1.02         | 3/3872 (0.1%)   | 1.61        | 78/5227 (1.5%)    |
| 1   | L     | 1.01         | 2/3872 (0.1%)   | 1.62        | 83/5227 (1.6%)    |
| 1   | M     | 1.01         | 2/3872 (0.1%)   | 1.60        | 78/5227 (1.5%)    |
| 1   | N     | 1.08         | 11/3872 (0.3%)  | 1.67        | 94/5227 (1.8%)    |
| All | All   | 0.94         | 73/54209 (0.1%) | 1.56        | 1144/73180 (1.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 19                  |
| 1   | B     | 0                   | 18                  |
| 1   | C     | 0                   | 18                  |
| 1   | D     | 0                   | 18                  |
| 1   | E     | 0                   | 19                  |
| 1   | F     | 0                   | 19                  |
| 1   | G     | 0                   | 18                  |
| 1   | H     | 1                   | 13                  |
| 1   | I     | 1                   | 14                  |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | J     | 1                   | 14                  |
| 1   | K     | 1                   | 15                  |
| 1   | L     | 1                   | 14                  |
| 1   | M     | 1                   | 14                  |
| 1   | N     | 1                   | 18                  |
| All | All   | 7                   | 231                 |

All (73) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | L     | 518 | GLU  | CA-CB | 13.48  | 1.83        | 1.53     |
| 1   | M     | 518 | GLU  | CA-CB | 13.48  | 1.83        | 1.53     |
| 1   | H     | 518 | GLU  | CA-CB | 13.48  | 1.83        | 1.53     |
| 1   | J     | 518 | GLU  | CA-CB | 13.48  | 1.83        | 1.53     |
| 1   | K     | 518 | GLU  | CA-CB | 13.47  | 1.83        | 1.53     |
| 1   | I     | 518 | GLU  | CA-CB | 13.46  | 1.83        | 1.53     |
| 1   | N     | 518 | GLU  | CA-CB | 13.45  | 1.83        | 1.53     |
| 1   | N     | 208 | PRO  | CA-C  | 11.95  | 1.76        | 1.52     |
| 1   | C     | 7   | LYS  | C-N   | -11.67 | 1.07        | 1.34     |
| 1   | A     | 7   | LYS  | C-N   | -11.66 | 1.07        | 1.34     |
| 1   | E     | 7   | LYS  | C-N   | -11.66 | 1.07        | 1.34     |
| 1   | G     | 7   | LYS  | C-N   | -11.66 | 1.07        | 1.34     |
| 1   | B     | 7   | LYS  | C-N   | -11.66 | 1.07        | 1.34     |
| 1   | D     | 7   | LYS  | C-N   | -11.66 | 1.07        | 1.34     |
| 1   | F     | 7   | LYS  | C-N   | -11.66 | 1.07        | 1.34     |
| 1   | C     | 213 | VAL  | C-N   | -11.26 | 1.08        | 1.34     |
| 1   | D     | 213 | VAL  | C-N   | -11.24 | 1.08        | 1.34     |
| 1   | F     | 213 | VAL  | C-N   | -11.24 | 1.08        | 1.34     |
| 1   | G     | 213 | VAL  | C-N   | -11.23 | 1.08        | 1.34     |
| 1   | B     | 213 | VAL  | C-N   | -11.23 | 1.08        | 1.34     |
| 1   | E     | 213 | VAL  | C-N   | -11.23 | 1.08        | 1.34     |
| 1   | N     | 207 | LYS  | CE-NZ | 8.36   | 1.70        | 1.49     |
| 1   | N     | 208 | PRO  | C-N   | 8.30   | 1.53        | 1.34     |
| 1   | N     | 207 | LYS  | CA-CB | 7.98   | 1.71        | 1.53     |
| 1   | D     | 11  | ASP  | C-N   | 7.91   | 1.52        | 1.34     |
| 1   | G     | 11  | ASP  | C-N   | 7.91   | 1.52        | 1.34     |
| 1   | A     | 11  | ASP  | C-N   | 7.90   | 1.52        | 1.34     |
| 1   | B     | 11  | ASP  | C-N   | 7.90   | 1.52        | 1.34     |
| 1   | E     | 11  | ASP  | C-N   | 7.90   | 1.52        | 1.34     |
| 1   | F     | 11  | ASP  | C-N   | 7.90   | 1.52        | 1.34     |
| 1   | C     | 11  | ASP  | C-N   | 7.89   | 1.52        | 1.34     |
| 1   | N     | 207 | LYS  | CB-CG | 7.55   | 1.73        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | I     | 243 | ALA  | CA-CB | 7.43  | 1.68        | 1.52     |
| 1   | J     | 243 | ALA  | CA-CB | 7.43  | 1.68        | 1.52     |
| 1   | L     | 243 | ALA  | CA-CB | 7.42  | 1.68        | 1.52     |
| 1   | N     | 243 | ALA  | CA-CB | 7.42  | 1.68        | 1.52     |
| 1   | M     | 243 | ALA  | CA-CB | 7.41  | 1.68        | 1.52     |
| 1   | H     | 243 | ALA  | CA-CB | 7.40  | 1.68        | 1.52     |
| 1   | K     | 243 | ALA  | CA-CB | 7.37  | 1.68        | 1.52     |
| 1   | N     | 207 | LYS  | CD-CE | 7.31  | 1.69        | 1.51     |
| 1   | B     | 52  | ASP  | C-N   | -7.22 | 1.20        | 1.33     |
| 1   | A     | 52  | ASP  | C-N   | -7.18 | 1.20        | 1.33     |
| 1   | E     | 52  | ASP  | C-N   | -7.18 | 1.20        | 1.33     |
| 1   | C     | 230 | ILE  | C-N   | 7.17  | 1.50        | 1.34     |
| 1   | D     | 52  | ASP  | C-N   | -7.17 | 1.20        | 1.33     |
| 1   | F     | 230 | ILE  | C-N   | 7.17  | 1.50        | 1.34     |
| 1   | G     | 230 | ILE  | C-N   | 7.17  | 1.50        | 1.34     |
| 1   | D     | 230 | ILE  | C-N   | 7.17  | 1.50        | 1.34     |
| 1   | F     | 52  | ASP  | C-N   | -7.17 | 1.20        | 1.33     |
| 1   | A     | 230 | ILE  | C-N   | 7.17  | 1.50        | 1.34     |
| 1   | B     | 230 | ILE  | C-N   | 7.17  | 1.50        | 1.34     |
| 1   | C     | 52  | ASP  | C-N   | -7.17 | 1.20        | 1.33     |
| 1   | E     | 230 | ILE  | C-N   | 7.17  | 1.50        | 1.34     |
| 1   | G     | 52  | ASP  | C-N   | -7.15 | 1.20        | 1.33     |
| 1   | B     | 513 | LEU  | C-N   | -6.61 | 1.18        | 1.34     |
| 1   | E     | 513 | LEU  | C-N   | -6.59 | 1.18        | 1.34     |
| 1   | A     | 513 | LEU  | C-N   | -6.58 | 1.19        | 1.34     |
| 1   | F     | 513 | LEU  | C-N   | -6.58 | 1.19        | 1.34     |
| 1   | C     | 513 | LEU  | C-N   | -6.58 | 1.19        | 1.34     |
| 1   | G     | 513 | LEU  | C-N   | -6.57 | 1.19        | 1.34     |
| 1   | D     | 513 | LEU  | C-N   | -6.56 | 1.19        | 1.34     |
| 1   | B     | 518 | GLU  | C-N   | -6.28 | 1.19        | 1.34     |
| 1   | F     | 518 | GLU  | C-N   | -6.25 | 1.19        | 1.34     |
| 1   | C     | 518 | GLU  | C-N   | -6.25 | 1.19        | 1.34     |
| 1   | A     | 518 | GLU  | C-N   | -6.24 | 1.19        | 1.34     |
| 1   | E     | 518 | GLU  | C-N   | -6.24 | 1.19        | 1.34     |
| 1   | G     | 518 | GLU  | C-N   | -6.24 | 1.19        | 1.34     |
| 1   | D     | 518 | GLU  | C-N   | -6.23 | 1.19        | 1.34     |
| 1   | H     | 242 | LYS  | CA-CB | 6.14  | 1.67        | 1.53     |
| 1   | K     | 242 | LYS  | CA-CB | 6.05  | 1.67        | 1.53     |
| 1   | N     | 207 | LYS  | CG-CD | 5.58  | 1.71        | 1.52     |
| 1   | N     | 208 | PRO  | N-CA  | 5.49  | 1.56        | 1.47     |
| 1   | N     | 207 | LYS  | C-N   | 5.29  | 1.44        | 1.34     |

All (1144) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | I     | 243 | ALA  | CB-CA-C  | -22.85 | 75.83       | 110.10   |
| 1   | L     | 243 | ALA  | CB-CA-C  | -22.84 | 75.83       | 110.10   |
| 1   | N     | 243 | ALA  | CB-CA-C  | -22.84 | 75.84       | 110.10   |
| 1   | J     | 243 | ALA  | CB-CA-C  | -22.84 | 75.85       | 110.10   |
| 1   | H     | 243 | ALA  | CB-CA-C  | -22.82 | 75.86       | 110.10   |
| 1   | K     | 243 | ALA  | CB-CA-C  | -22.80 | 75.90       | 110.10   |
| 1   | M     | 243 | ALA  | CB-CA-C  | -22.78 | 75.93       | 110.10   |
| 1   | K     | 242 | LYS  | N-CA-CB  | -22.64 | 69.85       | 110.60   |
| 1   | H     | 242 | LYS  | N-CA-CB  | -22.38 | 70.32       | 110.60   |
| 1   | J     | 518 | GLU  | N-CA-CB  | 20.19  | 146.95      | 110.60   |
| 1   | L     | 518 | GLU  | N-CA-CB  | 20.18  | 146.92      | 110.60   |
| 1   | I     | 518 | GLU  | N-CA-CB  | 20.16  | 146.89      | 110.60   |
| 1   | K     | 518 | GLU  | N-CA-CB  | 20.15  | 146.87      | 110.60   |
| 1   | H     | 518 | GLU  | N-CA-CB  | 20.13  | 146.84      | 110.60   |
| 1   | M     | 518 | GLU  | N-CA-CB  | 20.12  | 146.81      | 110.60   |
| 1   | N     | 518 | GLU  | N-CA-CB  | 20.12  | 146.81      | 110.60   |
| 1   | L     | 242 | LYS  | CB-CA-C  | 19.73  | 149.86      | 110.40   |
| 1   | J     | 242 | LYS  | CB-CA-C  | 19.25  | 148.90      | 110.40   |
| 1   | N     | 242 | LYS  | CB-CA-C  | 19.24  | 148.88      | 110.40   |
| 1   | I     | 242 | LYS  | CB-CA-C  | 19.21  | 148.81      | 110.40   |
| 1   | J     | 518 | GLU  | CB-CA-C  | -18.30 | 73.80       | 110.40   |
| 1   | K     | 518 | GLU  | CB-CA-C  | -18.29 | 73.82       | 110.40   |
| 1   | M     | 518 | GLU  | CB-CA-C  | -18.29 | 73.83       | 110.40   |
| 1   | L     | 518 | GLU  | CB-CA-C  | -18.28 | 73.84       | 110.40   |
| 1   | I     | 518 | GLU  | CB-CA-C  | -18.27 | 73.86       | 110.40   |
| 1   | N     | 518 | GLU  | CB-CA-C  | -18.27 | 73.87       | 110.40   |
| 1   | H     | 518 | GLU  | CB-CA-C  | -18.25 | 73.89       | 110.40   |
| 1   | N     | 260 | ALA  | N-CA-CB  | 18.12  | 135.47      | 110.10   |
| 1   | M     | 242 | LYS  | N-CA-CB  | -17.91 | 78.36       | 110.60   |
| 1   | M     | 260 | ALA  | N-CA-CB  | 17.64  | 134.79      | 110.10   |
| 1   | J     | 260 | ALA  | N-CA-CB  | 17.24  | 134.24      | 110.10   |
| 1   | H     | 260 | ALA  | N-CA-CB  | 17.24  | 134.23      | 110.10   |
| 1   | K     | 260 | ALA  | N-CA-CB  | 17.23  | 134.22      | 110.10   |
| 1   | I     | 260 | ALA  | N-CA-CB  | 14.68  | 130.65      | 110.10   |
| 1   | L     | 260 | ALA  | N-CA-CB  | 14.64  | 130.60      | 110.10   |
| 1   | J     | 242 | LYS  | N-CA-CB  | -14.60 | 84.31       | 110.60   |
| 1   | I     | 242 | LYS  | N-CA-CB  | -14.59 | 84.35       | 110.60   |
| 1   | N     | 242 | LYS  | N-CA-CB  | -14.57 | 84.37       | 110.60   |
| 1   | H     | 242 | LYS  | CA-CB-CG | 14.27  | 144.79      | 113.40   |
| 1   | L     | 242 | LYS  | N-CA-CB  | -14.21 | 85.02       | 110.60   |
| 1   | K     | 242 | LYS  | CA-CB-CG | 13.92  | 144.03      | 113.40   |
| 1   | I     | 260 | ALA  | CB-CA-C  | -13.22 | 90.27       | 110.10   |
| 1   | L     | 260 | ALA  | CB-CA-C  | -13.21 | 90.28       | 110.10   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | M     | 452 | ARG  | NE-CZ-NH1 | 11.69  | 126.14      | 120.30   |
| 1   | J     | 452 | ARG  | NE-CZ-NH1 | 11.64  | 126.12      | 120.30   |
| 1   | N     | 452 | ARG  | NE-CZ-NH1 | 11.64  | 126.12      | 120.30   |
| 1   | H     | 452 | ARG  | NE-CZ-NH1 | 11.63  | 126.11      | 120.30   |
| 1   | I     | 452 | ARG  | NE-CZ-NH1 | 11.57  | 126.09      | 120.30   |
| 1   | K     | 452 | ARG  | NE-CZ-NH1 | 11.55  | 126.08      | 120.30   |
| 1   | L     | 452 | ARG  | NE-CZ-NH1 | 11.55  | 126.08      | 120.30   |
| 1   | N     | 208 | PRO  | N-CA-C    | 11.52  | 142.06      | 112.10   |
| 1   | C     | 518 | GLU  | O-C-N     | -11.50 | 104.29      | 122.70   |
| 1   | E     | 518 | GLU  | O-C-N     | -11.50 | 104.30      | 122.70   |
| 1   | G     | 518 | GLU  | O-C-N     | -11.49 | 104.31      | 122.70   |
| 1   | F     | 518 | GLU  | O-C-N     | -11.49 | 104.32      | 122.70   |
| 1   | A     | 518 | GLU  | O-C-N     | -11.48 | 104.32      | 122.70   |
| 1   | D     | 518 | GLU  | O-C-N     | -11.48 | 104.33      | 122.70   |
| 1   | B     | 518 | GLU  | O-C-N     | -11.45 | 104.37      | 122.70   |
| 1   | N     | 208 | PRO  | CA-C-N    | 11.44  | 142.36      | 117.20   |
| 1   | N     | 207 | LYS  | CD-CE-NZ  | 11.34  | 137.79      | 111.70   |
| 1   | D     | 518 | GLU  | C-N-CA    | 11.34  | 150.05      | 121.70   |
| 1   | C     | 518 | GLU  | C-N-CA    | 11.34  | 150.04      | 121.70   |
| 1   | E     | 518 | GLU  | C-N-CA    | 11.34  | 150.04      | 121.70   |
| 1   | F     | 518 | GLU  | C-N-CA    | 11.34  | 150.04      | 121.70   |
| 1   | A     | 518 | GLU  | C-N-CA    | 11.33  | 150.03      | 121.70   |
| 1   | G     | 518 | GLU  | C-N-CA    | 11.33  | 150.03      | 121.70   |
| 1   | B     | 518 | GLU  | C-N-CA    | 11.32  | 150.00      | 121.70   |
| 1   | J     | 260 | ALA  | CB-CA-C   | -11.20 | 93.30       | 110.10   |
| 1   | H     | 260 | ALA  | CB-CA-C   | -11.20 | 93.31       | 110.10   |
| 1   | K     | 260 | ALA  | CB-CA-C   | -11.17 | 93.35       | 110.10   |
| 1   | F     | 29  | VAL  | CA-C-N    | -10.95 | 93.11       | 117.20   |
| 1   | A     | 29  | VAL  | CA-C-N    | -10.94 | 93.14       | 117.20   |
| 1   | E     | 29  | VAL  | CA-C-N    | -10.93 | 93.15       | 117.20   |
| 1   | M     | 242 | LYS  | CB-CA-C   | 10.93  | 132.26      | 110.40   |
| 1   | G     | 29  | VAL  | CA-C-N    | -10.93 | 93.15       | 117.20   |
| 1   | C     | 29  | VAL  | CA-C-N    | -10.93 | 93.16       | 117.20   |
| 1   | D     | 29  | VAL  | CA-C-N    | -10.93 | 93.16       | 117.20   |
| 1   | B     | 29  | VAL  | CA-C-N    | -10.93 | 93.16       | 117.20   |
| 1   | M     | 260 | ALA  | CB-CA-C   | -10.90 | 93.74       | 110.10   |
| 1   | N     | 260 | ALA  | CB-CA-C   | -10.32 | 94.62       | 110.10   |
| 1   | C     | 7   | LYS  | C-N-CA    | -10.31 | 95.93       | 121.70   |
| 1   | A     | 7   | LYS  | C-N-CA    | -10.29 | 95.96       | 121.70   |
| 1   | E     | 7   | LYS  | C-N-CA    | -10.29 | 95.96       | 121.70   |
| 1   | G     | 7   | LYS  | C-N-CA    | -10.29 | 95.97       | 121.70   |
| 1   | B     | 7   | LYS  | C-N-CA    | -10.29 | 95.98       | 121.70   |

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| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | D     | 7   | LYS  | C-N-CA   | -10.28 | 95.99       | 121.70   |
| 1   | F     | 7   | LYS  | C-N-CA   | -10.28 | 95.99       | 121.70   |
| 1   | C     | 7   | LYS  | O-C-N    | 10.28  | 139.14      | 122.70   |
| 1   | G     | 7   | LYS  | O-C-N    | 10.26  | 139.11      | 122.70   |
| 1   | A     | 7   | LYS  | O-C-N    | 10.26  | 139.11      | 122.70   |
| 1   | E     | 7   | LYS  | O-C-N    | 10.25  | 139.10      | 122.70   |
| 1   | B     | 7   | LYS  | O-C-N    | 10.24  | 139.08      | 122.70   |
| 1   | K     | 377 | ALA  | N-CA-CB  | 10.22  | 124.42      | 110.10   |
| 1   | F     | 7   | LYS  | O-C-N    | 10.22  | 139.05      | 122.70   |
| 1   | D     | 7   | LYS  | O-C-N    | 10.21  | 139.04      | 122.70   |
| 1   | N     | 377 | ALA  | N-CA-CB  | 10.21  | 124.39      | 110.10   |
| 1   | H     | 377 | ALA  | N-CA-CB  | 10.20  | 124.37      | 110.10   |
| 1   | I     | 377 | ALA  | N-CA-CB  | 10.20  | 124.37      | 110.10   |
| 1   | J     | 377 | ALA  | N-CA-CB  | 10.19  | 124.37      | 110.10   |
| 1   | L     | 377 | ALA  | N-CA-CB  | 10.19  | 124.37      | 110.10   |
| 1   | M     | 377 | ALA  | N-CA-CB  | 10.19  | 124.37      | 110.10   |
| 1   | E     | 29  | VAL  | O-C-N    | 9.97   | 138.66      | 122.70   |
| 1   | G     | 29  | VAL  | O-C-N    | 9.97   | 138.66      | 122.70   |
| 1   | N     | 207 | LYS  | CB-CG-CD | 9.97   | 137.51      | 111.60   |
| 1   | A     | 29  | VAL  | O-C-N    | 9.96   | 138.63      | 122.70   |
| 1   | F     | 29  | VAL  | O-C-N    | 9.96   | 138.63      | 122.70   |
| 1   | C     | 29  | VAL  | O-C-N    | 9.95   | 138.63      | 122.70   |
| 1   | B     | 29  | VAL  | O-C-N    | 9.95   | 138.62      | 122.70   |
| 1   | D     | 29  | VAL  | O-C-N    | 9.95   | 138.62      | 122.70   |
| 1   | E     | 214 | GLU  | CB-CA-C  | -9.85  | 90.71       | 110.40   |
| 1   | D     | 214 | GLU  | CB-CA-C  | -9.84  | 90.72       | 110.40   |
| 1   | F     | 214 | GLU  | CB-CA-C  | -9.84  | 90.72       | 110.40   |
| 1   | A     | 214 | GLU  | CB-CA-C  | -9.84  | 90.73       | 110.40   |
| 1   | B     | 214 | GLU  | CB-CA-C  | -9.83  | 90.74       | 110.40   |
| 1   | G     | 214 | GLU  | CB-CA-C  | -9.83  | 90.74       | 110.40   |
| 1   | C     | 214 | GLU  | CB-CA-C  | -9.82  | 90.76       | 110.40   |
| 1   | I     | 37  | ASN  | N-CA-CB  | 9.71   | 128.07      | 110.60   |
| 1   | K     | 37  | ASN  | N-CA-CB  | 9.69   | 128.03      | 110.60   |
| 1   | M     | 37  | ASN  | N-CA-CB  | 9.69   | 128.03      | 110.60   |
| 1   | H     | 37  | ASN  | N-CA-CB  | 9.68   | 128.03      | 110.60   |
| 1   | J     | 37  | ASN  | N-CA-CB  | 9.68   | 128.03      | 110.60   |
| 1   | N     | 37  | ASN  | N-CA-CB  | 9.68   | 128.03      | 110.60   |
| 1   | L     | 37  | ASN  | N-CA-CB  | 9.67   | 128.01      | 110.60   |
| 1   | D     | 41  | ASP  | N-CA-CB  | 9.66   | 127.99      | 110.60   |
| 1   | C     | 41  | ASP  | N-CA-CB  | 9.64   | 127.96      | 110.60   |
| 1   | B     | 41  | ASP  | N-CA-CB  | 9.64   | 127.95      | 110.60   |
| 1   | E     | 41  | ASP  | N-CA-CB  | 9.64   | 127.95      | 110.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 41  | ASP  | N-CA-CB   | 9.63  | 127.94      | 110.60   |
| 1   | G     | 41  | ASP  | N-CA-CB   | 9.63  | 127.94      | 110.60   |
| 1   | F     | 41  | ASP  | N-CA-CB   | 9.63  | 127.93      | 110.60   |
| 1   | F     | 501 | ARG  | NE-CZ-NH1 | 9.53  | 125.06      | 120.30   |
| 1   | B     | 501 | ARG  | NE-CZ-NH1 | 9.50  | 125.05      | 120.30   |
| 1   | G     | 501 | ARG  | NE-CZ-NH1 | 9.47  | 125.04      | 120.30   |
| 1   | J     | 18  | ARG  | NE-CZ-NH1 | 9.45  | 125.03      | 120.30   |
| 1   | L     | 18  | ARG  | NE-CZ-NH1 | 9.44  | 125.02      | 120.30   |
| 1   | A     | 501 | ARG  | NE-CZ-NH1 | 9.44  | 125.02      | 120.30   |
| 1   | C     | 7   | LYS  | CA-C-N    | -9.44 | 96.44       | 117.20   |
| 1   | D     | 501 | ARG  | NE-CZ-NH1 | 9.44  | 125.02      | 120.30   |
| 1   | E     | 501 | ARG  | NE-CZ-NH1 | 9.44  | 125.02      | 120.30   |
| 1   | A     | 7   | LYS  | CA-C-N    | -9.42 | 96.47       | 117.20   |
| 1   | E     | 7   | LYS  | CA-C-N    | -9.42 | 96.47       | 117.20   |
| 1   | G     | 7   | LYS  | CA-C-N    | -9.42 | 96.48       | 117.20   |
| 1   | B     | 7   | LYS  | CA-C-N    | -9.41 | 96.49       | 117.20   |
| 1   | D     | 7   | LYS  | CA-C-N    | -9.41 | 96.50       | 117.20   |
| 1   | F     | 7   | LYS  | CA-C-N    | -9.41 | 96.50       | 117.20   |
| 1   | C     | 501 | ARG  | NE-CZ-NH1 | 9.40  | 125.00      | 120.30   |
| 1   | N     | 207 | LYS  | CA-CB-CG  | 9.39  | 134.07      | 113.40   |
| 1   | N     | 219 | PHE  | N-CA-CB   | 9.39  | 127.50      | 110.60   |
| 1   | M     | 18  | ARG  | NE-CZ-NH1 | 9.37  | 124.98      | 120.30   |
| 1   | H     | 18  | ARG  | NE-CZ-NH1 | 9.37  | 124.98      | 120.30   |
| 1   | N     | 208 | PRO  | C-N-CA    | -9.36 | 98.31       | 121.70   |
| 1   | K     | 219 | PHE  | N-CA-CB   | 9.35  | 127.42      | 110.60   |
| 1   | N     | 18  | ARG  | NE-CZ-NH1 | 9.34  | 124.97      | 120.30   |
| 1   | L     | 219 | PHE  | N-CA-CB   | 9.29  | 127.31      | 110.60   |
| 1   | I     | 18  | ARG  | NE-CZ-NH1 | 9.28  | 124.94      | 120.30   |
| 1   | I     | 219 | PHE  | N-CA-CB   | 9.28  | 127.30      | 110.60   |
| 1   | M     | 219 | PHE  | N-CA-CB   | 9.28  | 127.30      | 110.60   |
| 1   | K     | 242 | LYS  | CB-CA-C   | 9.27  | 128.95      | 110.40   |
| 1   | J     | 219 | PHE  | N-CA-CB   | 9.27  | 127.28      | 110.60   |
| 1   | K     | 18  | ARG  | NE-CZ-NH1 | 9.25  | 124.93      | 120.30   |
| 1   | H     | 219 | PHE  | N-CA-CB   | 9.24  | 127.23      | 110.60   |
| 1   | G     | 199 | TYR  | C-N-CA    | -9.23 | 98.62       | 121.70   |
| 1   | J     | 18  | ARG  | NE-CZ-NH2 | -9.17 | 115.72      | 120.30   |
| 1   | L     | 18  | ARG  | NE-CZ-NH2 | -9.16 | 115.72      | 120.30   |
| 1   | M     | 18  | ARG  | NE-CZ-NH2 | -9.09 | 115.75      | 120.30   |
| 1   | N     | 18  | ARG  | NE-CZ-NH2 | -9.09 | 115.76      | 120.30   |
| 1   | H     | 242 | LYS  | CB-CA-C   | 9.04  | 128.48      | 110.40   |
| 1   | H     | 18  | ARG  | NE-CZ-NH2 | -9.03 | 115.78      | 120.30   |
| 1   | G     | 52  | ASP  | C-N-CA    | -9.03 | 103.34      | 122.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 52  | ASP  | C-N-CA    | -9.03 | 103.35      | 122.30   |
| 1   | C     | 52  | ASP  | C-N-CA    | -9.02 | 103.35      | 122.30   |
| 1   | I     | 18  | ARG  | NE-CZ-NH2 | -9.02 | 115.79      | 120.30   |
| 1   | A     | 52  | ASP  | C-N-CA    | -9.02 | 103.36      | 122.30   |
| 1   | D     | 52  | ASP  | C-N-CA    | -9.02 | 103.36      | 122.30   |
| 1   | K     | 18  | ARG  | NE-CZ-NH2 | -9.00 | 115.80      | 120.30   |
| 1   | B     | 52  | ASP  | C-N-CA    | -9.00 | 103.40      | 122.30   |
| 1   | E     | 52  | ASP  | C-N-CA    | -9.00 | 103.41      | 122.30   |
| 1   | H     | 243 | ALA  | N-CA-CB   | 8.94  | 122.62      | 110.10   |
| 1   | K     | 243 | ALA  | N-CA-CB   | 8.93  | 122.60      | 110.10   |
| 1   | M     | 243 | ALA  | N-CA-CB   | 8.89  | 122.55      | 110.10   |
| 1   | N     | 243 | ALA  | N-CA-CB   | 8.86  | 122.51      | 110.10   |
| 1   | J     | 243 | ALA  | N-CA-CB   | 8.86  | 122.51      | 110.10   |
| 1   | I     | 243 | ALA  | N-CA-CB   | 8.86  | 122.50      | 110.10   |
| 1   | L     | 243 | ALA  | N-CA-CB   | 8.85  | 122.49      | 110.10   |
| 1   | F     | 18  | ARG  | NE-CZ-NH1 | 8.84  | 124.72      | 120.30   |
| 1   | B     | 18  | ARG  | NE-CZ-NH1 | 8.80  | 124.70      | 120.30   |
| 1   | E     | 18  | ARG  | NE-CZ-NH1 | 8.79  | 124.69      | 120.30   |
| 1   | G     | 18  | ARG  | NE-CZ-NH1 | 8.77  | 124.69      | 120.30   |
| 1   | C     | 18  | ARG  | NE-CZ-NH1 | 8.76  | 124.68      | 120.30   |
| 1   | D     | 18  | ARG  | NE-CZ-NH1 | 8.72  | 124.66      | 120.30   |
| 1   | L     | 115 | ASP  | CB-CA-C   | 8.65  | 127.69      | 110.40   |
| 1   | N     | 115 | ASP  | CB-CA-C   | 8.64  | 127.68      | 110.40   |
| 1   | A     | 18  | ARG  | NE-CZ-NH1 | 8.64  | 124.62      | 120.30   |
| 1   | I     | 115 | ASP  | CB-CA-C   | 8.64  | 127.68      | 110.40   |
| 1   | H     | 115 | ASP  | CB-CA-C   | 8.63  | 127.67      | 110.40   |
| 1   | K     | 115 | ASP  | CB-CA-C   | 8.63  | 127.67      | 110.40   |
| 1   | J     | 115 | ASP  | CB-CA-C   | 8.63  | 127.66      | 110.40   |
| 1   | M     | 115 | ASP  | CB-CA-C   | 8.63  | 127.66      | 110.40   |
| 1   | N     | 240 | VAL  | CA-CB-CG2 | -8.58 | 98.04       | 110.90   |
| 1   | D     | 225 | LYS  | N-CA-CB   | 8.54  | 125.97      | 110.60   |
| 1   | M     | 240 | VAL  | CA-CB-CG2 | -8.54 | 98.09       | 110.90   |
| 1   | B     | 225 | LYS  | N-CA-CB   | 8.54  | 125.97      | 110.60   |
| 1   | G     | 225 | LYS  | N-CA-CB   | 8.54  | 125.96      | 110.60   |
| 1   | E     | 225 | LYS  | N-CA-CB   | 8.53  | 125.96      | 110.60   |
| 1   | A     | 225 | LYS  | N-CA-CB   | 8.53  | 125.96      | 110.60   |
| 1   | C     | 225 | LYS  | N-CA-CB   | 8.52  | 125.94      | 110.60   |
| 1   | F     | 225 | LYS  | N-CA-CB   | 8.52  | 125.94      | 110.60   |
| 1   | I     | 240 | VAL  | CA-CB-CG2 | -8.51 | 98.13       | 110.90   |
| 1   | L     | 240 | VAL  | CA-CB-CG2 | -8.51 | 98.14       | 110.90   |
| 1   | J     | 240 | VAL  | CA-CB-CG2 | -8.49 | 98.17       | 110.90   |
| 1   | G     | 213 | VAL  | O-C-N     | 8.48  | 136.27      | 122.70   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | H     | 240 | VAL  | CA-CB-CG2 | -8.48 | 98.17       | 110.90   |
| 1   | F     | 213 | VAL  | O-C-N     | 8.48  | 136.27      | 122.70   |
| 1   | K     | 240 | VAL  | CA-CB-CG2 | -8.48 | 98.19       | 110.90   |
| 1   | E     | 213 | VAL  | O-C-N     | 8.47  | 136.26      | 122.70   |
| 1   | C     | 213 | VAL  | O-C-N     | 8.47  | 136.26      | 122.70   |
| 1   | B     | 213 | VAL  | O-C-N     | 8.47  | 136.25      | 122.70   |
| 1   | D     | 213 | VAL  | O-C-N     | 8.44  | 136.20      | 122.70   |
| 1   | L     | 257 | GLU  | N-CA-CB   | -8.42 | 95.44       | 110.60   |
| 1   | F     | 29  | VAL  | C-N-CA    | -8.25 | 101.08      | 121.70   |
| 1   | A     | 29  | VAL  | C-N-CA    | -8.24 | 101.09      | 121.70   |
| 1   | B     | 29  | VAL  | C-N-CA    | -8.24 | 101.09      | 121.70   |
| 1   | C     | 29  | VAL  | C-N-CA    | -8.23 | 101.11      | 121.70   |
| 1   | D     | 29  | VAL  | C-N-CA    | -8.23 | 101.12      | 121.70   |
| 1   | E     | 29  | VAL  | C-N-CA    | -8.23 | 101.12      | 121.70   |
| 1   | G     | 29  | VAL  | C-N-CA    | -8.23 | 101.12      | 121.70   |
| 1   | N     | 207 | LYS  | CB-CA-C   | 8.16  | 126.73      | 110.40   |
| 1   | E     | 56  | VAL  | CB-CA-C   | -8.14 | 95.94       | 111.40   |
| 1   | G     | 56  | VAL  | CB-CA-C   | -8.13 | 95.96       | 111.40   |
| 1   | A     | 56  | VAL  | CB-CA-C   | -8.12 | 95.97       | 111.40   |
| 1   | D     | 56  | VAL  | CB-CA-C   | -8.12 | 95.97       | 111.40   |
| 1   | A     | 518 | GLU  | N-CA-CB   | 8.12  | 125.22      | 110.60   |
| 1   | F     | 56  | VAL  | CB-CA-C   | -8.12 | 95.98       | 111.40   |
| 1   | C     | 56  | VAL  | CB-CA-C   | -8.11 | 95.98       | 111.40   |
| 1   | B     | 56  | VAL  | CB-CA-C   | -8.11 | 95.99       | 111.40   |
| 1   | D     | 518 | GLU  | CA-C-N    | 8.11  | 135.04      | 117.20   |
| 1   | A     | 518 | GLU  | CA-C-N    | 8.10  | 135.03      | 117.20   |
| 1   | C     | 518 | GLU  | CA-C-N    | 8.10  | 135.03      | 117.20   |
| 1   | E     | 518 | GLU  | CA-C-N    | 8.10  | 135.03      | 117.20   |
| 1   | F     | 518 | GLU  | CA-C-N    | 8.10  | 135.03      | 117.20   |
| 1   | G     | 518 | GLU  | CA-C-N    | 8.10  | 135.02      | 117.20   |
| 1   | B     | 518 | GLU  | CA-C-N    | 8.09  | 135.00      | 117.20   |
| 1   | E     | 518 | GLU  | N-CA-CB   | 8.08  | 125.14      | 110.60   |
| 1   | C     | 518 | GLU  | N-CA-CB   | 8.06  | 125.11      | 110.60   |
| 1   | N     | 310 | GLU  | CB-CA-C   | -8.06 | 94.28       | 110.40   |
| 1   | J     | 284 | ARG  | NE-CZ-NH1 | 8.06  | 124.33      | 120.30   |
| 1   | H     | 310 | GLU  | CB-CA-C   | -8.06 | 94.29       | 110.40   |
| 1   | K     | 310 | GLU  | CB-CA-C   | -8.05 | 94.30       | 110.40   |
| 1   | N     | 284 | ARG  | NE-CZ-NH1 | 8.05  | 124.32      | 120.30   |
| 1   | F     | 518 | GLU  | N-CA-CB   | 8.04  | 125.07      | 110.60   |
| 1   | G     | 518 | GLU  | N-CA-CB   | 8.04  | 125.07      | 110.60   |
| 1   | H     | 284 | ARG  | NE-CZ-NH1 | 8.03  | 124.32      | 120.30   |
| 1   | D     | 518 | GLU  | N-CA-CB   | 8.03  | 125.06      | 110.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 518 | GLU  | N-CA-CB   | 8.03  | 125.05      | 110.60   |
| 1   | K     | 284 | ARG  | NE-CZ-NH1 | 8.02  | 124.31      | 120.30   |
| 1   | I     | 404 | ARG  | NE-CZ-NH2 | -8.02 | 116.29      | 120.30   |
| 1   | I     | 395 | ARG  | NE-CZ-NH2 | -8.01 | 116.30      | 120.30   |
| 1   | M     | 310 | GLU  | CB-CA-C   | -8.00 | 94.39       | 110.40   |
| 1   | I     | 284 | ARG  | NE-CZ-NH1 | 8.00  | 124.30      | 120.30   |
| 1   | J     | 310 | GLU  | CB-CA-C   | -8.00 | 94.40       | 110.40   |
| 1   | L     | 310 | GLU  | CB-CA-C   | -8.00 | 94.41       | 110.40   |
| 1   | L     | 284 | ARG  | NE-CZ-NH1 | 7.97  | 124.29      | 120.30   |
| 1   | M     | 395 | ARG  | NE-CZ-NH2 | -7.96 | 116.32      | 120.30   |
| 1   | M     | 284 | ARG  | NE-CZ-NH1 | 7.95  | 124.28      | 120.30   |
| 1   | I     | 310 | GLU  | CB-CA-C   | -7.95 | 94.50       | 110.40   |
| 1   | N     | 395 | ARG  | NE-CZ-NH2 | -7.94 | 116.33      | 120.30   |
| 1   | M     | 404 | ARG  | NE-CZ-NH2 | -7.94 | 116.33      | 120.30   |
| 1   | K     | 395 | ARG  | NE-CZ-NH2 | -7.92 | 116.34      | 120.30   |
| 1   | J     | 404 | ARG  | NE-CZ-NH2 | -7.92 | 116.34      | 120.30   |
| 1   | N     | 404 | ARG  | NE-CZ-NH2 | -7.92 | 116.34      | 120.30   |
| 1   | H     | 395 | ARG  | NE-CZ-NH2 | -7.92 | 116.34      | 120.30   |
| 1   | L     | 404 | ARG  | NE-CZ-NH2 | -7.91 | 116.34      | 120.30   |
| 1   | H     | 404 | ARG  | NE-CZ-NH2 | -7.90 | 116.35      | 120.30   |
| 1   | K     | 404 | ARG  | NE-CZ-NH2 | -7.88 | 116.36      | 120.30   |
| 1   | F     | 213 | VAL  | CA-C-N    | -7.86 | 99.92       | 117.20   |
| 1   | G     | 213 | VAL  | CA-C-N    | -7.85 | 99.92       | 117.20   |
| 1   | C     | 213 | VAL  | CA-C-N    | -7.85 | 99.92       | 117.20   |
| 1   | D     | 213 | VAL  | CA-C-N    | -7.85 | 99.93       | 117.20   |
| 1   | B     | 213 | VAL  | CA-C-N    | -7.85 | 99.94       | 117.20   |
| 1   | E     | 213 | VAL  | CA-C-N    | -7.84 | 99.95       | 117.20   |
| 1   | L     | 395 | ARG  | NE-CZ-NH2 | -7.83 | 116.38      | 120.30   |
| 1   | J     | 395 | ARG  | NE-CZ-NH2 | -7.80 | 116.40      | 120.30   |
| 1   | K     | 213 | VAL  | O-C-N     | -7.78 | 110.25      | 122.70   |
| 1   | I     | 213 | VAL  | O-C-N     | -7.76 | 110.28      | 122.70   |
| 1   | N     | 213 | VAL  | O-C-N     | -7.76 | 110.28      | 122.70   |
| 1   | J     | 213 | VAL  | O-C-N     | -7.76 | 110.28      | 122.70   |
| 1   | L     | 213 | VAL  | O-C-N     | -7.76 | 110.28      | 122.70   |
| 1   | H     | 213 | VAL  | O-C-N     | -7.74 | 110.32      | 122.70   |
| 1   | M     | 213 | VAL  | O-C-N     | -7.72 | 110.34      | 122.70   |
| 1   | B     | 258 | ALA  | N-CA-CB   | 7.72  | 120.91      | 110.10   |
| 1   | D     | 258 | ALA  | N-CA-CB   | 7.72  | 120.91      | 110.10   |
| 1   | A     | 258 | ALA  | N-CA-CB   | 7.72  | 120.91      | 110.10   |
| 1   | C     | 258 | ALA  | N-CA-CB   | 7.72  | 120.91      | 110.10   |
| 1   | E     | 258 | ALA  | N-CA-CB   | 7.71  | 120.89      | 110.10   |
| 1   | F     | 258 | ALA  | N-CA-CB   | 7.70  | 120.88      | 110.10   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | G     | 258 | ALA  | N-CA-CB   | 7.69  | 120.87      | 110.10   |
| 1   | F     | 18  | ARG  | NE-CZ-NH2 | -7.66 | 116.47      | 120.30   |
| 1   | G     | 18  | ARG  | NE-CZ-NH2 | -7.63 | 116.49      | 120.30   |
| 1   | A     | 18  | ARG  | NE-CZ-NH2 | -7.62 | 116.49      | 120.30   |
| 1   | D     | 18  | ARG  | NE-CZ-NH2 | -7.61 | 116.49      | 120.30   |
| 1   | L     | 77  | VAL  | CB-CA-C   | -7.61 | 96.94       | 111.40   |
| 1   | N     | 77  | VAL  | CB-CA-C   | -7.61 | 96.95       | 111.40   |
| 1   | I     | 77  | VAL  | CB-CA-C   | -7.61 | 96.95       | 111.40   |
| 1   | K     | 77  | VAL  | CB-CA-C   | -7.61 | 96.95       | 111.40   |
| 1   | B     | 18  | ARG  | NE-CZ-NH2 | -7.60 | 116.50      | 120.30   |
| 1   | J     | 77  | VAL  | CB-CA-C   | -7.60 | 96.96       | 111.40   |
| 1   | H     | 77  | VAL  | CB-CA-C   | -7.60 | 96.97       | 111.40   |
| 1   | E     | 18  | ARG  | NE-CZ-NH2 | -7.59 | 116.50      | 120.30   |
| 1   | M     | 77  | VAL  | CB-CA-C   | -7.59 | 96.98       | 111.40   |
| 1   | L     | 224 | ASP  | N-CA-CB   | 7.58  | 124.25      | 110.60   |
| 1   | N     | 224 | ASP  | N-CA-CB   | 7.58  | 124.23      | 110.60   |
| 1   | M     | 224 | ASP  | N-CA-CB   | 7.57  | 124.23      | 110.60   |
| 1   | N     | 208 | PRO  | O-C-N     | -7.56 | 110.60      | 122.70   |
| 1   | C     | 18  | ARG  | NE-CZ-NH2 | -7.56 | 116.52      | 120.30   |
| 1   | D     | 39  | VAL  | O-C-N     | 7.56  | 134.80      | 122.70   |
| 1   | F     | 39  | VAL  | O-C-N     | 7.54  | 134.77      | 122.70   |
| 1   | A     | 39  | VAL  | O-C-N     | 7.53  | 134.74      | 122.70   |
| 1   | B     | 39  | VAL  | O-C-N     | 7.52  | 134.74      | 122.70   |
| 1   | G     | 39  | VAL  | O-C-N     | 7.52  | 134.74      | 122.70   |
| 1   | I     | 303 | GLU  | CB-CA-C   | -7.52 | 95.35       | 110.40   |
| 1   | C     | 39  | VAL  | O-C-N     | 7.51  | 134.72      | 122.70   |
| 1   | E     | 39  | VAL  | O-C-N     | 7.51  | 134.71      | 122.70   |
| 1   | J     | 303 | GLU  | CB-CA-C   | -7.50 | 95.40       | 110.40   |
| 1   | F     | 452 | ARG  | NE-CZ-NH2 | -7.47 | 116.56      | 120.30   |
| 1   | G     | 452 | ARG  | NE-CZ-NH2 | -7.43 | 116.58      | 120.30   |
| 1   | A     | 316 | ASP  | N-CA-CB   | 7.42  | 123.95      | 110.60   |
| 1   | F     | 316 | ASP  | N-CA-CB   | 7.42  | 123.95      | 110.60   |
| 1   | B     | 316 | ASP  | N-CA-CB   | 7.41  | 123.94      | 110.60   |
| 1   | C     | 316 | ASP  | N-CA-CB   | 7.41  | 123.94      | 110.60   |
| 1   | E     | 316 | ASP  | N-CA-CB   | 7.41  | 123.93      | 110.60   |
| 1   | C     | 452 | ARG  | NE-CZ-NH2 | -7.41 | 116.60      | 120.30   |
| 1   | G     | 316 | ASP  | N-CA-CB   | 7.40  | 123.92      | 110.60   |
| 1   | E     | 452 | ARG  | NE-CZ-NH2 | -7.40 | 116.60      | 120.30   |
| 1   | D     | 316 | ASP  | N-CA-CB   | 7.40  | 123.91      | 110.60   |
| 1   | A     | 452 | ARG  | NE-CZ-NH2 | -7.39 | 116.61      | 120.30   |
| 1   | D     | 452 | ARG  | NE-CZ-NH2 | -7.39 | 116.61      | 120.30   |
| 1   | B     | 452 | ARG  | NE-CZ-NH2 | -7.37 | 116.61      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | N     | 345 | ARG  | NE-CZ-NH2 | -7.32 | 116.64      | 120.30   |
| 1   | M     | 345 | ARG  | NE-CZ-NH2 | -7.31 | 116.64      | 120.30   |
| 1   | J     | 224 | ASP  | N-CA-CB   | 7.30  | 123.74      | 110.60   |
| 1   | J     | 345 | ARG  | NE-CZ-NH2 | -7.30 | 116.65      | 120.30   |
| 1   | K     | 345 | ARG  | NE-CZ-NH2 | -7.30 | 116.65      | 120.30   |
| 1   | L     | 345 | ARG  | NE-CZ-NH2 | -7.30 | 116.65      | 120.30   |
| 1   | I     | 224 | ASP  | N-CA-CB   | 7.29  | 123.73      | 110.60   |
| 1   | H     | 345 | ARG  | NE-CZ-NH2 | -7.27 | 116.66      | 120.30   |
| 1   | H     | 18  | ARG  | CD-NE-CZ  | 7.17  | 133.63      | 123.60   |
| 1   | I     | 251 | ALA  | N-CA-CB   | 7.17  | 120.13      | 110.10   |
| 1   | A     | 289 | LEU  | CB-CG-CD1 | -7.15 | 98.84       | 111.00   |
| 1   | I     | 18  | ARG  | CD-NE-CZ  | 7.15  | 133.61      | 123.60   |
| 1   | J     | 251 | ALA  | N-CA-CB   | 7.15  | 120.11      | 110.10   |
| 1   | F     | 289 | LEU  | CB-CG-CD1 | -7.15 | 98.85       | 111.00   |
| 1   | C     | 289 | LEU  | CB-CG-CD1 | -7.14 | 98.86       | 111.00   |
| 1   | B     | 289 | LEU  | CB-CG-CD1 | -7.14 | 98.86       | 111.00   |
| 1   | G     | 289 | LEU  | CB-CG-CD1 | -7.14 | 98.86       | 111.00   |
| 1   | H     | 251 | ALA  | N-CA-CB   | 7.14  | 120.10      | 110.10   |
| 1   | E     | 289 | LEU  | CB-CG-CD1 | -7.14 | 98.87       | 111.00   |
| 1   | M     | 251 | ALA  | N-CA-CB   | 7.13  | 120.08      | 110.10   |
| 1   | I     | 345 | ARG  | NE-CZ-NH2 | -7.12 | 116.74      | 120.30   |
| 1   | D     | 289 | LEU  | CB-CG-CD1 | -7.12 | 98.90       | 111.00   |
| 1   | N     | 18  | ARG  | CD-NE-CZ  | 7.12  | 133.56      | 123.60   |
| 1   | H     | 303 | GLU  | CB-CA-C   | -7.11 | 96.18       | 110.40   |
| 1   | J     | 18  | ARG  | CD-NE-CZ  | 7.11  | 133.55      | 123.60   |
| 1   | L     | 18  | ARG  | CD-NE-CZ  | 7.11  | 133.56      | 123.60   |
| 1   | K     | 303 | GLU  | CB-CA-C   | -7.11 | 96.18       | 110.40   |
| 1   | M     | 18  | ARG  | CD-NE-CZ  | 7.11  | 133.55      | 123.60   |
| 1   | N     | 251 | ALA  | N-CA-CB   | 7.11  | 120.05      | 110.10   |
| 1   | K     | 251 | ALA  | N-CA-CB   | 7.10  | 120.04      | 110.10   |
| 1   | K     | 18  | ARG  | CD-NE-CZ  | 7.08  | 133.52      | 123.60   |
| 1   | L     | 251 | ALA  | N-CA-CB   | 7.08  | 120.01      | 110.10   |
| 1   | C     | 59  | GLU  | N-CA-CB   | -7.04 | 97.93       | 110.60   |
| 1   | D     | 59  | GLU  | N-CA-CB   | -7.04 | 97.93       | 110.60   |
| 1   | E     | 59  | GLU  | N-CA-CB   | -7.03 | 97.94       | 110.60   |
| 1   | K     | 362 | ARG  | NE-CZ-NH1 | 7.03  | 123.82      | 120.30   |
| 1   | A     | 59  | GLU  | N-CA-CB   | -7.03 | 97.95       | 110.60   |
| 1   | G     | 59  | GLU  | N-CA-CB   | -7.03 | 97.95       | 110.60   |
| 1   | H     | 362 | ARG  | NE-CZ-NH1 | 7.02  | 123.81      | 120.30   |
| 1   | B     | 59  | GLU  | N-CA-CB   | -7.01 | 97.97       | 110.60   |
| 1   | F     | 59  | GLU  | N-CA-CB   | -7.01 | 97.98       | 110.60   |
| 1   | I     | 362 | ARG  | NE-CZ-NH1 | 7.01  | 123.81      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1   | N     | 362 | ARG  | NE-CZ-NH1 | 6.99 | 123.80      | 120.30   |
| 1   | N     | 185 | ASP  | CB-CA-C   | 6.98 | 124.36      | 110.40   |
| 1   | H     | 185 | ASP  | CB-CA-C   | 6.98 | 124.36      | 110.40   |
| 1   | I     | 185 | ASP  | CB-CA-C   | 6.98 | 124.35      | 110.40   |
| 1   | L     | 185 | ASP  | CB-CA-C   | 6.97 | 124.35      | 110.40   |
| 1   | L     | 362 | ARG  | NE-CZ-NH1 | 6.97 | 123.79      | 120.30   |
| 1   | J     | 185 | ASP  | CB-CA-C   | 6.97 | 124.34      | 110.40   |
| 1   | M     | 185 | ASP  | CB-CA-C   | 6.97 | 124.34      | 110.40   |
| 1   | J     | 362 | ARG  | NE-CZ-NH1 | 6.96 | 123.78      | 120.30   |
| 1   | K     | 118 | ARG  | NE-CZ-NH1 | 6.96 | 123.78      | 120.30   |
| 1   | M     | 362 | ARG  | NE-CZ-NH1 | 6.95 | 123.78      | 120.30   |
| 1   | H     | 224 | ASP  | N-CA-CB   | 6.94 | 123.10      | 110.60   |
| 1   | K     | 224 | ASP  | N-CA-CB   | 6.93 | 123.07      | 110.60   |
| 1   | F     | 463 | SER  | N-CA-CB   | 6.92 | 120.89      | 110.50   |
| 1   | H     | 118 | ARG  | NE-CZ-NH1 | 6.89 | 123.75      | 120.30   |
| 1   | E     | 463 | SER  | N-CA-CB   | 6.89 | 120.83      | 110.50   |
| 1   | N     | 231 | ARG  | NE-CZ-NH1 | 6.89 | 123.75      | 120.30   |
| 1   | G     | 463 | SER  | N-CA-CB   | 6.89 | 120.83      | 110.50   |
| 1   | A     | 463 | SER  | N-CA-CB   | 6.89 | 120.83      | 110.50   |
| 1   | C     | 39  | VAL  | N-CA-CB   | 6.88 | 126.64      | 111.50   |
| 1   | F     | 39  | VAL  | N-CA-CB   | 6.88 | 126.63      | 111.50   |
| 1   | A     | 39  | VAL  | N-CA-CB   | 6.87 | 126.62      | 111.50   |
| 1   | D     | 463 | SER  | N-CA-CB   | 6.87 | 120.81      | 110.50   |
| 1   | J     | 118 | ARG  | NE-CZ-NH1 | 6.87 | 123.74      | 120.30   |
| 1   | G     | 39  | VAL  | N-CA-CB   | 6.87 | 126.62      | 111.50   |
| 1   | J     | 404 | ARG  | NE-CZ-NH1 | 6.87 | 123.73      | 120.30   |
| 1   | E     | 39  | VAL  | N-CA-CB   | 6.87 | 126.61      | 111.50   |
| 1   | B     | 463 | SER  | N-CA-CB   | 6.87 | 120.80      | 110.50   |
| 1   | D     | 39  | VAL  | N-CA-CB   | 6.86 | 126.60      | 111.50   |
| 1   | B     | 39  | VAL  | N-CA-CB   | 6.86 | 126.59      | 111.50   |
| 1   | L     | 404 | ARG  | NE-CZ-NH1 | 6.86 | 123.73      | 120.30   |
| 1   | I     | 118 | ARG  | NE-CZ-NH1 | 6.85 | 123.72      | 120.30   |
| 1   | C     | 463 | SER  | N-CA-CB   | 6.84 | 120.76      | 110.50   |
| 1   | M     | 34  | LYS  | CB-CA-C   | 6.83 | 124.05      | 110.40   |
| 1   | H     | 34  | LYS  | CB-CA-C   | 6.82 | 124.04      | 110.40   |
| 1   | K     | 404 | ARG  | NE-CZ-NH1 | 6.82 | 123.71      | 120.30   |
| 1   | L     | 118 | ARG  | NE-CZ-NH1 | 6.82 | 123.71      | 120.30   |
| 1   | J     | 34  | LYS  | CB-CA-C   | 6.81 | 124.03      | 110.40   |
| 1   | K     | 34  | LYS  | CB-CA-C   | 6.81 | 124.03      | 110.40   |
| 1   | I     | 34  | LYS  | CB-CA-C   | 6.81 | 124.02      | 110.40   |
| 1   | L     | 34  | LYS  | CB-CA-C   | 6.81 | 124.02      | 110.40   |
| 1   | I     | 404 | ARG  | NE-CZ-NH1 | 6.81 | 123.70      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | N     | 34  | LYS  | CB-CA-C   | 6.81  | 124.02      | 110.40   |
| 1   | M     | 118 | ARG  | NE-CZ-NH1 | 6.80  | 123.70      | 120.30   |
| 1   | F     | 247 | LEU  | CB-CA-C   | -6.80 | 97.28       | 110.20   |
| 1   | A     | 247 | LEU  | CB-CA-C   | -6.80 | 97.28       | 110.20   |
| 1   | D     | 247 | LEU  | CB-CA-C   | -6.80 | 97.28       | 110.20   |
| 1   | E     | 247 | LEU  | CB-CA-C   | -6.80 | 97.28       | 110.20   |
| 1   | N     | 404 | ARG  | NE-CZ-NH1 | 6.80  | 123.70      | 120.30   |
| 1   | B     | 247 | LEU  | CB-CA-C   | -6.79 | 97.29       | 110.20   |
| 1   | N     | 118 | ARG  | NE-CZ-NH1 | 6.79  | 123.69      | 120.30   |
| 1   | G     | 247 | LEU  | CB-CA-C   | -6.79 | 97.30       | 110.20   |
| 1   | C     | 247 | LEU  | CB-CA-C   | -6.78 | 97.31       | 110.20   |
| 1   | B     | 230 | ILE  | O-C-N     | 6.77  | 133.54      | 122.70   |
| 1   | C     | 87  | ASP  | N-CA-CB   | 6.77  | 122.79      | 110.60   |
| 1   | D     | 230 | ILE  | O-C-N     | 6.77  | 133.53      | 122.70   |
| 1   | G     | 87  | ASP  | N-CA-CB   | 6.77  | 122.78      | 110.60   |
| 1   | A     | 87  | ASP  | N-CA-CB   | 6.77  | 122.78      | 110.60   |
| 1   | A     | 230 | ILE  | O-C-N     | 6.77  | 133.53      | 122.70   |
| 1   | D     | 251 | ALA  | N-CA-CB   | -6.76 | 100.63      | 110.10   |
| 1   | D     | 362 | ARG  | NE-CZ-NH1 | 6.76  | 123.68      | 120.30   |
| 1   | E     | 87  | ASP  | N-CA-CB   | 6.76  | 122.77      | 110.60   |
| 1   | I     | 395 | ARG  | NE-CZ-NH1 | 6.76  | 123.68      | 120.30   |
| 1   | F     | 230 | ILE  | O-C-N     | 6.76  | 133.51      | 122.70   |
| 1   | G     | 230 | ILE  | O-C-N     | 6.75  | 133.51      | 122.70   |
| 1   | H     | 404 | ARG  | NE-CZ-NH1 | 6.75  | 123.68      | 120.30   |
| 1   | E     | 230 | ILE  | O-C-N     | 6.75  | 133.51      | 122.70   |
| 1   | A     | 251 | ALA  | N-CA-CB   | -6.75 | 100.65      | 110.10   |
| 1   | C     | 230 | ILE  | O-C-N     | 6.75  | 133.50      | 122.70   |
| 1   | E     | 251 | ALA  | N-CA-CB   | -6.75 | 100.65      | 110.10   |
| 1   | G     | 251 | ALA  | N-CA-CB   | -6.74 | 100.66      | 110.10   |
| 1   | B     | 251 | ALA  | N-CA-CB   | -6.73 | 100.67      | 110.10   |
| 1   | C     | 251 | ALA  | N-CA-CB   | -6.73 | 100.67      | 110.10   |
| 1   | F     | 251 | ALA  | N-CA-CB   | -6.73 | 100.67      | 110.10   |
| 1   | M     | 404 | ARG  | NE-CZ-NH1 | 6.72  | 123.66      | 120.30   |
| 1   | N     | 395 | ARG  | NE-CZ-NH1 | 6.72  | 123.66      | 120.30   |
| 1   | M     | 395 | ARG  | NE-CZ-NH1 | 6.71  | 123.66      | 120.30   |
| 1   | K     | 395 | ARG  | NE-CZ-NH1 | 6.69  | 123.64      | 120.30   |
| 1   | E     | 362 | ARG  | NE-CZ-NH1 | 6.68  | 123.64      | 120.30   |
| 1   | L     | 303 | GLU  | CB-CA-C   | -6.68 | 97.05       | 110.40   |
| 1   | N     | 303 | GLU  | CB-CA-C   | -6.68 | 97.05       | 110.40   |
| 1   | M     | 303 | GLU  | CB-CA-C   | -6.67 | 97.05       | 110.40   |
| 1   | B     | 362 | ARG  | NE-CZ-NH1 | 6.67  | 123.64      | 120.30   |
| 1   | C     | 362 | ARG  | NE-CZ-NH1 | 6.65  | 123.62      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | H     | 395 | ARG  | NE-CZ-NH1 | 6.64  | 123.62      | 120.30   |
| 1   | A     | 362 | ARG  | NE-CZ-NH1 | 6.63  | 123.61      | 120.30   |
| 1   | J     | 300 | VAL  | CB-CA-C   | -6.62 | 98.81       | 111.40   |
| 1   | J     | 395 | ARG  | NE-CZ-NH1 | 6.62  | 123.61      | 120.30   |
| 1   | I     | 300 | VAL  | CB-CA-C   | -6.62 | 98.83       | 111.40   |
| 1   | G     | 362 | ARG  | NE-CZ-NH1 | 6.61  | 123.61      | 120.30   |
| 1   | E     | 213 | VAL  | C-N-CA    | -6.61 | 105.17      | 121.70   |
| 1   | F     | 213 | VAL  | C-N-CA    | -6.61 | 105.18      | 121.70   |
| 1   | F     | 362 | ARG  | NE-CZ-NH1 | 6.61  | 123.60      | 120.30   |
| 1   | J     | 152 | ALA  | CB-CA-C   | 6.61  | 120.01      | 110.10   |
| 1   | I     | 383 | ALA  | N-CA-CB   | 6.60  | 119.34      | 110.10   |
| 1   | L     | 152 | ALA  | CB-CA-C   | 6.60  | 120.00      | 110.10   |
| 1   | L     | 383 | ALA  | N-CA-CB   | 6.60  | 119.34      | 110.10   |
| 1   | B     | 213 | VAL  | C-N-CA    | -6.60 | 105.21      | 121.70   |
| 1   | H     | 383 | ALA  | N-CA-CB   | 6.60  | 119.33      | 110.10   |
| 1   | G     | 213 | VAL  | C-N-CA    | -6.59 | 105.21      | 121.70   |
| 1   | H     | 152 | ALA  | CB-CA-C   | 6.59  | 119.99      | 110.10   |
| 1   | I     | 152 | ALA  | CB-CA-C   | 6.59  | 119.99      | 110.10   |
| 1   | J     | 383 | ALA  | N-CA-CB   | 6.59  | 119.33      | 110.10   |
| 1   | M     | 383 | ALA  | N-CA-CB   | 6.59  | 119.33      | 110.10   |
| 1   | N     | 383 | ALA  | N-CA-CB   | 6.59  | 119.33      | 110.10   |
| 1   | K     | 152 | ALA  | CB-CA-C   | 6.59  | 119.98      | 110.10   |
| 1   | K     | 383 | ALA  | N-CA-CB   | 6.59  | 119.32      | 110.10   |
| 1   | C     | 213 | VAL  | C-N-CA    | -6.58 | 105.24      | 121.70   |
| 1   | D     | 213 | VAL  | C-N-CA    | -6.58 | 105.24      | 121.70   |
| 1   | N     | 152 | ALA  | CB-CA-C   | 6.58  | 119.97      | 110.10   |
| 1   | M     | 152 | ALA  | CB-CA-C   | 6.57  | 119.96      | 110.10   |
| 1   | L     | 395 | ARG  | NE-CZ-NH1 | 6.57  | 123.58      | 120.30   |
| 1   | A     | 253 | ASP  | CB-CG-OD1 | 6.56  | 124.20      | 118.30   |
| 1   | L     | 300 | VAL  | CB-CA-C   | -6.54 | 98.97       | 111.40   |
| 1   | C     | 253 | ASP  | CB-CG-OD1 | 6.54  | 124.19      | 118.30   |
| 1   | N     | 300 | VAL  | CB-CA-C   | -6.54 | 98.97       | 111.40   |
| 1   | B     | 253 | ASP  | CB-CG-OD1 | 6.54  | 124.18      | 118.30   |
| 1   | I     | 242 | LYS  | CA-CB-CG  | 6.54  | 127.78      | 113.40   |
| 1   | K     | 37  | ASN  | CB-CA-C   | 6.53  | 123.46      | 110.40   |
| 1   | J     | 242 | LYS  | CA-CB-CG  | 6.53  | 127.76      | 113.40   |
| 1   | K     | 300 | VAL  | CB-CA-C   | -6.53 | 99.00       | 111.40   |
| 1   | D     | 252 | GLU  | N-CA-CB   | 6.52  | 122.34      | 110.60   |
| 1   | G     | 252 | GLU  | N-CA-CB   | 6.52  | 122.34      | 110.60   |
| 1   | G     | 253 | ASP  | CB-CG-OD1 | 6.52  | 124.17      | 118.30   |
| 1   | B     | 252 | GLU  | N-CA-CB   | 6.52  | 122.34      | 110.60   |
| 1   | C     | 252 | GLU  | N-CA-CB   | 6.52  | 122.34      | 110.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 252 | GLU  | N-CA-CB   | 6.51  | 122.33      | 110.60   |
| 1   | J     | 37  | ASN  | CB-CA-C   | 6.51  | 123.43      | 110.40   |
| 1   | L     | 37  | ASN  | CB-CA-C   | 6.51  | 123.43      | 110.40   |
| 1   | E     | 253 | ASP  | CB-CG-OD1 | 6.51  | 124.16      | 118.30   |
| 1   | F     | 252 | GLU  | N-CA-CB   | 6.51  | 122.32      | 110.60   |
| 1   | E     | 252 | GLU  | N-CA-CB   | 6.51  | 122.32      | 110.60   |
| 1   | F     | 253 | ASP  | CB-CG-OD1 | 6.51  | 124.16      | 118.30   |
| 1   | M     | 300 | VAL  | CB-CA-C   | -6.51 | 99.03       | 111.40   |
| 1   | N     | 37  | ASN  | CB-CA-C   | 6.51  | 123.42      | 110.40   |
| 1   | H     | 37  | ASN  | CB-CA-C   | 6.50  | 123.41      | 110.40   |
| 1   | H     | 300 | VAL  | CB-CA-C   | -6.50 | 99.05       | 111.40   |
| 1   | M     | 37  | ASN  | CB-CA-C   | 6.50  | 123.41      | 110.40   |
| 1   | N     | 242 | LYS  | CA-CB-CG  | 6.50  | 127.71      | 113.40   |
| 1   | I     | 37  | ASN  | CB-CA-C   | 6.50  | 123.40      | 110.40   |
| 1   | B     | 367 | GLU  | CB-CA-C   | -6.50 | 97.41       | 110.40   |
| 1   | D     | 253 | ASP  | CB-CG-OD1 | 6.50  | 124.15      | 118.30   |
| 1   | F     | 367 | GLU  | CB-CA-C   | -6.49 | 97.42       | 110.40   |
| 1   | D     | 367 | GLU  | CB-CA-C   | -6.49 | 97.42       | 110.40   |
| 1   | C     | 367 | GLU  | CB-CA-C   | -6.49 | 97.42       | 110.40   |
| 1   | A     | 367 | GLU  | CB-CA-C   | -6.48 | 97.43       | 110.40   |
| 1   | E     | 367 | GLU  | CB-CA-C   | -6.47 | 97.45       | 110.40   |
| 1   | G     | 367 | GLU  | CB-CA-C   | -6.47 | 97.45       | 110.40   |
| 1   | D     | 273 | VAL  | CB-CA-C   | -6.47 | 99.11       | 111.40   |
| 1   | L     | 242 | LYS  | CA-CB-CG  | 6.47  | 127.63      | 113.40   |
| 1   | B     | 273 | VAL  | CB-CA-C   | -6.46 | 99.13       | 111.40   |
| 1   | F     | 273 | VAL  | CB-CA-C   | -6.46 | 99.13       | 111.40   |
| 1   | A     | 273 | VAL  | CB-CA-C   | -6.46 | 99.13       | 111.40   |
| 1   | C     | 273 | VAL  | CB-CA-C   | -6.46 | 99.13       | 111.40   |
| 1   | G     | 273 | VAL  | CB-CA-C   | -6.46 | 99.13       | 111.40   |
| 1   | E     | 273 | VAL  | CB-CA-C   | -6.45 | 99.14       | 111.40   |
| 1   | H     | 365 | LEU  | CB-CA-C   | 6.45  | 122.45      | 110.20   |
| 1   | I     | 365 | LEU  | CB-CA-C   | 6.45  | 122.45      | 110.20   |
| 1   | J     | 365 | LEU  | CB-CA-C   | 6.45  | 122.45      | 110.20   |
| 1   | K     | 365 | LEU  | CB-CA-C   | 6.44  | 122.44      | 110.20   |
| 1   | M     | 365 | LEU  | CB-CA-C   | 6.44  | 122.44      | 110.20   |
| 1   | L     | 365 | LEU  | CB-CA-C   | 6.43  | 122.43      | 110.20   |
| 1   | N     | 365 | LEU  | CB-CA-C   | 6.43  | 122.42      | 110.20   |
| 1   | J     | 397 | GLU  | CB-CA-C   | 6.43  | 123.26      | 110.40   |
| 1   | H     | 397 | GLU  | CB-CA-C   | 6.43  | 123.25      | 110.40   |
| 1   | K     | 397 | GLU  | CB-CA-C   | 6.43  | 123.25      | 110.40   |
| 1   | M     | 397 | GLU  | CB-CA-C   | 6.42  | 123.25      | 110.40   |
| 1   | L     | 397 | GLU  | CB-CA-C   | 6.42  | 123.24      | 110.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | N     | 207 | LYS  | C-N-CD    | -6.42 | 106.47      | 120.60   |
| 1   | I     | 397 | GLU  | CB-CA-C   | 6.41  | 123.22      | 110.40   |
| 1   | D     | 153 | ASN  | CB-CA-C   | 6.41  | 123.21      | 110.40   |
| 1   | N     | 397 | GLU  | CB-CA-C   | 6.40  | 123.21      | 110.40   |
| 1   | D     | 39  | VAL  | CA-C-N    | -6.37 | 103.19      | 117.20   |
| 1   | F     | 39  | VAL  | CA-C-N    | -6.37 | 103.19      | 117.20   |
| 1   | F     | 153 | ASN  | CB-CA-C   | 6.37  | 123.13      | 110.40   |
| 1   | C     | 39  | VAL  | CA-C-N    | -6.36 | 103.21      | 117.20   |
| 1   | B     | 39  | VAL  | CA-C-N    | -6.36 | 103.21      | 117.20   |
| 1   | A     | 39  | VAL  | CA-C-N    | -6.36 | 103.22      | 117.20   |
| 1   | G     | 39  | VAL  | CA-C-N    | -6.35 | 103.23      | 117.20   |
| 1   | F     | 87  | ASP  | N-CA-CB   | 6.35  | 122.03      | 110.60   |
| 1   | E     | 39  | VAL  | CA-C-N    | -6.34 | 103.25      | 117.20   |
| 1   | D     | 87  | ASP  | N-CA-CB   | 6.33  | 121.98      | 110.60   |
| 1   | J     | 197 | ARG  | NE-CZ-NH1 | 6.25  | 123.43      | 120.30   |
| 1   | D     | 311 | LYS  | N-CA-CB   | 6.22  | 121.80      | 110.60   |
| 1   | C     | 311 | LYS  | N-CA-CB   | 6.22  | 121.79      | 110.60   |
| 1   | G     | 311 | LYS  | N-CA-CB   | 6.21  | 121.79      | 110.60   |
| 1   | M     | 266 | THR  | N-CA-CB   | 6.21  | 122.11      | 110.30   |
| 1   | C     | 34  | LYS  | N-CA-CB   | 6.21  | 121.78      | 110.60   |
| 1   | A     | 34  | LYS  | N-CA-CB   | 6.21  | 121.78      | 110.60   |
| 1   | A     | 311 | LYS  | N-CA-CB   | 6.21  | 121.78      | 110.60   |
| 1   | N     | 266 | THR  | N-CA-CB   | 6.21  | 122.09      | 110.30   |
| 1   | B     | 34  | LYS  | N-CA-CB   | 6.21  | 121.77      | 110.60   |
| 1   | D     | 34  | LYS  | N-CA-CB   | 6.21  | 121.77      | 110.60   |
| 1   | B     | 311 | LYS  | N-CA-CB   | 6.20  | 121.77      | 110.60   |
| 1   | E     | 311 | LYS  | N-CA-CB   | 6.20  | 121.76      | 110.60   |
| 1   | F     | 34  | LYS  | N-CA-CB   | 6.20  | 121.76      | 110.60   |
| 1   | F     | 311 | LYS  | N-CA-CB   | 6.20  | 121.76      | 110.60   |
| 1   | H     | 266 | THR  | N-CA-CB   | 6.20  | 122.08      | 110.30   |
| 1   | E     | 34  | LYS  | N-CA-CB   | 6.19  | 121.75      | 110.60   |
| 1   | G     | 34  | LYS  | N-CA-CB   | 6.19  | 121.75      | 110.60   |
| 1   | K     | 266 | THR  | N-CA-CB   | 6.19  | 122.06      | 110.30   |
| 1   | N     | 59  | GLU  | CB-CA-C   | 6.19  | 122.78      | 110.40   |
| 1   | I     | 266 | THR  | N-CA-CB   | 6.19  | 122.06      | 110.30   |
| 1   | J     | 59  | GLU  | CB-CA-C   | 6.19  | 122.77      | 110.40   |
| 1   | K     | 59  | GLU  | CB-CA-C   | 6.19  | 122.77      | 110.40   |
| 1   | H     | 59  | GLU  | CB-CA-C   | 6.18  | 122.76      | 110.40   |
| 1   | L     | 266 | THR  | N-CA-CB   | 6.18  | 122.04      | 110.30   |
| 1   | M     | 59  | GLU  | CB-CA-C   | 6.18  | 122.75      | 110.40   |
| 1   | L     | 59  | GLU  | CB-CA-C   | 6.17  | 122.75      | 110.40   |
| 1   | H     | 452 | ARG  | NE-CZ-NH2 | -6.17 | 117.22      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | I     | 59  | GLU  | CB-CA-C   | 6.17  | 122.73      | 110.40   |
| 1   | J     | 266 | THR  | N-CA-CB   | 6.16  | 122.01      | 110.30   |
| 1   | C     | 153 | ASN  | N-CA-CB   | 6.14  | 121.66      | 110.60   |
| 1   | A     | 153 | ASN  | N-CA-CB   | 6.13  | 121.64      | 110.60   |
| 1   | G     | 153 | ASN  | N-CA-CB   | 6.13  | 121.64      | 110.60   |
| 1   | E     | 153 | ASN  | N-CA-CB   | 6.13  | 121.63      | 110.60   |
| 1   | I     | 197 | ARG  | NE-CZ-NH1 | 6.11  | 123.36      | 120.30   |
| 1   | M     | 452 | ARG  | NE-CZ-NH2 | -6.11 | 117.25      | 120.30   |
| 1   | C     | 312 | ALA  | CB-CA-C   | 6.09  | 119.24      | 110.10   |
| 1   | N     | 452 | ARG  | NE-CZ-NH2 | -6.09 | 117.25      | 120.30   |
| 1   | B     | 312 | ALA  | CB-CA-C   | 6.08  | 119.22      | 110.10   |
| 1   | E     | 312 | ALA  | CB-CA-C   | 6.08  | 119.22      | 110.10   |
| 1   | F     | 312 | ALA  | CB-CA-C   | 6.08  | 119.21      | 110.10   |
| 1   | A     | 312 | ALA  | CB-CA-C   | 6.07  | 119.20      | 110.10   |
| 1   | G     | 312 | ALA  | CB-CA-C   | 6.07  | 119.20      | 110.10   |
| 1   | D     | 312 | ALA  | CB-CA-C   | 6.06  | 119.19      | 110.10   |
| 1   | H     | 482 | THR  | N-CA-CB   | 6.05  | 121.80      | 110.30   |
| 1   | K     | 482 | THR  | N-CA-CB   | 6.05  | 121.80      | 110.30   |
| 1   | M     | 482 | THR  | N-CA-CB   | 6.05  | 121.80      | 110.30   |
| 1   | N     | 482 | THR  | N-CA-CB   | 6.05  | 121.80      | 110.30   |
| 1   | E     | 231 | ARG  | NE-CZ-NH1 | 6.05  | 123.32      | 120.30   |
| 1   | J     | 482 | THR  | N-CA-CB   | 6.05  | 121.79      | 110.30   |
| 1   | L     | 482 | THR  | N-CA-CB   | 6.05  | 121.79      | 110.30   |
| 1   | N     | 197 | ARG  | NE-CZ-NH1 | 6.05  | 123.32      | 120.30   |
| 1   | F     | 231 | ARG  | NE-CZ-NH1 | 6.04  | 123.32      | 120.30   |
| 1   | B     | 87  | ASP  | N-CA-CB   | 6.03  | 121.46      | 110.60   |
| 1   | H     | 197 | ARG  | NE-CZ-NH1 | 6.03  | 123.31      | 120.30   |
| 1   | I     | 452 | ARG  | NE-CZ-NH2 | -6.02 | 117.29      | 120.30   |
| 1   | I     | 482 | THR  | N-CA-CB   | 6.02  | 121.74      | 110.30   |
| 1   | M     | 197 | ARG  | NE-CZ-NH1 | 6.01  | 123.31      | 120.30   |
| 1   | A     | 231 | ARG  | NE-CZ-NH1 | 6.01  | 123.31      | 120.30   |
| 1   | M     | 239 | ALA  | CB-CA-C   | 6.01  | 119.11      | 110.10   |
| 1   | J     | 452 | ARG  | NE-CZ-NH2 | -6.00 | 117.30      | 120.30   |
| 1   | L     | 452 | ARG  | NE-CZ-NH2 | -6.00 | 117.30      | 120.30   |
| 1   | I     | 363 | GLU  | CB-CA-C   | 5.99  | 122.39      | 110.40   |
| 1   | A     | 58  | ARG  | NE-CZ-NH1 | 5.99  | 123.29      | 120.30   |
| 1   | J     | 363 | GLU  | CB-CA-C   | 5.99  | 122.38      | 110.40   |
| 1   | D     | 231 | ARG  | NE-CZ-NH1 | 5.99  | 123.29      | 120.30   |
| 1   | J     | 197 | ARG  | NE-CZ-NH2 | -5.98 | 117.31      | 120.30   |
| 1   | E     | 402 | ALA  | N-CA-CB   | -5.98 | 101.73      | 110.10   |
| 1   | I     | 197 | ARG  | NE-CZ-NH2 | -5.98 | 117.31      | 120.30   |
| 1   | C     | 231 | ARG  | NE-CZ-NH1 | 5.97  | 123.29      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | H     | 363 | GLU  | CB-CA-C   | 5.97  | 122.34      | 110.40   |
| 1   | G     | 402 | ALA  | N-CA-CB   | -5.97 | 101.75      | 110.10   |
| 1   | L     | 363 | GLU  | CB-CA-C   | 5.97  | 122.33      | 110.40   |
| 1   | B     | 402 | ALA  | N-CA-CB   | -5.96 | 101.75      | 110.10   |
| 1   | A     | 402 | ALA  | N-CA-CB   | -5.96 | 101.75      | 110.10   |
| 1   | D     | 402 | ALA  | N-CA-CB   | -5.96 | 101.75      | 110.10   |
| 1   | M     | 363 | GLU  | CB-CA-C   | 5.96  | 122.33      | 110.40   |
| 1   | I     | 368 | ARG  | NE-CZ-NH1 | 5.96  | 123.28      | 120.30   |
| 1   | K     | 363 | GLU  | CB-CA-C   | 5.96  | 122.32      | 110.40   |
| 1   | K     | 452 | ARG  | NE-CZ-NH2 | -5.96 | 117.32      | 120.30   |
| 1   | N     | 363 | GLU  | CB-CA-C   | 5.96  | 122.32      | 110.40   |
| 1   | F     | 402 | ALA  | N-CA-CB   | -5.95 | 101.76      | 110.10   |
| 1   | A     | 371 | LYS  | CB-CA-C   | 5.95  | 122.30      | 110.40   |
| 1   | C     | 402 | ALA  | N-CA-CB   | -5.95 | 101.77      | 110.10   |
| 1   | F     | 371 | LYS  | CB-CA-C   | 5.95  | 122.30      | 110.40   |
| 1   | B     | 371 | LYS  | CB-CA-C   | 5.95  | 122.29      | 110.40   |
| 1   | M     | 379 | ILE  | CB-CA-C   | -5.95 | 99.71       | 111.60   |
| 1   | H     | 379 | ILE  | CB-CA-C   | -5.95 | 99.71       | 111.60   |
| 1   | C     | 371 | LYS  | CB-CA-C   | 5.94  | 122.29      | 110.40   |
| 1   | G     | 34  | LYS  | CB-CA-C   | 5.94  | 122.29      | 110.40   |
| 1   | G     | 231 | ARG  | NE-CZ-NH1 | 5.94  | 123.27      | 120.30   |
| 1   | G     | 371 | LYS  | CB-CA-C   | 5.94  | 122.29      | 110.40   |
| 1   | N     | 252 | GLU  | CB-CA-C   | -5.94 | 98.51       | 110.40   |
| 1   | E     | 371 | LYS  | CB-CA-C   | 5.94  | 122.28      | 110.40   |
| 1   | J     | 379 | ILE  | CB-CA-C   | -5.94 | 99.72       | 111.60   |
| 1   | I     | 379 | ILE  | CB-CA-C   | -5.94 | 99.72       | 111.60   |
| 1   | F     | 34  | LYS  | CB-CA-C   | 5.94  | 122.27      | 110.40   |
| 1   | L     | 252 | GLU  | CB-CA-C   | -5.94 | 98.53       | 110.40   |
| 1   | D     | 371 | LYS  | CB-CA-C   | 5.93  | 122.27      | 110.40   |
| 1   | E     | 34  | LYS  | CB-CA-C   | 5.93  | 122.27      | 110.40   |
| 1   | J     | 368 | ARG  | NE-CZ-NH1 | 5.93  | 123.27      | 120.30   |
| 1   | L     | 197 | ARG  | NE-CZ-NH1 | 5.93  | 123.27      | 120.30   |
| 1   | M     | 252 | GLU  | CB-CA-C   | -5.93 | 98.53       | 110.40   |
| 1   | A     | 34  | LYS  | CB-CA-C   | 5.93  | 122.27      | 110.40   |
| 1   | B     | 231 | ARG  | NE-CZ-NH1 | 5.93  | 123.27      | 120.30   |
| 1   | D     | 34  | LYS  | CB-CA-C   | 5.93  | 122.27      | 110.40   |
| 1   | K     | 379 | ILE  | CB-CA-C   | -5.93 | 99.73       | 111.60   |
| 1   | L     | 239 | ALA  | CB-CA-C   | 5.93  | 119.00      | 110.10   |
| 1   | L     | 379 | ILE  | CB-CA-C   | -5.93 | 99.74       | 111.60   |
| 1   | G     | 58  | ARG  | NE-CZ-NH1 | 5.93  | 123.26      | 120.30   |
| 1   | N     | 379 | ILE  | CB-CA-C   | -5.93 | 99.75       | 111.60   |
| 1   | C     | 34  | LYS  | CB-CA-C   | 5.92  | 122.25      | 110.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | L     | 368 | ARG  | NE-CZ-NH1 | 5.92  | 123.26      | 120.30   |
| 1   | B     | 34  | LYS  | CB-CA-C   | 5.91  | 122.23      | 110.40   |
| 1   | N     | 239 | ALA  | CB-CA-C   | 5.91  | 118.97      | 110.10   |
| 1   | H     | 239 | ALA  | CB-CA-C   | 5.91  | 118.97      | 110.10   |
| 1   | J     | 239 | ALA  | CB-CA-C   | 5.90  | 118.95      | 110.10   |
| 1   | H     | 368 | ARG  | NE-CZ-NH1 | 5.89  | 123.24      | 120.30   |
| 1   | I     | 239 | ALA  | CB-CA-C   | 5.89  | 118.93      | 110.10   |
| 1   | N     | 40  | LEU  | CB-CA-C   | -5.88 | 99.02       | 110.20   |
| 1   | K     | 40  | LEU  | CB-CA-C   | -5.88 | 99.02       | 110.20   |
| 1   | N     | 368 | ARG  | NE-CZ-NH1 | 5.88  | 123.24      | 120.30   |
| 1   | M     | 368 | ARG  | NE-CZ-NH1 | 5.88  | 123.24      | 120.30   |
| 1   | L     | 40  | LEU  | CB-CA-C   | -5.88 | 99.04       | 110.20   |
| 1   | H     | 40  | LEU  | CB-CA-C   | -5.87 | 99.04       | 110.20   |
| 1   | I     | 40  | LEU  | CB-CA-C   | -5.87 | 99.05       | 110.20   |
| 1   | M     | 40  | LEU  | CB-CA-C   | -5.87 | 99.05       | 110.20   |
| 1   | J     | 40  | LEU  | CB-CA-C   | -5.87 | 99.05       | 110.20   |
| 1   | K     | 368 | ARG  | NE-CZ-NH1 | 5.87  | 123.23      | 120.30   |
| 1   | A     | 40  | LEU  | CB-CA-C   | -5.86 | 99.07       | 110.20   |
| 1   | E     | 40  | LEU  | CB-CA-C   | -5.86 | 99.07       | 110.20   |
| 1   | F     | 11  | ASP  | O-C-N     | -5.86 | 113.33      | 122.70   |
| 1   | C     | 11  | ASP  | O-C-N     | -5.85 | 113.33      | 122.70   |
| 1   | B     | 40  | LEU  | CB-CA-C   | -5.85 | 99.08       | 110.20   |
| 1   | F     | 58  | ARG  | NE-CZ-NH1 | 5.85  | 123.23      | 120.30   |
| 1   | G     | 40  | LEU  | CB-CA-C   | -5.85 | 99.08       | 110.20   |
| 1   | N     | 208 | PRO  | N-CA-CB   | -5.85 | 96.16       | 102.60   |
| 1   | B     | 11  | ASP  | O-C-N     | -5.85 | 113.34      | 122.70   |
| 1   | C     | 40  | LEU  | CB-CA-C   | -5.85 | 99.09       | 110.20   |
| 1   | J     | 13  | ARG  | NE-CZ-NH1 | 5.85  | 123.22      | 120.30   |
| 1   | A     | 11  | ASP  | O-C-N     | -5.84 | 113.35      | 122.70   |
| 1   | D     | 40  | LEU  | CB-CA-C   | -5.84 | 99.09       | 110.20   |
| 1   | G     | 11  | ASP  | O-C-N     | -5.84 | 113.35      | 122.70   |
| 1   | D     | 11  | ASP  | O-C-N     | -5.84 | 113.35      | 122.70   |
| 1   | E     | 11  | ASP  | O-C-N     | -5.84 | 113.35      | 122.70   |
| 1   | E     | 58  | ARG  | NE-CZ-NH1 | 5.84  | 123.22      | 120.30   |
| 1   | F     | 40  | LEU  | CB-CA-C   | -5.84 | 99.11       | 110.20   |
| 1   | K     | 197 | ARG  | NE-CZ-NH1 | 5.83  | 123.22      | 120.30   |
| 1   | C     | 58  | ARG  | NE-CZ-NH1 | 5.83  | 123.21      | 120.30   |
| 1   | N     | 6   | VAL  | CB-CA-C   | -5.82 | 100.34      | 111.40   |
| 1   | I     | 6   | VAL  | CB-CA-C   | -5.82 | 100.35      | 111.40   |
| 1   | F     | 457 | ASN  | CB-CA-C   | 5.81  | 122.03      | 110.40   |
| 1   | C     | 452 | ARG  | NE-CZ-NH1 | 5.81  | 123.20      | 120.30   |
| 1   | H     | 6   | VAL  | CB-CA-C   | -5.81 | 100.36      | 111.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 457 | ASN  | CB-CA-C   | 5.81  | 122.02      | 110.40   |
| 1   | L     | 6   | VAL  | CB-CA-C   | -5.81 | 100.37      | 111.40   |
| 1   | E     | 197 | ARG  | CB-CA-C   | 5.81  | 122.01      | 110.40   |
| 1   | K     | 6   | VAL  | CB-CA-C   | -5.80 | 100.37      | 111.40   |
| 1   | M     | 6   | VAL  | CB-CA-C   | -5.80 | 100.37      | 111.40   |
| 1   | J     | 6   | VAL  | CB-CA-C   | -5.80 | 100.38      | 111.40   |
| 1   | J     | 401 | HIS  | CA-CB-CG  | 5.80  | 123.46      | 113.60   |
| 1   | L     | 401 | HIS  | CA-CB-CG  | 5.80  | 123.46      | 113.60   |
| 1   | H     | 334 | ASP  | CB-CA-C   | 5.80  | 122.00      | 110.40   |
| 1   | D     | 197 | ARG  | CB-CA-C   | 5.80  | 122.00      | 110.40   |
| 1   | G     | 197 | ARG  | CB-CA-C   | 5.80  | 122.00      | 110.40   |
| 1   | K     | 334 | ASP  | CB-CA-C   | 5.80  | 122.00      | 110.40   |
| 1   | A     | 197 | ARG  | CB-CA-C   | 5.80  | 122.00      | 110.40   |
| 1   | K     | 401 | HIS  | CA-CB-CG  | 5.80  | 123.45      | 113.60   |
| 1   | C     | 197 | ARG  | CB-CA-C   | 5.79  | 121.98      | 110.40   |
| 1   | N     | 401 | HIS  | CA-CB-CG  | 5.79  | 123.44      | 113.60   |
| 1   | J     | 334 | ASP  | CB-CA-C   | 5.79  | 121.98      | 110.40   |
| 1   | M     | 401 | HIS  | CA-CB-CG  | 5.79  | 123.44      | 113.60   |
| 1   | B     | 197 | ARG  | CB-CA-C   | 5.79  | 121.97      | 110.40   |
| 1   | I     | 401 | HIS  | CA-CB-CG  | 5.79  | 123.44      | 113.60   |
| 1   | F     | 197 | ARG  | CB-CA-C   | 5.78  | 121.97      | 110.40   |
| 1   | H     | 401 | HIS  | CA-CB-CG  | 5.78  | 123.43      | 113.60   |
| 1   | I     | 334 | ASP  | CB-CA-C   | 5.78  | 121.97      | 110.40   |
| 1   | G     | 452 | ARG  | NE-CZ-NH1 | 5.78  | 123.19      | 120.30   |
| 1   | L     | 334 | ASP  | CB-CA-C   | 5.78  | 121.96      | 110.40   |
| 1   | M     | 334 | ASP  | CB-CA-C   | 5.78  | 121.96      | 110.40   |
| 1   | G     | 296 | THR  | CA-CB-CG2 | -5.77 | 104.33      | 112.40   |
| 1   | N     | 334 | ASP  | CB-CA-C   | 5.76  | 121.93      | 110.40   |
| 1   | F     | 452 | ARG  | NE-CZ-NH1 | 5.76  | 123.18      | 120.30   |
| 1   | C     | 296 | THR  | CA-CB-CG2 | -5.76 | 104.34      | 112.40   |
| 1   | E     | 296 | THR  | CA-CB-CG2 | -5.76 | 104.34      | 112.40   |
| 1   | L     | 520 | MET  | N-CA-CB   | 5.76  | 120.96      | 110.60   |
| 1   | M     | 520 | MET  | N-CA-CB   | 5.75  | 120.95      | 110.60   |
| 1   | E     | 452 | ARG  | NE-CZ-NH1 | 5.75  | 123.17      | 120.30   |
| 1   | A     | 296 | THR  | CA-CB-CG2 | -5.75 | 104.36      | 112.40   |
| 1   | N     | 520 | MET  | N-CA-CB   | 5.74  | 120.94      | 110.60   |
| 1   | A     | 452 | ARG  | NE-CZ-NH1 | 5.74  | 123.17      | 120.30   |
| 1   | H     | 520 | MET  | N-CA-CB   | 5.74  | 120.93      | 110.60   |
| 1   | D     | 58  | ARG  | NE-CZ-NH1 | 5.74  | 123.17      | 120.30   |
| 1   | J     | 520 | MET  | N-CA-CB   | 5.74  | 120.92      | 110.60   |
| 1   | D     | 296 | THR  | CA-CB-CG2 | -5.73 | 104.38      | 112.40   |
| 1   | I     | 520 | MET  | N-CA-CB   | 5.73  | 120.91      | 110.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | K     | 520 | MET  | N-CA-CB   | 5.73  | 120.91      | 110.60   |
| 1   | C     | 445 | ARG  | NE-CZ-NH1 | 5.72  | 123.16      | 120.30   |
| 1   | A     | 277 | LYS  | CB-CA-C   | -5.71 | 98.97       | 110.40   |
| 1   | F     | 296 | THR  | CA-CB-CG2 | -5.71 | 104.40      | 112.40   |
| 1   | G     | 445 | ARG  | NE-CZ-NH1 | 5.71  | 123.16      | 120.30   |
| 1   | B     | 58  | ARG  | NE-CZ-NH1 | 5.71  | 123.16      | 120.30   |
| 1   | B     | 277 | LYS  | CB-CA-C   | -5.71 | 98.98       | 110.40   |
| 1   | B     | 296 | THR  | CA-CB-CG2 | -5.71 | 104.40      | 112.40   |
| 1   | D     | 452 | ARG  | NE-CZ-NH1 | 5.71  | 123.16      | 120.30   |
| 1   | E     | 277 | LYS  | CB-CA-C   | -5.71 | 98.98       | 110.40   |
| 1   | F     | 445 | ARG  | NE-CZ-NH1 | 5.71  | 123.16      | 120.30   |
| 1   | C     | 277 | LYS  | CB-CA-C   | -5.71 | 98.98       | 110.40   |
| 1   | G     | 277 | LYS  | CB-CA-C   | -5.71 | 98.99       | 110.40   |
| 1   | D     | 277 | LYS  | CB-CA-C   | -5.70 | 99.00       | 110.40   |
| 1   | J     | 87  | ASP  | CB-CG-OD2 | 5.70  | 123.43      | 118.30   |
| 1   | M     | 197 | ARG  | NE-CZ-NH2 | -5.70 | 117.45      | 120.30   |
| 1   | F     | 277 | LYS  | CB-CA-C   | -5.70 | 99.01       | 110.40   |
| 1   | D     | 411 | VAL  | CB-CA-C   | -5.69 | 100.60      | 111.40   |
| 1   | F     | 80  | LYS  | CB-CA-C   | 5.68  | 121.77      | 110.40   |
| 1   | F     | 411 | VAL  | CB-CA-C   | -5.68 | 100.61      | 111.40   |
| 1   | G     | 80  | LYS  | CB-CA-C   | 5.68  | 121.77      | 110.40   |
| 1   | G     | 411 | VAL  | CB-CA-C   | -5.68 | 100.60      | 111.40   |
| 1   | J     | 228 | SER  | N-CA-CB   | 5.68  | 119.02      | 110.50   |
| 1   | H     | 87  | ASP  | CB-CG-OD2 | 5.68  | 123.41      | 118.30   |
| 1   | A     | 80  | LYS  | CB-CA-C   | 5.68  | 121.76      | 110.40   |
| 1   | A     | 411 | VAL  | CB-CA-C   | -5.68 | 100.61      | 111.40   |
| 1   | E     | 80  | LYS  | CB-CA-C   | 5.68  | 121.76      | 110.40   |
| 1   | B     | 80  | LYS  | CB-CA-C   | 5.67  | 121.75      | 110.40   |
| 1   | C     | 80  | LYS  | CB-CA-C   | 5.67  | 121.75      | 110.40   |
| 1   | E     | 411 | VAL  | CB-CA-C   | -5.67 | 100.62      | 111.40   |
| 1   | A     | 445 | ARG  | NE-CZ-NH1 | 5.67  | 123.14      | 120.30   |
| 1   | B     | 452 | ARG  | NE-CZ-NH1 | 5.67  | 123.14      | 120.30   |
| 1   | B     | 411 | VAL  | CB-CA-C   | -5.67 | 100.63      | 111.40   |
| 1   | B     | 445 | ARG  | NE-CZ-NH1 | 5.67  | 123.14      | 120.30   |
| 1   | D     | 445 | ARG  | NE-CZ-NH1 | 5.67  | 123.14      | 120.30   |
| 1   | G     | 457 | ASN  | CB-CA-C   | 5.67  | 121.74      | 110.40   |
| 1   | D     | 80  | LYS  | CB-CA-C   | 5.67  | 121.74      | 110.40   |
| 1   | C     | 411 | VAL  | CB-CA-C   | -5.67 | 100.63      | 111.40   |
| 1   | K     | 197 | ARG  | CB-CA-C   | 5.67  | 121.73      | 110.40   |
| 1   | M     | 197 | ARG  | CB-CA-C   | 5.66  | 121.73      | 110.40   |
| 1   | I     | 87  | ASP  | CB-CG-OD2 | 5.66  | 123.39      | 118.30   |
| 1   | A     | 457 | ASN  | CB-CA-C   | 5.66  | 121.72      | 110.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 457 | ASN  | CB-CA-C    | 5.66  | 121.72      | 110.40   |
| 1   | K     | 87  | ASP  | CB-CG-OD2  | 5.66  | 123.39      | 118.30   |
| 1   | N     | 197 | ARG  | CB-CA-C    | 5.66  | 121.72      | 110.40   |
| 1   | H     | 236 | VAL  | CA-CB-CG1  | -5.66 | 102.42      | 110.90   |
| 1   | E     | 457 | ASN  | CB-CA-C    | 5.65  | 121.71      | 110.40   |
| 1   | J     | 236 | VAL  | CA-CB-CG1  | -5.65 | 102.42      | 110.90   |
| 1   | E     | 445 | ARG  | NE-CZ-NH1  | 5.65  | 123.12      | 120.30   |
| 1   | G     | 200 | LEU  | CA-CB-CG   | -5.65 | 102.30      | 115.30   |
| 1   | L     | 236 | VAL  | CA-CB-CG1  | -5.65 | 102.43      | 110.90   |
| 1   | M     | 236 | VAL  | CA-CB-CG1  | -5.65 | 102.42      | 110.90   |
| 1   | J     | 197 | ARG  | CB-CA-C    | 5.65  | 121.70      | 110.40   |
| 1   | I     | 87  | ASP  | OD1-CG-OD2 | -5.65 | 112.57      | 123.30   |
| 1   | H     | 197 | ARG  | CB-CA-C    | 5.65  | 121.69      | 110.40   |
| 1   | L     | 87  | ASP  | OD1-CG-OD2 | -5.65 | 112.57      | 123.30   |
| 1   | M     | 87  | ASP  | CB-CG-OD2  | 5.65  | 123.38      | 118.30   |
| 1   | H     | 87  | ASP  | OD1-CG-OD2 | -5.64 | 112.58      | 123.30   |
| 1   | I     | 236 | VAL  | CA-CB-CG1  | -5.64 | 102.44      | 110.90   |
| 1   | L     | 87  | ASP  | CB-CG-OD2  | 5.64  | 123.38      | 118.30   |
| 1   | L     | 197 | ARG  | CB-CA-C    | 5.64  | 121.68      | 110.40   |
| 1   | K     | 311 | LYS  | CB-CA-C    | 5.64  | 121.68      | 110.40   |
| 1   | H     | 368 | ARG  | CB-CA-C    | -5.63 | 99.13       | 110.40   |
| 1   | J     | 87  | ASP  | OD1-CG-OD2 | -5.63 | 112.60      | 123.30   |
| 1   | I     | 197 | ARG  | CB-CA-C    | 5.63  | 121.66      | 110.40   |
| 1   | K     | 87  | ASP  | OD1-CG-OD2 | -5.63 | 112.60      | 123.30   |
| 1   | B     | 457 | ASN  | CB-CA-C    | 5.63  | 121.66      | 110.40   |
| 1   | K     | 368 | ARG  | CB-CA-C    | -5.63 | 99.14       | 110.40   |
| 1   | M     | 368 | ARG  | CB-CA-C    | -5.63 | 99.14       | 110.40   |
| 1   | N     | 368 | ARG  | CB-CA-C    | -5.63 | 99.15       | 110.40   |
| 1   | H     | 311 | LYS  | CB-CA-C    | 5.62  | 121.65      | 110.40   |
| 1   | I     | 36  | ARG  | N-CA-CB    | 5.62  | 120.72      | 110.60   |
| 1   | M     | 87  | ASP  | OD1-CG-OD2 | -5.62 | 112.61      | 123.30   |
| 1   | L     | 368 | ARG  | CB-CA-C    | -5.62 | 99.17       | 110.40   |
| 1   | K     | 236 | VAL  | CA-CB-CG1  | -5.62 | 102.48      | 110.90   |
| 1   | H     | 197 | ARG  | NE-CZ-NH2  | -5.61 | 117.49      | 120.30   |
| 1   | N     | 87  | ASP  | OD1-CG-OD2 | -5.61 | 112.64      | 123.30   |
| 1   | N     | 87  | ASP  | CB-CG-OD2  | 5.61  | 123.35      | 118.30   |
| 1   | K     | 36  | ARG  | N-CA-CB    | 5.61  | 120.69      | 110.60   |
| 1   | L     | 13  | ARG  | NE-CZ-NH1  | 5.60  | 123.10      | 120.30   |
| 1   | N     | 236 | VAL  | CA-CB-CG1  | -5.60 | 102.50      | 110.90   |
| 1   | J     | 368 | ARG  | CB-CA-C    | -5.60 | 99.20       | 110.40   |
| 1   | J     | 445 | ARG  | NE-CZ-NH1  | 5.60  | 123.10      | 120.30   |
| 1   | I     | 368 | ARG  | CB-CA-C    | -5.59 | 99.22       | 110.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | J     | 36  | ARG  | N-CA-CB    | 5.59  | 120.66      | 110.60   |
| 1   | H     | 36  | ARG  | N-CA-CB    | 5.59  | 120.65      | 110.60   |
| 1   | I     | 445 | ARG  | NE-CZ-NH1  | 5.57  | 123.09      | 120.30   |
| 1   | N     | 36  | ARG  | N-CA-CB    | 5.57  | 120.63      | 110.60   |
| 1   | K     | 239 | ALA  | CB-CA-C    | 5.57  | 118.45      | 110.10   |
| 1   | L     | 36  | ARG  | N-CA-CB    | 5.57  | 120.62      | 110.60   |
| 1   | L     | 87  | ASP  | CB-CG-OD1  | 5.57  | 123.31      | 118.30   |
| 1   | L     | 197 | ARG  | NE-CZ-NH2  | -5.56 | 117.52      | 120.30   |
| 1   | N     | 208 | PRO  | CA-C-O     | -5.55 | 106.87      | 120.20   |
| 1   | M     | 36  | ARG  | N-CA-CB    | 5.55  | 120.59      | 110.60   |
| 1   | N     | 197 | ARG  | NE-CZ-NH2  | -5.55 | 117.53      | 120.30   |
| 1   | M     | 311 | LYS  | CB-CA-C    | 5.54  | 121.49      | 110.40   |
| 1   | L     | 311 | LYS  | CB-CA-C    | 5.54  | 121.48      | 110.40   |
| 1   | D     | 285 | ARG  | NE-CZ-NH2  | -5.54 | 117.53      | 120.30   |
| 1   | I     | 87  | ASP  | CB-CG-OD1  | 5.54  | 123.29      | 118.30   |
| 1   | D     | 87  | ASP  | CB-CG-OD2  | 5.53  | 123.28      | 118.30   |
| 1   | N     | 311 | LYS  | CB-CA-C    | 5.53  | 121.46      | 110.40   |
| 1   | L     | 445 | ARG  | NE-CZ-NH1  | 5.53  | 123.06      | 120.30   |
| 1   | F     | 87  | ASP  | CB-CG-OD2  | 5.52  | 123.27      | 118.30   |
| 1   | D     | 87  | ASP  | OD1-CG-OD2 | -5.51 | 112.82      | 123.30   |
| 1   | B     | 87  | ASP  | CB-CG-OD1  | 5.51  | 123.26      | 118.30   |
| 1   | N     | 87  | ASP  | CB-CG-OD1  | 5.51  | 123.26      | 118.30   |
| 1   | F     | 87  | ASP  | OD1-CG-OD2 | -5.51 | 112.83      | 123.30   |
| 1   | E     | 87  | ASP  | CB-CG-OD1  | 5.51  | 123.26      | 118.30   |
| 1   | K     | 87  | ASP  | CB-CG-OD1  | 5.50  | 123.25      | 118.30   |
| 1   | E     | 46  | ALA  | N-CA-CB    | -5.50 | 102.40      | 110.10   |
| 1   | B     | 285 | ARG  | NE-CZ-NH2  | -5.50 | 117.55      | 120.30   |
| 1   | E     | 87  | ASP  | OD1-CG-OD2 | -5.50 | 112.85      | 123.30   |
| 1   | D     | 46  | ALA  | N-CA-CB    | -5.50 | 102.41      | 110.10   |
| 1   | F     | 46  | ALA  | N-CA-CB    | -5.49 | 102.41      | 110.10   |
| 1   | H     | 87  | ASP  | CB-CG-OD1  | 5.49  | 123.24      | 118.30   |
| 1   | B     | 46  | ALA  | N-CA-CB    | -5.49 | 102.41      | 110.10   |
| 1   | M     | 87  | ASP  | CB-CG-OD1  | 5.49  | 123.24      | 118.30   |
| 1   | A     | 46  | ALA  | N-CA-CB    | -5.49 | 102.42      | 110.10   |
| 1   | J     | 311 | LYS  | CB-CA-C    | 5.49  | 121.38      | 110.40   |
| 1   | C     | 46  | ALA  | N-CA-CB    | -5.48 | 102.43      | 110.10   |
| 1   | F     | 285 | ARG  | NE-CZ-NH2  | -5.48 | 117.56      | 120.30   |
| 1   | G     | 46  | ALA  | N-CA-CB    | -5.48 | 102.43      | 110.10   |
| 1   | H     | 228 | SER  | N-CA-CB    | 5.48  | 118.72      | 110.50   |
| 1   | J     | 87  | ASP  | CB-CG-OD1  | 5.48  | 123.23      | 118.30   |
| 1   | H     | 239 | ALA  | N-CA-CB    | -5.47 | 102.44      | 110.10   |
| 1   | I     | 311 | LYS  | CB-CA-C    | 5.47  | 121.35      | 110.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | E     | 156 | GLU  | CB-CA-C    | -5.46 | 99.49       | 110.40   |
| 1   | E     | 251 | ALA  | CB-CA-C    | -5.46 | 101.92      | 110.10   |
| 1   | A     | 156 | GLU  | CB-CA-C    | -5.45 | 99.50       | 110.40   |
| 1   | C     | 156 | GLU  | CB-CA-C    | -5.45 | 99.50       | 110.40   |
| 1   | G     | 251 | ALA  | CB-CA-C    | -5.45 | 101.92      | 110.10   |
| 1   | C     | 87  | ASP  | OD1-CG-OD2 | -5.45 | 112.95      | 123.30   |
| 1   | G     | 156 | GLU  | CB-CA-C    | -5.45 | 99.50       | 110.40   |
| 1   | B     | 87  | ASP  | OD1-CG-OD2 | -5.45 | 112.95      | 123.30   |
| 1   | G     | 87  | ASP  | OD1-CG-OD2 | -5.44 | 112.96      | 123.30   |
| 1   | C     | 251 | ALA  | CB-CA-C    | -5.44 | 101.94      | 110.10   |
| 1   | D     | 251 | ALA  | CB-CA-C    | -5.44 | 101.94      | 110.10   |
| 1   | G     | 87  | ASP  | CB-CG-OD1  | 5.44  | 123.19      | 118.30   |
| 1   | A     | 87  | ASP  | OD1-CG-OD2 | -5.44 | 112.97      | 123.30   |
| 1   | K     | 13  | ARG  | NE-CZ-NH1  | 5.43  | 123.02      | 120.30   |
| 1   | C     | 87  | ASP  | CB-CG-OD1  | 5.43  | 123.19      | 118.30   |
| 1   | F     | 156 | GLU  | CB-CA-C    | -5.43 | 99.53       | 110.40   |
| 1   | I     | 239 | ALA  | N-CA-CB    | -5.43 | 102.50      | 110.10   |
| 1   | F     | 251 | ALA  | CB-CA-C    | -5.43 | 101.95      | 110.10   |
| 1   | L     | 239 | ALA  | N-CA-CB    | -5.43 | 102.50      | 110.10   |
| 1   | A     | 251 | ALA  | CB-CA-C    | -5.43 | 101.96      | 110.10   |
| 1   | K     | 197 | ARG  | NE-CZ-NH2  | -5.43 | 117.58      | 120.30   |
| 1   | A     | 285 | ARG  | NE-CZ-NH2  | -5.42 | 117.59      | 120.30   |
| 1   | B     | 251 | ALA  | CB-CA-C    | -5.42 | 101.96      | 110.10   |
| 1   | D     | 87  | ASP  | CB-CG-OD1  | 5.42  | 123.18      | 118.30   |
| 1   | G     | 285 | ARG  | NE-CZ-NH2  | -5.42 | 117.59      | 120.30   |
| 1   | B     | 18  | ARG  | CD-NE-CZ   | 5.42  | 131.19      | 123.60   |
| 1   | E     | 87  | ASP  | CB-CG-OD2  | 5.42  | 123.18      | 118.30   |
| 1   | F     | 345 | ARG  | NE-CZ-NH2  | -5.42 | 117.59      | 120.30   |
| 1   | N     | 445 | ARG  | NE-CZ-NH1  | 5.42  | 123.01      | 120.30   |
| 1   | C     | 18  | ARG  | CD-NE-CZ   | 5.42  | 131.18      | 123.60   |
| 1   | C     | 285 | ARG  | NE-CZ-NH2  | -5.42 | 117.59      | 120.30   |
| 1   | D     | 156 | GLU  | CB-CA-C    | -5.42 | 99.57       | 110.40   |
| 1   | E     | 18  | ARG  | CD-NE-CZ   | 5.41  | 131.18      | 123.60   |
| 1   | A     | 18  | ARG  | CD-NE-CZ   | 5.41  | 131.18      | 123.60   |
| 1   | F     | 140 | ASP  | N-CA-CB    | -5.41 | 100.87      | 110.60   |
| 1   | J     | 239 | ALA  | N-CA-CB    | -5.41 | 102.53      | 110.10   |
| 1   | B     | 156 | GLU  | CB-CA-C    | -5.41 | 99.59       | 110.40   |
| 1   | F     | 87  | ASP  | CB-CG-OD1  | 5.41  | 123.17      | 118.30   |
| 1   | M     | 239 | ALA  | N-CA-CB    | -5.41 | 102.53      | 110.10   |
| 1   | B     | 140 | ASP  | N-CA-CB    | -5.40 | 100.88      | 110.60   |
| 1   | C     | 140 | ASP  | N-CA-CB    | -5.40 | 100.88      | 110.60   |
| 1   | A     | 140 | ASP  | N-CA-CB    | -5.40 | 100.88      | 110.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | H     | 499 | VAL  | CG1-CB-CG2 | -5.40 | 102.26      | 110.90   |
| 1   | A     | 87  | ASP  | CB-CG-OD1  | 5.40  | 123.16      | 118.30   |
| 1   | A     | 345 | ARG  | NE-CZ-NH2  | -5.40 | 117.60      | 120.30   |
| 1   | B     | 345 | ARG  | NE-CZ-NH2  | -5.40 | 117.60      | 120.30   |
| 1   | G     | 18  | ARG  | CD-NE-CZ   | 5.40  | 131.16      | 123.60   |
| 1   | K     | 228 | SER  | N-CA-CB    | 5.40  | 118.59      | 110.50   |
| 1   | N     | 239 | ALA  | N-CA-CB    | -5.40 | 102.54      | 110.10   |
| 1   | D     | 18  | ARG  | CD-NE-CZ   | 5.39  | 131.15      | 123.60   |
| 1   | E     | 140 | ASP  | N-CA-CB    | -5.39 | 100.89      | 110.60   |
| 1   | G     | 200 | LEU  | CD1-CG-CD2 | 5.39  | 126.68      | 110.50   |
| 1   | K     | 499 | VAL  | CG1-CB-CG2 | -5.39 | 102.27      | 110.90   |
| 1   | M     | 499 | VAL  | CG1-CB-CG2 | -5.39 | 102.27      | 110.90   |
| 1   | D     | 140 | ASP  | N-CA-CB    | -5.39 | 100.89      | 110.60   |
| 1   | F     | 18  | ARG  | CD-NE-CZ   | 5.39  | 131.15      | 123.60   |
| 1   | E     | 285 | ARG  | NE-CZ-NH2  | -5.39 | 117.61      | 120.30   |
| 1   | N     | 296 | THR  | N-CA-CB    | 5.39  | 120.54      | 110.30   |
| 1   | B     | 254 | VAL  | CB-CA-C    | -5.38 | 101.17      | 111.40   |
| 1   | N     | 411 | VAL  | CB-CA-C    | -5.38 | 101.17      | 111.40   |
| 1   | G     | 140 | ASP  | N-CA-CB    | -5.38 | 100.91      | 110.60   |
| 1   | I     | 411 | VAL  | CB-CA-C    | -5.38 | 101.18      | 111.40   |
| 1   | L     | 296 | THR  | N-CA-CB    | 5.38  | 120.52      | 110.30   |
| 1   | M     | 445 | ARG  | NE-CZ-NH1  | 5.38  | 122.99      | 120.30   |
| 1   | H     | 296 | THR  | N-CA-CB    | 5.38  | 120.52      | 110.30   |
| 1   | J     | 296 | THR  | N-CA-CB    | 5.38  | 120.52      | 110.30   |
| 1   | K     | 296 | THR  | N-CA-CB    | 5.38  | 120.51      | 110.30   |
| 1   | M     | 296 | THR  | N-CA-CB    | 5.38  | 120.51      | 110.30   |
| 1   | A     | 254 | VAL  | CB-CA-C    | -5.37 | 101.19      | 111.40   |
| 1   | D     | 401 | HIS  | CA-CB-CG   | 5.37  | 122.74      | 113.60   |
| 1   | I     | 296 | THR  | N-CA-CB    | 5.37  | 120.51      | 110.30   |
| 1   | A     | 87  | ASP  | CB-CG-OD2  | 5.37  | 123.13      | 118.30   |
| 1   | E     | 254 | VAL  | CB-CA-C    | -5.37 | 101.20      | 111.40   |
| 1   | C     | 254 | VAL  | CB-CA-C    | -5.37 | 101.20      | 111.40   |
| 1   | L     | 499 | VAL  | CG1-CB-CG2 | -5.37 | 102.31      | 110.90   |
| 1   | C     | 87  | ASP  | CB-CG-OD2  | 5.37  | 123.13      | 118.30   |
| 1   | G     | 254 | VAL  | CB-CA-C    | -5.36 | 101.21      | 111.40   |
| 1   | J     | 188 | ASP  | CB-CG-OD1  | 5.36  | 123.13      | 118.30   |
| 1   | L     | 188 | ASP  | CB-CG-OD1  | 5.36  | 123.12      | 118.30   |
| 1   | D     | 254 | VAL  | CB-CA-C    | -5.36 | 101.21      | 111.40   |
| 1   | F     | 254 | VAL  | CB-CA-C    | -5.36 | 101.22      | 111.40   |
| 1   | F     | 401 | HIS  | CA-CB-CG   | 5.36  | 122.71      | 113.60   |
| 1   | J     | 499 | VAL  | CG1-CB-CG2 | -5.36 | 102.33      | 110.90   |
| 1   | H     | 445 | ARG  | NE-CZ-NH1  | 5.36  | 122.98      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | K     | 153 | ASN  | CA-CB-CG   | 5.36  | 125.18      | 113.40   |
| 1   | B     | 401 | HIS  | CA-CB-CG   | 5.35  | 122.70      | 113.60   |
| 1   | G     | 87  | ASP  | CB-CG-OD2  | 5.35  | 123.12      | 118.30   |
| 1   | D     | 345 | ARG  | NE-CZ-NH2  | -5.35 | 117.62      | 120.30   |
| 1   | D     | 381 | VAL  | CA-CB-CG2  | -5.35 | 102.87      | 110.90   |
| 1   | E     | 401 | HIS  | CA-CB-CG   | 5.35  | 122.70      | 113.60   |
| 1   | M     | 231 | ARG  | NE-CZ-NH1  | 5.35  | 122.98      | 120.30   |
| 1   | N     | 228 | SER  | N-CA-CB    | 5.35  | 118.53      | 110.50   |
| 1   | I     | 153 | ASN  | CA-CB-CG   | 5.35  | 125.17      | 113.40   |
| 1   | L     | 153 | ASN  | CA-CB-CG   | 5.35  | 125.17      | 113.40   |
| 1   | A     | 401 | HIS  | CA-CB-CG   | 5.35  | 122.69      | 113.60   |
| 1   | B     | 381 | VAL  | CA-CB-CG2  | -5.35 | 102.88      | 110.90   |
| 1   | C     | 381 | VAL  | CA-CB-CG2  | -5.35 | 102.88      | 110.90   |
| 1   | E     | 345 | ARG  | NE-CZ-NH2  | -5.35 | 117.63      | 120.30   |
| 1   | H     | 153 | ASN  | CA-CB-CG   | 5.35  | 125.16      | 113.40   |
| 1   | A     | 272 | LYS  | N-CA-CB    | -5.34 | 100.99      | 110.60   |
| 1   | I     | 499 | VAL  | CG1-CB-CG2 | -5.34 | 102.35      | 110.90   |
| 1   | C     | 401 | HIS  | CA-CB-CG   | 5.34  | 122.67      | 113.60   |
| 1   | J     | 153 | ASN  | CA-CB-CG   | 5.34  | 125.14      | 113.40   |
| 1   | E     | 272 | LYS  | N-CA-CB    | -5.33 | 101.00      | 110.60   |
| 1   | G     | 401 | HIS  | CA-CB-CG   | 5.33  | 122.67      | 113.60   |
| 1   | F     | 272 | LYS  | N-CA-CB    | -5.33 | 101.00      | 110.60   |
| 1   | G     | 272 | LYS  | N-CA-CB    | -5.33 | 101.00      | 110.60   |
| 1   | H     | 188 | ASP  | CB-CG-OD1  | 5.33  | 123.10      | 118.30   |
| 1   | K     | 445 | ARG  | NE-CZ-NH1  | 5.33  | 122.97      | 120.30   |
| 1   | M     | 153 | ASN  | CA-CB-CG   | 5.33  | 125.13      | 113.40   |
| 1   | D     | 272 | LYS  | N-CA-CB    | -5.33 | 101.01      | 110.60   |
| 1   | N     | 499 | VAL  | CG1-CB-CG2 | -5.33 | 102.38      | 110.90   |
| 1   | N     | 153 | ASN  | CA-CB-CG   | 5.33  | 125.12      | 113.40   |
| 1   | A     | 381 | VAL  | CA-CB-CG2  | -5.33 | 102.91      | 110.90   |
| 1   | B     | 272 | LYS  | N-CA-CB    | -5.33 | 101.02      | 110.60   |
| 1   | E     | 381 | VAL  | CA-CB-CG2  | -5.33 | 102.91      | 110.90   |
| 1   | G     | 345 | ARG  | NE-CZ-NH2  | -5.32 | 117.64      | 120.30   |
| 1   | I     | 188 | ASP  | CB-CG-OD1  | 5.32  | 123.09      | 118.30   |
| 1   | C     | 345 | ARG  | NE-CZ-NH2  | -5.32 | 117.64      | 120.30   |
| 1   | C     | 272 | LYS  | N-CA-CB    | -5.32 | 101.03      | 110.60   |
| 1   | K     | 188 | ASP  | CB-CG-OD1  | 5.32  | 123.09      | 118.30   |
| 1   | N     | 188 | ASP  | CB-CG-OD1  | 5.32  | 123.08      | 118.30   |
| 1   | F     | 381 | VAL  | CA-CB-CG2  | -5.31 | 102.93      | 110.90   |
| 1   | G     | 381 | VAL  | CA-CB-CG2  | -5.31 | 102.93      | 110.90   |
| 1   | I     | 228 | SER  | N-CA-CB    | 5.31  | 118.46      | 110.50   |
| 1   | H     | 310 | GLU  | CA-CB-CG   | 5.30  | 125.06      | 113.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | I     | 13  | ARG  | NE-CZ-NH1  | 5.30  | 122.95      | 120.30   |
| 1   | K     | 310 | GLU  | CA-CB-CG   | 5.30  | 125.06      | 113.40   |
| 1   | G     | 473 | ASP  | N-CA-CB    | 5.30  | 120.14      | 110.60   |
| 1   | C     | 359 | ASP  | CA-CB-CG   | -5.30 | 101.75      | 113.40   |
| 1   | G     | 359 | ASP  | CA-CB-CG   | -5.30 | 101.75      | 113.40   |
| 1   | K     | 239 | ALA  | N-CA-CB    | -5.29 | 102.69      | 110.10   |
| 1   | A     | 473 | ASP  | N-CA-CB    | 5.29  | 120.12      | 110.60   |
| 1   | F     | 359 | ASP  | CA-CB-CG   | -5.29 | 101.77      | 113.40   |
| 1   | F     | 473 | ASP  | N-CA-CB    | 5.29  | 120.11      | 110.60   |
| 1   | L     | 254 | VAL  | CG1-CB-CG2 | -5.29 | 102.44      | 110.90   |
| 1   | A     | 359 | ASP  | CA-CB-CG   | -5.28 | 101.78      | 113.40   |
| 1   | B     | 473 | ASP  | N-CA-CB    | 5.28  | 120.11      | 110.60   |
| 1   | D     | 359 | ASP  | CA-CB-CG   | -5.28 | 101.78      | 113.40   |
| 1   | E     | 359 | ASP  | CA-CB-CG   | -5.28 | 101.78      | 113.40   |
| 1   | N     | 52  | ASP  | CA-CB-CG   | -5.28 | 101.78      | 113.40   |
| 1   | B     | 359 | ASP  | CA-CB-CG   | -5.28 | 101.78      | 113.40   |
| 1   | D     | 473 | ASP  | N-CA-CB    | 5.28  | 120.10      | 110.60   |
| 1   | H     | 317 | LEU  | CB-CA-C    | -5.28 | 100.17      | 110.20   |
| 1   | K     | 52  | ASP  | CA-CB-CG   | -5.28 | 101.78      | 113.40   |
| 1   | M     | 52  | ASP  | CA-CB-CG   | -5.28 | 101.78      | 113.40   |
| 1   | J     | 317 | LEU  | CB-CA-C    | -5.28 | 100.17      | 110.20   |
| 1   | C     | 473 | ASP  | N-CA-CB    | 5.28  | 120.10      | 110.60   |
| 1   | H     | 52  | ASP  | CA-CB-CG   | -5.28 | 101.79      | 113.40   |
| 1   | E     | 473 | ASP  | N-CA-CB    | 5.28  | 120.10      | 110.60   |
| 1   | G     | 199 | TYR  | O-C-N      | -5.27 | 114.27      | 122.70   |
| 1   | L     | 52  | ASP  | CA-CB-CG   | -5.27 | 101.81      | 113.40   |
| 1   | J     | 52  | ASP  | CA-CB-CG   | -5.26 | 101.82      | 113.40   |
| 1   | N     | 310 | GLU  | CA-CB-CG   | 5.26  | 124.97      | 113.40   |
| 1   | G     | 73  | MET  | CB-CA-C    | -5.26 | 99.88       | 110.40   |
| 1   | I     | 52  | ASP  | CA-CB-CG   | -5.26 | 101.83      | 113.40   |
| 1   | M     | 390 | LYS  | CB-CA-C    | 5.26  | 120.92      | 110.40   |
| 1   | N     | 254 | VAL  | CG1-CB-CG2 | -5.26 | 102.49      | 110.90   |
| 1   | I     | 390 | LYS  | CB-CA-C    | 5.26  | 120.91      | 110.40   |
| 1   | D     | 73  | MET  | CB-CA-C    | -5.25 | 99.89       | 110.40   |
| 1   | A     | 73  | MET  | CB-CA-C    | -5.25 | 99.90       | 110.40   |
| 1   | J     | 390 | LYS  | CB-CA-C    | 5.25  | 120.90      | 110.40   |
| 1   | H     | 254 | VAL  | CG1-CB-CG2 | -5.25 | 102.50      | 110.90   |
| 1   | I     | 317 | LEU  | CB-CA-C    | -5.25 | 100.23      | 110.20   |
| 1   | H     | 390 | LYS  | CB-CA-C    | 5.24  | 120.89      | 110.40   |
| 1   | M     | 254 | VAL  | CG1-CB-CG2 | -5.24 | 102.51      | 110.90   |
| 1   | K     | 317 | LEU  | CB-CA-C    | -5.24 | 100.24      | 110.20   |
| 1   | B     | 73  | MET  | CB-CA-C    | -5.24 | 99.92       | 110.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | E     | 73  | MET  | CB-CA-C    | -5.24 | 99.92       | 110.40   |
| 1   | L     | 390 | LYS  | CB-CA-C    | 5.24  | 120.88      | 110.40   |
| 1   | N     | 390 | LYS  | CB-CA-C    | 5.24  | 120.88      | 110.40   |
| 1   | C     | 73  | MET  | CB-CA-C    | -5.24 | 99.92       | 110.40   |
| 1   | H     | 371 | LYS  | N-CA-CB    | -5.24 | 101.17      | 110.60   |
| 1   | K     | 254 | VAL  | CG1-CB-CG2 | -5.24 | 102.52      | 110.90   |
| 1   | F     | 73  | MET  | CB-CA-C    | -5.24 | 99.93       | 110.40   |
| 1   | K     | 390 | LYS  | CB-CA-C    | 5.24  | 120.87      | 110.40   |
| 1   | M     | 317 | LEU  | CB-CA-C    | -5.24 | 100.25      | 110.20   |
| 1   | K     | 371 | LYS  | N-CA-CB    | -5.23 | 101.18      | 110.60   |
| 1   | M     | 371 | LYS  | N-CA-CB    | -5.23 | 101.18      | 110.60   |
| 1   | M     | 310 | GLU  | CA-CB-CG   | 5.23  | 124.91      | 113.40   |
| 1   | J     | 371 | LYS  | N-CA-CB    | -5.23 | 101.19      | 110.60   |
| 1   | H     | 13  | ARG  | NE-CZ-NH1  | 5.23  | 122.91      | 120.30   |
| 1   | G     | 277 | LYS  | CA-CB-CG   | 5.22  | 124.89      | 113.40   |
| 1   | B     | 230 | ILE  | CA-C-N     | -5.22 | 105.72      | 117.20   |
| 1   | L     | 317 | LEU  | CB-CA-C    | -5.22 | 100.28      | 110.20   |
| 1   | D     | 230 | ILE  | CA-C-N     | -5.22 | 105.72      | 117.20   |
| 1   | N     | 371 | LYS  | N-CA-CB    | -5.22 | 101.21      | 110.60   |
| 1   | L     | 371 | LYS  | N-CA-CB    | -5.21 | 101.21      | 110.60   |
| 1   | B     | 277 | LYS  | CA-CB-CG   | 5.21  | 124.87      | 113.40   |
| 1   | C     | 277 | LYS  | CA-CB-CG   | 5.21  | 124.87      | 113.40   |
| 1   | A     | 230 | ILE  | CA-C-N     | -5.21 | 105.73      | 117.20   |
| 1   | G     | 230 | ILE  | CA-C-N     | -5.21 | 105.73      | 117.20   |
| 1   | F     | 230 | ILE  | CA-C-N     | -5.21 | 105.74      | 117.20   |
| 1   | D     | 277 | LYS  | CA-CB-CG   | 5.21  | 124.86      | 113.40   |
| 1   | I     | 254 | VAL  | CG1-CB-CG2 | -5.21 | 102.56      | 110.90   |
| 1   | A     | 277 | LYS  | CA-CB-CG   | 5.21  | 124.85      | 113.40   |
| 1   | E     | 230 | ILE  | CA-C-N     | -5.21 | 105.74      | 117.20   |
| 1   | F     | 277 | LYS  | CA-CB-CG   | 5.21  | 124.86      | 113.40   |
| 1   | I     | 371 | LYS  | N-CA-CB    | -5.21 | 101.23      | 110.60   |
| 1   | C     | 230 | ILE  | CA-C-N     | -5.20 | 105.76      | 117.20   |
| 1   | N     | 13  | ARG  | NE-CZ-NH1  | 5.20  | 122.90      | 120.30   |
| 1   | E     | 277 | LYS  | CA-CB-CG   | 5.20  | 124.83      | 113.40   |
| 1   | A     | 194 | GLN  | N-CA-CB    | -5.20 | 101.25      | 110.60   |
| 1   | E     | 194 | GLN  | N-CA-CB    | -5.20 | 101.25      | 110.60   |
| 1   | G     | 194 | GLN  | N-CA-CB    | -5.19 | 101.25      | 110.60   |
| 1   | D     | 194 | GLN  | N-CA-CB    | -5.19 | 101.26      | 110.60   |
| 1   | J     | 310 | GLU  | CA-CB-CG   | 5.19  | 124.81      | 113.40   |
| 1   | L     | 255 | GLU  | N-CA-CB    | 5.19  | 119.94      | 110.60   |
| 1   | L     | 310 | GLU  | CA-CB-CG   | 5.19  | 124.81      | 113.40   |
| 1   | B     | 87  | ASP  | CB-CG-OD2  | 5.18  | 122.97      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 194 | GLN  | N-CA-CB    | -5.18 | 101.27      | 110.60   |
| 1   | F     | 194 | GLN  | N-CA-CB    | -5.18 | 101.27      | 110.60   |
| 1   | J     | 254 | VAL  | CG1-CB-CG2 | -5.18 | 102.61      | 110.90   |
| 1   | I     | 389 | MET  | CB-CA-C    | 5.18  | 120.76      | 110.40   |
| 1   | N     | 389 | MET  | CB-CA-C    | 5.17  | 120.75      | 110.40   |
| 1   | J     | 389 | MET  | CB-CA-C    | 5.17  | 120.74      | 110.40   |
| 1   | L     | 389 | MET  | CB-CA-C    | 5.17  | 120.74      | 110.40   |
| 1   | K     | 389 | MET  | CB-CA-C    | 5.17  | 120.73      | 110.40   |
| 1   | M     | 389 | MET  | CB-CA-C    | 5.17  | 120.73      | 110.40   |
| 1   | H     | 389 | MET  | CB-CA-C    | 5.16  | 120.73      | 110.40   |
| 1   | I     | 310 | GLU  | CA-CB-CG   | 5.16  | 124.76      | 113.40   |
| 1   | B     | 153 | ASN  | N-CA-CB    | 5.15  | 119.88      | 110.60   |
| 1   | F     | 324 | VAL  | N-CA-CB    | -5.13 | 100.20      | 111.50   |
| 1   | G     | 324 | VAL  | N-CA-CB    | -5.13 | 100.21      | 111.50   |
| 1   | E     | 324 | VAL  | N-CA-CB    | -5.13 | 100.22      | 111.50   |
| 1   | A     | 324 | VAL  | N-CA-CB    | -5.12 | 100.23      | 111.50   |
| 1   | C     | 304 | GLU  | CB-CA-C    | -5.12 | 100.16      | 110.40   |
| 1   | C     | 324 | VAL  | N-CA-CB    | -5.12 | 100.23      | 111.50   |
| 1   | D     | 324 | VAL  | N-CA-CB    | -5.12 | 100.23      | 111.50   |
| 1   | L     | 228 | SER  | N-CA-CB    | 5.12  | 118.18      | 110.50   |
| 1   | B     | 324 | VAL  | N-CA-CB    | -5.12 | 100.24      | 111.50   |
| 1   | G     | 304 | GLU  | CB-CA-C    | -5.12 | 100.17      | 110.40   |
| 1   | I     | 268 | ARG  | NE-CZ-NH1  | 5.12  | 122.86      | 120.30   |
| 1   | D     | 304 | GLU  | CB-CA-C    | -5.11 | 100.17      | 110.40   |
| 1   | E     | 304 | GLU  | CB-CA-C    | -5.11 | 100.17      | 110.40   |
| 1   | A     | 304 | GLU  | CB-CA-C    | -5.10 | 100.20      | 110.40   |
| 1   | D     | 36  | ARG  | C-N-CA     | 5.10  | 134.45      | 121.70   |
| 1   | B     | 304 | GLU  | CB-CA-C    | -5.10 | 100.20      | 110.40   |
| 1   | F     | 304 | GLU  | CB-CA-C    | -5.10 | 100.21      | 110.40   |
| 1   | F     | 36  | ARG  | C-N-CA     | 5.09  | 134.43      | 121.70   |
| 1   | B     | 36  | ARG  | C-N-CA     | 5.09  | 134.43      | 121.70   |
| 1   | N     | 317 | LEU  | CB-CA-C    | -5.09 | 100.53      | 110.20   |
| 1   | C     | 36  | ARG  | C-N-CA     | 5.09  | 134.42      | 121.70   |
| 1   | E     | 36  | ARG  | C-N-CA     | 5.09  | 134.42      | 121.70   |
| 1   | M     | 13  | ARG  | NE-CZ-NH1  | 5.08  | 122.84      | 120.30   |
| 1   | J     | 523 | ASP  | N-CA-CB    | 5.08  | 119.74      | 110.60   |
| 1   | A     | 36  | ARG  | C-N-CA     | 5.07  | 134.39      | 121.70   |
| 1   | I     | 523 | ASP  | N-CA-CB    | 5.07  | 119.72      | 110.60   |
| 1   | L     | 523 | ASP  | N-CA-CB    | 5.07  | 119.72      | 110.60   |
| 1   | G     | 36  | ARG  | C-N-CA     | 5.06  | 134.36      | 121.70   |
| 1   | N     | 523 | ASP  | N-CA-CB    | 5.06  | 119.71      | 110.60   |
| 1   | M     | 523 | ASP  | N-CA-CB    | 5.06  | 119.71      | 110.60   |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | K     | 523 | ASP  | N-CA-CB | 5.05 | 119.70      | 110.60   |
| 1   | H     | 523 | ASP  | N-CA-CB | 5.05 | 119.68      | 110.60   |
| 1   | C     | 461 | GLU  | CB-CA-C | 5.03 | 120.46      | 110.40   |
| 1   | B     | 461 | GLU  | CB-CA-C | 5.02 | 120.44      | 110.40   |
| 1   | J     | 361 | ASP  | CB-CA-C | 5.02 | 120.44      | 110.40   |
| 1   | I     | 361 | ASP  | CB-CA-C | 5.01 | 120.43      | 110.40   |
| 1   | H     | 361 | ASP  | CB-CA-C | 5.01 | 120.41      | 110.40   |
| 1   | L     | 369 | VAL  | N-CA-CB | 5.00 | 122.50      | 111.50   |
| 1   | N     | 361 | ASP  | CB-CA-C | 5.00 | 120.40      | 110.40   |

All (7) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | H     | 37  | ASN  | CA   |
| 1   | I     | 37  | ASN  | CA   |
| 1   | J     | 37  | ASN  | CA   |
| 1   | K     | 37  | ASN  | CA   |
| 1   | L     | 37  | ASN  | CA   |
| 1   | M     | 37  | ASN  | CA   |
| 1   | N     | 37  | ASN  | CA   |

All (231) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 13  | ARG  | Sidechain         |
| 1   | A     | 18  | ARG  | Sidechain         |
| 1   | A     | 190 | VAL  | Peptide           |
| 1   | A     | 193 | MET  | Mainchain         |
| 1   | A     | 196 | ASP  | Peptide           |
| 1   | A     | 197 | ARG  | Mainchain,Peptide |
| 1   | A     | 231 | ARG  | Sidechain         |
| 1   | A     | 255 | GLU  | Peptide           |
| 1   | A     | 281 | PHE  | Peptide           |
| 1   | A     | 284 | ARG  | Sidechain         |
| 1   | A     | 285 | ARG  | Sidechain         |
| 1   | A     | 29  | VAL  | Mainchain         |
| 1   | A     | 296 | THR  | Peptide           |
| 1   | A     | 325 | ILE  | Peptide           |
| 1   | A     | 329 | THR  | Peptide           |
| 1   | A     | 368 | ARG  | Sidechain         |
| 1   | A     | 404 | ARG  | Sidechain         |
| 1   | A     | 52  | ASP  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | B     | 13  | ARG  | Sidechain         |
| 1   | B     | 18  | ARG  | Sidechain         |
| 1   | B     | 190 | VAL  | Peptide           |
| 1   | B     | 196 | ASP  | Peptide           |
| 1   | B     | 197 | ARG  | Mainchain,Peptide |
| 1   | B     | 231 | ARG  | Sidechain         |
| 1   | B     | 255 | GLU  | Peptide           |
| 1   | B     | 281 | PHE  | Peptide           |
| 1   | B     | 284 | ARG  | Sidechain         |
| 1   | B     | 285 | ARG  | Sidechain         |
| 1   | B     | 29  | VAL  | Mainchain         |
| 1   | B     | 296 | THR  | Peptide           |
| 1   | B     | 325 | ILE  | Peptide           |
| 1   | B     | 329 | THR  | Peptide           |
| 1   | B     | 368 | ARG  | Sidechain         |
| 1   | B     | 404 | ARG  | Sidechain         |
| 1   | B     | 52  | ASP  | Mainchain         |
| 1   | C     | 13  | ARG  | Sidechain         |
| 1   | C     | 18  | ARG  | Sidechain         |
| 1   | C     | 190 | VAL  | Peptide           |
| 1   | C     | 196 | ASP  | Peptide           |
| 1   | C     | 197 | ARG  | Mainchain,Peptide |
| 1   | C     | 231 | ARG  | Sidechain         |
| 1   | C     | 255 | GLU  | Peptide           |
| 1   | C     | 281 | PHE  | Peptide           |
| 1   | C     | 284 | ARG  | Sidechain         |
| 1   | C     | 285 | ARG  | Sidechain         |
| 1   | C     | 29  | VAL  | Mainchain         |
| 1   | C     | 296 | THR  | Peptide           |
| 1   | C     | 325 | ILE  | Peptide           |
| 1   | C     | 329 | THR  | Peptide           |
| 1   | C     | 368 | ARG  | Sidechain         |
| 1   | C     | 404 | ARG  | Sidechain         |
| 1   | C     | 52  | ASP  | Mainchain         |
| 1   | D     | 13  | ARG  | Sidechain         |
| 1   | D     | 18  | ARG  | Sidechain         |
| 1   | D     | 193 | MET  | Mainchain         |
| 1   | D     | 196 | ASP  | Peptide           |
| 1   | D     | 197 | ARG  | Mainchain,Peptide |
| 1   | D     | 231 | ARG  | Sidechain         |
| 1   | D     | 255 | GLU  | Peptide           |
| 1   | D     | 281 | PHE  | Peptide           |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | D     | 284 | ARG  | Sidechain         |
| 1   | D     | 285 | ARG  | Sidechain         |
| 1   | D     | 29  | VAL  | Mainchain         |
| 1   | D     | 296 | THR  | Peptide           |
| 1   | D     | 325 | ILE  | Peptide           |
| 1   | D     | 329 | THR  | Peptide           |
| 1   | D     | 368 | ARG  | Sidechain         |
| 1   | D     | 404 | ARG  | Sidechain         |
| 1   | D     | 52  | ASP  | Mainchain         |
| 1   | E     | 13  | ARG  | Sidechain         |
| 1   | E     | 18  | ARG  | Sidechain         |
| 1   | E     | 190 | VAL  | Peptide           |
| 1   | E     | 193 | MET  | Mainchain         |
| 1   | E     | 196 | ASP  | Peptide           |
| 1   | E     | 197 | ARG  | Mainchain,Peptide |
| 1   | E     | 231 | ARG  | Sidechain         |
| 1   | E     | 255 | GLU  | Peptide           |
| 1   | E     | 281 | PHE  | Peptide           |
| 1   | E     | 284 | ARG  | Sidechain         |
| 1   | E     | 285 | ARG  | Sidechain         |
| 1   | E     | 29  | VAL  | Mainchain         |
| 1   | E     | 296 | THR  | Peptide           |
| 1   | E     | 325 | ILE  | Peptide           |
| 1   | E     | 329 | THR  | Peptide           |
| 1   | E     | 368 | ARG  | Sidechain         |
| 1   | E     | 404 | ARG  | Sidechain         |
| 1   | E     | 52  | ASP  | Mainchain         |
| 1   | F     | 13  | ARG  | Sidechain         |
| 1   | F     | 18  | ARG  | Sidechain         |
| 1   | F     | 190 | VAL  | Peptide           |
| 1   | F     | 193 | MET  | Mainchain         |
| 1   | F     | 196 | ASP  | Peptide           |
| 1   | F     | 197 | ARG  | Mainchain,Peptide |
| 1   | F     | 231 | ARG  | Sidechain         |
| 1   | F     | 255 | GLU  | Peptide           |
| 1   | F     | 281 | PHE  | Peptide           |
| 1   | F     | 284 | ARG  | Sidechain         |
| 1   | F     | 285 | ARG  | Sidechain         |
| 1   | F     | 29  | VAL  | Mainchain         |
| 1   | F     | 296 | THR  | Peptide           |
| 1   | F     | 325 | ILE  | Peptide           |
| 1   | F     | 329 | THR  | Peptide           |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | F     | 368 | ARG  | Sidechain         |
| 1   | F     | 404 | ARG  | Sidechain         |
| 1   | F     | 52  | ASP  | Mainchain         |
| 1   | G     | 13  | ARG  | Sidechain         |
| 1   | G     | 18  | ARG  | Sidechain         |
| 1   | G     | 190 | VAL  | Peptide           |
| 1   | G     | 197 | ARG  | Mainchain,Peptide |
| 1   | G     | 199 | TYR  | Mainchain         |
| 1   | G     | 231 | ARG  | Sidechain         |
| 1   | G     | 255 | GLU  | Peptide           |
| 1   | G     | 281 | PHE  | Peptide           |
| 1   | G     | 284 | ARG  | Sidechain         |
| 1   | G     | 285 | ARG  | Sidechain         |
| 1   | G     | 29  | VAL  | Mainchain         |
| 1   | G     | 296 | THR  | Peptide           |
| 1   | G     | 325 | ILE  | Peptide           |
| 1   | G     | 329 | THR  | Peptide           |
| 1   | G     | 368 | ARG  | Sidechain         |
| 1   | G     | 404 | ARG  | Sidechain         |
| 1   | G     | 52  | ASP  | Mainchain         |
| 1   | H     | 213 | VAL  | Mainchain         |
| 1   | H     | 219 | PHE  | Sidechain         |
| 1   | H     | 285 | ARG  | Sidechain         |
| 1   | H     | 345 | ARG  | Sidechain         |
| 1   | H     | 350 | ARG  | Sidechain         |
| 1   | H     | 368 | ARG  | Sidechain         |
| 1   | H     | 395 | ARG  | Sidechain         |
| 1   | H     | 404 | ARG  | Sidechain         |
| 1   | H     | 421 | ARG  | Sidechain         |
| 1   | H     | 452 | ARG  | Sidechain         |
| 1   | H     | 50  | THR  | Peptide           |
| 1   | H     | 506 | TYR  | Sidechain         |
| 1   | H     | 58  | ARG  | Sidechain         |
| 1   | I     | 197 | ARG  | Mainchain         |
| 1   | I     | 213 | VAL  | Mainchain         |
| 1   | I     | 219 | PHE  | Sidechain         |
| 1   | I     | 285 | ARG  | Sidechain         |
| 1   | I     | 345 | ARG  | Sidechain         |
| 1   | I     | 350 | ARG  | Sidechain         |
| 1   | I     | 368 | ARG  | Sidechain         |
| 1   | I     | 395 | ARG  | Sidechain         |
| 1   | I     | 404 | ARG  | Sidechain         |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | I     | 421 | ARG  | Sidechain |
| 1   | I     | 452 | ARG  | Sidechain |
| 1   | I     | 50  | THR  | Peptide   |
| 1   | I     | 506 | TYR  | Sidechain |
| 1   | I     | 58  | ARG  | Sidechain |
| 1   | J     | 197 | ARG  | Mainchain |
| 1   | J     | 213 | VAL  | Mainchain |
| 1   | J     | 219 | PHE  | Sidechain |
| 1   | J     | 285 | ARG  | Sidechain |
| 1   | J     | 345 | ARG  | Sidechain |
| 1   | J     | 350 | ARG  | Sidechain |
| 1   | J     | 368 | ARG  | Sidechain |
| 1   | J     | 395 | ARG  | Sidechain |
| 1   | J     | 404 | ARG  | Sidechain |
| 1   | J     | 421 | ARG  | Sidechain |
| 1   | J     | 452 | ARG  | Sidechain |
| 1   | J     | 50  | THR  | Peptide   |
| 1   | J     | 506 | TYR  | Sidechain |
| 1   | J     | 58  | ARG  | Sidechain |
| 1   | K     | 18  | ARG  | Sidechain |
| 1   | K     | 197 | ARG  | Mainchain |
| 1   | K     | 213 | VAL  | Mainchain |
| 1   | K     | 219 | PHE  | Sidechain |
| 1   | K     | 285 | ARG  | Sidechain |
| 1   | K     | 345 | ARG  | Sidechain |
| 1   | K     | 350 | ARG  | Sidechain |
| 1   | K     | 368 | ARG  | Sidechain |
| 1   | K     | 395 | ARG  | Sidechain |
| 1   | K     | 404 | ARG  | Sidechain |
| 1   | K     | 421 | ARG  | Sidechain |
| 1   | K     | 452 | ARG  | Sidechain |
| 1   | K     | 50  | THR  | Peptide   |
| 1   | K     | 506 | TYR  | Sidechain |
| 1   | K     | 58  | ARG  | Sidechain |
| 1   | L     | 197 | ARG  | Mainchain |
| 1   | L     | 213 | VAL  | Mainchain |
| 1   | L     | 219 | PHE  | Sidechain |
| 1   | L     | 285 | ARG  | Sidechain |
| 1   | L     | 345 | ARG  | Sidechain |
| 1   | L     | 350 | ARG  | Sidechain |
| 1   | L     | 368 | ARG  | Sidechain |
| 1   | L     | 395 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | L     | 404 | ARG  | Sidechain         |
| 1   | L     | 421 | ARG  | Sidechain         |
| 1   | L     | 452 | ARG  | Sidechain         |
| 1   | L     | 50  | THR  | Peptide           |
| 1   | L     | 506 | TYR  | Sidechain         |
| 1   | L     | 58  | ARG  | Sidechain         |
| 1   | M     | 197 | ARG  | Mainchain         |
| 1   | M     | 213 | VAL  | Mainchain         |
| 1   | M     | 219 | PHE  | Sidechain         |
| 1   | M     | 285 | ARG  | Sidechain         |
| 1   | M     | 345 | ARG  | Sidechain         |
| 1   | M     | 350 | ARG  | Sidechain         |
| 1   | M     | 368 | ARG  | Sidechain         |
| 1   | M     | 395 | ARG  | Sidechain         |
| 1   | M     | 404 | ARG  | Sidechain         |
| 1   | M     | 421 | ARG  | Sidechain         |
| 1   | M     | 452 | ARG  | Sidechain         |
| 1   | M     | 50  | THR  | Peptide           |
| 1   | M     | 506 | TYR  | Sidechain         |
| 1   | M     | 58  | ARG  | Sidechain         |
| 1   | N     | 197 | ARG  | Mainchain,Peptide |
| 1   | N     | 206 | ASN  | Peptide           |
| 1   | N     | 207 | LYS  | Peptide           |
| 1   | N     | 208 | PRO  | Peptide           |
| 1   | N     | 213 | VAL  | Mainchain         |
| 1   | N     | 219 | PHE  | Sidechain         |
| 1   | N     | 285 | ARG  | Sidechain         |
| 1   | N     | 345 | ARG  | Sidechain         |
| 1   | N     | 350 | ARG  | Sidechain         |
| 1   | N     | 368 | ARG  | Sidechain         |
| 1   | N     | 395 | ARG  | Sidechain         |
| 1   | N     | 404 | ARG  | Sidechain         |
| 1   | N     | 421 | ARG  | Sidechain         |
| 1   | N     | 452 | ARG  | Sidechain         |
| 1   | N     | 50  | THR  | Peptide           |
| 1   | N     | 506 | TYR  | Sidechain         |
| 1   | N     | 58  | ARG  | Sidechain         |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3846  | 0        | 3967     | 219     | 0            |
| 1   | B     | 3845  | 0        | 3962     | 231     | 0            |
| 1   | C     | 3845  | 0        | 3962     | 229     | 0            |
| 1   | D     | 3845  | 0        | 3962     | 233     | 0            |
| 1   | E     | 3845  | 0        | 3962     | 222     | 0            |
| 1   | F     | 3845  | 0        | 3962     | 232     | 0            |
| 1   | G     | 3845  | 0        | 3962     | 228     | 0            |
| 1   | H     | 3845  | 0        | 3965     | 254     | 0            |
| 1   | I     | 3845  | 0        | 3965     | 251     | 0            |
| 1   | J     | 3845  | 0        | 3965     | 259     | 0            |
| 1   | K     | 3845  | 0        | 3965     | 264     | 0            |
| 1   | L     | 3845  | 0        | 3965     | 262     | 0            |
| 1   | M     | 3845  | 0        | 3965     | 258     | 0            |
| 1   | N     | 3845  | 0        | 3965     | 272     | 0            |
| 2   | A     | 1     | 0        | 0        | 3       | 0            |
| 2   | B     | 1     | 0        | 0        | 3       | 0            |
| 2   | C     | 1     | 0        | 0        | 4       | 0            |
| 2   | D     | 1     | 0        | 0        | 3       | 0            |
| 2   | E     | 1     | 0        | 0        | 4       | 0            |
| 2   | F     | 1     | 0        | 0        | 3       | 0            |
| 2   | G     | 1     | 0        | 0        | 3       | 0            |
| 2   | H     | 1     | 0        | 0        | 5       | 0            |
| 2   | I     | 1     | 0        | 0        | 5       | 0            |
| 2   | J     | 1     | 0        | 0        | 5       | 0            |
| 2   | K     | 1     | 0        | 0        | 5       | 0            |
| 2   | L     | 1     | 0        | 0        | 5       | 0            |
| 2   | M     | 1     | 0        | 0        | 5       | 0            |
| 2   | N     | 1     | 0        | 0        | 5       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 3   | H     | 1     | 0        | 0        | 0       | 0            |
| 3   | I     | 1     | 0        | 0        | 0       | 0            |
| 3   | J     | 1     | 0        | 0        | 0       | 0            |
| 3   | K     | 1     | 0        | 0        | 0       | 0            |
| 3   | L     | 1     | 0        | 0        | 0       | 0            |
| 3   | M     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | N     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 31    | 0        | 12       | 2       | 0            |
| 4   | B     | 31    | 0        | 12       | 2       | 0            |
| 4   | C     | 31    | 0        | 12       | 3       | 0            |
| 4   | D     | 31    | 0        | 12       | 2       | 0            |
| 4   | E     | 31    | 0        | 12       | 3       | 0            |
| 4   | F     | 31    | 0        | 12       | 2       | 0            |
| 4   | G     | 31    | 0        | 12       | 2       | 0            |
| 4   | H     | 31    | 0        | 12       | 4       | 0            |
| 4   | I     | 31    | 0        | 12       | 4       | 0            |
| 4   | J     | 31    | 0        | 12       | 5       | 0            |
| 4   | K     | 31    | 0        | 12       | 4       | 0            |
| 4   | L     | 31    | 0        | 12       | 5       | 0            |
| 4   | M     | 31    | 0        | 12       | 5       | 0            |
| 4   | N     | 31    | 0        | 12       | 5       | 0            |
| All | All   | 54293 | 0        | 55662    | 3207    | 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 29.

All (3207) 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:D:249:ILE:HD12 | 1:D:262:LEU:CD1 | 1.30                     | 1.62              |
| 1:C:249:ILE:HD12 | 1:C:262:LEU:CD1 | 1.30                     | 1.61              |
| 1:E:249:ILE:HD12 | 1:E:262:LEU:CD1 | 1.30                     | 1.60              |
| 1:B:249:ILE:HD12 | 1:B:262:LEU:CD1 | 1.30                     | 1.59              |
| 1:A:249:ILE:HD12 | 1:A:262:LEU:CD1 | 1.29                     | 1.57              |
| 1:M:518:GLU:CB   | 1:M:518:GLU:CA  | 1.83                     | 1.57              |
| 1:F:249:ILE:HD12 | 1:F:262:LEU:CD1 | 1.30                     | 1.57              |
| 1:H:518:GLU:CB   | 1:H:518:GLU:CA  | 1.83                     | 1.56              |
| 1:N:518:GLU:CA   | 1:N:518:GLU:CB  | 1.83                     | 1.56              |
| 1:G:249:ILE:HD12 | 1:G:262:LEU:CD1 | 1.30                     | 1.55              |
| 1:I:518:GLU:CB   | 1:I:518:GLU:CA  | 1.83                     | 1.55              |
| 1:L:518:GLU:CB   | 1:L:518:GLU:CA  | 1.83                     | 1.54              |
| 1:N:207:LYS:NZ   | 1:N:207:LYS:CE  | 1.70                     | 1.53              |
| 1:N:208:PRO:CA   | 1:N:208:PRO:C   | 1.76                     | 1.51              |
| 1:K:518:GLU:CB   | 1:K:518:GLU:CA  | 1.83                     | 1.51              |
| 1:J:518:GLU:CB   | 1:J:518:GLU:CA  | 1.83                     | 1.51              |
| 1:F:200:LEU:HD21 | 1:F:254:VAL:CG2 | 1.12                     | 1.46              |
| 1:D:200:LEU:HD21 | 1:D:254:VAL:CG2 | 1.12                     | 1.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:200:LEU:HD21 | 1:E:254:VAL:CG2  | 1.12                     | 1.45              |
| 1:A:200:LEU:HD21 | 1:A:254:VAL:CG2  | 1.12                     | 1.44              |
| 1:C:200:LEU:HD21 | 1:C:254:VAL:CG2  | 1.12                     | 1.42              |
| 1:B:200:LEU:HD21 | 1:B:254:VAL:CG2  | 1.12                     | 1.42              |
| 1:A:200:LEU:CD2  | 1:A:254:VAL:CG2  | 1.87                     | 1.41              |
| 1:C:200:LEU:CD2  | 1:C:254:VAL:HG21 | 1.32                     | 1.40              |
| 1:D:200:LEU:CD2  | 1:D:254:VAL:HG21 | 1.32                     | 1.39              |
| 1:B:200:LEU:CD2  | 1:B:254:VAL:HG21 | 1.32                     | 1.39              |
| 1:A:200:LEU:CD2  | 1:A:254:VAL:HG21 | 1.32                     | 1.37              |
| 1:E:200:LEU:CD2  | 1:E:254:VAL:HG21 | 1.32                     | 1.36              |
| 1:F:200:LEU:CD2  | 1:F:254:VAL:HG21 | 1.32                     | 1.35              |
| 1:M:23:LEU:CD1   | 1:M:60:ILE:HD12  | 1.58                     | 1.34              |
| 1:C:249:ILE:CD1  | 1:C:262:LEU:HD11 | 1.59                     | 1.33              |
| 1:B:249:ILE:CD1  | 1:B:262:LEU:HD11 | 1.59                     | 1.33              |
| 1:D:249:ILE:CD1  | 1:D:262:LEU:HD11 | 1.59                     | 1.33              |
| 1:K:23:LEU:CD1   | 1:K:60:ILE:HD12  | 1.58                     | 1.32              |
| 1:N:23:LEU:CD1   | 1:N:60:ILE:HD12  | 1.58                     | 1.32              |
| 1:H:23:LEU:CD1   | 1:H:60:ILE:HD12  | 1.58                     | 1.32              |
| 1:L:23:LEU:CD1   | 1:L:60:ILE:HD12  | 1.58                     | 1.32              |
| 1:I:233:MET:CE   | 1:I:249:ILE:HD13 | 1.60                     | 1.32              |
| 1:J:23:LEU:CD1   | 1:J:60:ILE:HD12  | 1.58                     | 1.32              |
| 1:A:249:ILE:CD1  | 1:A:262:LEU:HD11 | 1.58                     | 1.31              |
| 1:E:249:ILE:CD1  | 1:E:262:LEU:HD11 | 1.59                     | 1.31              |
| 1:I:23:LEU:CD1   | 1:I:60:ILE:HD12  | 1.58                     | 1.31              |
| 1:J:233:MET:CE   | 1:J:249:ILE:HD13 | 1.60                     | 1.30              |
| 1:F:249:ILE:CD1  | 1:F:262:LEU:HD11 | 1.58                     | 1.29              |
| 1:G:249:ILE:CD1  | 1:G:262:LEU:HD11 | 1.59                     | 1.29              |
| 1:D:200:LEU:CD2  | 1:D:254:VAL:CG2  | 1.87                     | 1.29              |
| 1:M:518:GLU:C    | 1:M:518:GLU:CB   | 2.01                     | 1.29              |
| 1:L:518:GLU:CB   | 1:L:518:GLU:C    | 2.01                     | 1.28              |
| 1:K:233:MET:CE   | 1:K:249:ILE:HD13 | 1.62                     | 1.28              |
| 1:N:518:GLU:CB   | 1:N:518:GLU:C    | 2.01                     | 1.28              |
| 1:N:233:MET:CE   | 1:N:249:ILE:HD13 | 1.63                     | 1.28              |
| 1:H:233:MET:CE   | 1:H:249:ILE:HD13 | 1.63                     | 1.27              |
| 1:I:518:GLU:CB   | 1:I:518:GLU:C    | 2.01                     | 1.27              |
| 1:L:233:MET:CE   | 1:L:249:ILE:HD13 | 1.65                     | 1.27              |
| 1:J:518:GLU:CB   | 1:J:518:GLU:C    | 2.01                     | 1.26              |
| 1:H:518:GLU:CB   | 1:H:518:GLU:C    | 2.02                     | 1.26              |
| 1:K:518:GLU:CB   | 1:K:518:GLU:C    | 2.01                     | 1.25              |
| 1:M:233:MET:CE   | 1:M:249:ILE:HD13 | 1.66                     | 1.25              |
| 1:C:200:LEU:CD2  | 1:C:254:VAL:CG2  | 1.87                     | 1.24              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:301:ILE:CD1  | 1:K:312:ALA:HB2  | 1.69                     | 1.23              |
| 1:L:301:ILE:CD1  | 1:L:312:ALA:HB2  | 1.69                     | 1.23              |
| 1:J:301:ILE:CD1  | 1:J:312:ALA:HB2  | 1.69                     | 1.23              |
| 1:M:301:ILE:CD1  | 1:M:312:ALA:HB2  | 1.69                     | 1.23              |
| 1:I:301:ILE:CD1  | 1:I:312:ALA:HB2  | 1.69                     | 1.22              |
| 1:N:301:ILE:CD1  | 1:N:312:ALA:HB2  | 1.68                     | 1.21              |
| 1:I:23:LEU:HD12  | 1:I:60:ILE:CD1   | 1.71                     | 1.21              |
| 1:B:200:LEU:CD2  | 1:B:254:VAL:CG2  | 1.87                     | 1.21              |
| 1:H:23:LEU:HD12  | 1:H:60:ILE:CD1   | 1.71                     | 1.21              |
| 1:J:23:LEU:HD12  | 1:J:60:ILE:CD1   | 1.71                     | 1.20              |
| 1:H:301:ILE:CD1  | 1:H:312:ALA:HB2  | 1.69                     | 1.20              |
| 1:N:23:LEU:HD12  | 1:N:60:ILE:CD1   | 1.71                     | 1.20              |
| 1:K:23:LEU:HD12  | 1:K:60:ILE:CD1   | 1.71                     | 1.20              |
| 1:M:23:LEU:HD12  | 1:M:60:ILE:CD1   | 1.71                     | 1.19              |
| 1:L:23:LEU:HD12  | 1:L:60:ILE:CD1   | 1.71                     | 1.19              |
| 1:G:23:LEU:HG    | 1:G:60:ILE:HD12  | 1.21                     | 1.18              |
| 1:F:23:LEU:HG    | 1:F:60:ILE:HD12  | 1.21                     | 1.18              |
| 1:C:193:MET:HG2  | 1:C:295:LEU:HG   | 1.23                     | 1.18              |
| 1:G:249:ILE:HD11 | 1:G:262:LEU:HD21 | 1.23                     | 1.17              |
| 1:C:249:ILE:HD11 | 1:C:262:LEU:HD21 | 1.22                     | 1.17              |
| 1:L:37:ASN:N     | 1:M:518:GLU:HA   | 1.60                     | 1.17              |
| 1:D:249:ILE:HD11 | 1:D:262:LEU:HD21 | 1.22                     | 1.17              |
| 1:J:37:ASN:N     | 1:K:518:GLU:HA   | 1.59                     | 1.17              |
| 1:E:249:ILE:CD1  | 1:E:262:LEU:CD1  | 2.20                     | 1.16              |
| 1:B:249:ILE:HD11 | 1:B:262:LEU:HD21 | 1.23                     | 1.16              |
| 1:A:249:ILE:HD11 | 1:A:262:LEU:HD21 | 1.22                     | 1.16              |
| 1:I:37:ASN:N     | 1:J:518:GLU:HA   | 1.59                     | 1.16              |
| 1:K:37:ASN:N     | 1:L:518:GLU:HA   | 1.59                     | 1.15              |
| 1:M:37:ASN:N     | 1:N:518:GLU:HA   | 1.59                     | 1.15              |
| 1:A:23:LEU:HG    | 1:A:60:ILE:HD12  | 1.21                     | 1.15              |
| 1:E:249:ILE:HD11 | 1:E:262:LEU:HD21 | 1.23                     | 1.15              |
| 1:A:249:ILE:CD1  | 1:A:262:LEU:CD1  | 2.20                     | 1.15              |
| 1:J:233:MET:HE2  | 1:J:249:ILE:HD13 | 1.30                     | 1.14              |
| 1:B:249:ILE:CD1  | 1:B:262:LEU:CD1  | 2.21                     | 1.14              |
| 1:I:233:MET:HE2  | 1:I:249:ILE:HD13 | 1.29                     | 1.14              |
| 1:E:200:LEU:CD2  | 1:E:254:VAL:CG2  | 1.87                     | 1.14              |
| 1:F:249:ILE:HD11 | 1:F:262:LEU:HD21 | 1.22                     | 1.14              |
| 1:A:193:MET:HE3  | 1:A:332:ILE:HD12 | 1.28                     | 1.14              |
| 1:G:249:ILE:CD1  | 1:G:262:LEU:CD1  | 2.21                     | 1.13              |
| 1:E:23:LEU:HG    | 1:E:60:ILE:HD12  | 1.21                     | 1.13              |
| 1:D:193:MET:HE3  | 1:D:332:ILE:HD12 | 1.27                     | 1.12              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:23:LEU:HG    | 1:B:60:ILE:HD12  | 1.21                     | 1.12              |
| 1:D:249:ILE:CD1  | 1:D:262:LEU:CD1  | 2.20                     | 1.12              |
| 1:E:193:MET:HE3  | 1:E:332:ILE:HD12 | 1.30                     | 1.11              |
| 1:L:301:ILE:HD13 | 1:L:312:ALA:HB2  | 1.29                     | 1.11              |
| 1:F:200:LEU:CD2  | 1:F:254:VAL:CG2  | 1.87                     | 1.11              |
| 1:H:301:ILE:HD13 | 1:H:312:ALA:HB2  | 1.28                     | 1.11              |
| 1:F:193:MET:HE3  | 1:F:332:ILE:HD12 | 1.28                     | 1.10              |
| 1:I:301:ILE:HD13 | 1:I:312:ALA:HB2  | 1.29                     | 1.10              |
| 1:H:518:GLU:HA   | 1:N:37:ASN:N     | 1.59                     | 1.10              |
| 1:H:37:ASN:N     | 1:I:518:GLU:HA   | 1.59                     | 1.10              |
| 1:M:38:VAL:HA    | 1:N:519:CYS:H    | 1.11                     | 1.10              |
| 1:B:193:MET:HE3  | 1:B:332:ILE:HD12 | 1.31                     | 1.10              |
| 1:H:38:VAL:HA    | 1:I:519:CYS:H    | 1.11                     | 1.10              |
| 1:C:199:TYR:HB3  | 1:C:325:ILE:HD11 | 1.33                     | 1.10              |
| 1:E:249:ILE:HD11 | 1:E:262:LEU:CD2  | 1.82                     | 1.10              |
| 1:I:38:VAL:HA    | 1:J:519:CYS:H    | 1.11                     | 1.10              |
| 1:B:199:TYR:HB3  | 1:B:325:ILE:HD11 | 1.33                     | 1.10              |
| 1:F:249:ILE:HD11 | 1:F:262:LEU:CD2  | 1.82                     | 1.09              |
| 1:C:23:LEU:HG    | 1:C:60:ILE:HD12  | 1.21                     | 1.09              |
| 1:K:38:VAL:HA    | 1:L:519:CYS:H    | 1.11                     | 1.09              |
| 1:D:249:ILE:HD11 | 1:D:262:LEU:CD2  | 1.82                     | 1.09              |
| 1:G:200:LEU:HD11 | 1:G:254:VAL:HG21 | 1.34                     | 1.09              |
| 1:A:150:ILE:CD1  | 1:A:493:ILE:HA   | 1.83                     | 1.09              |
| 1:I:301:ILE:CD1  | 1:I:312:ALA:CB   | 2.31                     | 1.09              |
| 1:J:301:ILE:CD1  | 1:J:312:ALA:CB   | 2.31                     | 1.09              |
| 1:F:249:ILE:CD1  | 1:F:262:LEU:CD1  | 2.20                     | 1.09              |
| 1:K:301:ILE:HD13 | 1:K:312:ALA:HB2  | 1.29                     | 1.09              |
| 1:D:23:LEU:HG    | 1:D:60:ILE:HD12  | 1.21                     | 1.08              |
| 1:C:150:ILE:CD1  | 1:C:493:ILE:HA   | 1.83                     | 1.08              |
| 1:G:150:ILE:CD1  | 1:G:493:ILE:HA   | 1.83                     | 1.08              |
| 1:H:301:ILE:CD1  | 1:H:312:ALA:CB   | 2.31                     | 1.08              |
| 1:G:249:ILE:HD11 | 1:G:262:LEU:CD2  | 1.82                     | 1.08              |
| 1:H:233:MET:HE2  | 1:H:249:ILE:HD13 | 1.29                     | 1.08              |
| 1:H:519:CYS:H    | 1:N:38:VAL:HA    | 1.11                     | 1.08              |
| 1:L:38:VAL:HA    | 1:M:519:CYS:H    | 1.11                     | 1.08              |
| 1:N:301:ILE:CD1  | 1:N:312:ALA:CB   | 2.31                     | 1.08              |
| 1:K:301:ILE:CD1  | 1:K:312:ALA:CB   | 2.31                     | 1.08              |
| 1:A:249:ILE:HD11 | 1:A:262:LEU:CD2  | 1.82                     | 1.08              |
| 1:M:301:ILE:CD1  | 1:M:312:ALA:CB   | 2.31                     | 1.08              |
| 1:A:199:TYR:HB3  | 1:A:325:ILE:HD11 | 1.33                     | 1.07              |
| 1:N:301:ILE:HD13 | 1:N:312:ALA:HB2  | 1.29                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:301:ILE:HD13 | 1:J:312:ALA:HB2  | 1.28                     | 1.07              |
| 1:B:150:ILE:CD1  | 1:B:493:ILE:HA   | 1.84                     | 1.07              |
| 1:C:249:ILE:HD11 | 1:C:262:LEU:CD2  | 1.82                     | 1.07              |
| 1:E:150:ILE:CD1  | 1:E:493:ILE:HA   | 1.83                     | 1.07              |
| 1:B:249:ILE:HD11 | 1:B:262:LEU:CD2  | 1.82                     | 1.07              |
| 1:L:233:MET:HE1  | 1:L:249:ILE:HD13 | 1.32                     | 1.07              |
| 1:L:301:ILE:CD1  | 1:L:312:ALA:CB   | 2.31                     | 1.07              |
| 1:N:208:PRO:HA   | 1:N:208:PRO:C    | 1.63                     | 1.07              |
| 1:J:38:VAL:HA    | 1:K:519:CYS:H    | 1.11                     | 1.07              |
| 1:M:233:MET:HE2  | 1:M:249:ILE:HD13 | 1.31                     | 1.07              |
| 1:C:249:ILE:CD1  | 1:C:262:LEU:CD1  | 2.20                     | 1.06              |
| 1:D:150:ILE:CD1  | 1:D:493:ILE:HA   | 1.84                     | 1.06              |
| 1:F:150:ILE:CD1  | 1:F:493:ILE:HA   | 1.84                     | 1.06              |
| 1:D:199:TYR:HB3  | 1:D:325:ILE:HD11 | 1.30                     | 1.05              |
| 1:F:199:TYR:HB3  | 1:F:325:ILE:HD11 | 1.33                     | 1.05              |
| 1:E:199:TYR:HB3  | 1:E:325:ILE:HD11 | 1.33                     | 1.05              |
| 1:K:233:MET:HE2  | 1:K:249:ILE:HD13 | 1.35                     | 1.04              |
| 1:G:199:TYR:HB3  | 1:G:325:ILE:HD11 | 1.33                     | 1.04              |
| 1:K:233:MET:HE1  | 1:K:249:ILE:HD13 | 1.37                     | 1.04              |
| 1:M:301:ILE:HD13 | 1:M:312:ALA:HB2  | 1.29                     | 1.04              |
| 1:J:203:TYR:CG   | 1:J:267:MET:SD   | 2.52                     | 1.03              |
| 1:C:249:ILE:HD12 | 1:C:262:LEU:HD13 | 1.38                     | 1.03              |
| 1:I:203:TYR:CG   | 1:I:267:MET:SD   | 2.52                     | 1.03              |
| 1:M:203:TYR:CG   | 1:M:267:MET:SD   | 2.51                     | 1.03              |
| 1:N:233:MET:HE2  | 1:N:249:ILE:HD13 | 1.33                     | 1.03              |
| 1:K:203:TYR:CG   | 1:K:267:MET:SD   | 2.52                     | 1.03              |
| 1:H:203:TYR:CG   | 1:H:267:MET:SD   | 2.52                     | 1.02              |
| 1:L:203:TYR:CG   | 1:L:267:MET:SD   | 2.51                     | 1.02              |
| 1:N:203:TYR:CG   | 1:N:267:MET:SD   | 2.51                     | 1.02              |
| 1:A:249:ILE:HD12 | 1:A:262:LEU:HD13 | 1.38                     | 1.02              |
| 1:N:182:GLY:HA3  | 1:N:383:ALA:H    | 1.24                     | 1.02              |
| 1:J:233:MET:HE1  | 1:J:249:ILE:HD13 | 1.41                     | 1.01              |
| 1:J:233:MET:CE   | 1:J:249:ILE:CD1  | 2.37                     | 1.01              |
| 1:H:233:MET:HE2  | 1:H:249:ILE:CD1  | 1.90                     | 1.01              |
| 1:F:249:ILE:HD12 | 1:F:262:LEU:HD13 | 1.38                     | 1.01              |
| 1:I:233:MET:CE   | 1:I:249:ILE:CD1  | 2.37                     | 1.00              |
| 1:M:233:MET:HE2  | 1:M:249:ILE:CD1  | 1.90                     | 1.00              |
| 1:L:182:GLY:HA3  | 1:L:383:ALA:H    | 1.24                     | 1.00              |
| 1:H:233:MET:CE   | 1:H:249:ILE:CD1  | 2.39                     | 1.00              |
| 1:N:233:MET:CE   | 1:N:249:ILE:CD1  | 2.40                     | 1.00              |
| 1:N:233:MET:HE1  | 1:N:249:ILE:HD13 | 1.40                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:249:ILE:HD12 | 1:B:262:LEU:HD13 | 1.38                     | 1.00              |
| 1:G:249:ILE:HD12 | 1:G:262:LEU:HD13 | 1.39                     | 1.00              |
| 1:L:233:MET:HE2  | 1:L:249:ILE:HD13 | 1.44                     | 1.00              |
| 1:E:249:ILE:HD12 | 1:E:262:LEU:HD13 | 1.38                     | 1.00              |
| 1:N:233:MET:HE2  | 1:N:249:ILE:CD1  | 1.92                     | 1.00              |
| 1:G:200:LEU:HD22 | 1:G:259:LEU:HD22 | 1.45                     | 0.99              |
| 1:I:233:MET:HE2  | 1:I:249:ILE:CD1  | 1.91                     | 0.99              |
| 1:J:182:GLY:HA3  | 1:J:383:ALA:H    | 1.24                     | 0.99              |
| 1:K:233:MET:CE   | 1:K:249:ILE:CD1  | 2.39                     | 0.99              |
| 1:D:249:ILE:CD1  | 1:D:262:LEU:HD21 | 1.93                     | 0.99              |
| 1:J:223:ALA:HB2  | 1:J:309:LEU:HD21 | 1.44                     | 0.99              |
| 1:J:233:MET:HE2  | 1:J:249:ILE:CD1  | 1.91                     | 0.99              |
| 1:K:223:ALA:HB2  | 1:K:309:LEU:HD21 | 1.44                     | 0.99              |
| 1:D:249:ILE:HD12 | 1:D:262:LEU:HD13 | 1.38                     | 0.99              |
| 1:G:200:LEU:CD1  | 1:G:254:VAL:HG11 | 1.93                     | 0.98              |
| 1:K:518:GLU:C    | 1:K:518:GLU:HB3  | 1.83                     | 0.98              |
| 1:I:223:ALA:HB2  | 1:I:309:LEU:HD21 | 1.45                     | 0.98              |
| 1:I:233:MET:HE1  | 1:I:249:ILE:HD13 | 1.42                     | 0.98              |
| 1:F:249:ILE:CD1  | 1:F:262:LEU:HD21 | 1.93                     | 0.98              |
| 1:N:518:GLU:C    | 1:N:518:GLU:HB3  | 1.83                     | 0.98              |
| 1:I:182:GLY:HA3  | 1:I:383:ALA:H    | 1.24                     | 0.98              |
| 1:M:223:ALA:HB2  | 1:M:309:LEU:HD21 | 1.43                     | 0.98              |
| 1:A:249:ILE:CD1  | 1:A:262:LEU:HD21 | 1.93                     | 0.98              |
| 1:H:223:ALA:HB2  | 1:H:309:LEU:HD21 | 1.44                     | 0.98              |
| 1:H:227:ILE:HD13 | 1:H:233:MET:SD   | 2.05                     | 0.97              |
| 1:M:182:GLY:HA3  | 1:M:383:ALA:H    | 1.24                     | 0.97              |
| 1:C:249:ILE:CD1  | 1:C:262:LEU:HD21 | 1.93                     | 0.97              |
| 1:I:518:GLU:HB3  | 1:I:518:GLU:C    | 1.83                     | 0.97              |
| 1:L:223:ALA:HB2  | 1:L:309:LEU:HD21 | 1.43                     | 0.97              |
| 1:E:249:ILE:CD1  | 1:E:262:LEU:HD21 | 1.93                     | 0.97              |
| 1:J:227:ILE:HD13 | 1:J:233:MET:SD   | 2.04                     | 0.97              |
| 1:L:233:MET:CE   | 1:L:249:ILE:CD1  | 2.42                     | 0.97              |
| 1:M:233:MET:CE   | 1:M:249:ILE:CD1  | 2.43                     | 0.97              |
| 1:J:518:GLU:HB3  | 1:J:518:GLU:C    | 1.83                     | 0.97              |
| 1:K:227:ILE:HD13 | 1:K:233:MET:SD   | 2.05                     | 0.97              |
| 1:M:233:MET:HE1  | 1:M:249:ILE:HD13 | 1.46                     | 0.97              |
| 1:G:200:LEU:HD11 | 1:G:254:VAL:CG2  | 1.94                     | 0.97              |
| 1:H:233:MET:HE1  | 1:H:249:ILE:HD13 | 1.44                     | 0.97              |
| 1:K:233:MET:HE2  | 1:K:249:ILE:CD1  | 1.93                     | 0.97              |
| 1:B:249:ILE:CD1  | 1:B:262:LEU:HD21 | 1.93                     | 0.97              |
| 1:G:249:ILE:CD1  | 1:G:262:LEU:HD21 | 1.93                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:227:ILE:HD13 | 1:I:233:MET:SD   | 2.05                     | 0.97              |
| 1:N:223:ALA:HB2  | 1:N:309:LEU:HD21 | 1.42                     | 0.97              |
| 1:H:182:GLY:HA3  | 1:H:383:ALA:H    | 1.27                     | 0.97              |
| 1:A:249:ILE:HD12 | 1:A:262:LEU:HD11 | 0.97                     | 0.97              |
| 1:E:249:ILE:HD12 | 1:E:262:LEU:HD11 | 0.97                     | 0.96              |
| 1:F:249:ILE:HD12 | 1:F:262:LEU:HD11 | 0.97                     | 0.96              |
| 1:K:182:GLY:HA3  | 1:K:383:ALA:H    | 1.24                     | 0.96              |
| 1:A:249:ILE:CD1  | 1:A:262:LEU:CD2  | 2.44                     | 0.96              |
| 1:B:249:ILE:CD1  | 1:B:262:LEU:CD2  | 2.44                     | 0.96              |
| 1:M:227:ILE:HD13 | 1:M:233:MET:SD   | 2.06                     | 0.96              |
| 1:L:227:ILE:HD13 | 1:L:233:MET:SD   | 2.06                     | 0.95              |
| 1:C:249:ILE:CD1  | 1:C:262:LEU:CD2  | 2.44                     | 0.95              |
| 1:G:249:ILE:CD1  | 1:G:262:LEU:CD2  | 2.44                     | 0.95              |
| 1:G:249:ILE:HD12 | 1:G:262:LEU:HD11 | 0.97                     | 0.95              |
| 1:M:518:GLU:HB3  | 1:M:518:GLU:C    | 1.83                     | 0.95              |
| 1:C:249:ILE:HD12 | 1:C:262:LEU:HD11 | 0.97                     | 0.95              |
| 1:N:227:ILE:HD13 | 1:N:233:MET:SD   | 2.05                     | 0.95              |
| 1:B:249:ILE:HD12 | 1:B:262:LEU:HD11 | 0.97                     | 0.94              |
| 1:L:518:GLU:HB3  | 1:L:518:GLU:C    | 1.83                     | 0.94              |
| 1:H:518:GLU:HB3  | 1:H:518:GLU:C    | 1.83                     | 0.94              |
| 1:L:233:MET:HE2  | 1:L:249:ILE:CD1  | 1.97                     | 0.94              |
| 1:D:249:ILE:CD1  | 1:D:262:LEU:CD2  | 2.44                     | 0.94              |
| 1:D:249:ILE:HD12 | 1:D:262:LEU:HD11 | 0.97                     | 0.94              |
| 1:E:249:ILE:CD1  | 1:E:262:LEU:CD2  | 2.44                     | 0.94              |
| 1:C:200:LEU:HD23 | 1:C:254:VAL:HG21 | 1.49                     | 0.93              |
| 1:B:200:LEU:HD23 | 1:B:254:VAL:HG21 | 1.49                     | 0.93              |
| 1:F:249:ILE:CD1  | 1:F:262:LEU:CD2  | 2.44                     | 0.93              |
| 1:F:220:ILE:HD13 | 1:F:332:ILE:HD13 | 1.49                     | 0.93              |
| 1:G:220:ILE:HD13 | 1:G:332:ILE:HD13 | 1.49                     | 0.93              |
| 1:L:242:LYS:CA   | 1:M:257:GLU:HA   | 1.99                     | 0.93              |
| 1:M:242:LYS:CA   | 1:N:257:GLU:HA   | 1.99                     | 0.93              |
| 1:F:200:LEU:HD23 | 1:F:254:VAL:HG21 | 1.49                     | 0.93              |
| 1:J:203:TYR:CD2  | 1:J:267:MET:SD   | 2.62                     | 0.93              |
| 1:N:203:TYR:CD2  | 1:N:267:MET:SD   | 2.62                     | 0.93              |
| 1:D:23:LEU:HG    | 1:D:60:ILE:CD1   | 1.99                     | 0.93              |
| 1:K:203:TYR:CD2  | 1:K:267:MET:SD   | 2.62                     | 0.93              |
| 1:C:23:LEU:HG    | 1:C:60:ILE:CD1   | 1.99                     | 0.93              |
| 1:J:242:LYS:CA   | 1:K:257:GLU:HA   | 1.99                     | 0.93              |
| 1:L:203:TYR:CD2  | 1:L:267:MET:SD   | 2.62                     | 0.92              |
| 1:A:200:LEU:HD23 | 1:A:254:VAL:HG21 | 1.49                     | 0.92              |
| 1:A:220:ILE:HD13 | 1:A:332:ILE:HD13 | 1.50                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:257:GLU:HA   | 1:N:242:LYS:CA   | 1.99                     | 0.92              |
| 1:H:242:LYS:CA   | 1:I:257:GLU:HA   | 1.99                     | 0.92              |
| 1:M:203:TYR:CD2  | 1:M:267:MET:SD   | 2.62                     | 0.92              |
| 1:D:200:LEU:HD23 | 1:D:254:VAL:HG21 | 1.49                     | 0.92              |
| 1:I:203:TYR:CD2  | 1:I:267:MET:SD   | 2.62                     | 0.92              |
| 1:E:23:LEU:HG    | 1:E:60:ILE:CD1   | 1.99                     | 0.92              |
| 1:H:203:TYR:CD2  | 1:H:267:MET:SD   | 2.62                     | 0.92              |
| 1:G:23:LEU:HG    | 1:G:60:ILE:CD1   | 1.98                     | 0.92              |
| 1:B:220:ILE:HD13 | 1:B:332:ILE:HD13 | 1.49                     | 0.92              |
| 1:B:23:LEU:HG    | 1:B:60:ILE:CD1   | 1.98                     | 0.92              |
| 1:E:220:ILE:HD13 | 1:E:332:ILE:HD13 | 1.49                     | 0.91              |
| 1:I:242:LYS:CA   | 1:J:257:GLU:HA   | 1.99                     | 0.91              |
| 1:A:23:LEU:HG    | 1:A:60:ILE:CD1   | 1.98                     | 0.91              |
| 1:C:23:LEU:HA    | 1:C:60:ILE:HD13  | 1.52                     | 0.91              |
| 1:D:23:LEU:HA    | 1:D:60:ILE:HD13  | 1.52                     | 0.91              |
| 1:F:23:LEU:HG    | 1:F:60:ILE:CD1   | 1.99                     | 0.91              |
| 1:C:213:VAL:CG1  | 1:C:325:ILE:HG12 | 2.01                     | 0.91              |
| 1:B:23:LEU:HA    | 1:B:60:ILE:HD13  | 1.52                     | 0.91              |
| 1:E:213:VAL:CG1  | 1:E:325:ILE:HG12 | 2.01                     | 0.91              |
| 1:C:220:ILE:HD13 | 1:C:332:ILE:HD13 | 1.49                     | 0.90              |
| 1:E:23:LEU:HA    | 1:E:60:ILE:HD13  | 1.52                     | 0.90              |
| 1:F:213:VAL:CG1  | 1:F:325:ILE:HG12 | 2.01                     | 0.90              |
| 1:D:220:ILE:HD13 | 1:D:332:ILE:HD13 | 1.49                     | 0.90              |
| 1:D:213:VAL:CG1  | 1:D:325:ILE:HG12 | 2.01                     | 0.90              |
| 1:G:213:VAL:CG1  | 1:G:325:ILE:HG12 | 2.01                     | 0.90              |
| 1:E:200:LEU:HD23 | 1:E:254:VAL:HG21 | 1.49                     | 0.90              |
| 1:K:242:LYS:CA   | 1:L:257:GLU:HA   | 2.01                     | 0.90              |
| 1:A:23:LEU:HA    | 1:A:60:ILE:HD13  | 1.52                     | 0.90              |
| 1:B:213:VAL:CG1  | 1:B:325:ILE:HG12 | 2.01                     | 0.90              |
| 1:F:23:LEU:HA    | 1:F:60:ILE:HD13  | 1.52                     | 0.90              |
| 1:J:23:LEU:HD12  | 1:J:60:ILE:HD12  | 0.89                     | 0.89              |
| 1:K:223:ALA:HB3  | 1:K:251:ALA:HB2  | 1.53                     | 0.89              |
| 1:K:193:MET:SD   | 1:K:292:ILE:HA   | 2.12                     | 0.89              |
| 1:K:23:LEU:HD12  | 1:K:60:ILE:HD12  | 0.89                     | 0.89              |
| 1:G:23:LEU:HA    | 1:G:60:ILE:HD13  | 1.52                     | 0.89              |
| 1:L:223:ALA:HB3  | 1:L:251:ALA:HB2  | 1.54                     | 0.89              |
| 1:M:23:LEU:HD12  | 1:M:60:ILE:HD12  | 0.89                     | 0.89              |
| 1:I:23:LEU:HD12  | 1:I:60:ILE:HD12  | 0.90                     | 0.89              |
| 1:L:23:LEU:HD12  | 1:L:60:ILE:HD12  | 0.89                     | 0.89              |
| 1:N:223:ALA:HB3  | 1:N:251:ALA:HB2  | 1.54                     | 0.89              |
| 1:N:206:ASN:HA   | 1:N:207:LYS:HG2  | 1.55                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:206:ASN:HA   | 1:N:207:LYS:CG   | 2.04                     | 0.88              |
| 1:I:223:ALA:HB3  | 1:I:251:ALA:HB2  | 1.52                     | 0.88              |
| 1:H:23:LEU:HD12  | 1:H:60:ILE:HD12  | 0.89                     | 0.88              |
| 1:J:223:ALA:HB3  | 1:J:251:ALA:HB2  | 1.52                     | 0.88              |
| 1:C:193:MET:HE3  | 1:C:292:ILE:HG23 | 1.56                     | 0.88              |
| 1:H:223:ALA:HB3  | 1:H:251:ALA:HB2  | 1.53                     | 0.87              |
| 1:M:223:ALA:HB3  | 1:M:251:ALA:HB2  | 1.54                     | 0.87              |
| 1:N:23:LEU:HD12  | 1:N:60:ILE:HD12  | 0.89                     | 0.87              |
| 1:C:193:MET:HE3  | 1:C:332:ILE:HD12 | 1.57                     | 0.87              |
| 1:A:249:ILE:HD12 | 1:A:262:LEU:CG   | 2.05                     | 0.87              |
| 1:F:150:ILE:HD12 | 1:F:493:ILE:HA   | 1.57                     | 0.86              |
| 1:G:200:LEU:N    | 1:G:200:LEU:HD12 | 1.88                     | 0.86              |
| 1:G:249:ILE:HD12 | 1:G:262:LEU:CG   | 2.05                     | 0.86              |
| 1:H:242:LYS:C    | 1:I:257:GLU:HA   | 1.96                     | 0.86              |
| 1:M:242:LYS:C    | 1:N:257:GLU:HA   | 1.96                     | 0.86              |
| 1:B:249:ILE:HD12 | 1:B:262:LEU:CG   | 2.05                     | 0.86              |
| 1:N:204:PHE:HA   | 1:N:207:LYS:NZ   | 1.89                     | 0.86              |
| 1:H:219:PHE:HB2  | 1:H:240:VAL:HG13 | 1.57                     | 0.85              |
| 1:K:219:PHE:HB2  | 1:K:240:VAL:HG13 | 1.57                     | 0.85              |
| 1:L:242:LYS:C    | 1:M:257:GLU:HA   | 1.97                     | 0.85              |
| 1:B:150:ILE:HD12 | 1:B:493:ILE:HA   | 1.57                     | 0.85              |
| 1:F:249:ILE:HD12 | 1:F:262:LEU:CG   | 2.05                     | 0.85              |
| 1:J:219:PHE:HB2  | 1:J:240:VAL:HG13 | 1.57                     | 0.85              |
| 1:N:219:PHE:HB2  | 1:N:240:VAL:HG13 | 1.57                     | 0.85              |
| 1:E:249:ILE:HD12 | 1:E:262:LEU:CG   | 2.05                     | 0.85              |
| 1:I:219:PHE:HB2  | 1:I:240:VAL:HG13 | 1.57                     | 0.85              |
| 1:M:301:ILE:HD12 | 1:M:312:ALA:CB   | 2.07                     | 0.85              |
| 1:C:249:ILE:HD12 | 1:C:262:LEU:CG   | 2.05                     | 0.85              |
| 1:L:219:PHE:HB2  | 1:L:240:VAL:HG13 | 1.57                     | 0.85              |
| 1:D:150:ILE:HD12 | 1:D:493:ILE:HA   | 1.58                     | 0.85              |
| 1:D:249:ILE:HD12 | 1:D:262:LEU:CG   | 2.05                     | 0.85              |
| 1:L:301:ILE:HD12 | 1:L:312:ALA:CB   | 2.07                     | 0.84              |
| 1:N:208:PRO:O    | 1:N:208:PRO:HA   | 1.76                     | 0.84              |
| 1:H:257:GLU:HA   | 1:N:242:LYS:C    | 1.98                     | 0.84              |
| 1:K:37:ASN:N     | 1:L:518:GLU:CA   | 2.36                     | 0.84              |
| 1:K:199:TYR:HB3  | 1:K:325:ILE:HD11 | 1.58                     | 0.84              |
| 1:J:301:ILE:HD12 | 1:J:312:ALA:CB   | 2.07                     | 0.83              |
| 1:M:219:PHE:HB2  | 1:M:240:VAL:HG13 | 1.57                     | 0.83              |
| 1:E:150:ILE:HD12 | 1:E:493:ILE:HA   | 1.60                     | 0.83              |
| 1:I:301:ILE:HD12 | 1:I:312:ALA:CB   | 2.07                     | 0.83              |
| 1:H:301:ILE:HD12 | 1:H:312:ALA:CB   | 2.07                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:242:LYS:C    | 1:J:257:GLU:HA   | 1.98                     | 0.83              |
| 1:C:150:ILE:HD12 | 1:C:493:ILE:HA   | 1.60                     | 0.83              |
| 1:K:301:ILE:HD12 | 1:K:312:ALA:CB   | 2.07                     | 0.83              |
| 1:J:242:LYS:C    | 1:K:257:GLU:HA   | 1.98                     | 0.83              |
| 1:L:207:LYS:HE2  | 1:L:207:LYS:HA   | 1.61                     | 0.83              |
| 1:K:242:LYS:C    | 1:L:257:GLU:HA   | 1.98                     | 0.83              |
| 1:N:301:ILE:HD12 | 1:N:312:ALA:CB   | 2.07                     | 0.82              |
| 1:M:37:ASN:N     | 1:N:518:GLU:CA   | 2.36                     | 0.82              |
| 1:C:223:ALA:O    | 1:C:251:ALA:HA   | 1.80                     | 0.82              |
| 1:A:223:ALA:O    | 1:A:251:ALA:HA   | 1.80                     | 0.82              |
| 1:N:138:CYS:N    | 1:N:410:GLY:HA2  | 1.95                     | 0.82              |
| 1:H:138:CYS:N    | 1:H:410:GLY:HA2  | 1.95                     | 0.82              |
| 1:L:150:ILE:HD11 | 1:L:493:ILE:HA   | 1.62                     | 0.82              |
| 1:M:138:CYS:N    | 1:M:410:GLY:HA2  | 1.95                     | 0.82              |
| 1:C:192:GLY:HA2  | 1:C:332:ILE:O    | 1.80                     | 0.82              |
| 1:F:249:ILE:HD13 | 1:F:262:LEU:HD11 | 1.62                     | 0.82              |
| 1:K:150:ILE:HD11 | 1:K:493:ILE:HA   | 1.62                     | 0.82              |
| 1:L:38:VAL:HA    | 1:M:519:CYS:N    | 1.95                     | 0.82              |
| 1:M:38:VAL:HA    | 1:N:519:CYS:N    | 1.94                     | 0.82              |
| 1:G:200:LEU:CD2  | 1:G:254:VAL:HG11 | 2.10                     | 0.81              |
| 1:G:150:ILE:HD12 | 1:G:493:ILE:HA   | 1.60                     | 0.81              |
| 1:A:150:ILE:HD12 | 1:A:493:ILE:HA   | 1.60                     | 0.81              |
| 1:K:38:VAL:HA    | 1:L:519:CYS:N    | 1.95                     | 0.81              |
| 1:L:162:ILE:HD13 | 1:L:400:LEU:HA   | 1.62                     | 0.81              |
| 1:C:193:MET:CE   | 1:C:292:ILE:HG23 | 2.11                     | 0.81              |
| 1:I:138:CYS:N    | 1:I:410:GLY:HA2  | 1.95                     | 0.81              |
| 1:L:183:LEU:HD23 | 1:L:183:LEU:H    | 1.45                     | 0.81              |
| 1:L:138:CYS:N    | 1:L:410:GLY:HA2  | 1.95                     | 0.81              |
| 1:M:150:ILE:HD11 | 1:M:493:ILE:HA   | 1.61                     | 0.81              |
| 1:I:38:VAL:HA    | 1:J:519:CYS:N    | 1.95                     | 0.81              |
| 1:K:162:ILE:HD13 | 1:K:400:LEU:HA   | 1.62                     | 0.81              |
| 1:M:36:ARG:C     | 1:N:518:GLU:HA   | 2.01                     | 0.81              |
| 1:H:38:VAL:HA    | 1:I:519:CYS:N    | 1.95                     | 0.81              |
| 1:J:150:ILE:HD11 | 1:J:493:ILE:HA   | 1.62                     | 0.81              |
| 1:M:162:ILE:HD13 | 1:M:400:LEU:HA   | 1.62                     | 0.81              |
| 1:J:38:VAL:HA    | 1:K:519:CYS:N    | 1.95                     | 0.81              |
| 1:F:223:ALA:O    | 1:F:251:ALA:HA   | 1.80                     | 0.81              |
| 1:F:186:GLU:HB2  | 1:F:380:LYS:HB2  | 1.63                     | 0.81              |
| 1:J:162:ILE:HD13 | 1:J:400:LEU:HA   | 1.62                     | 0.81              |
| 1:N:208:PRO:HB2  | 1:N:209:GLU:OE2  | 1.80                     | 0.81              |
| 1:E:223:ALA:O    | 1:E:251:ALA:HA   | 1.80                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:162:ILE:HD13 | 1:I:400:LEU:HA   | 1.62                     | 0.80              |
| 1:H:150:ILE:HD11 | 1:H:493:ILE:HA   | 1.61                     | 0.80              |
| 1:N:162:ILE:HD13 | 1:N:400:LEU:HA   | 1.62                     | 0.80              |
| 1:J:138:CYS:N    | 1:J:410:GLY:HA2  | 1.95                     | 0.80              |
| 1:J:36:ARG:C     | 1:K:518:GLU:HA   | 2.01                     | 0.80              |
| 1:K:36:ARG:C     | 1:L:518:GLU:HA   | 2.01                     | 0.80              |
| 1:K:138:CYS:N    | 1:K:410:GLY:HA2  | 1.95                     | 0.80              |
| 1:L:36:ARG:C     | 1:M:518:GLU:HA   | 2.01                     | 0.80              |
| 1:H:162:ILE:HD13 | 1:H:400:LEU:HA   | 1.62                     | 0.80              |
| 1:I:150:ILE:HD11 | 1:I:493:ILE:HA   | 1.62                     | 0.80              |
| 1:L:38:VAL:CA    | 1:M:519:CYS:H    | 1.94                     | 0.80              |
| 1:D:137:PRO:HA   | 1:D:410:GLY:HA2  | 1.63                     | 0.80              |
| 1:G:223:ALA:O    | 1:G:251:ALA:HA   | 1.80                     | 0.80              |
| 1:B:223:ALA:O    | 1:B:251:ALA:HA   | 1.80                     | 0.80              |
| 1:D:223:ALA:O    | 1:D:251:ALA:HA   | 1.80                     | 0.80              |
| 1:D:193:MET:HE3  | 1:D:332:ILE:CD1  | 2.09                     | 0.79              |
| 1:G:137:PRO:HA   | 1:G:410:GLY:CA   | 2.12                     | 0.79              |
| 1:B:249:ILE:HD13 | 1:B:262:LEU:HD11 | 1.62                     | 0.79              |
| 1:B:137:PRO:HA   | 1:B:410:GLY:CA   | 2.12                     | 0.79              |
| 1:D:137:PRO:HA   | 1:D:410:GLY:CA   | 2.12                     | 0.79              |
| 1:E:137:PRO:HA   | 1:E:410:GLY:HA2  | 1.63                     | 0.79              |
| 1:E:199:TYR:HB3  | 1:E:325:ILE:CD1  | 2.12                     | 0.79              |
| 1:N:206:ASN:HA   | 1:N:207:LYS:CB   | 2.11                     | 0.79              |
| 1:H:518:GLU:CA   | 1:N:37:ASN:N     | 2.36                     | 0.79              |
| 1:N:150:ILE:HD11 | 1:N:493:ILE:HA   | 1.62                     | 0.79              |
| 1:A:137:PRO:HA   | 1:A:410:GLY:CA   | 2.12                     | 0.79              |
| 1:H:36:ARG:C     | 1:I:518:GLU:HA   | 2.01                     | 0.79              |
| 1:H:38:VAL:CA    | 1:I:519:CYS:H    | 1.94                     | 0.79              |
| 1:N:204:PHE:HD1  | 1:N:207:LYS:HZ1  | 1.29                     | 0.79              |
| 1:H:519:CYS:N    | 1:N:38:VAL:HA    | 1.94                     | 0.79              |
| 1:F:137:PRO:HA   | 1:F:410:GLY:CA   | 2.12                     | 0.79              |
| 1:I:199:TYR:HB3  | 1:I:325:ILE:HD11 | 1.65                     | 0.79              |
| 1:C:199:TYR:HB3  | 1:C:325:ILE:CD1  | 2.12                     | 0.79              |
| 1:C:137:PRO:HA   | 1:C:410:GLY:CA   | 2.12                     | 0.79              |
| 1:C:137:PRO:HA   | 1:C:410:GLY:HA2  | 1.63                     | 0.79              |
| 1:H:518:GLU:HA   | 1:N:36:ARG:C     | 2.01                     | 0.79              |
| 1:I:36:ARG:C     | 1:J:518:GLU:HA   | 2.01                     | 0.79              |
| 1:C:249:ILE:HD13 | 1:C:262:LEU:HD11 | 1.62                     | 0.79              |
| 1:E:137:PRO:HA   | 1:E:410:GLY:CA   | 2.12                     | 0.79              |
| 1:M:199:TYR:HB3  | 1:M:325:ILE:HD11 | 1.65                     | 0.79              |
| 1:N:199:TYR:HB3  | 1:N:325:ILE:HD11 | 1.65                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:207:LYS:H    | 1:C:207:LYS:HE3  | 1.47                     | 0.78              |
| 1:F:137:PRO:HA   | 1:F:410:GLY:HA2  | 1.63                     | 0.78              |
| 1:I:38:VAL:CA    | 1:J:519:CYS:H    | 1.94                     | 0.78              |
| 1:A:193:MET:HE3  | 1:A:332:ILE:CD1  | 2.10                     | 0.78              |
| 1:I:301:ILE:HD12 | 1:I:312:ALA:HB2  | 1.65                     | 0.78              |
| 1:J:199:TYR:HB3  | 1:J:325:ILE:HD11 | 1.65                     | 0.78              |
| 1:A:137:PRO:HA   | 1:A:410:GLY:HA2  | 1.63                     | 0.78              |
| 1:G:137:PRO:HA   | 1:G:410:GLY:HA2  | 1.63                     | 0.78              |
| 1:L:199:TYR:HB3  | 1:L:325:ILE:HD11 | 1.65                     | 0.78              |
| 1:B:199:TYR:HB3  | 1:B:325:ILE:CD1  | 2.12                     | 0.78              |
| 1:H:519:CYS:H    | 1:N:38:VAL:CA    | 1.94                     | 0.78              |
| 1:I:30:THR:O     | 1:I:35:GLY:HA3   | 1.84                     | 0.78              |
| 1:K:30:THR:O     | 1:K:35:GLY:HA3   | 1.84                     | 0.78              |
| 1:D:300:VAL:HG23 | 1:D:312:ALA:HB2  | 1.66                     | 0.78              |
| 1:F:193:MET:HE3  | 1:F:332:ILE:CD1  | 2.10                     | 0.78              |
| 1:J:37:ASN:N     | 1:K:518:GLU:CA   | 2.36                     | 0.78              |
| 1:E:200:LEU:HB2  | 1:E:259:LEU:HD13 | 1.66                     | 0.78              |
| 1:C:300:VAL:HG23 | 1:C:312:ALA:HB2  | 1.66                     | 0.78              |
| 1:F:200:LEU:HB2  | 1:F:259:LEU:HD13 | 1.66                     | 0.77              |
| 1:F:300:VAL:HG23 | 1:F:312:ALA:HB2  | 1.66                     | 0.77              |
| 1:G:300:VAL:HG23 | 1:G:312:ALA:HB2  | 1.66                     | 0.77              |
| 1:A:249:ILE:HD13 | 1:A:262:LEU:HD11 | 1.62                     | 0.77              |
| 1:B:137:PRO:HA   | 1:B:410:GLY:HA2  | 1.63                     | 0.77              |
| 1:F:199:TYR:HB3  | 1:F:325:ILE:CD1  | 2.12                     | 0.77              |
| 1:G:23:LEU:CG    | 1:G:60:ILE:HD12  | 2.11                     | 0.77              |
| 1:M:295:LEU:HA   | 1:M:342:ILE:HD11 | 1.66                     | 0.77              |
| 1:M:30:THR:O     | 1:M:35:GLY:HA3   | 1.84                     | 0.77              |
| 1:E:249:ILE:HD13 | 1:E:262:LEU:HD11 | 1.62                     | 0.77              |
| 1:E:300:VAL:HG23 | 1:E:312:ALA:HB2  | 1.66                     | 0.77              |
| 1:A:200:LEU:HB2  | 1:A:259:LEU:HD13 | 1.66                     | 0.77              |
| 1:C:200:LEU:HD12 | 1:C:275:ALA:HB3  | 1.66                     | 0.77              |
| 1:D:23:LEU:CG    | 1:D:60:ILE:HD12  | 2.11                     | 0.77              |
| 1:J:38:VAL:CA    | 1:K:519:CYS:H    | 1.94                     | 0.77              |
| 1:N:295:LEU:HA   | 1:N:342:ILE:HD11 | 1.66                     | 0.77              |
| 1:A:200:LEU:HD12 | 1:A:275:ALA:HB3  | 1.66                     | 0.77              |
| 1:F:192:GLY:HA2  | 1:F:332:ILE:O    | 1.85                     | 0.77              |
| 1:H:295:LEU:HA   | 1:H:342:ILE:HD11 | 1.66                     | 0.77              |
| 1:H:38:VAL:HA    | 1:I:519:CYS:O    | 1.85                     | 0.77              |
| 1:L:30:THR:O     | 1:L:35:GLY:HA3   | 1.84                     | 0.77              |
| 1:K:38:VAL:CA    | 1:L:519:CYS:H    | 1.94                     | 0.77              |
| 1:C:150:ILE:HD13 | 1:C:493:ILE:HG23 | 1.67                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:200:LEU:HD12 | 1:D:275:ALA:HB3  | 1.66                     | 0.77              |
| 1:K:182:GLY:CA   | 1:K:383:ALA:H    | 1.98                     | 0.77              |
| 1:A:300:VAL:HG23 | 1:A:312:ALA:HB2  | 1.66                     | 0.77              |
| 1:A:199:TYR:HB3  | 1:A:325:ILE:CD1  | 2.12                     | 0.77              |
| 1:B:300:VAL:HG23 | 1:B:312:ALA:HB2  | 1.66                     | 0.77              |
| 1:D:200:LEU:HB2  | 1:D:259:LEU:HD13 | 1.66                     | 0.77              |
| 1:F:150:ILE:CD1  | 1:F:493:ILE:HG23 | 2.15                     | 0.77              |
| 1:F:200:LEU:HD12 | 1:F:275:ALA:HB3  | 1.66                     | 0.77              |
| 1:J:301:ILE:HD12 | 1:J:312:ALA:HB2  | 1.65                     | 0.77              |
| 1:J:30:THR:O     | 1:J:35:GLY:HA3   | 1.84                     | 0.77              |
| 1:L:295:LEU:HA   | 1:L:342:ILE:HD11 | 1.66                     | 0.77              |
| 1:N:187:LEU:HD12 | 1:N:378:VAL:O    | 1.85                     | 0.77              |
| 1:D:150:ILE:CD1  | 1:D:493:ILE:HG23 | 2.15                     | 0.77              |
| 1:G:200:LEU:CG   | 1:G:254:VAL:HG11 | 2.14                     | 0.77              |
| 1:G:249:ILE:HD13 | 1:G:262:LEU:HD11 | 1.62                     | 0.77              |
| 1:K:177:VAL:HG22 | 1:K:379:ILE:HB   | 1.67                     | 0.77              |
| 1:N:30:THR:O     | 1:N:35:GLY:HA3   | 1.84                     | 0.77              |
| 1:B:200:LEU:HB2  | 1:B:259:LEU:HD13 | 1.66                     | 0.77              |
| 1:I:182:GLY:CA   | 1:I:383:ALA:H    | 1.98                     | 0.77              |
| 1:B:150:ILE:CD1  | 1:B:493:ILE:HG23 | 2.15                     | 0.76              |
| 1:E:192:GLY:HA2  | 1:E:332:ILE:O    | 1.85                     | 0.76              |
| 1:G:150:ILE:HD13 | 1:G:493:ILE:HG23 | 1.67                     | 0.76              |
| 1:I:38:VAL:HA    | 1:J:519:CYS:O    | 1.85                     | 0.76              |
| 1:H:519:CYS:O    | 1:N:38:VAL:HA    | 1.85                     | 0.76              |
| 1:B:356:ALA:HB1  | 1:B:361:ASP:HB2  | 1.68                     | 0.76              |
| 1:F:23:LEU:CG    | 1:F:60:ILE:HD12  | 2.11                     | 0.76              |
| 1:H:30:THR:O     | 1:H:35:GLY:HA3   | 1.84                     | 0.76              |
| 1:I:295:LEU:HA   | 1:I:342:ILE:HD11 | 1.66                     | 0.76              |
| 1:J:38:VAL:HA    | 1:K:519:CYS:O    | 1.84                     | 0.76              |
| 1:E:150:ILE:HD13 | 1:E:493:ILE:HG23 | 1.67                     | 0.76              |
| 1:B:200:LEU:HD12 | 1:B:275:ALA:HB3  | 1.66                     | 0.76              |
| 1:C:356:ALA:HB1  | 1:C:361:ASP:HB2  | 1.68                     | 0.76              |
| 1:D:192:GLY:HA2  | 1:D:332:ILE:O    | 1.85                     | 0.76              |
| 1:K:38:VAL:HA    | 1:L:519:CYS:O    | 1.85                     | 0.76              |
| 1:A:192:GLY:HA2  | 1:A:332:ILE:O    | 1.85                     | 0.76              |
| 1:D:200:LEU:HD12 | 1:D:275:ALA:CB   | 2.16                     | 0.76              |
| 1:L:249:ILE:HB   | 1:L:275:ALA:HB2  | 1.68                     | 0.76              |
| 1:C:200:LEU:HB2  | 1:C:259:LEU:HD13 | 1.66                     | 0.76              |
| 1:E:193:MET:HE3  | 1:E:332:ILE:CD1  | 2.12                     | 0.76              |
| 1:G:192:GLY:HA2  | 1:G:332:ILE:O    | 1.85                     | 0.76              |
| 1:G:193:MET:SD   | 1:G:292:ILE:HA   | 2.26                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:249:ILE:HB   | 1:H:275:ALA:HB2  | 1.68                     | 0.76              |
| 1:A:240:VAL:HG11 | 1:A:247:LEU:HB2  | 1.68                     | 0.76              |
| 1:C:200:LEU:HD12 | 1:C:275:ALA:CB   | 2.16                     | 0.76              |
| 1:F:200:LEU:HD12 | 1:F:275:ALA:CB   | 2.16                     | 0.76              |
| 1:F:150:ILE:HD13 | 1:F:493:ILE:HG23 | 1.68                     | 0.76              |
| 1:G:199:TYR:HB3  | 1:G:325:ILE:CD1  | 2.12                     | 0.76              |
| 1:M:249:ILE:HB   | 1:M:275:ALA:HB2  | 1.68                     | 0.76              |
| 1:N:206:ASN:OD1  | 1:N:213:VAL:HG23 | 1.84                     | 0.76              |
| 1:D:150:ILE:HD13 | 1:D:493:ILE:HG23 | 1.68                     | 0.76              |
| 1:E:200:LEU:HD12 | 1:E:275:ALA:CB   | 2.16                     | 0.76              |
| 1:H:37:ASN:N     | 1:I:518:GLU:CA   | 2.36                     | 0.76              |
| 1:J:182:GLY:CA   | 1:J:383:ALA:H    | 1.98                     | 0.76              |
| 1:L:279:PRO:O    | 1:L:285:ARG:HA   | 1.85                     | 0.76              |
| 1:M:169:VAL:CG1  | 1:M:377:ALA:HB3  | 2.16                     | 0.76              |
| 1:L:38:VAL:HA    | 1:M:519:CYS:O    | 1.85                     | 0.76              |
| 1:N:249:ILE:HB   | 1:N:275:ALA:HB2  | 1.68                     | 0.76              |
| 1:A:200:LEU:HD12 | 1:A:275:ALA:CB   | 2.16                     | 0.76              |
| 1:A:356:ALA:HB1  | 1:A:361:ASP:HB2  | 1.68                     | 0.76              |
| 1:B:192:GLY:HA2  | 1:B:332:ILE:O    | 1.85                     | 0.76              |
| 1:E:200:LEU:HD12 | 1:E:275:ALA:HB3  | 1.66                     | 0.76              |
| 1:K:137:PRO:HA   | 1:K:410:GLY:HA3  | 1.66                     | 0.76              |
| 1:K:249:ILE:HB   | 1:K:275:ALA:HB2  | 1.68                     | 0.76              |
| 1:K:279:PRO:O    | 1:K:285:ARG:HA   | 1.85                     | 0.76              |
| 1:L:182:GLY:CA   | 1:L:383:ALA:H    | 1.98                     | 0.76              |
| 1:L:137:PRO:HA   | 1:L:410:GLY:HA3  | 1.66                     | 0.76              |
| 1:M:279:PRO:O    | 1:M:285:ARG:HA   | 1.85                     | 0.76              |
| 1:M:137:PRO:HA   | 1:M:410:GLY:HA3  | 1.66                     | 0.76              |
| 1:M:38:VAL:HA    | 1:N:519:CYS:O    | 1.85                     | 0.76              |
| 1:B:240:VAL:HG11 | 1:B:247:LEU:HB2  | 1.68                     | 0.76              |
| 1:B:200:LEU:HD12 | 1:B:275:ALA:CB   | 2.16                     | 0.76              |
| 1:D:249:ILE:HD13 | 1:D:262:LEU:HD11 | 1.62                     | 0.76              |
| 1:H:137:PRO:HA   | 1:H:410:GLY:HA3  | 1.66                     | 0.76              |
| 1:I:279:PRO:O    | 1:I:285:ARG:HA   | 1.86                     | 0.76              |
| 1:I:137:PRO:HA   | 1:I:410:GLY:HA3  | 1.66                     | 0.76              |
| 1:J:137:PRO:HA   | 1:J:410:GLY:HA3  | 1.66                     | 0.76              |
| 1:K:295:LEU:HA   | 1:K:342:ILE:HD11 | 1.66                     | 0.76              |
| 1:N:137:PRO:HA   | 1:N:410:GLY:HA3  | 1.66                     | 0.76              |
| 1:M:38:VAL:CA    | 1:N:519:CYS:H    | 1.94                     | 0.76              |
| 1:C:23:LEU:CG    | 1:C:60:ILE:HD12  | 2.11                     | 0.75              |
| 1:J:279:PRO:O    | 1:J:285:ARG:HA   | 1.86                     | 0.75              |
| 1:J:295:LEU:HA   | 1:J:342:ILE:HD11 | 1.66                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:182:GLY:CA   | 1:M:383:ALA:H    | 1.98                     | 0.75              |
| 1:B:193:MET:HE3  | 1:B:332:ILE:CD1  | 2.13                     | 0.75              |
| 1:G:240:VAL:HG11 | 1:G:247:LEU:HB2  | 1.68                     | 0.75              |
| 1:N:182:GLY:CA   | 1:N:383:ALA:H    | 1.98                     | 0.75              |
| 1:D:356:ALA:HB1  | 1:D:361:ASP:HB2  | 1.68                     | 0.75              |
| 1:J:169:VAL:CG1  | 1:J:377:ALA:HB3  | 2.16                     | 0.75              |
| 1:H:279:PRO:O    | 1:H:285:ARG:HA   | 1.85                     | 0.75              |
| 1:H:182:GLY:CA   | 1:H:383:ALA:H    | 1.98                     | 0.75              |
| 1:I:169:VAL:CG1  | 1:I:377:ALA:HB3  | 2.16                     | 0.75              |
| 1:K:169:VAL:CG1  | 1:K:377:ALA:HB3  | 2.16                     | 0.75              |
| 1:C:207:LYS:HB2  | 1:C:208:PRO:HD3  | 1.68                     | 0.75              |
| 1:L:169:VAL:CG1  | 1:L:377:ALA:HB3  | 2.16                     | 0.75              |
| 1:H:169:VAL:CG1  | 1:H:377:ALA:HB3  | 2.16                     | 0.75              |
| 1:D:240:VAL:HG11 | 1:D:247:LEU:HB2  | 1.68                     | 0.75              |
| 1:G:356:ALA:HB1  | 1:G:361:ASP:HB2  | 1.68                     | 0.75              |
| 1:I:249:ILE:HB   | 1:I:275:ALA:HB2  | 1.68                     | 0.75              |
| 1:M:301:ILE:HD12 | 1:M:312:ALA:HB2  | 1.65                     | 0.75              |
| 1:N:169:VAL:CG1  | 1:N:377:ALA:HB3  | 2.16                     | 0.75              |
| 1:B:150:ILE:HD13 | 1:B:493:ILE:HG23 | 1.68                     | 0.74              |
| 1:H:138:CYS:H    | 1:H:410:GLY:HA2  | 1.52                     | 0.74              |
| 1:J:249:ILE:HB   | 1:J:275:ALA:HB2  | 1.68                     | 0.74              |
| 1:N:138:CYS:H    | 1:N:410:GLY:HA2  | 1.52                     | 0.74              |
| 1:F:240:VAL:HG11 | 1:F:247:LEU:HB2  | 1.68                     | 0.74              |
| 1:A:150:ILE:HD13 | 1:A:493:ILE:HG23 | 1.67                     | 0.74              |
| 1:D:150:ILE:HD11 | 1:D:493:ILE:HA   | 1.68                     | 0.74              |
| 1:E:240:VAL:HG11 | 1:E:247:LEU:HB2  | 1.68                     | 0.74              |
| 1:E:356:ALA:HB1  | 1:E:361:ASP:HB2  | 1.68                     | 0.74              |
| 1:M:138:CYS:H    | 1:M:410:GLY:HA2  | 1.52                     | 0.74              |
| 1:N:204:PHE:HA   | 1:N:207:LYS:HZ1  | 1.49                     | 0.74              |
| 1:C:240:VAL:HG11 | 1:C:247:LEU:HB2  | 1.68                     | 0.74              |
| 1:E:381:VAL:HG21 | 1:E:393:LYS:N    | 2.03                     | 0.74              |
| 1:F:356:ALA:HB1  | 1:F:361:ASP:HB2  | 1.68                     | 0.74              |
| 1:E:23:LEU:CG    | 1:E:60:ILE:HD12  | 2.11                     | 0.74              |
| 1:N:279:PRO:O    | 1:N:285:ARG:HA   | 1.85                     | 0.74              |
| 1:D:381:VAL:HG21 | 1:D:393:LYS:N    | 2.03                     | 0.74              |
| 1:A:38:VAL:HG21  | 1:A:56:VAL:CG2   | 2.18                     | 0.74              |
| 1:B:38:VAL:HG21  | 1:B:56:VAL:CG2   | 2.18                     | 0.74              |
| 1:C:38:VAL:HG21  | 1:C:56:VAL:CG2   | 2.18                     | 0.74              |
| 1:D:38:VAL:HG21  | 1:D:56:VAL:CG2   | 2.18                     | 0.74              |
| 1:G:38:VAL:HG21  | 1:G:56:VAL:CG2   | 2.18                     | 0.74              |
| 1:N:301:ILE:HD12 | 1:N:312:ALA:HB2  | 1.65                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:150:ILE:HD11 | 1:A:493:ILE:HA   | 1.69                     | 0.73              |
| 1:B:222:LEU:HD21 | 1:B:292:ILE:HG22 | 1.70                     | 0.73              |
| 1:E:38:VAL:HG21  | 1:E:56:VAL:CG2   | 2.18                     | 0.73              |
| 1:F:222:LEU:HD21 | 1:F:292:ILE:HG22 | 1.70                     | 0.73              |
| 1:G:150:ILE:HD11 | 1:G:493:ILE:HA   | 1.69                     | 0.73              |
| 1:B:150:ILE:HD11 | 1:B:493:ILE:HA   | 1.68                     | 0.73              |
| 1:B:23:LEU:CG    | 1:B:60:ILE:HD12  | 2.11                     | 0.73              |
| 1:C:381:VAL:HG21 | 1:C:393:LYS:N    | 2.03                     | 0.73              |
| 1:F:38:VAL:HG21  | 1:F:56:VAL:CG2   | 2.18                     | 0.73              |
| 1:I:301:ILE:CD1  | 1:I:312:ALA:HB1  | 2.18                     | 0.73              |
| 1:C:222:LEU:HD21 | 1:C:292:ILE:HG22 | 1.70                     | 0.73              |
| 1:G:222:LEU:HD21 | 1:G:292:ILE:HG22 | 1.70                     | 0.73              |
| 1:K:301:ILE:CD1  | 1:K:312:ALA:HB1  | 2.18                     | 0.73              |
| 1:L:301:ILE:CD1  | 1:L:312:ALA:HB1  | 2.18                     | 0.73              |
| 1:A:222:LEU:HD21 | 1:A:292:ILE:HG22 | 1.70                     | 0.73              |
| 1:C:262:LEU:HD22 | 1:C:273:VAL:HG11 | 1.71                     | 0.73              |
| 1:E:222:LEU:HD21 | 1:E:292:ILE:HG22 | 1.70                     | 0.73              |
| 1:F:381:VAL:HG21 | 1:F:393:LYS:N    | 2.03                     | 0.73              |
| 1:H:301:ILE:CD1  | 1:H:312:ALA:HB1  | 2.18                     | 0.73              |
| 1:A:313:THR:H    | 1:A:316:ASP:HB3  | 1.54                     | 0.73              |
| 1:B:313:THR:H    | 1:B:316:ASP:HB3  | 1.54                     | 0.73              |
| 1:G:313:THR:H    | 1:G:316:ASP:HB3  | 1.54                     | 0.73              |
| 1:I:138:CYS:H    | 1:I:410:GLY:HA2  | 1.52                     | 0.73              |
| 1:F:150:ILE:HD11 | 1:F:493:ILE:HA   | 1.68                     | 0.73              |
| 1:A:262:LEU:HD22 | 1:A:273:VAL:HG11 | 1.71                     | 0.73              |
| 1:A:381:VAL:HG21 | 1:A:393:LYS:N    | 2.03                     | 0.73              |
| 1:B:381:VAL:HG21 | 1:B:393:LYS:N    | 2.03                     | 0.73              |
| 1:D:222:LEU:HD21 | 1:D:292:ILE:HG22 | 1.71                     | 0.73              |
| 1:I:37:ASN:N     | 1:J:518:GLU:CA   | 2.36                     | 0.73              |
| 1:G:262:LEU:HD22 | 1:G:273:VAL:HG11 | 1.71                     | 0.73              |
| 1:L:138:CYS:H    | 1:L:410:GLY:HA2  | 1.52                     | 0.73              |
| 1:C:313:THR:H    | 1:C:316:ASP:HB3  | 1.54                     | 0.72              |
| 1:G:381:VAL:HG21 | 1:G:393:LYS:N    | 2.03                     | 0.72              |
| 1:F:313:THR:H    | 1:F:316:ASP:HB3  | 1.54                     | 0.72              |
| 1:E:313:THR:H    | 1:E:316:ASP:HB3  | 1.54                     | 0.72              |
| 1:N:301:ILE:CD1  | 1:N:312:ALA:HB1  | 2.18                     | 0.72              |
| 1:G:150:ILE:CD1  | 1:G:493:ILE:HG23 | 2.20                     | 0.72              |
| 1:K:207:LYS:HE3  | 1:K:207:LYS:HA   | 1.70                     | 0.72              |
| 1:C:150:ILE:CD1  | 1:C:493:ILE:HG23 | 2.20                     | 0.72              |
| 1:D:262:LEU:HD22 | 1:D:273:VAL:HG11 | 1.71                     | 0.72              |
| 1:D:313:THR:H    | 1:D:316:ASP:HB3  | 1.54                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:150:ILE:CD1  | 1:E:493:ILE:HG23 | 2.20                     | 0.72              |
| 1:G:193:MET:HE1  | 1:G:295:LEU:HB3  | 1.72                     | 0.72              |
| 1:G:193:MET:HG2  | 1:G:295:LEU:HG   | 1.71                     | 0.72              |
| 1:M:301:ILE:CD1  | 1:M:312:ALA:HB1  | 2.18                     | 0.72              |
| 1:N:205:ILE:O    | 1:N:207:LYS:HG2  | 1.89                     | 0.72              |
| 1:A:162:ILE:HD13 | 1:A:400:LEU:CA   | 2.20                     | 0.72              |
| 1:J:223:ALA:HB1  | 1:J:225:LYS:HD2  | 1.72                     | 0.72              |
| 1:G:200:LEU:CD1  | 1:G:254:VAL:CG1  | 2.68                     | 0.72              |
| 1:B:206:ASN:HB3  | 1:B:208:PRO:HD2  | 1.70                     | 0.71              |
| 1:B:262:LEU:HD22 | 1:B:273:VAL:HG11 | 1.71                     | 0.71              |
| 1:A:23:LEU:CG    | 1:A:60:ILE:HD12  | 2.11                     | 0.71              |
| 1:K:243:ALA:HB2  | 1:L:256:GLY:O    | 1.90                     | 0.71              |
| 1:A:150:ILE:CD1  | 1:A:493:ILE:HG23 | 2.20                     | 0.71              |
| 1:H:243:ALA:HB2  | 1:I:256:GLY:O    | 1.90                     | 0.71              |
| 1:J:138:CYS:H    | 1:J:410:GLY:HA2  | 1.52                     | 0.71              |
| 1:L:243:ALA:HB2  | 1:M:256:GLY:O    | 1.90                     | 0.71              |
| 1:M:243:ALA:HB2  | 1:N:256:GLY:O    | 1.90                     | 0.71              |
| 1:C:162:ILE:HD13 | 1:C:400:LEU:CA   | 2.20                     | 0.71              |
| 1:E:162:ILE:HD13 | 1:E:400:LEU:CA   | 2.20                     | 0.71              |
| 1:H:256:GLY:O    | 1:N:243:ALA:HB2  | 1.90                     | 0.71              |
| 1:F:262:LEU:HD22 | 1:F:273:VAL:HG11 | 1.71                     | 0.71              |
| 1:F:162:ILE:HD13 | 1:F:400:LEU:CA   | 2.20                     | 0.71              |
| 1:I:223:ALA:HB1  | 1:I:225:LYS:HD2  | 1.72                     | 0.71              |
| 1:N:23:LEU:HD13  | 1:N:60:ILE:HD12  | 1.70                     | 0.71              |
| 1:E:150:ILE:HD11 | 1:E:493:ILE:HA   | 1.70                     | 0.71              |
| 1:F:249:ILE:CD1  | 1:F:262:LEU:CG   | 2.67                     | 0.71              |
| 1:H:199:TYR:HB3  | 1:H:325:ILE:HD11 | 1.72                     | 0.71              |
| 1:D:162:ILE:HD13 | 1:D:400:LEU:CA   | 2.20                     | 0.70              |
| 1:E:262:LEU:HD22 | 1:E:273:VAL:HG11 | 1.71                     | 0.70              |
| 1:J:301:ILE:CD1  | 1:J:312:ALA:HB1  | 2.18                     | 0.70              |
| 1:C:150:ILE:HD11 | 1:C:493:ILE:HA   | 1.70                     | 0.70              |
| 1:H:217:SER:HA   | 1:H:320:ALA:O    | 1.91                     | 0.70              |
| 1:K:223:ALA:HB1  | 1:K:225:LYS:HD2  | 1.73                     | 0.70              |
| 1:J:243:ALA:HB2  | 1:K:256:GLY:O    | 1.90                     | 0.70              |
| 1:H:301:ILE:HD12 | 1:H:312:ALA:HB2  | 1.65                     | 0.70              |
| 1:J:23:LEU:HD13  | 1:J:60:ILE:HD12  | 1.70                     | 0.70              |
| 1:B:162:ILE:HD13 | 1:B:400:LEU:CA   | 2.20                     | 0.70              |
| 1:B:195:PHE:CE1  | 1:B:330:THR:HB   | 2.26                     | 0.70              |
| 2:C:1525:PO4:P   | 4:C:1527:ATP:O1G | 2.50                     | 0.70              |
| 1:K:138:CYS:H    | 1:K:410:GLY:HA2  | 1.52                     | 0.70              |
| 1:B:200:LEU:CB   | 1:B:259:LEU:HD13 | 2.22                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:1525:PO4:P   | 4:D:1527:ATP:O1G | 2.49                     | 0.70              |
| 1:C:200:LEU:CB   | 1:C:259:LEU:HD13 | 2.22                     | 0.70              |
| 1:F:207:LYS:HE2  | 1:F:207:LYS:H    | 1.55                     | 0.70              |
| 1:H:223:ALA:HB1  | 1:H:225:LYS:HD2  | 1.73                     | 0.70              |
| 1:K:153:ASN:N    | 1:K:154:SER:HA   | 2.06                     | 0.70              |
| 1:N:223:ALA:O    | 1:N:251:ALA:HA   | 1.92                     | 0.70              |
| 1:A:220:ILE:HD12 | 1:A:296:THR:HG21 | 1.74                     | 0.70              |
| 1:A:200:LEU:CB   | 1:A:259:LEU:HD13 | 2.22                     | 0.70              |
| 2:F:1525:PO4:P   | 4:F:1527:ATP:O1G | 2.49                     | 0.70              |
| 1:H:153:ASN:N    | 1:H:154:SER:HA   | 2.06                     | 0.70              |
| 1:D:199:TYR:HB3  | 1:D:325:ILE:CD1  | 2.16                     | 0.70              |
| 1:F:200:LEU:CB   | 1:F:259:LEU:HD13 | 2.22                     | 0.70              |
| 1:I:223:ALA:O    | 1:I:251:ALA:HA   | 1.92                     | 0.70              |
| 1:G:162:ILE:HD13 | 1:G:400:LEU:CA   | 2.20                     | 0.70              |
| 1:N:153:ASN:N    | 1:N:154:SER:HA   | 2.06                     | 0.70              |
| 1:N:217:SER:HA   | 1:N:320:ALA:O    | 1.91                     | 0.70              |
| 2:A:1525:PO4:P   | 4:A:1527:ATP:O1G | 2.50                     | 0.69              |
| 1:G:309:LEU:HD22 | 1:G:312:ALA:HB3  | 1.74                     | 0.69              |
| 1:K:192:GLY:O    | 1:K:375:GLY:HA2  | 1.92                     | 0.69              |
| 1:K:52:ASP:OD1   | 2:K:1525:PO4:P   | 2.50                     | 0.69              |
| 1:L:223:ALA:O    | 1:L:251:ALA:HA   | 1.92                     | 0.69              |
| 1:A:309:LEU:HD22 | 1:A:312:ALA:HB3  | 1.74                     | 0.69              |
| 1:C:192:GLY:HA3  | 1:C:376:VAL:HG23 | 1.73                     | 0.69              |
| 1:G:220:ILE:HD12 | 1:G:296:THR:HG21 | 1.74                     | 0.69              |
| 1:I:243:ALA:HB2  | 1:J:256:GLY:O    | 1.90                     | 0.69              |
| 1:K:223:ALA:O    | 1:K:251:ALA:HA   | 1.92                     | 0.69              |
| 1:L:242:LYS:HB2  | 1:M:257:GLU:O    | 1.92                     | 0.69              |
| 1:N:52:ASP:OD1   | 2:N:1525:PO4:P   | 2.50                     | 0.69              |
| 1:B:220:ILE:HD12 | 1:B:296:THR:HG21 | 1.74                     | 0.69              |
| 1:C:309:LEU:HD22 | 1:C:312:ALA:HB3  | 1.74                     | 0.69              |
| 2:E:1525:PO4:P   | 4:E:1527:ATP:O1G | 2.50                     | 0.69              |
| 1:L:52:ASP:OD1   | 2:L:1525:PO4:P   | 2.50                     | 0.69              |
| 1:M:153:ASN:N    | 1:M:154:SER:HA   | 2.06                     | 0.69              |
| 1:D:200:LEU:CB   | 1:D:259:LEU:HD13 | 2.22                     | 0.69              |
| 1:E:200:LEU:CB   | 1:E:259:LEU:HD13 | 2.22                     | 0.69              |
| 1:I:217:SER:HA   | 1:I:320:ALA:O    | 1.91                     | 0.69              |
| 1:J:217:SER:HA   | 1:J:320:ALA:O    | 1.91                     | 0.69              |
| 2:B:1525:PO4:P   | 4:B:1527:ATP:O1G | 2.50                     | 0.69              |
| 1:D:309:LEU:HD22 | 1:D:312:ALA:HB3  | 1.74                     | 0.69              |
| 1:E:202:PRO:O    | 1:E:205:ILE:HG13 | 1.92                     | 0.69              |
| 1:F:309:LEU:HD22 | 1:F:312:ALA:HB3  | 1.74                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:249:ILE:CD1  | 1:G:262:LEU:CG   | 2.67                     | 0.69              |
| 1:I:52:ASP:OD1   | 2:I:1525:PO4:P   | 2.50                     | 0.69              |
| 1:M:52:ASP:OD1   | 2:M:1525:PO4:P   | 2.50                     | 0.69              |
| 1:B:309:LEU:HD22 | 1:B:312:ALA:HB3  | 1.75                     | 0.69              |
| 1:D:249:ILE:CD1  | 1:D:262:LEU:CG   | 2.67                     | 0.69              |
| 1:L:223:ALA:HB2  | 1:L:309:LEU:CD2  | 2.20                     | 0.69              |
| 2:G:1525:PO4:P   | 4:G:1527:ATP:O1G | 2.50                     | 0.69              |
| 1:H:23:LEU:HD13  | 1:H:60:ILE:HD12  | 1.71                     | 0.69              |
| 1:L:153:ASN:N    | 1:L:154:SER:HA   | 2.06                     | 0.69              |
| 1:M:217:SER:HA   | 1:M:320:ALA:O    | 1.91                     | 0.69              |
| 1:E:309:LEU:HD22 | 1:E:312:ALA:HB3  | 1.74                     | 0.69              |
| 1:J:223:ALA:O    | 1:J:251:ALA:HA   | 1.92                     | 0.69              |
| 1:L:137:PRO:HA   | 1:L:410:GLY:CA   | 2.23                     | 0.69              |
| 1:M:223:ALA:O    | 1:M:251:ALA:HA   | 1.92                     | 0.69              |
| 1:H:223:ALA:O    | 1:H:251:ALA:HA   | 1.92                     | 0.69              |
| 1:J:153:ASN:N    | 1:J:154:SER:HA   | 2.06                     | 0.69              |
| 1:H:257:GLU:O    | 1:N:242:LYS:HB2  | 1.93                     | 0.69              |
| 1:J:242:LYS:HB2  | 1:K:257:GLU:O    | 1.93                     | 0.69              |
| 1:A:270:ILE:HG22 | 1:A:271:VAL:HG23 | 1.75                     | 0.69              |
| 1:C:220:ILE:HD12 | 1:C:296:THR:HG21 | 1.74                     | 0.69              |
| 1:H:52:ASP:OD1   | 2:H:1525:PO4:P   | 2.50                     | 0.69              |
| 1:K:217:SER:HA   | 1:K:320:ALA:O    | 1.91                     | 0.69              |
| 1:L:217:SER:HA   | 1:L:320:ALA:O    | 1.91                     | 0.69              |
| 1:M:223:ALA:HB2  | 1:M:309:LEU:CD2  | 2.20                     | 0.69              |
| 1:M:36:ARG:C     | 1:N:518:GLU:CA   | 2.62                     | 0.69              |
| 1:I:36:ARG:C     | 1:J:518:GLU:CA   | 2.62                     | 0.68              |
| 1:K:177:VAL:HG22 | 1:K:379:ILE:CG2  | 2.23                     | 0.68              |
| 1:L:37:ASN:N     | 1:M:518:GLU:CA   | 2.36                     | 0.68              |
| 1:B:270:ILE:HG22 | 1:B:271:VAL:HG23 | 1.76                     | 0.68              |
| 1:K:36:ARG:C     | 1:L:518:GLU:CA   | 2.62                     | 0.68              |
| 1:N:223:ALA:HB2  | 1:N:309:LEU:CD2  | 2.20                     | 0.68              |
| 1:E:249:ILE:CD1  | 1:E:262:LEU:CG   | 2.67                     | 0.68              |
| 1:G:193:MET:CG   | 1:G:295:LEU:HG   | 2.22                     | 0.68              |
| 1:H:518:GLU:CA   | 1:N:36:ARG:C     | 2.62                     | 0.68              |
| 1:I:153:ASN:N    | 1:I:154:SER:HA   | 2.06                     | 0.68              |
| 1:K:137:PRO:HA   | 1:K:410:GLY:CA   | 2.23                     | 0.68              |
| 1:L:23:LEU:HD13  | 1:L:60:ILE:HD12  | 1.71                     | 0.68              |
| 1:C:270:ILE:HG22 | 1:C:271:VAL:HG23 | 1.75                     | 0.68              |
| 1:F:220:ILE:HD12 | 1:F:296:THR:HG21 | 1.74                     | 0.68              |
| 1:G:183:LEU:HA   | 1:G:383:ALA:H    | 1.59                     | 0.68              |
| 1:G:270:ILE:HG22 | 1:G:271:VAL:HG23 | 1.76                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:52:ASP:OD1   | 2:J:1525:PO4:P   | 2.50                     | 0.68              |
| 1:K:223:ALA:HB2  | 1:K:309:LEU:CD2  | 2.21                     | 0.68              |
| 1:D:220:ILE:HD12 | 1:D:296:THR:HG21 | 1.74                     | 0.68              |
| 1:E:220:ILE:HD12 | 1:E:296:THR:HG21 | 1.74                     | 0.68              |
| 1:H:169:VAL:HG23 | 1:H:170:GLY:O    | 1.93                     | 0.68              |
| 1:A:183:LEU:HA   | 1:A:383:ALA:H    | 1.59                     | 0.68              |
| 1:F:183:LEU:HA   | 1:F:383:ALA:H    | 1.59                     | 0.68              |
| 1:H:137:PRO:HA   | 1:H:410:GLY:CA   | 2.23                     | 0.68              |
| 1:I:242:LYS:HB2  | 1:J:257:GLU:O    | 1.93                     | 0.68              |
| 1:M:178:GLU:O    | 1:M:380:LYS:HA   | 1.94                     | 0.68              |
| 1:N:137:PRO:HA   | 1:N:410:GLY:CA   | 2.23                     | 0.68              |
| 1:G:193:MET:CE   | 1:G:296:THR:HG23 | 2.24                     | 0.68              |
| 1:I:178:GLU:O    | 1:I:380:LYS:HA   | 1.94                     | 0.68              |
| 1:K:178:GLU:O    | 1:K:380:LYS:HA   | 1.94                     | 0.68              |
| 1:L:178:GLU:O    | 1:L:380:LYS:HA   | 1.94                     | 0.68              |
| 1:M:223:ALA:HB1  | 1:M:225:LYS:HD2  | 1.76                     | 0.68              |
| 1:N:223:ALA:HB1  | 1:N:225:LYS:HD2  | 1.76                     | 0.68              |
| 1:E:183:LEU:HA   | 1:E:383:ALA:H    | 1.59                     | 0.68              |
| 1:I:137:PRO:HA   | 1:I:410:GLY:CA   | 2.23                     | 0.68              |
| 1:J:168:LYS:CG   | 1:J:187:LEU:HD21 | 2.24                     | 0.68              |
| 1:H:203:TYR:CD1  | 1:H:267:MET:SD   | 2.88                     | 0.67              |
| 1:I:169:VAL:HG23 | 1:I:170:GLY:O    | 1.93                     | 0.67              |
| 1:J:169:VAL:HG23 | 1:J:170:GLY:O    | 1.93                     | 0.67              |
| 1:J:137:PRO:HA   | 1:J:410:GLY:CA   | 2.23                     | 0.67              |
| 1:I:203:TYR:CD1  | 1:I:267:MET:SD   | 2.87                     | 0.67              |
| 1:L:223:ALA:HB1  | 1:L:225:LYS:HD2  | 1.76                     | 0.67              |
| 1:B:183:LEU:HA   | 1:B:383:ALA:H    | 1.59                     | 0.67              |
| 1:D:183:LEU:HA   | 1:D:383:ALA:H    | 1.59                     | 0.67              |
| 1:F:270:ILE:HG22 | 1:F:271:VAL:HG23 | 1.75                     | 0.67              |
| 1:G:312:ALA:HB1  | 1:G:316:ASP:CG   | 2.15                     | 0.67              |
| 1:J:223:ALA:HB2  | 1:J:309:LEU:CD2  | 2.22                     | 0.67              |
| 1:K:169:VAL:HG23 | 1:K:170:GLY:O    | 1.93                     | 0.67              |
| 1:M:137:PRO:HA   | 1:M:410:GLY:CA   | 2.23                     | 0.67              |
| 1:N:203:TYR:CD1  | 1:N:267:MET:SD   | 2.87                     | 0.67              |
| 1:D:270:ILE:HG22 | 1:D:271:VAL:HG23 | 1.75                     | 0.67              |
| 1:H:36:ARG:C     | 1:I:518:GLU:CA   | 2.62                     | 0.67              |
| 1:L:169:VAL:HG23 | 1:L:170:GLY:O    | 1.93                     | 0.67              |
| 1:G:227:ILE:HB   | 1:G:258:ALA:HB2  | 1.77                     | 0.67              |
| 1:K:203:TYR:CD1  | 1:K:267:MET:SD   | 2.87                     | 0.67              |
| 1:K:243:ALA:HA   | 1:L:260:ALA:HB2  | 1.77                     | 0.67              |
| 1:M:169:VAL:HG23 | 1:M:170:GLY:O    | 1.93                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:162:ILE:HD13 | 1:A:400:LEU:HA   | 1.77                     | 0.67              |
| 1:A:249:ILE:CD1  | 1:A:262:LEU:CG   | 2.67                     | 0.67              |
| 1:C:183:LEU:HA   | 1:C:383:ALA:H    | 1.59                     | 0.67              |
| 1:G:162:ILE:HD13 | 1:G:400:LEU:HA   | 1.77                     | 0.67              |
| 1:A:227:ILE:HB   | 1:A:258:ALA:HB2  | 1.77                     | 0.67              |
| 1:B:227:ILE:HB   | 1:B:258:ALA:HB2  | 1.77                     | 0.67              |
| 1:E:162:ILE:HD13 | 1:E:400:LEU:HA   | 1.77                     | 0.67              |
| 1:H:243:ALA:HA   | 1:I:260:ALA:HB2  | 1.77                     | 0.67              |
| 1:H:178:GLU:O    | 1:H:380:LYS:HA   | 1.94                     | 0.67              |
| 1:N:178:GLU:O    | 1:N:380:LYS:HA   | 1.94                     | 0.67              |
| 1:E:270:ILE:HG22 | 1:E:271:VAL:HG23 | 1.75                     | 0.67              |
| 1:H:223:ALA:HB2  | 1:H:309:LEU:CD2  | 2.21                     | 0.67              |
| 1:B:312:ALA:HB1  | 1:B:316:ASP:CG   | 2.15                     | 0.67              |
| 1:C:227:ILE:HB   | 1:C:258:ALA:HB2  | 1.77                     | 0.67              |
| 1:F:312:ALA:HB1  | 1:F:316:ASP:CG   | 2.15                     | 0.67              |
| 1:L:243:ALA:CA   | 1:M:256:GLY:O    | 2.43                     | 0.67              |
| 1:B:194:GLN:CG   | 1:B:329:THR:HG21 | 2.25                     | 0.67              |
| 1:B:193:MET:CE   | 1:B:332:ILE:HD12 | 2.18                     | 0.67              |
| 1:C:249:ILE:CD1  | 1:C:262:LEU:CG   | 2.67                     | 0.67              |
| 1:C:312:ALA:HB1  | 1:C:316:ASP:CG   | 2.15                     | 0.67              |
| 1:D:213:VAL:HG13 | 1:D:325:ILE:HG12 | 1.76                     | 0.67              |
| 1:E:312:ALA:HB1  | 1:E:316:ASP:CG   | 2.15                     | 0.67              |
| 1:L:203:TYR:CD1  | 1:L:267:MET:SD   | 2.87                     | 0.67              |
| 1:M:203:TYR:CD1  | 1:M:267:MET:SD   | 2.87                     | 0.67              |
| 1:J:36:ARG:C     | 1:K:518:GLU:CA   | 2.62                     | 0.66              |
| 1:F:162:ILE:HD13 | 1:F:400:LEU:HA   | 1.77                     | 0.66              |
| 1:F:227:ILE:HB   | 1:F:258:ALA:HB2  | 1.77                     | 0.66              |
| 1:F:213:VAL:HG13 | 1:F:325:ILE:HG12 | 1.77                     | 0.66              |
| 1:H:256:GLY:O    | 1:N:243:ALA:CA   | 2.43                     | 0.66              |
| 1:H:295:LEU:HD23 | 1:H:342:ILE:HD13 | 1.78                     | 0.66              |
| 1:N:295:LEU:HD23 | 1:N:342:ILE:HD13 | 1.77                     | 0.66              |
| 1:B:271:VAL:HG12 | 1:B:273:VAL:CG2  | 2.26                     | 0.66              |
| 1:B:162:ILE:HD13 | 1:B:400:LEU:HA   | 1.77                     | 0.66              |
| 1:D:162:ILE:HD13 | 1:D:400:LEU:HA   | 1.77                     | 0.66              |
| 1:E:279:PRO:O    | 1:E:285:ARG:HA   | 1.95                     | 0.66              |
| 1:F:279:PRO:O    | 1:F:285:ARG:HA   | 1.95                     | 0.66              |
| 1:I:223:ALA:HB2  | 1:I:309:LEU:CD2  | 2.22                     | 0.66              |
| 1:J:203:TYR:CD1  | 1:J:267:MET:SD   | 2.87                     | 0.66              |
| 1:K:243:ALA:CA   | 1:L:256:GLY:O    | 2.43                     | 0.66              |
| 1:L:36:ARG:C     | 1:M:518:GLU:CA   | 2.62                     | 0.66              |
| 1:A:271:VAL:HG12 | 1:A:273:VAL:CG2  | 2.26                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:312:ALA:HB1  | 1:A:316:ASP:CG   | 2.15                     | 0.66              |
| 1:D:227:ILE:HB   | 1:D:258:ALA:HB2  | 1.77                     | 0.66              |
| 1:M:243:ALA:CA   | 1:N:256:GLY:O    | 2.43                     | 0.66              |
| 1:C:271:VAL:HG12 | 1:C:273:VAL:CG2  | 2.26                     | 0.66              |
| 1:C:279:PRO:O    | 1:C:285:ARG:HA   | 1.95                     | 0.66              |
| 1:D:271:VAL:HG12 | 1:D:273:VAL:CG2  | 2.26                     | 0.66              |
| 1:D:312:ALA:HB1  | 1:D:316:ASP:CG   | 2.15                     | 0.66              |
| 1:E:271:VAL:HG12 | 1:E:273:VAL:CG2  | 2.26                     | 0.66              |
| 1:G:213:VAL:HG13 | 1:G:325:ILE:HG12 | 1.76                     | 0.66              |
| 1:H:243:ALA:CA   | 1:I:256:GLY:O    | 2.43                     | 0.66              |
| 1:N:206:ASN:CA   | 1:N:207:LYS:HG2  | 2.24                     | 0.66              |
| 1:A:200:LEU:HB2  | 1:A:259:LEU:CD1  | 2.25                     | 0.66              |
| 1:E:227:ILE:HB   | 1:E:258:ALA:HB2  | 1.77                     | 0.66              |
| 1:F:271:VAL:HG12 | 1:F:273:VAL:CG2  | 2.26                     | 0.66              |
| 1:G:271:VAL:HG12 | 1:G:273:VAL:CG2  | 2.26                     | 0.66              |
| 1:H:199:TYR:CE1  | 1:H:202:PRO:HA   | 2.31                     | 0.66              |
| 1:K:223:ALA:CB   | 1:K:309:LEU:HD21 | 2.25                     | 0.66              |
| 1:D:200:LEU:HB2  | 1:D:259:LEU:CD1  | 2.25                     | 0.66              |
| 1:B:249:ILE:CD1  | 1:B:262:LEU:CG   | 2.67                     | 0.66              |
| 1:E:200:LEU:HB2  | 1:E:259:LEU:CD1  | 2.25                     | 0.66              |
| 1:B:213:VAL:HG13 | 1:B:325:ILE:HG12 | 1.76                     | 0.66              |
| 1:C:162:ILE:HD13 | 1:C:400:LEU:HA   | 1.77                     | 0.66              |
| 1:I:295:LEU:HD23 | 1:I:342:ILE:HD13 | 1.78                     | 0.66              |
| 1:B:200:LEU:HB2  | 1:B:259:LEU:CD1  | 2.26                     | 0.65              |
| 1:B:279:PRO:O    | 1:B:285:ARG:HA   | 1.95                     | 0.65              |
| 1:D:279:PRO:O    | 1:D:285:ARG:HA   | 1.95                     | 0.65              |
| 1:E:195:PHE:CE2  | 1:E:292:ILE:HD13 | 2.31                     | 0.65              |
| 1:G:279:PRO:O    | 1:G:285:ARG:HA   | 1.95                     | 0.65              |
| 1:K:27:VAL:HG12  | 1:K:90:THR:HG23  | 1.78                     | 0.65              |
| 1:I:243:ALA:CA   | 1:J:256:GLY:O    | 2.43                     | 0.65              |
| 1:L:27:VAL:HG12  | 1:L:90:THR:HG23  | 1.78                     | 0.65              |
| 1:E:213:VAL:HG13 | 1:E:325:ILE:HG12 | 1.76                     | 0.65              |
| 1:H:149:THR:O    | 1:H:154:SER:HA   | 1.97                     | 0.65              |
| 1:I:249:ILE:O    | 1:I:275:ALA:HA   | 1.97                     | 0.65              |
| 1:J:27:VAL:HG12  | 1:J:90:THR:HG23  | 1.78                     | 0.65              |
| 1:J:243:ALA:CA   | 1:K:256:GLY:O    | 2.43                     | 0.65              |
| 1:L:149:THR:O    | 1:L:154:SER:HA   | 1.97                     | 0.65              |
| 1:M:249:ILE:O    | 1:M:275:ALA:HA   | 1.97                     | 0.65              |
| 1:A:162:ILE:HD13 | 1:A:400:LEU:N    | 2.12                     | 0.65              |
| 1:B:162:ILE:HD13 | 1:B:400:LEU:N    | 2.12                     | 0.65              |
| 1:G:193:MET:SD   | 1:G:295:LEU:HG   | 2.36                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:149:THR:O    | 1:K:154:SER:HA   | 1.97                     | 0.65              |
| 1:H:249:ILE:O    | 1:H:275:ALA:HA   | 1.97                     | 0.65              |
| 1:J:249:ILE:O    | 1:J:275:ALA:HA   | 1.97                     | 0.65              |
| 1:C:200:LEU:HB2  | 1:C:259:LEU:CD1  | 2.26                     | 0.65              |
| 1:F:200:LEU:HB2  | 1:F:259:LEU:CD1  | 2.25                     | 0.65              |
| 1:J:149:THR:O    | 1:J:154:SER:HA   | 1.97                     | 0.65              |
| 1:K:249:ILE:O    | 1:K:275:ALA:HA   | 1.97                     | 0.65              |
| 1:M:295:LEU:HD23 | 1:M:342:ILE:HD13 | 1.78                     | 0.65              |
| 1:A:279:PRO:O    | 1:A:285:ARG:HA   | 1.95                     | 0.65              |
| 1:J:295:LEU:HD23 | 1:J:342:ILE:HD13 | 1.78                     | 0.65              |
| 1:M:223:ALA:CB   | 1:M:309:LEU:HD21 | 2.23                     | 0.65              |
| 1:C:195:PHE:CE2  | 1:C:292:ILE:HD13 | 2.31                     | 0.65              |
| 1:M:149:THR:O    | 1:M:154:SER:HA   | 1.97                     | 0.65              |
| 1:A:195:PHE:CE2  | 1:A:292:ILE:HD13 | 2.31                     | 0.65              |
| 1:D:195:PHE:CE2  | 1:D:292:ILE:HD13 | 2.31                     | 0.65              |
| 1:G:161:LEU:HD11 | 1:G:185:ASP:HB3  | 1.79                     | 0.65              |
| 1:G:195:PHE:CE2  | 1:G:292:ILE:HD13 | 2.31                     | 0.65              |
| 1:I:27:VAL:HG12  | 1:I:90:THR:HG23  | 1.78                     | 0.65              |
| 1:D:223:ALA:HA   | 1:D:309:LEU:HD23 | 1.79                     | 0.64              |
| 1:I:23:LEU:HD13  | 1:I:60:ILE:HD12  | 1.70                     | 0.64              |
| 1:J:168:LYS:HG3  | 1:J:187:LEU:HD21 | 1.78                     | 0.64              |
| 1:C:162:ILE:HD13 | 1:C:400:LEU:N    | 2.12                     | 0.64              |
| 1:M:27:VAL:HG12  | 1:M:90:THR:HG23  | 1.78                     | 0.64              |
| 1:N:149:THR:O    | 1:N:154:SER:HA   | 1.97                     | 0.64              |
| 1:C:223:ALA:HA   | 1:C:309:LEU:HD23 | 1.79                     | 0.64              |
| 1:K:223:ALA:HB3  | 1:K:251:ALA:CB   | 2.25                     | 0.64              |
| 1:E:162:ILE:HD13 | 1:E:400:LEU:N    | 2.12                     | 0.64              |
| 1:L:249:ILE:O    | 1:L:275:ALA:HA   | 1.97                     | 0.64              |
| 1:M:223:ALA:HB3  | 1:M:251:ALA:CB   | 2.26                     | 0.64              |
| 1:N:223:ALA:CB   | 1:N:309:LEU:HD21 | 2.23                     | 0.64              |
| 1:B:197:ARG:HG3  | 1:B:198:GLY:O    | 1.97                     | 0.64              |
| 1:E:223:ALA:HA   | 1:E:309:LEU:HD23 | 1.79                     | 0.64              |
| 1:L:223:ALA:CB   | 1:L:309:LEU:HD21 | 2.23                     | 0.64              |
| 1:G:162:ILE:HD13 | 1:G:400:LEU:N    | 2.12                     | 0.64              |
| 1:M:301:ILE:HD11 | 1:M:316:ASP:OD2  | 1.98                     | 0.64              |
| 1:N:202:PRO:O    | 1:N:205:ILE:HG13 | 1.98                     | 0.64              |
| 1:C:213:VAL:HG13 | 1:C:325:ILE:HG12 | 1.76                     | 0.64              |
| 1:J:202:PRO:O    | 1:J:205:ILE:HG13 | 1.98                     | 0.64              |
| 1:L:202:PRO:O    | 1:L:205:ILE:HG13 | 1.98                     | 0.64              |
| 1:L:223:ALA:HB3  | 1:L:251:ALA:CB   | 2.26                     | 0.64              |
| 1:L:295:LEU:HD23 | 1:L:342:ILE:HD13 | 1.78                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:301:ILE:HD11 | 1:L:316:ASP:OD2  | 1.97                     | 0.64              |
| 1:A:223:ALA:HA   | 1:A:309:LEU:HD23 | 1.79                     | 0.64              |
| 1:D:162:ILE:HD13 | 1:D:400:LEU:N    | 2.12                     | 0.64              |
| 1:G:202:PRO:O    | 1:G:205:ILE:HG13 | 1.98                     | 0.64              |
| 1:J:223:ALA:CB   | 1:J:309:LEU:HD21 | 2.26                     | 0.64              |
| 1:K:295:LEU:HD23 | 1:K:342:ILE:HD13 | 1.77                     | 0.64              |
| 1:G:223:ALA:HA   | 1:G:309:LEU:HD23 | 1.79                     | 0.64              |
| 1:J:223:ALA:HB3  | 1:J:251:ALA:CB   | 2.25                     | 0.64              |
| 1:K:301:ILE:HD11 | 1:K:316:ASP:OD2  | 1.98                     | 0.64              |
| 1:K:295:LEU:HA   | 1:K:342:ILE:CD1  | 2.27                     | 0.64              |
| 1:N:249:ILE:O    | 1:N:275:ALA:HA   | 1.97                     | 0.64              |
| 1:N:27:VAL:HG12  | 1:N:90:THR:HG23  | 1.78                     | 0.64              |
| 1:C:221:LEU:HD11 | 1:C:309:LEU:HD21 | 1.80                     | 0.64              |
| 2:H:1525:PO4:P   | 4:H:1527:ATP:O3G | 2.56                     | 0.64              |
| 1:H:27:VAL:HG12  | 1:H:90:THR:HG23  | 1.78                     | 0.64              |
| 1:A:227:ILE:HD12 | 1:A:258:ALA:CB   | 2.29                     | 0.63              |
| 1:B:223:ALA:HA   | 1:B:309:LEU:HD23 | 1.79                     | 0.63              |
| 1:C:202:PRO:O    | 1:C:205:ILE:HG13 | 1.98                     | 0.63              |
| 1:D:221:LEU:HD11 | 1:D:309:LEU:HD21 | 1.80                     | 0.63              |
| 1:F:162:ILE:HD13 | 1:F:400:LEU:N    | 2.12                     | 0.63              |
| 1:I:149:THR:O    | 1:I:154:SER:HA   | 1.97                     | 0.63              |
| 1:I:202:PRO:O    | 1:I:205:ILE:HG13 | 1.98                     | 0.63              |
| 1:K:23:LEU:HD13  | 1:K:60:ILE:HD12  | 1.71                     | 0.63              |
| 1:N:223:ALA:HB3  | 1:N:251:ALA:CB   | 2.26                     | 0.63              |
| 1:N:295:LEU:HA   | 1:N:342:ILE:CD1  | 2.27                     | 0.63              |
| 1:G:200:LEU:HD13 | 1:G:254:VAL:HG11 | 1.79                     | 0.63              |
| 1:H:295:LEU:HA   | 1:H:342:ILE:CD1  | 2.27                     | 0.63              |
| 1:J:295:LEU:HA   | 1:J:342:ILE:CD1  | 2.27                     | 0.63              |
| 2:L:1525:PO4:P   | 4:L:1527:ATP:O3G | 2.56                     | 0.63              |
| 2:M:1525:PO4:P   | 4:M:1527:ATP:O3G | 2.56                     | 0.63              |
| 1:M:295:LEU:HA   | 1:M:342:ILE:CD1  | 2.27                     | 0.63              |
| 2:N:1525:PO4:P   | 4:N:1527:ATP:O3G | 2.56                     | 0.63              |
| 1:B:202:PRO:O    | 1:B:205:ILE:HG13 | 1.98                     | 0.63              |
| 1:G:221:LEU:HD11 | 1:G:309:LEU:HD21 | 1.80                     | 0.63              |
| 1:H:301:ILE:HD11 | 1:H:316:ASP:OD2  | 1.99                     | 0.63              |
| 2:K:1525:PO4:P   | 4:K:1527:ATP:O3G | 2.56                     | 0.63              |
| 1:L:221:LEU:HA   | 1:L:317:LEU:HG   | 1.80                     | 0.63              |
| 1:A:199:TYR:CB   | 1:A:325:ILE:HD11 | 2.21                     | 0.63              |
| 1:F:221:LEU:HD11 | 1:F:309:LEU:HD21 | 1.80                     | 0.63              |
| 1:M:202:PRO:O    | 1:M:205:ILE:HG13 | 1.98                     | 0.63              |
| 1:M:242:LYS:CB   | 1:N:257:GLU:HA   | 2.27                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:221:LEU:HD11 | 1:B:309:LEU:HD21 | 1.80                     | 0.63              |
| 1:F:223:ALA:HA   | 1:F:309:LEU:HD23 | 1.79                     | 0.63              |
| 1:F:227:ILE:HD12 | 1:F:258:ALA:CB   | 2.29                     | 0.63              |
| 1:N:221:LEU:HA   | 1:N:317:LEU:HG   | 1.79                     | 0.63              |
| 1:N:196:ASP:OD1  | 1:N:329:THR:HG22 | 1.99                     | 0.63              |
| 1:D:227:ILE:HD12 | 1:D:258:ALA:CB   | 2.29                     | 0.63              |
| 1:H:202:PRO:O    | 1:H:205:ILE:HG13 | 1.98                     | 0.63              |
| 1:I:223:ALA:HB3  | 1:I:251:ALA:CB   | 2.25                     | 0.63              |
| 2:J:1525:PO4:P   | 4:J:1527:ATP:O3G | 2.56                     | 0.63              |
| 1:L:295:LEU:HA   | 1:L:342:ILE:CD1  | 2.27                     | 0.63              |
| 1:M:221:LEU:HA   | 1:M:317:LEU:HG   | 1.80                     | 0.63              |
| 1:N:301:ILE:HD11 | 1:N:316:ASP:OD2  | 1.98                     | 0.63              |
| 1:E:227:ILE:HD12 | 1:E:258:ALA:CB   | 2.29                     | 0.63              |
| 1:F:224:ASP:O    | 1:F:303:GLU:HB2  | 1.99                     | 0.63              |
| 1:G:227:ILE:HD12 | 1:G:258:ALA:CB   | 2.29                     | 0.63              |
| 1:C:145:ALA:HA   | 1:C:159:GLY:O    | 1.99                     | 0.63              |
| 1:D:197:ARG:HG3  | 1:D:198:GLY:O    | 1.99                     | 0.63              |
| 1:E:224:ASP:O    | 1:E:303:GLU:HB2  | 1.99                     | 0.63              |
| 1:D:145:ALA:HA   | 1:D:159:GLY:O    | 1.99                     | 0.63              |
| 1:D:224:ASP:O    | 1:D:303:GLU:HB2  | 1.99                     | 0.63              |
| 1:G:224:ASP:O    | 1:G:303:GLU:HB2  | 1.99                     | 0.63              |
| 1:H:223:ALA:HB3  | 1:H:251:ALA:CB   | 2.25                     | 0.63              |
| 1:I:301:ILE:HD11 | 1:I:316:ASP:OD2  | 1.98                     | 0.63              |
| 1:I:295:LEU:HA   | 1:I:342:ILE:CD1  | 2.27                     | 0.63              |
| 1:J:301:ILE:HD11 | 1:J:316:ASP:OD2  | 1.99                     | 0.63              |
| 1:K:202:PRO:O    | 1:K:205:ILE:HG13 | 1.98                     | 0.63              |
| 1:C:224:ASP:O    | 1:C:303:GLU:HB2  | 1.99                     | 0.62              |
| 1:E:145:ALA:HA   | 1:E:159:GLY:O    | 1.99                     | 0.62              |
| 1:I:149:THR:HA   | 1:I:155:ASP:O    | 1.99                     | 0.62              |
| 1:A:511:ALA:O    | 1:A:515:ILE:HG13 | 2.00                     | 0.62              |
| 1:B:227:ILE:HD12 | 1:B:258:ALA:CB   | 2.29                     | 0.62              |
| 1:D:202:PRO:O    | 1:D:205:ILE:HG13 | 1.98                     | 0.62              |
| 1:E:221:LEU:HD11 | 1:E:309:LEU:HD21 | 1.80                     | 0.62              |
| 1:K:203:TYR:CD1  | 1:K:267:MET:HE1  | 2.34                     | 0.62              |
| 1:N:149:THR:HA   | 1:N:155:ASP:O    | 2.00                     | 0.62              |
| 1:B:224:ASP:O    | 1:B:303:GLU:HB2  | 1.99                     | 0.62              |
| 1:C:227:ILE:HD12 | 1:C:258:ALA:CB   | 2.29                     | 0.62              |
| 1:E:511:ALA:O    | 1:E:515:ILE:HG13 | 2.00                     | 0.62              |
| 1:F:511:ALA:O    | 1:F:515:ILE:HG13 | 2.00                     | 0.62              |
| 1:G:511:ALA:O    | 1:G:515:ILE:HG13 | 2.00                     | 0.62              |
| 1:K:221:LEU:HA   | 1:K:317:LEU:HG   | 1.80                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:221:LEU:HD11 | 1:A:309:LEU:HD21 | 1.80                     | 0.62              |
| 1:B:145:ALA:HA   | 1:B:159:GLY:O    | 1.99                     | 0.62              |
| 1:I:223:ALA:CB   | 1:I:309:LEU:HD21 | 2.26                     | 0.62              |
| 1:J:192:GLY:O    | 1:J:375:GLY:HA2  | 1.99                     | 0.62              |
| 1:A:145:ALA:HA   | 1:A:159:GLY:O    | 1.99                     | 0.62              |
| 1:H:149:THR:HA   | 1:H:155:ASP:O    | 2.00                     | 0.62              |
| 1:N:240:VAL:CG2  | 1:N:317:LEU:HD22 | 2.30                     | 0.62              |
| 1:F:145:ALA:HA   | 1:F:159:GLY:O    | 1.99                     | 0.62              |
| 1:F:207:LYS:CE   | 1:F:207:LYS:H    | 2.12                     | 0.62              |
| 2:I:1525:PO4:P   | 4:I:1527:ATP:O3G | 2.56                     | 0.62              |
| 1:J:149:THR:HA   | 1:J:155:ASP:O    | 2.00                     | 0.62              |
| 1:J:151:SER:CB   | 1:J:399:ALA:HA   | 2.30                     | 0.62              |
| 1:M:149:THR:HA   | 1:M:155:ASP:O    | 2.00                     | 0.62              |
| 1:A:224:ASP:O    | 1:A:303:GLU:HB2  | 1.99                     | 0.62              |
| 1:B:511:ALA:O    | 1:B:515:ILE:HG13 | 2.00                     | 0.62              |
| 1:N:204:PHE:C    | 1:N:207:LYS:HE2  | 2.20                     | 0.62              |
| 1:C:511:ALA:O    | 1:C:515:ILE:HG13 | 2.00                     | 0.62              |
| 1:D:240:VAL:CG1  | 1:D:271:VAL:HG13 | 2.30                     | 0.62              |
| 1:G:145:ALA:HA   | 1:G:159:GLY:O    | 1.99                     | 0.62              |
| 1:G:240:VAL:CG1  | 1:G:271:VAL:HG13 | 2.30                     | 0.62              |
| 1:J:240:VAL:CG2  | 1:J:317:LEU:HD22 | 2.30                     | 0.62              |
| 1:K:72:GLN:HA    | 1:K:75:LYS:HD2   | 1.82                     | 0.62              |
| 1:L:192:GLY:O    | 1:L:375:GLY:HA2  | 1.99                     | 0.62              |
| 1:D:511:ALA:O    | 1:D:515:ILE:HG13 | 2.00                     | 0.62              |
| 1:M:240:VAL:CG2  | 1:M:317:LEU:HD22 | 2.30                     | 0.62              |
| 1:B:204:PHE:CE1  | 1:B:273:VAL:O    | 2.53                     | 0.61              |
| 1:E:240:VAL:CG1  | 1:E:271:VAL:HG13 | 2.30                     | 0.61              |
| 1:F:165:ALA:HB2  | 1:F:187:LEU:HD11 | 1.82                     | 0.61              |
| 1:F:240:VAL:CG1  | 1:F:271:VAL:HG13 | 2.30                     | 0.61              |
| 1:I:151:SER:CB   | 1:I:399:ALA:HA   | 2.30                     | 0.61              |
| 1:J:72:GLN:HA    | 1:J:75:LYS:HD2   | 1.82                     | 0.61              |
| 1:L:72:GLN:HA    | 1:L:75:LYS:HD2   | 1.82                     | 0.61              |
| 1:H:223:ALA:CB   | 1:H:309:LEU:HD21 | 2.25                     | 0.61              |
| 1:I:72:GLN:HA    | 1:I:75:LYS:HD2   | 1.82                     | 0.61              |
| 1:K:151:SER:CB   | 1:K:399:ALA:HA   | 2.30                     | 0.61              |
| 1:M:151:SER:CB   | 1:M:399:ALA:HA   | 2.30                     | 0.61              |
| 1:N:192:GLY:O    | 1:N:375:GLY:HA2  | 1.99                     | 0.61              |
| 1:N:151:SER:CB   | 1:N:399:ALA:HA   | 2.30                     | 0.61              |
| 1:C:204:PHE:CE1  | 1:C:273:VAL:O    | 2.53                     | 0.61              |
| 1:F:204:PHE:CE1  | 1:F:273:VAL:O    | 2.53                     | 0.61              |
| 1:H:192:GLY:O    | 1:H:375:GLY:HA2  | 1.99                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:151:SER:CB   | 1:L:399:ALA:HA   | 2.30                     | 0.61              |
| 1:H:151:SER:CB   | 1:H:399:ALA:HA   | 2.30                     | 0.61              |
| 1:B:240:VAL:CG1  | 1:B:271:VAL:HG13 | 2.30                     | 0.61              |
| 1:H:221:LEU:HA   | 1:H:317:LEU:HG   | 1.81                     | 0.61              |
| 1:H:72:GLN:HA    | 1:H:75:LYS:HD2   | 1.82                     | 0.61              |
| 1:K:177:VAL:HG22 | 1:K:379:ILE:CB   | 2.30                     | 0.61              |
| 1:K:240:VAL:CG2  | 1:K:317:LEU:HD22 | 2.30                     | 0.61              |
| 1:L:149:THR:HA   | 1:L:155:ASP:O    | 1.99                     | 0.61              |
| 1:L:240:VAL:CG2  | 1:L:317:LEU:HD22 | 2.30                     | 0.61              |
| 1:L:189:VAL:HA   | 1:L:377:ALA:HA   | 1.83                     | 0.61              |
| 1:D:169:VAL:HB   | 1:D:173:GLY:HA3  | 1.82                     | 0.61              |
| 1:I:192:GLY:O    | 1:I:375:GLY:HA2  | 1.99                     | 0.61              |
| 1:A:204:PHE:CE1  | 1:A:273:VAL:O    | 2.53                     | 0.61              |
| 1:H:189:VAL:HA   | 1:H:377:ALA:HA   | 1.83                     | 0.61              |
| 1:M:23:LEU:HD13  | 1:M:60:ILE:HD12  | 1.70                     | 0.61              |
| 1:E:169:VAL:HB   | 1:E:173:GLY:HA3  | 1.82                     | 0.61              |
| 1:G:204:PHE:CE1  | 1:G:273:VAL:O    | 2.53                     | 0.61              |
| 1:N:189:VAL:HA   | 1:N:377:ALA:HA   | 1.83                     | 0.61              |
| 1:C:169:VAL:HB   | 1:C:173:GLY:HA3  | 1.83                     | 0.61              |
| 1:D:204:PHE:CE1  | 1:D:273:VAL:O    | 2.53                     | 0.61              |
| 1:H:203:TYR:CD1  | 1:H:267:MET:HE1  | 2.36                     | 0.61              |
| 1:I:221:LEU:HA   | 1:I:317:LEU:HG   | 1.81                     | 0.61              |
| 1:J:221:LEU:HA   | 1:J:317:LEU:HG   | 1.80                     | 0.61              |
| 1:M:203:TYR:CD1  | 1:M:267:MET:HE1  | 2.36                     | 0.61              |
| 1:B:200:LEU:CD1  | 1:B:259:LEU:HD13 | 2.31                     | 0.61              |
| 1:E:220:ILE:HD13 | 1:E:332:ILE:CD1  | 2.27                     | 0.61              |
| 1:F:220:ILE:HD13 | 1:F:332:ILE:CD1  | 2.27                     | 0.61              |
| 1:K:189:VAL:HA   | 1:K:377:ALA:HA   | 1.83                     | 0.61              |
| 1:K:480:ALA:O    | 1:K:483:GLU:HG2  | 2.01                     | 0.61              |
| 1:M:192:GLY:O    | 1:M:375:GLY:HA2  | 1.99                     | 0.61              |
| 1:N:72:GLN:HA    | 1:N:75:LYS:HD2   | 1.82                     | 0.61              |
| 1:B:169:VAL:HB   | 1:B:173:GLY:HA3  | 1.82                     | 0.60              |
| 1:I:240:VAL:CG2  | 1:I:317:LEU:HD22 | 2.30                     | 0.60              |
| 1:K:149:THR:HA   | 1:K:155:ASP:O    | 2.00                     | 0.60              |
| 1:A:169:VAL:HB   | 1:A:173:GLY:HA3  | 1.82                     | 0.60              |
| 1:D:200:LEU:CD1  | 1:D:259:LEU:HD13 | 2.31                     | 0.60              |
| 1:H:240:VAL:HG22 | 1:H:317:LEU:HD22 | 1.84                     | 0.60              |
| 1:J:203:TYR:CD1  | 1:J:267:MET:HE1  | 2.35                     | 0.60              |
| 1:L:480:ALA:O    | 1:L:483:GLU:HG2  | 2.01                     | 0.60              |
| 1:M:72:GLN:HA    | 1:M:75:LYS:HD2   | 1.82                     | 0.60              |
| 1:N:480:ALA:O    | 1:N:483:GLU:HG2  | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:199:TYR:CB   | 1:B:325:ILE:HD11 | 2.21                     | 0.60              |
| 1:D:52:ASP:OD1   | 2:D:1525:PO4:P   | 2.60                     | 0.60              |
| 1:F:169:VAL:HB   | 1:F:173:GLY:HA3  | 1.83                     | 0.60              |
| 1:G:169:VAL:HB   | 1:G:173:GLY:HA3  | 1.82                     | 0.60              |
| 1:G:217:SER:HA   | 1:G:320:ALA:O    | 2.02                     | 0.60              |
| 1:H:240:VAL:CG2  | 1:H:317:LEU:HD22 | 2.30                     | 0.60              |
| 1:M:480:ALA:O    | 1:M:483:GLU:HG2  | 2.01                     | 0.60              |
| 1:I:240:VAL:HG22 | 1:I:317:LEU:HD22 | 1.84                     | 0.60              |
| 1:I:169:VAL:HG12 | 1:I:377:ALA:HB3  | 1.83                     | 0.60              |
| 1:J:189:VAL:HA   | 1:J:377:ALA:HA   | 1.83                     | 0.60              |
| 1:J:169:VAL:HG12 | 1:J:377:ALA:HB3  | 1.83                     | 0.60              |
| 1:A:217:SER:HA   | 1:A:320:ALA:O    | 2.02                     | 0.60              |
| 1:C:200:LEU:CD1  | 1:C:259:LEU:HD13 | 2.31                     | 0.60              |
| 1:C:240:VAL:CG1  | 1:C:271:VAL:HG13 | 2.30                     | 0.60              |
| 1:D:199:TYR:CB   | 1:D:325:ILE:HD11 | 2.20                     | 0.60              |
| 1:F:217:SER:HA   | 1:F:320:ALA:O    | 2.02                     | 0.60              |
| 1:L:203:TYR:CD1  | 1:L:267:MET:HE1  | 2.37                     | 0.60              |
| 1:A:240:VAL:CG1  | 1:A:271:VAL:HG13 | 2.30                     | 0.60              |
| 1:D:220:ILE:HD13 | 1:D:332:ILE:CD1  | 2.27                     | 0.60              |
| 1:E:200:LEU:CD1  | 1:E:259:LEU:HD13 | 2.31                     | 0.60              |
| 1:F:52:ASP:OD1   | 2:F:1525:PO4:P   | 2.60                     | 0.60              |
| 1:G:220:ILE:HD13 | 1:G:332:ILE:CD1  | 2.27                     | 0.60              |
| 1:K:192:GLY:HA3  | 1:K:332:ILE:O    | 2.02                     | 0.60              |
| 1:A:200:LEU:CD1  | 1:A:259:LEU:HD13 | 2.31                     | 0.60              |
| 1:H:480:ALA:O    | 1:H:483:GLU:HG2  | 2.01                     | 0.60              |
| 1:I:480:ALA:O    | 1:I:483:GLU:HG2  | 2.01                     | 0.60              |
| 1:B:52:ASP:OD1   | 2:B:1525:PO4:P   | 2.60                     | 0.60              |
| 1:F:200:LEU:CD1  | 1:F:259:LEU:HD13 | 2.31                     | 0.60              |
| 1:K:127:ALA:HB2  | 1:K:426:LEU:HD11 | 1.84                     | 0.60              |
| 1:A:200:LEU:HB3  | 1:A:259:LEU:HD22 | 1.84                     | 0.60              |
| 1:F:199:TYR:CB   | 1:F:325:ILE:HD11 | 2.21                     | 0.60              |
| 1:J:240:VAL:HG22 | 1:J:317:LEU:HD22 | 1.84                     | 0.60              |
| 1:M:193:MET:SD   | 1:M:292:ILE:HA   | 2.42                     | 0.60              |
| 1:N:240:VAL:HG22 | 1:N:317:LEU:HD22 | 1.83                     | 0.60              |
| 1:A:220:ILE:HD13 | 1:A:332:ILE:CD1  | 2.27                     | 0.59              |
| 1:B:220:ILE:HD13 | 1:B:332:ILE:CD1  | 2.27                     | 0.59              |
| 1:B:217:SER:HA   | 1:B:320:ALA:O    | 2.02                     | 0.59              |
| 1:J:193:MET:SD   | 1:J:292:ILE:HA   | 2.42                     | 0.59              |
| 1:M:127:ALA:HB2  | 1:M:426:LEU:HD11 | 1.84                     | 0.59              |
| 1:N:127:ALA:HB2  | 1:N:426:LEU:HD11 | 1.84                     | 0.59              |
| 1:C:220:ILE:HD13 | 1:C:332:ILE:CD1  | 2.27                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:127:ALA:HB2  | 1:J:426:LEU:HD11 | 1.84                     | 0.59              |
| 1:K:204:PHE:CD1  | 1:K:273:VAL:O    | 2.55                     | 0.59              |
| 1:L:127:ALA:HB2  | 1:L:426:LEU:HD11 | 1.84                     | 0.59              |
| 1:M:242:LYS:HB3  | 1:N:257:GLU:HA   | 1.83                     | 0.59              |
| 1:N:204:PHE:CD1  | 1:N:273:VAL:O    | 2.55                     | 0.59              |
| 1:D:200:LEU:HB3  | 1:D:259:LEU:HD22 | 1.84                     | 0.59              |
| 1:G:193:MET:HE1  | 1:G:296:THR:HG23 | 1.84                     | 0.59              |
| 1:J:204:PHE:CD1  | 1:J:273:VAL:O    | 2.55                     | 0.59              |
| 1:L:193:MET:SD   | 1:L:292:ILE:HA   | 2.42                     | 0.59              |
| 1:C:200:LEU:HB3  | 1:C:259:LEU:HD22 | 1.84                     | 0.59              |
| 1:E:217:SER:HA   | 1:E:320:ALA:O    | 2.02                     | 0.59              |
| 1:I:193:MET:SD   | 1:I:292:ILE:HA   | 2.42                     | 0.59              |
| 1:I:204:PHE:CD1  | 1:I:273:VAL:O    | 2.55                     | 0.59              |
| 1:L:174:VAL:HG12 | 1:L:376:VAL:HG13 | 1.83                     | 0.59              |
| 1:H:193:MET:SD   | 1:H:292:ILE:HA   | 2.42                     | 0.59              |
| 1:H:301:ILE:HD11 | 1:H:312:ALA:CB   | 2.32                     | 0.59              |
| 1:I:127:ALA:HB2  | 1:I:426:LEU:HD11 | 1.84                     | 0.59              |
| 1:J:192:GLY:HA3  | 1:J:332:ILE:O    | 2.03                     | 0.59              |
| 1:K:169:VAL:HG12 | 1:K:377:ALA:HB3  | 1.83                     | 0.59              |
| 1:K:240:VAL:HG22 | 1:K:317:LEU:HD22 | 1.83                     | 0.59              |
| 1:N:193:MET:SD   | 1:N:292:ILE:HA   | 2.42                     | 0.59              |
| 1:G:52:ASP:OD1   | 2:G:1525:PO4:P   | 2.61                     | 0.59              |
| 1:I:203:TYR:CD1  | 1:I:267:MET:HE1  | 2.37                     | 0.59              |
| 1:J:480:ALA:O    | 1:J:483:GLU:HG2  | 2.01                     | 0.59              |
| 1:L:204:PHE:CD1  | 1:L:273:VAL:O    | 2.55                     | 0.59              |
| 1:M:23:LEU:HD23  | 1:M:74:VAL:HG13  | 1.85                     | 0.59              |
| 1:M:204:PHE:CD1  | 1:M:273:VAL:O    | 2.55                     | 0.59              |
| 1:A:52:ASP:OD1   | 2:A:1525:PO4:P   | 2.61                     | 0.59              |
| 1:H:169:VAL:HG12 | 1:H:377:ALA:HB3  | 1.83                     | 0.59              |
| 1:H:127:ALA:HB2  | 1:H:426:LEU:HD11 | 1.84                     | 0.59              |
| 1:N:23:LEU:HD23  | 1:N:74:VAL:HG13  | 1.84                     | 0.59              |
| 1:H:23:LEU:HD23  | 1:H:74:VAL:HG13  | 1.84                     | 0.59              |
| 1:K:242:LYS:HG3  | 1:L:257:GLU:O    | 2.03                     | 0.59              |
| 1:L:192:GLY:HA3  | 1:L:332:ILE:O    | 2.03                     | 0.59              |
| 1:H:165:ALA:O    | 1:H:169:VAL:HG22 | 2.03                     | 0.59              |
| 1:H:204:PHE:CD1  | 1:H:273:VAL:O    | 2.55                     | 0.59              |
| 2:J:1525:PO4:P   | 4:J:1527:ATP:O1A | 2.61                     | 0.59              |
| 1:M:165:ALA:O    | 1:M:169:VAL:HG22 | 2.03                     | 0.59              |
| 1:M:240:VAL:HG22 | 1:M:317:LEU:HD22 | 1.83                     | 0.59              |
| 1:M:243:ALA:CB   | 1:N:256:GLY:O    | 2.51                     | 0.59              |
| 2:N:1525:PO4:P   | 4:N:1527:ATP:O1A | 2.61                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:199:TYR:CB   | 1:G:325:ILE:HD11 | 2.21                     | 0.59              |
| 1:L:165:ALA:O    | 1:L:169:VAL:HG22 | 2.03                     | 0.59              |
| 2:M:1525:PO4:P   | 4:M:1527:ATP:O1A | 2.61                     | 0.59              |
| 1:M:169:VAL:HG12 | 1:M:377:ALA:HB3  | 1.83                     | 0.59              |
| 1:M:420:ILE:HD12 | 1:M:451:LEU:HD13 | 1.85                     | 0.59              |
| 1:N:165:ALA:O    | 1:N:169:VAL:HG22 | 2.03                     | 0.59              |
| 1:E:52:ASP:OD1   | 2:E:1525:PO4:P   | 2.61                     | 0.58              |
| 1:H:298:GLY:HA3  | 1:H:318:GLY:HA3  | 1.86                     | 0.58              |
| 1:J:243:ALA:CB   | 1:K:256:GLY:O    | 2.51                     | 0.58              |
| 1:I:243:ALA:CB   | 1:J:256:GLY:O    | 2.51                     | 0.58              |
| 1:J:298:GLY:HA3  | 1:J:318:GLY:HA3  | 1.85                     | 0.58              |
| 1:K:165:ALA:O    | 1:K:169:VAL:HG22 | 2.03                     | 0.58              |
| 1:L:175:ILE:HG22 | 1:L:176:THR:N    | 2.17                     | 0.58              |
| 1:N:169:VAL:HG12 | 1:N:377:ALA:HB3  | 1.83                     | 0.58              |
| 1:H:256:GLY:O    | 1:N:243:ALA:CB   | 2.51                     | 0.58              |
| 1:M:242:LYS:HB3  | 1:N:257:GLU:CA   | 2.31                     | 0.58              |
| 1:B:195:PHE:CZ   | 1:B:330:THR:HB   | 2.38                     | 0.58              |
| 1:H:243:ALA:CB   | 1:I:256:GLY:O    | 2.51                     | 0.58              |
| 2:I:1525:PO4:P   | 4:I:1527:ATP:O1A | 2.61                     | 0.58              |
| 2:K:1525:PO4:P   | 4:K:1527:ATP:O1A | 2.61                     | 0.58              |
| 1:K:301:ILE:HD12 | 1:K:312:ALA:HB2  | 1.65                     | 0.58              |
| 2:L:1525:PO4:P   | 4:L:1527:ATP:O1A | 2.61                     | 0.58              |
| 1:L:240:VAL:HG22 | 1:L:317:LEU:HD22 | 1.84                     | 0.58              |
| 1:L:23:LEU:HD23  | 1:L:74:VAL:HG13  | 1.85                     | 0.58              |
| 1:N:192:GLY:HA3  | 1:N:332:ILE:O    | 2.03                     | 0.58              |
| 1:I:169:VAL:HB   | 1:I:173:GLY:HA3  | 1.85                     | 0.58              |
| 1:N:420:ILE:HD12 | 1:N:451:LEU:HD13 | 1.86                     | 0.58              |
| 1:C:52:ASP:OD1   | 2:C:1525:PO4:P   | 2.61                     | 0.58              |
| 1:G:221:LEU:HD13 | 1:G:236:VAL:HG21 | 1.86                     | 0.58              |
| 2:H:1525:PO4:P   | 4:H:1527:ATP:O1A | 2.61                     | 0.58              |
| 1:H:169:VAL:HB   | 1:H:173:GLY:HA3  | 1.85                     | 0.58              |
| 1:I:298:GLY:HA3  | 1:I:318:GLY:HA3  | 1.85                     | 0.58              |
| 1:J:169:VAL:HB   | 1:J:173:GLY:HA3  | 1.85                     | 0.58              |
| 1:N:203:TYR:CD1  | 1:N:267:MET:HE1  | 2.39                     | 0.58              |
| 1:A:221:LEU:HD13 | 1:A:236:VAL:HG21 | 1.86                     | 0.58              |
| 1:D:217:SER:HA   | 1:D:320:ALA:O    | 2.02                     | 0.58              |
| 1:E:199:TYR:CB   | 1:E:325:ILE:HD11 | 2.21                     | 0.58              |
| 1:G:200:LEU:N    | 1:G:200:LEU:CD1  | 2.64                     | 0.58              |
| 1:I:165:ALA:O    | 1:I:169:VAL:HG22 | 2.03                     | 0.58              |
| 1:K:298:GLY:HA3  | 1:K:318:GLY:HA3  | 1.86                     | 0.58              |
| 1:B:200:LEU:HB3  | 1:B:259:LEU:HD22 | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:199:TYR:CB   | 1:C:325:ILE:HD11 | 2.21                     | 0.58              |
| 1:E:200:LEU:HB3  | 1:E:259:LEU:HD22 | 1.84                     | 0.58              |
| 1:F:221:LEU:HD13 | 1:F:236:VAL:HG21 | 1.86                     | 0.58              |
| 1:F:200:LEU:HB3  | 1:F:259:LEU:HD22 | 1.84                     | 0.58              |
| 1:H:192:GLY:HA3  | 1:H:332:ILE:O    | 2.03                     | 0.58              |
| 1:L:152:ALA:HB3  | 1:L:155:ASP:H    | 1.69                     | 0.58              |
| 1:L:169:VAL:HG12 | 1:L:377:ALA:HB3  | 1.83                     | 0.58              |
| 1:L:420:ILE:HD12 | 1:L:451:LEU:HD13 | 1.86                     | 0.58              |
| 1:L:243:ALA:CB   | 1:M:256:GLY:O    | 2.51                     | 0.58              |
| 1:N:199:TYR:CB   | 1:N:325:ILE:HD11 | 2.34                     | 0.58              |
| 1:N:298:GLY:HA3  | 1:N:318:GLY:HA3  | 1.85                     | 0.58              |
| 1:E:193:MET:CE   | 1:E:332:ILE:HD12 | 2.19                     | 0.58              |
| 1:I:192:GLY:HA3  | 1:I:332:ILE:O    | 2.02                     | 0.58              |
| 1:J:162:ILE:HD13 | 1:J:400:LEU:CA   | 2.34                     | 0.58              |
| 1:C:217:SER:HA   | 1:C:320:ALA:O    | 2.02                     | 0.58              |
| 1:I:301:ILE:HD11 | 1:I:312:ALA:CB   | 2.32                     | 0.58              |
| 1:K:169:VAL:HB   | 1:K:173:GLY:HA3  | 1.85                     | 0.58              |
| 1:H:519:CYS:O    | 1:N:39:VAL:N     | 2.37                     | 0.58              |
| 1:G:200:LEU:HD11 | 1:G:254:VAL:CG1  | 2.33                     | 0.58              |
| 1:I:152:ALA:HB3  | 1:I:155:ASP:H    | 1.69                     | 0.58              |
| 1:H:38:VAL:CA    | 1:I:519:CYS:O    | 2.52                     | 0.58              |
| 1:J:152:ALA:HB3  | 1:J:155:ASP:H    | 1.69                     | 0.58              |
| 1:J:165:ALA:O    | 1:J:169:VAL:HG22 | 2.03                     | 0.58              |
| 1:J:23:LEU:HD23  | 1:J:74:VAL:HG13  | 1.84                     | 0.58              |
| 1:K:162:ILE:HD13 | 1:K:400:LEU:CA   | 2.34                     | 0.58              |
| 1:N:169:VAL:HB   | 1:N:173:GLY:HA3  | 1.85                     | 0.58              |
| 1:B:293:ALA:HB1  | 1:B:299:THR:HA   | 1.85                     | 0.58              |
| 1:F:293:ALA:HB1  | 1:F:299:THR:HA   | 1.86                     | 0.58              |
| 1:G:293:ALA:HB1  | 1:G:299:THR:HA   | 1.85                     | 0.58              |
| 1:H:420:ILE:HD12 | 1:H:451:LEU:HD13 | 1.85                     | 0.58              |
| 1:I:23:LEU:HD23  | 1:I:74:VAL:HG13  | 1.84                     | 0.58              |
| 1:K:242:LYS:CB   | 1:L:257:GLU:HA   | 2.34                     | 0.58              |
| 1:K:420:ILE:HD12 | 1:K:451:LEU:HD13 | 1.85                     | 0.58              |
| 1:K:23:LEU:HD23  | 1:K:74:VAL:HG13  | 1.84                     | 0.58              |
| 1:K:39:VAL:N     | 1:L:519:CYS:O    | 2.37                     | 0.58              |
| 1:M:192:GLY:HA3  | 1:M:332:ILE:O    | 2.03                     | 0.58              |
| 1:C:293:ALA:HB1  | 1:C:299:THR:HA   | 1.85                     | 0.57              |
| 1:H:39:VAL:N     | 1:I:519:CYS:O    | 2.37                     | 0.57              |
| 1:I:38:VAL:CA    | 1:J:519:CYS:O    | 2.52                     | 0.57              |
| 1:K:152:ALA:HB3  | 1:K:155:ASP:H    | 1.69                     | 0.57              |
| 1:L:298:GLY:HA3  | 1:L:318:GLY:HA3  | 1.85                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:199:TYR:CB   | 1:M:325:ILE:HD11 | 2.34                     | 0.57              |
| 1:I:162:ILE:HD13 | 1:I:400:LEU:CA   | 2.34                     | 0.57              |
| 1:M:298:GLY:HA3  | 1:M:318:GLY:HA3  | 1.85                     | 0.57              |
| 1:B:221:LEU:HD13 | 1:B:236:VAL:HG21 | 1.86                     | 0.57              |
| 1:C:224:ASP:HA   | 1:C:289:LEU:HD13 | 1.86                     | 0.57              |
| 1:F:381:VAL:HG22 | 1:F:382:GLY:N    | 2.20                     | 0.57              |
| 1:G:300:VAL:CG2  | 1:G:312:ALA:HB2  | 2.33                     | 0.57              |
| 1:H:353:ILE:HD11 | 1:H:369:VAL:CG2  | 2.35                     | 0.57              |
| 1:I:353:ILE:HD11 | 1:I:369:VAL:CG2  | 2.35                     | 0.57              |
| 1:I:420:ILE:HD12 | 1:I:451:LEU:HD13 | 1.85                     | 0.57              |
| 1:J:39:VAL:N     | 1:K:519:CYS:O    | 2.37                     | 0.57              |
| 1:D:224:ASP:HA   | 1:D:289:LEU:HD13 | 1.86                     | 0.57              |
| 1:F:193:MET:CE   | 1:F:332:ILE:HD12 | 2.19                     | 0.57              |
| 1:G:381:VAL:HG22 | 1:G:382:GLY:N    | 2.20                     | 0.57              |
| 1:I:301:ILE:HD11 | 1:I:312:ALA:HB1  | 1.85                     | 0.57              |
| 1:I:524:LEU:HG   | 1:I:525:PRO:N    | 2.20                     | 0.57              |
| 1:K:243:ALA:CB   | 1:L:256:GLY:O    | 2.51                     | 0.57              |
| 1:N:152:ALA:HB3  | 1:N:155:ASP:H    | 1.69                     | 0.57              |
| 1:E:221:LEU:HD13 | 1:E:236:VAL:HG21 | 1.86                     | 0.57              |
| 1:E:300:VAL:CG2  | 1:E:312:ALA:HB2  | 2.33                     | 0.57              |
| 1:F:300:VAL:CG2  | 1:F:312:ALA:HB2  | 2.33                     | 0.57              |
| 1:G:200:LEU:CD1  | 1:G:254:VAL:HG21 | 2.22                     | 0.57              |
| 1:J:207:LYS:HE2  | 1:J:207:LYS:CA   | 2.34                     | 0.57              |
| 1:I:39:VAL:N     | 1:J:519:CYS:O    | 2.37                     | 0.57              |
| 1:L:301:ILE:HD12 | 1:L:312:ALA:HB2  | 1.65                     | 0.57              |
| 1:M:353:ILE:HD11 | 1:M:369:VAL:CG2  | 2.35                     | 0.57              |
| 1:M:39:VAL:N     | 1:N:519:CYS:O    | 2.37                     | 0.57              |
| 1:E:381:VAL:HG22 | 1:E:382:GLY:N    | 2.20                     | 0.57              |
| 1:J:301:ILE:HD11 | 1:J:312:ALA:HB1  | 1.85                     | 0.57              |
| 1:J:420:ILE:HD12 | 1:J:451:LEU:HD13 | 1.86                     | 0.57              |
| 1:K:353:ILE:HD11 | 1:K:369:VAL:CG2  | 2.35                     | 0.57              |
| 1:L:384:ALA:HA   | 1:L:385:THR:C    | 2.25                     | 0.57              |
| 1:L:36:ARG:O     | 1:M:518:GLU:HB2  | 2.05                     | 0.57              |
| 1:A:300:VAL:CG2  | 1:A:312:ALA:HB2  | 2.33                     | 0.57              |
| 1:E:200:LEU:HB3  | 1:E:259:LEU:CD2  | 2.35                     | 0.57              |
| 1:E:293:ALA:HB1  | 1:E:299:THR:HA   | 1.86                     | 0.57              |
| 1:F:23:LEU:HA    | 1:F:60:ILE:CD1   | 2.32                     | 0.57              |
| 1:H:301:ILE:HD11 | 1:H:312:ALA:HB1  | 1.85                     | 0.57              |
| 1:I:240:VAL:HG11 | 1:I:247:LEU:HA   | 1.87                     | 0.57              |
| 1:J:240:VAL:HG11 | 1:J:247:LEU:HA   | 1.87                     | 0.57              |
| 1:J:524:LEU:HG   | 1:J:525:PRO:N    | 2.20                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:301:ILE:HD11 | 1:K:312:ALA:CB   | 2.32                     | 0.57              |
| 1:J:36:ARG:O     | 1:K:518:GLU:HB2  | 2.05                     | 0.57              |
| 1:K:524:LEU:HG   | 1:K:525:PRO:N    | 2.20                     | 0.57              |
| 1:L:199:TYR:CB   | 1:L:325:ILE:HD11 | 2.34                     | 0.57              |
| 1:M:524:LEU:HG   | 1:M:525:PRO:N    | 2.20                     | 0.57              |
| 1:N:240:VAL:HG11 | 1:N:247:LEU:HA   | 1.87                     | 0.57              |
| 1:N:353:ILE:HD11 | 1:N:369:VAL:CG2  | 2.35                     | 0.57              |
| 1:C:221:LEU:HD13 | 1:C:236:VAL:HG21 | 1.86                     | 0.57              |
| 1:D:293:ALA:HB1  | 1:D:299:THR:HA   | 1.86                     | 0.57              |
| 1:E:240:VAL:HG21 | 1:E:247:LEU:HB2  | 1.87                     | 0.57              |
| 1:F:240:VAL:HG21 | 1:F:247:LEU:HB2  | 1.87                     | 0.57              |
| 1:F:192:GLY:HA3  | 1:F:376:VAL:HG23 | 1.86                     | 0.57              |
| 1:G:224:ASP:HA   | 1:G:289:LEU:HD13 | 1.86                     | 0.57              |
| 1:G:240:VAL:HG21 | 1:G:247:LEU:HB2  | 1.87                     | 0.57              |
| 1:H:518:GLU:HB2  | 1:N:36:ARG:O     | 2.05                     | 0.57              |
| 1:L:524:LEU:HG   | 1:L:525:PRO:N    | 2.20                     | 0.57              |
| 1:A:240:VAL:HG21 | 1:A:247:LEU:HB2  | 1.87                     | 0.57              |
| 1:D:221:LEU:HD13 | 1:D:236:VAL:HG21 | 1.86                     | 0.57              |
| 1:D:240:VAL:HG21 | 1:D:247:LEU:HB2  | 1.87                     | 0.57              |
| 1:E:192:GLY:HA3  | 1:E:376:VAL:HG23 | 1.86                     | 0.57              |
| 1:H:240:VAL:HG11 | 1:H:247:LEU:HA   | 1.87                     | 0.57              |
| 1:H:524:LEU:HG   | 1:H:525:PRO:N    | 2.20                     | 0.57              |
| 1:A:293:ALA:HB1  | 1:A:299:THR:HA   | 1.86                     | 0.57              |
| 1:D:381:VAL:HG22 | 1:D:382:GLY:N    | 2.20                     | 0.57              |
| 1:E:38:VAL:HG21  | 1:E:56:VAL:HG22  | 1.87                     | 0.57              |
| 1:G:192:GLY:HA3  | 1:G:376:VAL:HG23 | 1.86                     | 0.57              |
| 1:H:519:CYS:O    | 1:N:38:VAL:CA    | 2.52                     | 0.57              |
| 1:I:384:ALA:HA   | 1:I:385:THR:C    | 2.25                     | 0.57              |
| 1:I:518:GLU:HB3  | 1:I:519:CYS:N    | 2.19                     | 0.57              |
| 1:J:353:ILE:HD11 | 1:J:369:VAL:CG2  | 2.35                     | 0.57              |
| 1:J:518:GLU:HB3  | 1:J:519:CYS:N    | 2.19                     | 0.57              |
| 1:L:206:ASN:OD1  | 1:L:207:LYS:HD2  | 2.05                     | 0.57              |
| 1:L:162:ILE:HD13 | 1:L:400:LEU:CA   | 2.34                     | 0.57              |
| 1:L:39:VAL:N     | 1:M:519:CYS:O    | 2.37                     | 0.57              |
| 1:B:300:VAL:CG2  | 1:B:312:ALA:HB2  | 2.33                     | 0.56              |
| 1:D:300:VAL:CG2  | 1:D:312:ALA:HB2  | 2.33                     | 0.56              |
| 1:F:224:ASP:HA   | 1:F:289:LEU:HD13 | 1.86                     | 0.56              |
| 1:I:36:ARG:O     | 1:J:518:GLU:HB2  | 2.05                     | 0.56              |
| 1:H:36:ARG:O     | 1:I:518:GLU:HB2  | 2.05                     | 0.56              |
| 1:N:524:LEU:HG   | 1:N:525:LEU:N    | 2.20                     | 0.56              |
| 1:B:224:ASP:HA   | 1:B:289:LEU:HD13 | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:192:GLY:HA3  | 1:B:376:VAL:HG23 | 1.86                     | 0.56              |
| 1:C:200:LEU:HB3  | 1:C:259:LEU:CD2  | 2.35                     | 0.56              |
| 1:H:152:ALA:HB3  | 1:H:155:ASP:H    | 1.69                     | 0.56              |
| 1:N:518:GLU:HB3  | 1:N:519:CYS:N    | 2.19                     | 0.56              |
| 1:A:224:ASP:HA   | 1:A:289:LEU:HD13 | 1.86                     | 0.56              |
| 1:C:38:VAL:HG21  | 1:C:56:VAL:HG22  | 1.86                     | 0.56              |
| 1:J:384:ALA:HA   | 1:J:385:THR:C    | 2.25                     | 0.56              |
| 1:K:384:ALA:HA   | 1:K:385:THR:C    | 2.25                     | 0.56              |
| 1:M:384:ALA:HA   | 1:M:385:THR:C    | 2.25                     | 0.56              |
| 1:B:200:LEU:HB3  | 1:B:259:LEU:CD2  | 2.35                     | 0.56              |
| 1:B:38:VAL:HG21  | 1:B:56:VAL:HG22  | 1.87                     | 0.56              |
| 1:D:200:LEU:HB3  | 1:D:259:LEU:CD2  | 2.35                     | 0.56              |
| 1:F:38:VAL:HG21  | 1:F:56:VAL:HG22  | 1.87                     | 0.56              |
| 1:K:518:GLU:HB3  | 1:K:519:CYS:N    | 2.19                     | 0.56              |
| 1:M:240:VAL:HG11 | 1:M:247:LEU:HA   | 1.87                     | 0.56              |
| 1:L:38:VAL:CA    | 1:M:519:CYS:O    | 2.52                     | 0.56              |
| 1:A:207:LYS:HB2  | 1:A:208:PRO:HD3  | 1.87                     | 0.56              |
| 1:A:381:VAL:HG22 | 1:A:382:GLY:N    | 2.20                     | 0.56              |
| 1:B:240:VAL:HG21 | 1:B:247:LEU:HB2  | 1.87                     | 0.56              |
| 1:C:23:LEU:HA    | 1:C:60:ILE:CD1   | 2.32                     | 0.56              |
| 1:E:200:LEU:HD12 | 1:E:259:LEU:HD13 | 1.88                     | 0.56              |
| 1:E:224:ASP:HA   | 1:E:289:LEU:HD13 | 1.86                     | 0.56              |
| 1:F:200:LEU:HD12 | 1:F:259:LEU:HD13 | 1.88                     | 0.56              |
| 1:K:240:VAL:HG11 | 1:K:247:LEU:HA   | 1.87                     | 0.56              |
| 1:K:38:VAL:CA    | 1:L:519:CYS:O    | 2.52                     | 0.56              |
| 1:L:169:VAL:HB   | 1:L:173:GLY:HA3  | 1.85                     | 0.56              |
| 1:K:36:ARG:O     | 1:L:518:GLU:HB2  | 2.05                     | 0.56              |
| 1:M:152:ALA:HB3  | 1:M:155:ASP:H    | 1.69                     | 0.56              |
| 1:A:38:VAL:HG21  | 1:A:56:VAL:HG22  | 1.87                     | 0.56              |
| 1:C:300:VAL:CG2  | 1:C:312:ALA:HB2  | 2.33                     | 0.56              |
| 1:H:518:GLU:HB3  | 1:H:519:CYS:N    | 2.19                     | 0.56              |
| 1:J:100:ILE:HD13 | 1:J:514:MET:SD   | 2.46                     | 0.56              |
| 1:L:100:ILE:HD13 | 1:L:514:MET:SD   | 2.46                     | 0.56              |
| 1:D:150:ILE:HD11 | 1:D:493:ILE:HG23 | 1.88                     | 0.56              |
| 1:D:192:GLY:HA3  | 1:D:376:VAL:HG23 | 1.86                     | 0.56              |
| 1:D:193:MET:CE   | 1:D:332:ILE:HD12 | 2.19                     | 0.56              |
| 1:H:240:VAL:HG21 | 1:H:247:LEU:HD13 | 1.88                     | 0.56              |
| 1:K:301:ILE:HD11 | 1:K:312:ALA:HB1  | 1.85                     | 0.56              |
| 1:M:36:ARG:O     | 1:N:518:GLU:HB2  | 2.05                     | 0.56              |
| 1:A:192:GLY:HA3  | 1:A:376:VAL:HG23 | 1.86                     | 0.56              |
| 1:D:38:VAL:HG21  | 1:D:56:VAL:HG22  | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:521:VAL:CG1  | 1:E:59:GLU:HB3   | 2.36                     | 0.56              |
| 1:F:200:LEU:HB3  | 1:F:259:LEU:CD2  | 2.35                     | 0.56              |
| 1:F:187:LEU:CD1  | 1:F:379:ILE:HG12 | 2.35                     | 0.56              |
| 1:E:521:VAL:CG1  | 1:F:59:GLU:HB3   | 2.36                     | 0.56              |
| 1:H:100:ILE:HD13 | 1:H:514:MET:SD   | 2.46                     | 0.56              |
| 1:L:240:VAL:HG11 | 1:L:247:LEU:HA   | 1.87                     | 0.56              |
| 1:N:301:ILE:HD11 | 1:N:312:ALA:HB1  | 1.86                     | 0.56              |
| 1:B:31:LEU:HB2   | 1:B:90:THR:HG21  | 1.88                     | 0.56              |
| 1:C:240:VAL:HG21 | 1:C:247:LEU:HB2  | 1.87                     | 0.56              |
| 1:C:312:ALA:HB1  | 1:C:316:ASP:OD2  | 2.06                     | 0.56              |
| 1:D:200:LEU:HD12 | 1:D:259:LEU:HD13 | 1.88                     | 0.56              |
| 1:F:521:VAL:CG1  | 1:G:59:GLU:HB3   | 2.36                     | 0.56              |
| 1:H:384:ALA:HA   | 1:H:385:THR:C    | 2.25                     | 0.56              |
| 1:J:243:ALA:HA   | 1:K:260:ALA:HB2  | 1.88                     | 0.56              |
| 1:L:301:ILE:HD11 | 1:L:312:ALA:HB1  | 1.86                     | 0.56              |
| 1:M:518:GLU:HB3  | 1:M:519:CYS:N    | 2.19                     | 0.56              |
| 1:A:200:LEU:HB3  | 1:A:259:LEU:CD2  | 2.35                     | 0.56              |
| 1:B:312:ALA:HB1  | 1:B:316:ASP:OD2  | 2.06                     | 0.56              |
| 1:H:302:SER:HB2  | 1:H:305:ILE:H    | 1.71                     | 0.56              |
| 1:I:240:VAL:HG21 | 1:I:247:LEU:HD13 | 1.88                     | 0.56              |
| 1:K:206:ASN:HB2  | 1:K:213:VAL:HG23 | 1.88                     | 0.56              |
| 1:L:353:ILE:HD11 | 1:L:369:VAL:CG2  | 2.35                     | 0.56              |
| 1:B:381:VAL:HG22 | 1:B:382:GLY:N    | 2.19                     | 0.56              |
| 1:F:312:ALA:HB1  | 1:F:316:ASP:OD2  | 2.06                     | 0.56              |
| 1:F:150:ILE:HD11 | 1:F:493:ILE:HG23 | 1.87                     | 0.56              |
| 1:H:239:ALA:HB1  | 1:H:314:LEU:HB3  | 1.88                     | 0.56              |
| 1:M:100:ILE:HD13 | 1:M:514:MET:SD   | 2.46                     | 0.56              |
| 1:M:301:ILE:HD11 | 1:M:312:ALA:HB1  | 1.86                     | 0.56              |
| 1:N:240:VAL:HG21 | 1:N:247:LEU:HD13 | 1.87                     | 0.56              |
| 1:M:38:VAL:CA    | 1:N:519:CYS:O    | 2.52                     | 0.56              |
| 1:C:200:LEU:HD12 | 1:C:259:LEU:HD13 | 1.88                     | 0.55              |
| 1:C:521:VAL:CG1  | 1:D:59:GLU:HB3   | 2.36                     | 0.55              |
| 1:I:239:ALA:HB1  | 1:I:314:LEU:HB3  | 1.88                     | 0.55              |
| 1:J:240:VAL:HG21 | 1:J:247:LEU:HD13 | 1.88                     | 0.55              |
| 1:A:200:LEU:HD21 | 1:A:254:VAL:HG21 | 1.04                     | 0.55              |
| 1:D:191:GLU:HG3  | 1:D:342:ILE:CD1  | 2.37                     | 0.55              |
| 1:F:202:PRO:O    | 1:F:205:ILE:HG13 | 2.05                     | 0.55              |
| 1:G:312:ALA:HB1  | 1:G:316:ASP:OD2  | 2.06                     | 0.55              |
| 1:A:59:GLU:HB3   | 1:G:521:VAL:CG1  | 2.36                     | 0.55              |
| 1:G:38:VAL:HG21  | 1:G:56:VAL:HG22  | 1.87                     | 0.55              |
| 1:K:193:MET:HE1  | 1:K:295:LEU:HD12 | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:183:LEU:O    | 1:L:183:LEU:HG   | 2.06                     | 0.55              |
| 1:N:239:ALA:HB1  | 1:N:314:LEU:HB3  | 1.88                     | 0.55              |
| 1:D:312:ALA:HB1  | 1:D:316:ASP:OD2  | 2.06                     | 0.55              |
| 1:J:290:GLN:HA   | 1:J:300:VAL:CG2  | 2.37                     | 0.55              |
| 1:K:302:SER:HB2  | 1:K:305:ILE:H    | 1.71                     | 0.55              |
| 1:K:100:ILE:HD13 | 1:K:514:MET:SD   | 2.46                     | 0.55              |
| 1:M:162:ILE:HD13 | 1:M:400:LEU:CA   | 2.34                     | 0.55              |
| 1:B:150:ILE:HD11 | 1:B:493:ILE:HG23 | 1.88                     | 0.55              |
| 1:I:100:ILE:HD13 | 1:I:514:MET:SD   | 2.46                     | 0.55              |
| 1:N:384:ALA:HA   | 1:N:385:THR:C    | 2.25                     | 0.55              |
| 1:C:381:VAL:HG22 | 1:C:382:GLY:N    | 2.20                     | 0.55              |
| 1:K:240:VAL:HG11 | 1:K:247:LEU:CB   | 2.37                     | 0.55              |
| 1:K:240:VAL:HG21 | 1:K:247:LEU:HD13 | 1.88                     | 0.55              |
| 1:L:518:GLU:HB3  | 1:L:519:CYS:N    | 2.19                     | 0.55              |
| 1:N:100:ILE:HD13 | 1:N:514:MET:SD   | 2.46                     | 0.55              |
| 1:N:221:LEU:HD13 | 1:N:317:LEU:HD11 | 1.89                     | 0.55              |
| 1:B:200:LEU:HD12 | 1:B:259:LEU:HD13 | 1.88                     | 0.55              |
| 1:J:240:VAL:HG11 | 1:J:247:LEU:CB   | 2.37                     | 0.55              |
| 1:I:243:ALA:HA   | 1:J:260:ALA:HB2  | 1.88                     | 0.55              |
| 1:K:193:MET:CE   | 1:K:295:LEU:HD12 | 2.36                     | 0.55              |
| 1:J:38:VAL:CA    | 1:K:519:CYS:O    | 2.52                     | 0.55              |
| 1:A:521:VAL:CG1  | 1:B:59:GLU:HB3   | 2.36                     | 0.55              |
| 1:B:521:VAL:CG1  | 1:C:59:GLU:HB3   | 2.36                     | 0.55              |
| 1:D:190:VAL:HB   | 1:D:334:ASP:HB2  | 1.89                     | 0.55              |
| 1:D:23:LEU:HA    | 1:D:60:ILE:CD1   | 2.32                     | 0.55              |
| 1:D:406:ALA:HB1  | 1:D:411:VAL:HG13 | 1.89                     | 0.55              |
| 1:M:240:VAL:HG11 | 1:M:247:LEU:CB   | 2.37                     | 0.55              |
| 1:E:312:ALA:HB1  | 1:E:316:ASP:OD2  | 2.06                     | 0.55              |
| 1:F:31:LEU:HB2   | 1:F:90:THR:HG21  | 1.89                     | 0.55              |
| 1:N:240:VAL:HG11 | 1:N:247:LEU:CB   | 2.35                     | 0.55              |
| 1:A:200:LEU:HD12 | 1:A:259:LEU:HD13 | 1.88                     | 0.55              |
| 1:A:312:ALA:HB1  | 1:A:316:ASP:OD2  | 2.06                     | 0.55              |
| 1:D:31:LEU:HB2   | 1:D:90:THR:HG21  | 1.89                     | 0.55              |
| 1:F:207:LYS:HE2  | 1:F:207:LYS:N    | 2.21                     | 0.55              |
| 1:G:193:MET:CE   | 1:G:295:LEU:HB3  | 2.37                     | 0.55              |
| 1:H:240:VAL:HG11 | 1:H:247:LEU:CB   | 2.37                     | 0.55              |
| 1:H:243:ALA:CA   | 1:I:260:ALA:HB2  | 2.37                     | 0.55              |
| 1:J:199:TYR:CB   | 1:J:325:ILE:HD11 | 2.34                     | 0.55              |
| 1:A:197:ARG:HG3  | 1:A:198:GLY:O    | 2.07                     | 0.54              |
| 1:I:240:VAL:HG11 | 1:I:247:LEU:CB   | 2.37                     | 0.54              |
| 1:I:181:THR:O    | 1:I:383:ALA:HB3  | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:239:ALA:HB1  | 1:J:314:LEU:HB3  | 1.88                     | 0.54              |
| 1:L:240:VAL:HG21 | 1:L:247:LEU:HD13 | 1.87                     | 0.54              |
| 1:A:213:VAL:HG13 | 1:A:325:ILE:HG12 | 1.89                     | 0.54              |
| 1:E:406:ALA:HB1  | 1:E:411:VAL:HG13 | 1.89                     | 0.54              |
| 1:F:150:ILE:CD1  | 1:F:493:ILE:CA   | 2.74                     | 0.54              |
| 1:F:150:ILE:HD13 | 1:F:493:ILE:CG2  | 2.36                     | 0.54              |
| 1:L:301:ILE:HD11 | 1:L:312:ALA:CB   | 2.32                     | 0.54              |
| 1:M:239:ALA:HB1  | 1:M:314:LEU:HB3  | 1.88                     | 0.54              |
| 1:H:207:LYS:CA   | 1:H:207:LYS:HE2  | 2.38                     | 0.54              |
| 1:I:221:LEU:HD13 | 1:I:317:LEU:HD11 | 1.89                     | 0.54              |
| 1:M:240:VAL:HG21 | 1:M:247:LEU:HD13 | 1.87                     | 0.54              |
| 1:M:290:GLN:HA   | 1:M:300:VAL:CG2  | 2.38                     | 0.54              |
| 1:K:221:LEU:HD13 | 1:K:317:LEU:HD11 | 1.90                     | 0.54              |
| 1:N:221:LEU:HD21 | 1:N:309:LEU:HD22 | 1.88                     | 0.54              |
| 1:B:137:PRO:HA   | 1:B:410:GLY:HA3  | 1.90                     | 0.54              |
| 1:C:406:ALA:HB1  | 1:C:411:VAL:HG13 | 1.89                     | 0.54              |
| 1:F:206:ASN:HB3  | 1:F:208:PRO:HD2  | 1.90                     | 0.54              |
| 1:G:241:ALA:HA   | 1:G:271:VAL:HG22 | 1.90                     | 0.54              |
| 1:L:240:VAL:HG11 | 1:L:247:LEU:CB   | 2.37                     | 0.54              |
| 1:I:290:GLN:HA   | 1:I:300:VAL:CG2  | 2.37                     | 0.54              |
| 1:J:302:SER:HB2  | 1:J:305:ILE:H    | 1.72                     | 0.54              |
| 1:K:137:PRO:CA   | 1:K:410:GLY:HA3  | 2.36                     | 0.54              |
| 1:A:241:ALA:HA   | 1:A:271:VAL:HG22 | 1.90                     | 0.54              |
| 1:B:150:ILE:HD13 | 1:B:493:ILE:CG2  | 2.37                     | 0.54              |
| 1:E:200:LEU:CB   | 1:E:259:LEU:CD1  | 2.86                     | 0.54              |
| 1:J:221:LEU:HD13 | 1:J:317:LEU:HD11 | 1.90                     | 0.54              |
| 1:N:221:LEU:HD22 | 1:N:236:VAL:HG11 | 1.90                     | 0.54              |
| 1:H:260:ALA:HB2  | 1:N:243:ALA:CA   | 2.38                     | 0.54              |
| 1:H:260:ALA:HB2  | 1:N:243:ALA:HA   | 1.88                     | 0.54              |
| 1:D:150:ILE:CD1  | 1:D:493:ILE:CA   | 2.74                     | 0.54              |
| 1:I:189:VAL:HA   | 1:I:377:ALA:HA   | 1.89                     | 0.54              |
| 1:C:464:VAL:HG22 | 1:J:464:VAL:HG22 | 1.90                     | 0.54              |
| 1:L:239:ALA:HB1  | 1:L:314:LEU:HB3  | 1.88                     | 0.54              |
| 1:M:60:ILE:HA    | 1:N:6:VAL:HG21   | 1.90                     | 0.54              |
| 1:A:150:ILE:HD13 | 1:A:493:ILE:CG2  | 2.37                     | 0.54              |
| 1:C:144:ILE:HG23 | 1:C:403:THR:CG2  | 2.38                     | 0.54              |
| 1:C:31:LEU:HB2   | 1:C:90:THR:HG21  | 1.90                     | 0.54              |
| 1:D:464:VAL:HG22 | 1:K:464:VAL:HG22 | 1.90                     | 0.54              |
| 1:E:23:LEU:HA    | 1:E:60:ILE:CD1   | 2.32                     | 0.54              |
| 1:H:6:VAL:HG21   | 1:N:60:ILE:HA    | 1.90                     | 0.54              |
| 1:H:242:LYS:HG3  | 1:I:257:GLU:O    | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:221:LEU:HD13 | 1:L:317:LEU:HD11 | 1.90                     | 0.54              |
| 1:A:31:LEU:HB2   | 1:A:90:THR:HG21  | 1.90                     | 0.54              |
| 1:E:213:VAL:HG11 | 1:E:325:ILE:HG12 | 1.87                     | 0.54              |
| 1:E:31:LEU:HB2   | 1:E:90:THR:HG21  | 1.90                     | 0.54              |
| 1:F:193:MET:SD   | 1:F:292:ILE:HG23 | 2.48                     | 0.54              |
| 1:H:221:LEU:HD13 | 1:H:317:LEU:HD11 | 1.90                     | 0.54              |
| 1:I:243:ALA:CA   | 1:J:260:ALA:HB2  | 2.38                     | 0.54              |
| 1:J:243:ALA:CA   | 1:K:260:ALA:HB2  | 2.38                     | 0.54              |
| 1:D:137:PRO:HA   | 1:D:410:GLY:HA3  | 1.90                     | 0.53              |
| 1:F:406:ALA:HB1  | 1:F:411:VAL:HG13 | 1.88                     | 0.53              |
| 1:G:193:MET:SD   | 1:G:295:LEU:HB3  | 2.48                     | 0.53              |
| 1:G:31:LEU:HB2   | 1:G:90:THR:HG21  | 1.90                     | 0.53              |
| 1:I:23:LEU:HA    | 1:I:60:ILE:HD13  | 1.90                     | 0.53              |
| 1:K:150:ILE:CD1  | 1:K:494:LEU:H    | 2.22                     | 0.53              |
| 1:N:290:GLN:HA   | 1:N:300:VAL:CG2  | 2.38                     | 0.53              |
| 1:A:23:LEU:HA    | 1:A:60:ILE:CD1   | 2.32                     | 0.53              |
| 1:B:144:ILE:HG23 | 1:B:403:THR:CG2  | 2.39                     | 0.53              |
| 1:B:464:VAL:HG22 | 1:I:464:VAL:HG22 | 1.90                     | 0.53              |
| 1:D:144:ILE:HG23 | 1:D:403:THR:CG2  | 2.39                     | 0.53              |
| 1:F:241:ALA:HA   | 1:F:271:VAL:HG22 | 1.90                     | 0.53              |
| 1:I:199:TYR:CB   | 1:I:325:ILE:HD11 | 2.34                     | 0.53              |
| 1:I:206:ASN:CG   | 1:I:207:LYS:H    | 2.12                     | 0.53              |
| 1:J:221:LEU:HD21 | 1:J:309:LEU:HD22 | 1.90                     | 0.53              |
| 1:J:23:LEU:HA    | 1:J:60:ILE:HD13  | 1.90                     | 0.53              |
| 1:K:243:ALA:CA   | 1:L:260:ALA:HB2  | 2.37                     | 0.53              |
| 1:K:290:GLN:HA   | 1:K:300:VAL:CG2  | 2.38                     | 0.53              |
| 1:N:162:ILE:HD13 | 1:N:400:LEU:CA   | 2.34                     | 0.53              |
| 1:A:144:ILE:HG23 | 1:A:403:THR:CG2  | 2.38                     | 0.53              |
| 1:D:193:MET:SD   | 1:D:292:ILE:HG23 | 2.48                     | 0.53              |
| 1:E:144:ILE:HG23 | 1:E:403:THR:CG2  | 2.38                     | 0.53              |
| 1:E:193:MET:SD   | 1:E:292:ILE:HA   | 2.49                     | 0.53              |
| 1:G:150:ILE:HD13 | 1:G:493:ILE:CG2  | 2.37                     | 0.53              |
| 1:H:290:GLN:HA   | 1:H:300:VAL:CG2  | 2.38                     | 0.53              |
| 1:L:221:LEU:HD22 | 1:L:236:VAL:HG11 | 1.90                     | 0.53              |
| 1:L:290:GLN:HA   | 1:L:300:VAL:CG2  | 2.38                     | 0.53              |
| 1:M:221:LEU:HD13 | 1:M:317:LEU:HD11 | 1.90                     | 0.53              |
| 1:A:200:LEU:HD11 | 1:A:254:VAL:CA   | 2.12                     | 0.53              |
| 1:A:406:ALA:HB1  | 1:A:411:VAL:HG13 | 1.89                     | 0.53              |
| 1:B:193:MET:SD   | 1:B:292:ILE:HG23 | 2.48                     | 0.53              |
| 1:C:38:VAL:HG11  | 1:C:56:VAL:HG22  | 1.91                     | 0.53              |
| 1:F:137:PRO:HA   | 1:F:410:GLY:HA3  | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:200:LEU:CB   | 1:F:259:LEU:CD1  | 2.86                     | 0.53              |
| 1:H:221:LEU:HD21 | 1:H:309:LEU:HD22 | 1.90                     | 0.53              |
| 1:H:137:PRO:CA   | 1:H:410:GLY:HA3  | 2.36                     | 0.53              |
| 1:I:221:LEU:HD21 | 1:I:309:LEU:HD22 | 1.90                     | 0.53              |
| 1:K:221:LEU:HD21 | 1:K:309:LEU:HD22 | 1.89                     | 0.53              |
| 1:L:150:ILE:CD1  | 1:L:494:LEU:H    | 2.22                     | 0.53              |
| 1:L:243:ALA:CA   | 1:M:260:ALA:HB2  | 2.39                     | 0.53              |
| 1:A:193:MET:SD   | 1:A:292:ILE:HG23 | 2.48                     | 0.53              |
| 1:B:406:ALA:HB1  | 1:B:411:VAL:HG13 | 1.88                     | 0.53              |
| 1:H:60:ILE:HA    | 1:I:6:VAL:HG21   | 1.90                     | 0.53              |
| 1:L:60:ILE:HA    | 1:M:6:VAL:HG21   | 1.90                     | 0.53              |
| 1:M:229:ASN:HD22 | 1:M:230:ILE:H    | 1.56                     | 0.53              |
| 1:M:518:GLU:CB   | 1:M:518:GLU:O    | 2.54                     | 0.53              |
| 1:N:137:PRO:CA   | 1:N:410:GLY:HA3  | 2.36                     | 0.53              |
| 1:D:200:LEU:CB   | 1:D:259:LEU:CD1  | 2.86                     | 0.53              |
| 1:D:241:ALA:HA   | 1:D:271:VAL:HG22 | 1.90                     | 0.53              |
| 1:D:213:VAL:HG11 | 1:D:325:ILE:HG12 | 1.88                     | 0.53              |
| 1:H:242:LYS:CB   | 1:I:257:GLU:HA   | 2.38                     | 0.53              |
| 1:H:31:LEU:CB    | 1:H:90:THR:HG21  | 2.39                     | 0.53              |
| 1:J:221:LEU:CG   | 1:J:309:LEU:HD22 | 2.39                     | 0.53              |
| 1:K:221:LEU:HD22 | 1:K:236:VAL:HG11 | 1.91                     | 0.53              |
| 1:K:239:ALA:HB1  | 1:K:314:LEU:HB3  | 1.89                     | 0.53              |
| 1:L:221:LEU:HD21 | 1:L:309:LEU:HD22 | 1.89                     | 0.53              |
| 1:M:221:LEU:HD21 | 1:M:309:LEU:HD22 | 1.89                     | 0.53              |
| 1:B:193:MET:SD   | 1:B:292:ILE:HA   | 2.49                     | 0.53              |
| 1:G:406:ALA:HB1  | 1:G:411:VAL:HG13 | 1.89                     | 0.53              |
| 1:I:302:SER:HB2  | 1:I:305:ILE:H    | 1.72                     | 0.53              |
| 1:I:31:LEU:CB    | 1:I:90:THR:HG21  | 2.39                     | 0.53              |
| 1:A:137:PRO:HA   | 1:A:410:GLY:HA3  | 1.90                     | 0.53              |
| 1:C:241:ALA:HA   | 1:C:271:VAL:HG22 | 1.90                     | 0.53              |
| 1:E:241:ALA:HA   | 1:E:271:VAL:HG22 | 1.90                     | 0.53              |
| 1:E:464:VAL:HG22 | 1:L:464:VAL:HG22 | 1.91                     | 0.53              |
| 1:F:193:MET:SD   | 1:F:292:ILE:HA   | 2.49                     | 0.53              |
| 1:K:31:LEU:CB    | 1:K:90:THR:HG21  | 2.39                     | 0.53              |
| 1:M:221:LEU:HD22 | 1:M:236:VAL:HG11 | 1.91                     | 0.53              |
| 1:M:243:ALA:CA   | 1:N:260:ALA:HB2  | 2.39                     | 0.53              |
| 1:M:150:ILE:CD1  | 1:M:494:LEU:H    | 2.22                     | 0.53              |
| 1:N:518:GLU:O    | 1:N:518:GLU:CB   | 2.54                     | 0.53              |
| 1:N:31:LEU:CB    | 1:N:90:THR:HG21  | 2.39                     | 0.53              |
| 1:A:193:MET:SD   | 1:A:292:ILE:HA   | 2.49                     | 0.53              |
| 1:B:200:LEU:CB   | 1:B:259:LEU:CD1  | 2.86                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:241:ALA:HA   | 1:B:271:VAL:HG22 | 1.90                     | 0.53              |
| 1:D:196:ASP:OD1  | 1:D:329:THR:HG22 | 2.08                     | 0.53              |
| 1:D:38:VAL:HG11  | 1:D:56:VAL:HG22  | 1.91                     | 0.53              |
| 1:E:193:MET:SD   | 1:E:292:ILE:HG23 | 2.48                     | 0.53              |
| 1:F:144:ILE:HG23 | 1:F:403:THR:CG2  | 2.39                     | 0.53              |
| 1:G:144:ILE:HG23 | 1:G:403:THR:CG2  | 2.38                     | 0.53              |
| 1:I:60:ILE:HA    | 1:J:6:VAL:HG21   | 1.90                     | 0.53              |
| 1:J:60:ILE:HA    | 1:K:6:VAL:HG21   | 1.90                     | 0.53              |
| 1:M:302:SER:HB2  | 1:M:305:ILE:H    | 1.74                     | 0.53              |
| 1:G:199:TYR:C    | 1:G:200:LEU:HD12 | 2.29                     | 0.53              |
| 1:G:240:VAL:HG12 | 1:G:271:VAL:HG13 | 1.91                     | 0.53              |
| 1:L:23:LEU:HA    | 1:L:60:ILE:HD13  | 1.90                     | 0.53              |
| 1:M:23:LEU:HA    | 1:M:60:ILE:HD13  | 1.90                     | 0.53              |
| 1:A:174:VAL:H    | 1:A:376:VAL:HG22 | 1.74                     | 0.52              |
| 1:A:464:VAL:HG22 | 1:H:464:VAL:HG22 | 1.91                     | 0.52              |
| 1:E:240:VAL:HG12 | 1:E:271:VAL:HG13 | 1.91                     | 0.52              |
| 1:H:162:ILE:HD13 | 1:H:400:LEU:CA   | 2.34                     | 0.52              |
| 1:H:23:LEU:HA    | 1:H:60:ILE:HD13  | 1.90                     | 0.52              |
| 1:J:31:LEU:CB    | 1:J:90:THR:HG21  | 2.39                     | 0.52              |
| 1:J:150:ILE:CD1  | 1:J:494:LEU:H    | 2.22                     | 0.52              |
| 1:D:193:MET:SD   | 1:D:292:ILE:HA   | 2.49                     | 0.52              |
| 1:F:174:VAL:H    | 1:F:376:VAL:HG22 | 1.74                     | 0.52              |
| 1:I:221:LEU:CG   | 1:I:309:LEU:HD22 | 2.39                     | 0.52              |
| 1:N:150:ILE:CD1  | 1:N:494:LEU:H    | 2.22                     | 0.52              |
| 1:D:150:ILE:HD13 | 1:D:493:ILE:CG2  | 2.37                     | 0.52              |
| 1:I:137:PRO:CA   | 1:I:410:GLY:HA3  | 2.36                     | 0.52              |
| 1:K:60:ILE:HA    | 1:L:6:VAL:HG21   | 1.90                     | 0.52              |
| 1:L:31:LEU:CB    | 1:L:90:THR:HG21  | 2.39                     | 0.52              |
| 1:L:243:ALA:HA   | 1:M:260:ALA:HB2  | 1.90                     | 0.52              |
| 1:E:220:ILE:CD1  | 1:E:332:ILE:HD13 | 2.33                     | 0.52              |
| 1:F:213:VAL:HG11 | 1:F:325:ILE:HG12 | 1.88                     | 0.52              |
| 1:G:197:ARG:HG3  | 1:G:198:GLY:O    | 2.10                     | 0.52              |
| 1:H:150:ILE:CD1  | 1:H:494:LEU:H    | 2.22                     | 0.52              |
| 1:K:23:LEU:HA    | 1:K:60:ILE:HD13  | 1.90                     | 0.52              |
| 1:M:31:LEU:CB    | 1:M:90:THR:HG21  | 2.39                     | 0.52              |
| 1:N:221:LEU:HB2  | 1:N:317:LEU:HD21 | 1.91                     | 0.52              |
| 1:A:328:ASP:O    | 1:A:329:THR:HG23 | 2.10                     | 0.52              |
| 1:B:328:ASP:O    | 1:B:329:THR:HG23 | 2.10                     | 0.52              |
| 1:B:381:VAL:HB   | 1:B:393:LYS:HA   | 1.92                     | 0.52              |
| 1:C:381:VAL:HB   | 1:C:393:LYS:HA   | 1.92                     | 0.52              |
| 1:E:150:ILE:HD13 | 1:E:493:ILE:CG2  | 2.37                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:183:LEU:HA   | 1:F:383:ALA:N    | 2.25                     | 0.52              |
| 1:H:220:ILE:HD12 | 1:H:296:THR:CG2  | 2.40                     | 0.52              |
| 1:B:38:VAL:HG11  | 1:B:56:VAL:HG22  | 1.91                     | 0.52              |
| 1:E:174:VAL:H    | 1:E:376:VAL:HG22 | 1.74                     | 0.52              |
| 1:D:521:VAL:O    | 1:E:41:ASP:CB    | 2.58                     | 0.52              |
| 1:F:464:VAL:HG22 | 1:M:464:VAL:HG22 | 1.91                     | 0.52              |
| 1:J:221:LEU:HD22 | 1:J:236:VAL:HG11 | 1.92                     | 0.52              |
| 1:L:191:GLU:CG   | 1:L:192:GLY:H    | 2.21                     | 0.52              |
| 1:L:220:ILE:HD12 | 1:L:296:THR:CG2  | 2.40                     | 0.52              |
| 1:M:137:PRO:CA   | 1:M:410:GLY:HA3  | 2.36                     | 0.52              |
| 1:N:221:LEU:CG   | 1:N:309:LEU:HD22 | 2.40                     | 0.52              |
| 1:N:23:LEU:HA    | 1:N:60:ILE:HD13  | 1.89                     | 0.52              |
| 1:A:521:VAL:O    | 1:B:41:ASP:CB    | 2.58                     | 0.52              |
| 1:B:27:VAL:HG12  | 1:B:90:THR:HG23  | 1.92                     | 0.52              |
| 1:F:27:VAL:HG12  | 1:F:90:THR:HG23  | 1.92                     | 0.52              |
| 1:G:183:LEU:HA   | 1:G:383:ALA:N    | 2.25                     | 0.52              |
| 1:I:247:LEU:O    | 1:I:273:VAL:HA   | 2.10                     | 0.52              |
| 1:E:38:VAL:HG11  | 1:E:56:VAL:HG22  | 1.91                     | 0.52              |
| 1:G:328:ASP:O    | 1:G:329:THR:HG23 | 2.10                     | 0.52              |
| 1:J:194:GLN:OE1  | 1:J:329:THR:HG21 | 2.09                     | 0.52              |
| 1:K:207:LYS:CE   | 1:K:207:LYS:HA   | 2.35                     | 0.52              |
| 1:K:247:LEU:O    | 1:K:273:VAL:HA   | 2.10                     | 0.52              |
| 1:K:221:LEU:HB2  | 1:K:317:LEU:HD21 | 1.92                     | 0.52              |
| 1:L:233:MET:HE2  | 1:L:249:ILE:HD11 | 1.90                     | 0.52              |
| 1:L:247:LEU:O    | 1:L:273:VAL:HA   | 2.10                     | 0.52              |
| 1:M:247:LEU:O    | 1:M:273:VAL:HA   | 2.10                     | 0.52              |
| 1:A:200:LEU:CB   | 1:A:259:LEU:CD1  | 2.86                     | 0.52              |
| 1:B:37:ASN:ND2   | 1:B:49:ILE:HG23  | 2.25                     | 0.52              |
| 1:B:521:VAL:O    | 1:C:41:ASP:CB    | 2.58                     | 0.52              |
| 1:C:328:ASP:O    | 1:C:329:THR:HG23 | 2.10                     | 0.52              |
| 1:E:183:LEU:HA   | 1:E:383:ALA:N    | 2.25                     | 0.52              |
| 1:F:521:VAL:O    | 1:G:41:ASP:CB    | 2.58                     | 0.52              |
| 1:G:464:VAL:HG22 | 1:N:464:VAL:HG22 | 1.91                     | 0.52              |
| 1:H:221:LEU:CG   | 1:H:309:LEU:HD22 | 2.39                     | 0.52              |
| 1:K:221:LEU:CG   | 1:K:309:LEU:HD22 | 2.39                     | 0.52              |
| 1:L:221:LEU:HB2  | 1:L:317:LEU:HD21 | 1.92                     | 0.52              |
| 1:N:302:SER:HB2  | 1:N:305:ILE:H    | 1.74                     | 0.52              |
| 1:A:41:ASP:CB    | 1:G:521:VAL:O    | 2.58                     | 0.52              |
| 1:A:37:ASN:ND2   | 1:A:49:ILE:HG23  | 2.25                     | 0.52              |
| 1:C:37:ASN:ND2   | 1:C:49:ILE:HG23  | 2.25                     | 0.52              |
| 1:K:220:ILE:HD12 | 1:K:296:THR:CG2  | 2.40                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:518:GLU:O    | 1:L:518:GLU:CB   | 2.54                     | 0.52              |
| 1:M:221:LEU:CG   | 1:M:309:LEU:HD22 | 2.40                     | 0.52              |
| 1:D:381:VAL:HB   | 1:D:393:LYS:HA   | 1.92                     | 0.51              |
| 1:C:521:VAL:O    | 1:D:41:ASP:CB    | 2.58                     | 0.51              |
| 1:J:221:LEU:HB2  | 1:J:317:LEU:HD21 | 1.92                     | 0.51              |
| 1:A:193:MET:CE   | 1:A:332:ILE:HD12 | 2.18                     | 0.51              |
| 1:B:158:VAL:HG22 | 1:B:396:VAL:HG22 | 1.92                     | 0.51              |
| 1:D:37:ASN:ND2   | 1:D:49:ILE:HG23  | 2.25                     | 0.51              |
| 1:D:521:VAL:HG11 | 1:E:59:GLU:HB3   | 1.93                     | 0.51              |
| 1:E:150:ILE:CD1  | 1:E:493:ILE:CA   | 2.74                     | 0.51              |
| 1:E:521:VAL:HG11 | 1:F:59:GLU:HB3   | 1.92                     | 0.51              |
| 1:E:521:VAL:O    | 1:F:41:ASP:CB    | 2.58                     | 0.51              |
| 1:N:204:PHE:HA   | 1:N:207:LYS:CE   | 2.40                     | 0.51              |
| 1:A:34:LYS:HB2   | 1:A:458:CYS:HA   | 1.92                     | 0.51              |
| 1:A:521:VAL:HG11 | 1:B:59:GLU:HB3   | 1.93                     | 0.51              |
| 1:C:174:VAL:H    | 1:C:376:VAL:HG22 | 1.74                     | 0.51              |
| 1:C:521:VAL:HG11 | 1:D:59:GLU:HB3   | 1.93                     | 0.51              |
| 1:D:174:VAL:H    | 1:D:376:VAL:HG22 | 1.74                     | 0.51              |
| 1:D:27:VAL:HG12  | 1:D:90:THR:HG23  | 1.92                     | 0.51              |
| 1:G:174:VAL:H    | 1:G:376:VAL:HG22 | 1.74                     | 0.51              |
| 1:H:247:LEU:O    | 1:H:273:VAL:HA   | 2.10                     | 0.51              |
| 1:I:221:LEU:HD22 | 1:I:236:VAL:HG11 | 1.91                     | 0.51              |
| 1:J:511:ALA:O    | 1:J:515:ILE:HG13 | 2.11                     | 0.51              |
| 1:B:207:LYS:HB2  | 1:B:208:PRO:HD3  | 1.92                     | 0.51              |
| 1:C:207:LYS:CB   | 1:C:208:PRO:HD3  | 2.40                     | 0.51              |
| 1:C:27:VAL:HG12  | 1:C:90:THR:HG23  | 1.93                     | 0.51              |
| 1:C:150:ILE:HD13 | 1:C:493:ILE:CG2  | 2.37                     | 0.51              |
| 1:G:34:LYS:HB2   | 1:G:458:CYS:HA   | 1.92                     | 0.51              |
| 1:H:221:LEU:HD22 | 1:H:236:VAL:HG11 | 1.91                     | 0.51              |
| 1:I:221:LEU:HB2  | 1:I:317:LEU:HD21 | 1.92                     | 0.51              |
| 1:N:247:LEU:O    | 1:N:273:VAL:HA   | 2.10                     | 0.51              |
| 1:B:174:VAL:H    | 1:B:376:VAL:HG22 | 1.74                     | 0.51              |
| 1:B:195:PHE:CZ   | 1:B:330:THR:CB   | 2.94                     | 0.51              |
| 1:B:521:VAL:HG11 | 1:C:59:GLU:HB3   | 1.93                     | 0.51              |
| 1:E:475:ASN:ND2  | 1:E:489:ILE:HD11 | 2.26                     | 0.51              |
| 1:E:37:ASN:ND2   | 1:E:49:ILE:HG23  | 2.25                     | 0.51              |
| 1:F:161:LEU:HD11 | 1:F:185:ASP:HB3  | 1.93                     | 0.51              |
| 1:G:23:LEU:HA    | 1:G:60:ILE:CD1   | 2.32                     | 0.51              |
| 1:G:38:VAL:HG11  | 1:G:56:VAL:HG22  | 1.91                     | 0.51              |
| 1:G:52:ASP:CB    | 1:G:55:SER:H     | 2.24                     | 0.51              |
| 1:H:221:LEU:HB2  | 1:H:317:LEU:HD21 | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:511:ALA:O    | 1:H:515:ILE:HG13 | 2.11                     | 0.51              |
| 1:J:220:ILE:HD12 | 1:J:296:THR:CG2  | 2.40                     | 0.51              |
| 2:K:1525:PO4:P   | 4:K:1527:ATP:PG  | 3.09                     | 0.51              |
| 1:L:137:PRO:CA   | 1:L:410:GLY:HA3  | 2.36                     | 0.51              |
| 1:M:220:ILE:HD12 | 1:M:296:THR:CG2  | 2.40                     | 0.51              |
| 1:M:221:LEU:HB2  | 1:M:317:LEU:HD21 | 1.92                     | 0.51              |
| 1:A:183:LEU:HA   | 1:A:383:ALA:N    | 2.25                     | 0.51              |
| 1:A:59:GLU:HB3   | 1:G:521:VAL:HG11 | 1.93                     | 0.51              |
| 1:A:27:VAL:HG12  | 1:A:90:THR:HG23  | 1.93                     | 0.51              |
| 1:B:240:VAL:HG12 | 1:B:271:VAL:HG13 | 1.91                     | 0.51              |
| 1:C:141:SER:O    | 1:C:163:ALA:HB1  | 2.11                     | 0.51              |
| 1:C:158:VAL:HG22 | 1:C:396:VAL:HG22 | 1.93                     | 0.51              |
| 1:C:213:VAL:HG11 | 1:C:325:ILE:HG12 | 1.87                     | 0.51              |
| 1:D:183:LEU:HA   | 1:D:383:ALA:N    | 2.25                     | 0.51              |
| 1:D:34:LYS:HB2   | 1:D:458:CYS:HA   | 1.92                     | 0.51              |
| 1:D:158:VAL:HG22 | 1:D:396:VAL:HG22 | 1.93                     | 0.51              |
| 1:F:328:ASP:O    | 1:F:329:THR:HG23 | 2.10                     | 0.51              |
| 1:F:52:ASP:HB3   | 1:F:55:SER:H     | 1.75                     | 0.51              |
| 1:G:37:ASN:ND2   | 1:G:49:ILE:HG23  | 2.25                     | 0.51              |
| 1:F:521:VAL:HG11 | 1:G:59:GLU:HB3   | 1.92                     | 0.51              |
| 2:I:1525:PO4:P   | 4:I:1527:ATP:PG  | 3.09                     | 0.51              |
| 2:J:1525:PO4:P   | 4:J:1527:ATP:PG  | 3.09                     | 0.51              |
| 1:K:183:LEU:HD23 | 1:K:183:LEU:H    | 1.76                     | 0.51              |
| 1:A:158:VAL:HG22 | 1:A:396:VAL:HG22 | 1.93                     | 0.51              |
| 1:A:475:ASN:ND2  | 1:A:489:ILE:HD11 | 2.26                     | 0.51              |
| 1:C:34:LYS:HB2   | 1:C:458:CYS:HA   | 1.92                     | 0.51              |
| 1:D:225:LYS:CB   | 1:D:308:GLU:HA   | 2.41                     | 0.51              |
| 1:D:328:ASP:O    | 1:D:329:THR:HG23 | 2.10                     | 0.51              |
| 1:E:27:VAL:HG12  | 1:E:90:THR:HG23  | 1.93                     | 0.51              |
| 1:H:77:VAL:HG22  | 1:H:510:VAL:HB   | 1.92                     | 0.51              |
| 1:I:150:ILE:CD1  | 1:I:494:LEU:H    | 2.22                     | 0.51              |
| 1:J:137:PRO:CA   | 1:J:410:GLY:HA3  | 2.37                     | 0.51              |
| 1:K:511:ALA:O    | 1:K:515:ILE:HG13 | 2.11                     | 0.51              |
| 2:L:1525:PO4:P   | 4:L:1527:ATP:PG  | 3.09                     | 0.51              |
| 1:M:189:VAL:HA   | 1:M:377:ALA:HA   | 1.93                     | 0.51              |
| 1:N:169:VAL:HG23 | 1:N:170:GLY:O    | 2.10                     | 0.51              |
| 1:N:240:VAL:HG11 | 1:N:247:LEU:CA   | 2.40                     | 0.51              |
| 1:N:77:VAL:HG22  | 1:N:510:VAL:HB   | 1.92                     | 0.51              |
| 1:A:141:SER:O    | 1:A:163:ALA:HB1  | 2.11                     | 0.51              |
| 1:C:183:LEU:HA   | 1:C:383:ALA:N    | 2.25                     | 0.51              |
| 1:C:225:LYS:CB   | 1:C:308:GLU:HA   | 2.41                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:475:ASN:ND2  | 1:C:489:ILE:HD11 | 2.26                     | 0.51              |
| 1:D:52:ASP:HB3   | 1:D:55:SER:H     | 1.75                     | 0.51              |
| 1:E:141:SER:O    | 1:E:163:ALA:HB1  | 2.11                     | 0.51              |
| 1:E:328:ASP:O    | 1:E:329:THR:HG23 | 2.10                     | 0.51              |
| 1:E:52:ASP:CB    | 1:E:55:SER:H     | 2.24                     | 0.51              |
| 1:F:34:LYS:HB2   | 1:F:458:CYS:HA   | 1.92                     | 0.51              |
| 1:G:27:VAL:HG12  | 1:G:90:THR:HG23  | 1.93                     | 0.51              |
| 2:H:1525:PO4:P   | 4:H:1527:ATP:PG  | 3.09                     | 0.51              |
| 1:I:220:ILE:HD12 | 1:I:296:THR:CG2  | 2.40                     | 0.51              |
| 1:L:240:VAL:HG11 | 1:L:247:LEU:CA   | 2.41                     | 0.51              |
| 1:N:240:VAL:HG11 | 1:N:247:LEU:HB2  | 1.93                     | 0.51              |
| 1:B:141:SER:O    | 1:B:163:ALA:HB1  | 2.11                     | 0.51              |
| 1:B:225:LYS:CB   | 1:B:308:GLU:HA   | 2.41                     | 0.51              |
| 1:C:240:VAL:HG12 | 1:C:271:VAL:HG13 | 1.91                     | 0.51              |
| 1:E:225:LYS:CB   | 1:E:308:GLU:HA   | 2.41                     | 0.51              |
| 1:F:240:VAL:HG12 | 1:F:271:VAL:HG13 | 1.91                     | 0.51              |
| 1:F:37:ASN:ND2   | 1:F:49:ILE:HG23  | 2.25                     | 0.51              |
| 1:G:475:ASN:ND2  | 1:G:489:ILE:HD11 | 2.26                     | 0.51              |
| 1:H:207:LYS:HE2  | 1:H:207:LYS:N    | 2.24                     | 0.51              |
| 1:H:518:GLU:O    | 1:H:518:GLU:CB   | 2.54                     | 0.51              |
| 1:J:183:LEU:HD23 | 1:J:183:LEU:H    | 1.76                     | 0.51              |
| 1:L:302:SER:HB2  | 1:L:305:ILE:H    | 1.74                     | 0.51              |
| 1:M:77:VAL:HG22  | 1:M:510:VAL:HB   | 1.92                     | 0.51              |
| 1:N:511:ALA:O    | 1:N:515:ILE:HG13 | 2.11                     | 0.51              |
| 1:A:381:VAL:HB   | 1:A:393:LYS:HA   | 1.92                     | 0.51              |
| 1:B:52:ASP:CB    | 1:B:55:SER:H     | 2.24                     | 0.51              |
| 1:C:194:GLN:CG   | 1:C:329:THR:HG21 | 2.41                     | 0.51              |
| 1:C:200:LEU:CB   | 1:C:259:LEU:CD1  | 2.86                     | 0.51              |
| 1:C:52:ASP:CB    | 1:C:55:SER:H     | 2.24                     | 0.51              |
| 1:F:381:VAL:HB   | 1:F:393:LYS:HA   | 1.92                     | 0.51              |
| 1:G:141:SER:O    | 1:G:163:ALA:HB1  | 2.11                     | 0.51              |
| 1:L:221:LEU:CG   | 1:L:309:LEU:HD22 | 2.40                     | 0.51              |
| 1:N:220:ILE:HD12 | 1:N:296:THR:CG2  | 2.40                     | 0.51              |
| 1:N:221:LEU:CD2  | 1:N:309:LEU:HD22 | 2.41                     | 0.51              |
| 1:A:38:VAL:HG11  | 1:A:56:VAL:HG22  | 1.91                     | 0.50              |
| 1:D:475:ASN:ND2  | 1:D:489:ILE:HD11 | 2.26                     | 0.50              |
| 1:E:161:LEU:HD11 | 1:E:185:ASP:HB3  | 1.93                     | 0.50              |
| 1:F:141:SER:O    | 1:F:163:ALA:HB1  | 2.11                     | 0.50              |
| 1:F:38:VAL:HG11  | 1:F:56:VAL:HG22  | 1.91                     | 0.50              |
| 1:H:240:VAL:HG11 | 1:H:247:LEU:CA   | 2.42                     | 0.50              |
| 1:J:247:LEU:O    | 1:J:273:VAL:HA   | 2.10                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:249:ILE:HB   | 1:M:275:ALA:CB   | 2.40                     | 0.50              |
| 1:A:161:LEU:HD11 | 1:A:185:ASP:HB3  | 1.93                     | 0.50              |
| 1:B:100:ILE:HD13 | 1:B:514:MET:SD   | 2.52                     | 0.50              |
| 1:B:34:LYS:HB2   | 1:B:458:CYS:HA   | 1.92                     | 0.50              |
| 1:D:194:GLN:CG   | 1:D:329:THR:HG21 | 2.41                     | 0.50              |
| 1:G:100:ILE:HD13 | 1:G:514:MET:SD   | 2.52                     | 0.50              |
| 1:I:206:ASN:HB3  | 1:I:208:PRO:HD2  | 1.93                     | 0.50              |
| 1:J:206:ASN:CG   | 1:J:207:LYS:H    | 2.15                     | 0.50              |
| 1:J:240:VAL:HG11 | 1:J:247:LEU:CA   | 2.41                     | 0.50              |
| 1:K:177:VAL:HG12 | 1:K:393:LYS:HE2  | 1.93                     | 0.50              |
| 1:M:183:LEU:H    | 1:M:183:LEU:HD23 | 1.76                     | 0.50              |
| 1:M:240:VAL:HG11 | 1:M:247:LEU:CA   | 2.41                     | 0.50              |
| 1:A:100:ILE:HD13 | 1:A:514:MET:SD   | 2.52                     | 0.50              |
| 1:G:158:VAL:HG22 | 1:G:396:VAL:HG22 | 1.93                     | 0.50              |
| 1:L:511:ALA:O    | 1:L:515:ILE:HG13 | 2.11                     | 0.50              |
| 1:L:77:VAL:HG22  | 1:L:510:VAL:HB   | 1.92                     | 0.50              |
| 1:A:240:VAL:HG12 | 1:A:271:VAL:HG13 | 1.91                     | 0.50              |
| 1:C:137:PRO:HA   | 1:C:410:GLY:HA3  | 1.90                     | 0.50              |
| 1:C:100:ILE:HD13 | 1:C:514:MET:SD   | 2.52                     | 0.50              |
| 1:D:166:MET:O    | 1:D:170:GLY:HA2  | 2.12                     | 0.50              |
| 1:F:158:VAL:HG22 | 1:F:396:VAL:HG22 | 1.93                     | 0.50              |
| 1:G:166:MET:O    | 1:G:170:GLY:HA2  | 2.12                     | 0.50              |
| 1:G:213:VAL:HG11 | 1:G:325:ILE:HG12 | 1.88                     | 0.50              |
| 2:M:1525:PO4:P   | 4:M:1527:ATP:PG  | 3.09                     | 0.50              |
| 2:N:1525:PO4:P   | 4:N:1527:ATP:PG  | 3.09                     | 0.50              |
| 1:A:166:MET:O    | 1:A:170:GLY:HA2  | 2.12                     | 0.50              |
| 1:A:200:LEU:HD11 | 1:A:254:VAL:HA   | 1.94                     | 0.50              |
| 1:B:183:LEU:HA   | 1:B:383:ALA:N    | 2.25                     | 0.50              |
| 1:B:194:GLN:O    | 1:B:371:LYS:HB3  | 2.12                     | 0.50              |
| 1:D:161:LEU:HD11 | 1:D:185:ASP:HB3  | 1.93                     | 0.50              |
| 1:D:240:VAL:HG12 | 1:D:271:VAL:HG13 | 1.91                     | 0.50              |
| 1:E:158:VAL:HG22 | 1:E:396:VAL:HG22 | 1.93                     | 0.50              |
| 1:F:100:ILE:HD13 | 1:F:514:MET:SD   | 2.52                     | 0.50              |
| 1:F:475:ASN:ND2  | 1:F:489:ILE:HD11 | 2.26                     | 0.50              |
| 1:G:194:GLN:CG   | 1:G:329:THR:HG21 | 2.41                     | 0.50              |
| 1:G:381:VAL:HB   | 1:G:393:LYS:HA   | 1.92                     | 0.50              |
| 1:K:190:VAL:HG21 | 1:K:333:ILE:HD13 | 1.94                     | 0.50              |
| 1:B:52:ASP:HB3   | 1:B:55:SER:H     | 1.76                     | 0.50              |
| 1:G:255:GLU:HB2  | 1:G:259:LEU:H    | 1.77                     | 0.50              |
| 1:G:225:LYS:CB   | 1:G:308:GLU:HA   | 2.41                     | 0.50              |
| 1:I:77:VAL:HG22  | 1:I:510:VAL:HB   | 1.92                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:77:VAL:HG22  | 1:J:510:VAL:HB   | 1.92                     | 0.50              |
| 1:K:221:LEU:CD2  | 1:K:309:LEU:HD22 | 2.42                     | 0.50              |
| 1:L:191:GLU:HG2  | 1:L:192:GLY:H    | 1.75                     | 0.50              |
| 1:L:221:LEU:CD2  | 1:L:309:LEU:HD22 | 2.42                     | 0.50              |
| 1:N:204:PHE:HD1  | 1:N:207:LYS:NZ   | 2.06                     | 0.50              |
| 1:N:249:ILE:HB   | 1:N:275:ALA:CB   | 2.40                     | 0.50              |
| 1:A:194:GLN:CG   | 1:A:329:THR:HG21 | 2.41                     | 0.50              |
| 1:B:255:GLU:HB2  | 1:B:259:LEU:H    | 1.77                     | 0.50              |
| 1:C:166:MET:O    | 1:C:170:GLY:HA2  | 2.12                     | 0.50              |
| 1:E:194:GLN:CG   | 1:E:329:THR:HG21 | 2.41                     | 0.50              |
| 1:E:34:LYS:HB2   | 1:E:458:CYS:HA   | 1.92                     | 0.50              |
| 1:E:381:VAL:HB   | 1:E:393:LYS:HA   | 1.92                     | 0.50              |
| 1:F:200:LEU:HD12 | 1:F:275:ALA:HB1  | 1.93                     | 0.50              |
| 1:G:150:ILE:CD1  | 1:G:493:ILE:CA   | 2.74                     | 0.50              |
| 1:G:406:ALA:HB1  | 1:G:411:VAL:CG1  | 2.42                     | 0.50              |
| 1:J:168:LYS:HG2  | 1:J:187:LEU:HD21 | 1.93                     | 0.50              |
| 1:M:511:ALA:O    | 1:M:515:ILE:HG13 | 2.11                     | 0.50              |
| 1:N:183:LEU:HD23 | 1:N:183:LEU:H    | 1.76                     | 0.50              |
| 1:C:249:ILE:HD11 | 1:C:262:LEU:HD22 | 1.87                     | 0.50              |
| 1:C:224:ASP:HA   | 1:C:289:LEU:CD1  | 2.42                     | 0.50              |
| 1:D:255:GLU:HB2  | 1:D:259:LEU:H    | 1.77                     | 0.50              |
| 1:E:147:VAL:HG22 | 1:E:494:LEU:HB2  | 1.94                     | 0.50              |
| 1:E:166:MET:O    | 1:E:170:GLY:HA2  | 2.12                     | 0.50              |
| 1:F:147:VAL:HG22 | 1:F:494:LEU:HB2  | 1.94                     | 0.50              |
| 1:G:382:GLY:O    | 1:G:389:MET:HA   | 2.12                     | 0.50              |
| 1:I:511:ALA:O    | 1:I:515:ILE:HG13 | 2.11                     | 0.50              |
| 1:J:190:VAL:HG21 | 1:J:333:ILE:HD13 | 1.94                     | 0.50              |
| 1:K:182:GLY:HA3  | 1:K:383:ALA:N    | 2.09                     | 0.50              |
| 1:J:242:LYS:CB   | 1:K:257:GLU:HA   | 2.41                     | 0.50              |
| 1:A:225:LYS:CB   | 1:A:308:GLU:HA   | 2.41                     | 0.50              |
| 1:A:224:ASP:HA   | 1:A:289:LEU:CD1  | 2.42                     | 0.50              |
| 1:A:52:ASP:CB    | 1:A:55:SER:H     | 2.24                     | 0.50              |
| 1:B:147:VAL:HG22 | 1:B:494:LEU:HB2  | 1.94                     | 0.50              |
| 1:B:213:VAL:HG11 | 1:B:325:ILE:HG12 | 1.88                     | 0.50              |
| 1:B:406:ALA:HB1  | 1:B:411:VAL:CG1  | 2.42                     | 0.50              |
| 1:C:382:GLY:O    | 1:C:389:MET:HA   | 2.12                     | 0.50              |
| 1:D:141:SER:O    | 1:D:163:ALA:HB1  | 2.11                     | 0.50              |
| 1:E:240:VAL:HG21 | 1:E:247:LEU:HD13 | 1.94                     | 0.50              |
| 1:E:382:GLY:O    | 1:E:389:MET:HA   | 2.12                     | 0.50              |
| 1:F:224:ASP:HA   | 1:F:289:LEU:CD1  | 2.42                     | 0.50              |
| 1:K:240:VAL:HG11 | 1:K:247:LEU:CA   | 2.41                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:221:LEU:CD2  | 1:M:309:LEU:HD22 | 2.42                     | 0.50              |
| 1:A:225:LYS:HB2  | 1:A:308:GLU:HA   | 1.94                     | 0.49              |
| 1:B:475:ASN:ND2  | 1:B:489:ILE:HD11 | 2.26                     | 0.49              |
| 1:C:224:ASP:CG   | 1:C:302:SER:HA   | 2.33                     | 0.49              |
| 1:D:100:ILE:HD13 | 1:D:514:MET:SD   | 2.52                     | 0.49              |
| 1:D:191:GLU:HG3  | 1:D:342:ILE:HD12 | 1.93                     | 0.49              |
| 1:G:200:LEU:CD2  | 1:G:254:VAL:CG1  | 2.86                     | 0.49              |
| 1:I:190:VAL:HG21 | 1:I:333:ILE:HD13 | 1.94                     | 0.49              |
| 1:I:221:LEU:HG   | 1:I:309:LEU:HD22 | 1.94                     | 0.49              |
| 1:K:152:ALA:HB3  | 1:K:155:ASP:N    | 2.27                     | 0.49              |
| 1:M:152:ALA:HB3  | 1:M:155:ASP:N    | 2.27                     | 0.49              |
| 1:M:190:VAL:HG21 | 1:M:333:ILE:HD13 | 1.94                     | 0.49              |
| 1:M:301:ILE:HD11 | 1:M:312:ALA:CB   | 2.32                     | 0.49              |
| 1:A:224:ASP:CG   | 1:A:302:SER:HA   | 2.33                     | 0.49              |
| 1:A:147:VAL:HG22 | 1:A:494:LEU:HB2  | 1.94                     | 0.49              |
| 1:B:161:LEU:HD11 | 1:B:185:ASP:HB3  | 1.93                     | 0.49              |
| 1:B:224:ASP:HA   | 1:B:289:LEU:CD1  | 2.42                     | 0.49              |
| 1:B:225:LYS:HB2  | 1:B:308:GLU:HA   | 1.94                     | 0.49              |
| 1:C:161:LEU:HD11 | 1:C:185:ASP:HB3  | 1.93                     | 0.49              |
| 1:C:192:GLY:HA3  | 1:C:376:VAL:CG2  | 2.40                     | 0.49              |
| 1:C:25:ASP:CG    | 1:C:28:LYS:HZ3   | 2.16                     | 0.49              |
| 1:D:220:ILE:CD1  | 1:D:332:ILE:HD13 | 2.33                     | 0.49              |
| 1:F:240:VAL:HG21 | 1:F:247:LEU:HD13 | 1.94                     | 0.49              |
| 1:F:225:LYS:CB   | 1:F:308:GLU:HA   | 2.41                     | 0.49              |
| 1:G:225:LYS:HB2  | 1:G:308:GLU:HA   | 1.94                     | 0.49              |
| 1:J:224:ASP:HB2  | 1:J:303:GLU:H    | 1.77                     | 0.49              |
| 1:K:240:VAL:HG11 | 1:K:247:LEU:HB2  | 1.94                     | 0.49              |
| 1:L:249:ILE:HB   | 1:L:275:ALA:CB   | 2.40                     | 0.49              |
| 1:L:31:LEU:HB2   | 1:L:90:THR:HG21  | 1.95                     | 0.49              |
| 1:M:243:ALA:HA   | 1:N:260:ALA:HB2  | 1.93                     | 0.49              |
| 1:N:182:GLY:HA3  | 1:N:383:ALA:N    | 2.09                     | 0.49              |
| 1:B:166:MET:O    | 1:B:170:GLY:HA2  | 2.12                     | 0.49              |
| 1:B:240:VAL:HG21 | 1:B:247:LEU:HD13 | 1.94                     | 0.49              |
| 1:C:147:VAL:HG22 | 1:C:494:LEU:HB2  | 1.94                     | 0.49              |
| 1:D:190:VAL:HG23 | 1:D:333:ILE:CG2  | 2.42                     | 0.49              |
| 1:D:224:ASP:HA   | 1:D:289:LEU:CD1  | 2.42                     | 0.49              |
| 1:D:240:VAL:HG21 | 1:D:247:LEU:HD13 | 1.94                     | 0.49              |
| 1:D:382:GLY:O    | 1:D:389:MET:HA   | 2.12                     | 0.49              |
| 1:E:25:ASP:CG    | 1:E:28:LYS:HZ3   | 2.15                     | 0.49              |
| 1:F:225:LYS:HB2  | 1:F:308:GLU:HA   | 1.94                     | 0.49              |
| 1:H:152:ALA:HB3  | 1:H:155:ASP:N    | 2.27                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:178:GLU:O    | 1:J:380:LYS:HA   | 2.12                     | 0.49              |
| 1:K:77:VAL:HG22  | 1:K:510:VAL:HB   | 1.92                     | 0.49              |
| 1:K:518:GLU:CB   | 1:K:518:GLU:O    | 2.54                     | 0.49              |
| 1:H:257:GLU:HA   | 1:N:242:LYS:CB   | 2.41                     | 0.49              |
| 1:C:240:VAL:HG21 | 1:C:247:LEU:HD13 | 1.94                     | 0.49              |
| 1:D:52:ASP:CB    | 1:D:55:SER:H     | 2.25                     | 0.49              |
| 1:E:221:LEU:HD21 | 1:E:309:LEU:HD11 | 1.95                     | 0.49              |
| 1:F:166:MET:O    | 1:F:170:GLY:HA2  | 2.12                     | 0.49              |
| 1:F:255:GLU:HB2  | 1:F:259:LEU:H    | 1.77                     | 0.49              |
| 1:F:406:ALA:HB1  | 1:F:411:VAL:CG1  | 2.42                     | 0.49              |
| 1:H:236:VAL:O    | 1:H:240:VAL:HG23 | 2.13                     | 0.49              |
| 1:I:31:LEU:HB2   | 1:I:90:THR:HG21  | 1.95                     | 0.49              |
| 1:I:243:ALA:N    | 1:J:256:GLY:C    | 2.66                     | 0.49              |
| 1:K:249:ILE:HB   | 1:K:275:ALA:CB   | 2.40                     | 0.49              |
| 1:K:31:LEU:HB2   | 1:K:90:THR:HG21  | 1.95                     | 0.49              |
| 1:N:224:ASP:HB2  | 1:N:303:GLU:H    | 1.78                     | 0.49              |
| 1:A:240:VAL:HG21 | 1:A:247:LEU:HD13 | 1.94                     | 0.49              |
| 1:A:382:GLY:O    | 1:A:389:MET:HA   | 2.12                     | 0.49              |
| 1:A:406:ALA:HB1  | 1:A:411:VAL:CG1  | 2.42                     | 0.49              |
| 1:B:200:LEU:HD11 | 1:B:254:VAL:HA   | 1.94                     | 0.49              |
| 1:C:221:LEU:HD21 | 1:C:309:LEU:HD11 | 1.95                     | 0.49              |
| 1:C:193:MET:CE   | 1:C:332:ILE:HD12 | 2.36                     | 0.49              |
| 1:D:147:VAL:HG22 | 1:D:494:LEU:HB2  | 1.94                     | 0.49              |
| 1:E:85:ALA:HB1   | 1:E:499:VAL:HG12 | 1.95                     | 0.49              |
| 1:G:224:ASP:CG   | 1:G:302:SER:HA   | 2.33                     | 0.49              |
| 1:G:25:ASP:CG    | 1:G:28:LYS:HZ3   | 2.15                     | 0.49              |
| 1:I:183:LEU:HD23 | 1:I:183:LEU:H    | 1.76                     | 0.49              |
| 1:J:227:ILE:CD1  | 1:J:233:MET:SD   | 2.92                     | 0.49              |
| 1:J:242:LYS:HG3  | 1:K:257:GLU:HB2  | 1.94                     | 0.49              |
| 1:J:240:VAL:HG11 | 1:J:247:LEU:HB2  | 1.94                     | 0.49              |
| 1:K:406:ALA:HB1  | 1:K:411:VAL:CG1  | 2.43                     | 0.49              |
| 1:L:406:ALA:HB1  | 1:L:411:VAL:CG1  | 2.43                     | 0.49              |
| 1:B:224:ASP:CG   | 1:B:302:SER:HA   | 2.33                     | 0.49              |
| 1:C:200:LEU:HD12 | 1:C:275:ALA:HB1  | 1.93                     | 0.49              |
| 1:C:406:ALA:HB1  | 1:C:411:VAL:CG1  | 2.42                     | 0.49              |
| 1:D:521:VAL:HG21 | 1:E:59:GLU:CB    | 2.43                     | 0.49              |
| 1:E:100:ILE:HD13 | 1:E:514:MET:SD   | 2.52                     | 0.49              |
| 1:E:137:PRO:HA   | 1:E:410:GLY:HA3  | 1.90                     | 0.49              |
| 1:F:194:GLN:CG   | 1:F:329:THR:HG21 | 2.41                     | 0.49              |
| 1:H:221:LEU:HG   | 1:H:309:LEU:HD22 | 1.95                     | 0.49              |
| 1:H:406:ALA:HB1  | 1:H:411:VAL:CG1  | 2.43                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:242:LYS:CB   | 1:J:257:GLU:HA   | 2.41                     | 0.49              |
| 1:I:242:LYS:HG3  | 1:J:257:GLU:HB2  | 1.93                     | 0.49              |
| 1:I:240:VAL:HG11 | 1:I:247:LEU:CA   | 2.41                     | 0.49              |
| 1:J:221:LEU:HG   | 1:J:309:LEU:HD22 | 1.95                     | 0.49              |
| 1:J:31:LEU:HB2   | 1:J:90:THR:HG21  | 1.95                     | 0.49              |
| 1:A:255:GLU:HB2  | 1:A:259:LEU:H    | 1.77                     | 0.49              |
| 1:D:383:ALA:HA   | 1:D:389:MET:HB2  | 1.95                     | 0.49              |
| 1:E:224:ASP:CG   | 1:E:302:SER:HA   | 2.33                     | 0.49              |
| 1:F:383:ALA:HA   | 1:F:389:MET:HB2  | 1.95                     | 0.49              |
| 1:F:85:ALA:HB1   | 1:F:499:VAL:HG12 | 1.95                     | 0.49              |
| 1:G:240:VAL:HG21 | 1:G:247:LEU:HD13 | 1.94                     | 0.49              |
| 1:H:190:VAL:HG21 | 1:H:333:ILE:HD13 | 1.94                     | 0.49              |
| 1:H:249:ILE:HB   | 1:H:275:ALA:CB   | 2.40                     | 0.49              |
| 1:J:290:GLN:HA   | 1:J:300:VAL:HG21 | 1.95                     | 0.49              |
| 1:K:242:LYS:C    | 1:L:257:GLU:CA   | 2.78                     | 0.49              |
| 1:L:182:GLY:HA3  | 1:L:383:ALA:N    | 2.09                     | 0.49              |
| 1:L:224:ASP:HB2  | 1:L:303:GLU:H    | 1.78                     | 0.49              |
| 1:H:256:GLY:C    | 1:N:243:ALA:N    | 2.66                     | 0.49              |
| 1:B:200:LEU:HD12 | 1:B:275:ALA:HB1  | 1.93                     | 0.49              |
| 1:B:382:GLY:O    | 1:B:389:MET:HA   | 2.12                     | 0.49              |
| 1:C:225:LYS:HB2  | 1:C:308:GLU:HA   | 1.94                     | 0.49              |
| 1:D:224:ASP:CG   | 1:D:302:SER:HA   | 2.33                     | 0.49              |
| 1:D:85:ALA:HB1   | 1:D:499:VAL:HG12 | 1.95                     | 0.49              |
| 1:E:383:ALA:HA   | 1:E:389:MET:HB2  | 1.95                     | 0.49              |
| 1:F:227:ILE:HG12 | 1:F:309:LEU:HG   | 1.95                     | 0.49              |
| 1:F:52:ASP:CB    | 1:F:55:SER:H     | 2.25                     | 0.49              |
| 1:I:236:VAL:O    | 1:I:240:VAL:HG23 | 2.13                     | 0.49              |
| 1:J:243:ALA:N    | 1:K:256:GLY:C    | 2.66                     | 0.49              |
| 1:J:406:ALA:HB1  | 1:J:411:VAL:CG1  | 2.43                     | 0.49              |
| 1:M:31:LEU:HB2   | 1:M:90:THR:HG21  | 1.95                     | 0.49              |
| 1:N:206:ASN:HB2  | 1:N:213:VAL:HA   | 1.94                     | 0.49              |
| 1:A:220:ILE:CD1  | 1:A:332:ILE:HD13 | 2.33                     | 0.49              |
| 1:B:221:LEU:HD21 | 1:B:309:LEU:HD11 | 1.95                     | 0.49              |
| 1:C:255:GLU:HB2  | 1:C:259:LEU:H    | 1.77                     | 0.49              |
| 1:D:406:ALA:HB1  | 1:D:411:VAL:CG1  | 2.42                     | 0.49              |
| 1:E:225:LYS:HB2  | 1:E:308:GLU:HA   | 1.94                     | 0.49              |
| 1:E:249:ILE:HD11 | 1:E:262:LEU:HD22 | 1.87                     | 0.49              |
| 1:E:521:VAL:HG21 | 1:F:59:GLU:CB    | 2.43                     | 0.49              |
| 1:G:137:PRO:HA   | 1:G:410:GLY:HA3  | 1.90                     | 0.49              |
| 1:H:136:VAL:O    | 1:H:410:GLY:HA3  | 2.13                     | 0.49              |
| 1:H:31:LEU:HB2   | 1:H:90:THR:HG21  | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:221:LEU:HD13 | 1:I:317:LEU:CD1  | 2.43                     | 0.49              |
| 1:I:290:GLN:HA   | 1:I:300:VAL:HG21 | 1.95                     | 0.49              |
| 1:J:242:LYS:C    | 1:K:257:GLU:CA   | 2.78                     | 0.49              |
| 1:K:243:ALA:N    | 1:L:256:GLY:C    | 2.66                     | 0.49              |
| 1:M:182:GLY:HA3  | 1:M:383:ALA:N    | 2.09                     | 0.49              |
| 1:A:383:ALA:HA   | 1:A:389:MET:HB2  | 1.95                     | 0.49              |
| 1:B:383:ALA:HA   | 1:B:389:MET:HB2  | 1.95                     | 0.49              |
| 1:C:383:ALA:HA   | 1:C:389:MET:HB2  | 1.95                     | 0.49              |
| 1:D:221:LEU:HD21 | 1:D:309:LEU:HD11 | 1.95                     | 0.49              |
| 1:E:240:VAL:CG1  | 1:E:247:LEU:HB2  | 2.42                     | 0.49              |
| 1:G:227:ILE:HG12 | 1:G:309:LEU:HG   | 1.94                     | 0.49              |
| 1:H:257:GLU:HB2  | 1:N:242:LYS:HG3  | 1.94                     | 0.49              |
| 1:H:221:LEU:CD2  | 1:H:309:LEU:HD22 | 2.42                     | 0.49              |
| 1:H:427:ALA:HA   | 1:H:444:LEU:HD11 | 1.95                     | 0.49              |
| 1:L:240:VAL:HG11 | 1:L:247:LEU:HB2  | 1.94                     | 0.49              |
| 1:M:243:ALA:N    | 1:N:256:GLY:C    | 2.66                     | 0.49              |
| 1:M:136:VAL:O    | 1:M:410:GLY:HA3  | 2.13                     | 0.49              |
| 1:N:206:ASN:C    | 1:N:208:PRO:N    | 2.66                     | 0.49              |
| 1:C:247:LEU:HB3  | 1:C:273:VAL:HG22 | 1.96                     | 0.48              |
| 1:E:227:ILE:HG12 | 1:E:309:LEU:HG   | 1.94                     | 0.48              |
| 1:G:383:ALA:HA   | 1:G:389:MET:HB2  | 1.95                     | 0.48              |
| 1:I:224:ASP:HB2  | 1:I:303:GLU:H    | 1.78                     | 0.48              |
| 1:K:221:LEU:HG   | 1:K:309:LEU:HD22 | 1.95                     | 0.48              |
| 1:L:255:GLU:CD   | 1:L:256:GLY:H    | 2.16                     | 0.48              |
| 1:L:290:GLN:HA   | 1:L:300:VAL:HG21 | 1.95                     | 0.48              |
| 1:M:240:VAL:HG11 | 1:M:247:LEU:HB2  | 1.94                     | 0.48              |
| 1:L:243:ALA:N    | 1:M:256:GLY:C    | 2.66                     | 0.48              |
| 1:M:290:GLN:HA   | 1:M:300:VAL:HG21 | 1.95                     | 0.48              |
| 1:M:406:ALA:HB1  | 1:M:411:VAL:CG1  | 2.43                     | 0.48              |
| 1:N:152:ALA:HB3  | 1:N:155:ASP:N    | 2.27                     | 0.48              |
| 1:N:190:VAL:HG21 | 1:N:333:ILE:HD13 | 1.94                     | 0.48              |
| 1:N:31:LEU:HB2   | 1:N:90:THR:HG21  | 1.95                     | 0.48              |
| 1:A:59:GLU:CB    | 1:G:521:VAL:HG21 | 2.43                     | 0.48              |
| 1:D:225:LYS:HB2  | 1:D:308:GLU:HA   | 1.94                     | 0.48              |
| 1:E:200:LEU:HD12 | 1:E:275:ALA:HB1  | 1.93                     | 0.48              |
| 1:E:224:ASP:HA   | 1:E:289:LEU:CD1  | 2.42                     | 0.48              |
| 1:G:206:ASN:HB3  | 1:G:208:PRO:HD2  | 1.94                     | 0.48              |
| 1:H:243:ALA:N    | 1:I:256:GLY:C    | 2.66                     | 0.48              |
| 1:I:152:ALA:HB3  | 1:I:155:ASP:N    | 2.27                     | 0.48              |
| 1:I:427:ALA:HA   | 1:I:444:LEU:HD11 | 1.95                     | 0.48              |
| 1:J:221:LEU:HD13 | 1:J:317:LEU:CD1  | 2.44                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:350:ARG:HD2  | 1:N:353:ILE:HD12 | 1.96                     | 0.48              |
| 1:N:427:ALA:HA   | 1:N:444:LEU:HD11 | 1.95                     | 0.48              |
| 1:B:247:LEU:HB3  | 1:B:273:VAL:HG22 | 1.96                     | 0.48              |
| 1:E:255:GLU:HB2  | 1:E:259:LEU:H    | 1.77                     | 0.48              |
| 1:F:382:GLY:O    | 1:F:389:MET:HA   | 2.12                     | 0.48              |
| 1:G:220:ILE:CD1  | 1:G:332:ILE:HD13 | 2.33                     | 0.48              |
| 1:H:350:ARG:HD2  | 1:H:353:ILE:HD12 | 1.95                     | 0.48              |
| 1:I:221:LEU:CD2  | 1:I:309:LEU:HD22 | 2.42                     | 0.48              |
| 1:I:518:GLU:CB   | 1:I:518:GLU:O    | 2.54                     | 0.48              |
| 1:J:152:ALA:HB3  | 1:J:155:ASP:N    | 2.27                     | 0.48              |
| 1:N:290:GLN:HA   | 1:N:300:VAL:HG21 | 1.95                     | 0.48              |
| 1:B:521:VAL:HG21 | 1:C:59:GLU:CB    | 2.43                     | 0.48              |
| 1:E:200:LEU:HD11 | 1:E:254:VAL:CA   | 2.12                     | 0.48              |
| 1:E:406:ALA:HB1  | 1:E:411:VAL:CG1  | 2.42                     | 0.48              |
| 1:G:85:ALA:HB1   | 1:G:499:VAL:HG12 | 1.95                     | 0.48              |
| 1:I:240:VAL:HG11 | 1:I:247:LEU:HB2  | 1.94                     | 0.48              |
| 1:K:221:LEU:HD13 | 1:K:317:LEU:CD1  | 2.44                     | 0.48              |
| 1:L:152:ALA:HB3  | 1:L:155:ASP:N    | 2.27                     | 0.48              |
| 1:M:350:ARG:HD2  | 1:M:353:ILE:HD12 | 1.96                     | 0.48              |
| 1:A:247:LEU:HB3  | 1:A:273:VAL:HG22 | 1.96                     | 0.48              |
| 1:D:190:VAL:HG23 | 1:D:333:ILE:HG23 | 1.96                     | 0.48              |
| 1:G:147:VAL:HG22 | 1:G:494:LEU:HB2  | 1.94                     | 0.48              |
| 1:K:290:GLN:HA   | 1:K:300:VAL:HG21 | 1.95                     | 0.48              |
| 1:A:227:ILE:HG12 | 1:A:309:LEU:HG   | 1.95                     | 0.48              |
| 1:A:311:LYS:HA   | 1:A:311:LYS:HD3  | 1.93                     | 0.48              |
| 1:B:150:ILE:CD1  | 1:B:493:ILE:CA   | 2.74                     | 0.48              |
| 1:B:23:LEU:HA    | 1:B:60:ILE:CD1   | 2.32                     | 0.48              |
| 1:D:200:LEU:HD11 | 1:D:254:VAL:CA   | 2.12                     | 0.48              |
| 1:D:240:VAL:CG1  | 1:D:247:LEU:HB2  | 2.42                     | 0.48              |
| 1:F:247:LEU:HB3  | 1:F:273:VAL:HG22 | 1.95                     | 0.48              |
| 1:F:224:ASP:CG   | 1:F:302:SER:HA   | 2.33                     | 0.48              |
| 1:F:521:VAL:HG21 | 1:G:59:GLU:CB    | 2.43                     | 0.48              |
| 1:G:162:ILE:CD1  | 1:G:400:LEU:N    | 2.77                     | 0.48              |
| 1:G:224:ASP:HA   | 1:G:289:LEU:CD1  | 2.42                     | 0.48              |
| 1:H:240:VAL:HG11 | 1:H:247:LEU:HB2  | 1.95                     | 0.48              |
| 1:H:290:GLN:HA   | 1:H:300:VAL:HG21 | 1.95                     | 0.48              |
| 1:H:221:LEU:HD13 | 1:H:317:LEU:CD1  | 2.44                     | 0.48              |
| 1:J:221:LEU:CD2  | 1:J:309:LEU:HD22 | 2.42                     | 0.48              |
| 1:J:249:ILE:HB   | 1:J:275:ALA:CB   | 2.40                     | 0.48              |
| 1:J:427:ALA:HA   | 1:J:444:LEU:HD11 | 1.95                     | 0.48              |
| 1:K:274:ALA:HB1  | 1:K:325:ILE:HD13 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:224:ASP:HB2  | 1:M:303:GLU:H    | 1.78                     | 0.48              |
| 1:A:227:ILE:HD12 | 1:A:258:ALA:HB1  | 1.96                     | 0.48              |
| 1:B:222:LEU:CD2  | 1:B:292:ILE:HG22 | 2.42                     | 0.48              |
| 1:C:162:ILE:CD1  | 1:C:400:LEU:N    | 2.77                     | 0.48              |
| 1:C:85:ALA:HB1   | 1:C:499:VAL:HG12 | 1.95                     | 0.48              |
| 1:D:25:ASP:CG    | 1:D:28:LYS:HZ3   | 2.17                     | 0.48              |
| 1:D:309:LEU:O    | 1:D:312:ALA:HB3  | 2.14                     | 0.48              |
| 1:E:158:VAL:HG13 | 1:E:396:VAL:HA   | 1.96                     | 0.48              |
| 1:F:309:LEU:O    | 1:F:312:ALA:HB3  | 2.14                     | 0.48              |
| 1:G:241:ALA:CA   | 1:G:271:VAL:HG22 | 2.44                     | 0.48              |
| 1:G:247:LEU:HB3  | 1:G:273:VAL:HG22 | 1.96                     | 0.48              |
| 1:I:182:GLY:HA3  | 1:I:383:ALA:N    | 2.09                     | 0.48              |
| 1:I:136:VAL:O    | 1:I:410:GLY:HA3  | 2.13                     | 0.48              |
| 1:L:236:VAL:O    | 1:L:240:VAL:HG23 | 2.13                     | 0.48              |
| 1:M:236:VAL:O    | 1:M:240:VAL:HG23 | 2.13                     | 0.48              |
| 1:A:200:LEU:HD12 | 1:A:275:ALA:HB1  | 1.93                     | 0.48              |
| 1:D:158:VAL:HG13 | 1:D:396:VAL:HA   | 1.96                     | 0.48              |
| 1:D:190:VAL:CG2  | 1:D:333:ILE:HG22 | 2.43                     | 0.48              |
| 1:D:247:LEU:HB3  | 1:D:273:VAL:HG22 | 1.96                     | 0.48              |
| 1:F:158:VAL:HG13 | 1:F:396:VAL:HA   | 1.96                     | 0.48              |
| 1:G:184:GLN:HG2  | 1:G:185:ASP:O    | 2.14                     | 0.48              |
| 1:H:203:TYR:CD1  | 1:H:267:MET:CE   | 2.97                     | 0.48              |
| 1:L:196:ASP:OD1  | 1:L:329:THR:HG22 | 2.14                     | 0.48              |
| 1:L:136:VAL:O    | 1:L:410:GLY:HA3  | 2.13                     | 0.48              |
| 1:A:222:LEU:CD2  | 1:A:292:ILE:HG22 | 2.42                     | 0.48              |
| 1:D:162:ILE:CD1  | 1:D:400:LEU:N    | 2.77                     | 0.48              |
| 1:E:247:LEU:HB3  | 1:E:273:VAL:HG22 | 1.96                     | 0.48              |
| 1:E:222:LEU:CD2  | 1:E:292:ILE:HG22 | 2.42                     | 0.48              |
| 1:J:207:LYS:HE2  | 1:J:207:LYS:N    | 2.28                     | 0.48              |
| 1:J:518:GLU:CB   | 1:J:518:GLU:O    | 2.54                     | 0.48              |
| 1:L:298:GLY:HA3  | 1:L:318:GLY:CA   | 2.44                     | 0.48              |
| 1:M:183:LEU:HA   | 1:M:382:GLY:CA   | 2.44                     | 0.48              |
| 1:N:236:VAL:O    | 1:N:240:VAL:HG23 | 2.14                     | 0.48              |
| 1:A:99:ILE:CG2   | 1:A:120:ILE:HD13 | 2.44                     | 0.48              |
| 1:A:249:ILE:HD11 | 1:A:262:LEU:HD22 | 1.87                     | 0.48              |
| 1:A:309:LEU:O    | 1:A:312:ALA:HB3  | 2.14                     | 0.48              |
| 1:A:85:ALA:HB1   | 1:A:499:VAL:HG12 | 1.95                     | 0.48              |
| 1:B:85:ALA:HB1   | 1:B:499:VAL:HG12 | 1.95                     | 0.48              |
| 1:C:213:VAL:CG2  | 1:C:214:GLU:N    | 2.77                     | 0.48              |
| 1:E:309:LEU:O    | 1:E:312:ALA:HB3  | 2.14                     | 0.48              |
| 1:F:221:LEU:HD21 | 1:F:309:LEU:HD11 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:207:LYS:HE2  | 1:G:207:LYS:HB2  | 1.49                     | 0.48              |
| 1:G:311:LYS:HA   | 1:G:311:LYS:HD3  | 1.93                     | 0.48              |
| 1:I:350:ARG:HD2  | 1:I:353:ILE:HD12 | 1.95                     | 0.48              |
| 1:K:236:VAL:O    | 1:K:240:VAL:HG23 | 2.13                     | 0.48              |
| 1:L:183:LEU:N    | 1:L:183:LEU:HD23 | 2.22                     | 0.48              |
| 1:L:350:ARG:HD2  | 1:L:353:ILE:HD12 | 1.96                     | 0.48              |
| 1:B:220:ILE:CD1  | 1:B:332:ILE:HD13 | 2.33                     | 0.47              |
| 1:B:99:ILE:CG2   | 1:B:120:ILE:HD13 | 2.44                     | 0.47              |
| 1:C:200:LEU:HD11 | 1:C:254:VAL:HA   | 1.94                     | 0.47              |
| 1:D:190:VAL:HB   | 1:D:334:ASP:CB   | 2.44                     | 0.47              |
| 1:D:241:ALA:CA   | 1:D:271:VAL:HG22 | 2.44                     | 0.47              |
| 1:C:521:VAL:HG21 | 1:D:59:GLU:CB    | 2.43                     | 0.47              |
| 1:E:180:GLY:HA2  | 1:E:380:LYS:HB3  | 1.96                     | 0.47              |
| 1:E:240:VAL:HG11 | 1:E:247:LEU:CB   | 2.43                     | 0.47              |
| 1:F:25:ASP:CG    | 1:F:28:LYS:HZ3   | 2.18                     | 0.47              |
| 1:G:200:LEU:HD22 | 1:G:259:LEU:CD2  | 2.30                     | 0.47              |
| 1:J:183:LEU:HA   | 1:J:382:GLY:CA   | 2.44                     | 0.47              |
| 1:K:427:ALA:HA   | 1:K:444:LEU:HD11 | 1.95                     | 0.47              |
| 1:L:427:ALA:HA   | 1:L:444:LEU:HD11 | 1.95                     | 0.47              |
| 1:N:221:LEU:HD13 | 1:N:317:LEU:CD1  | 2.44                     | 0.47              |
| 1:A:384:ALA:HA   | 1:A:385:THR:HA   | 1.68                     | 0.47              |
| 1:A:162:ILE:CD1  | 1:A:400:LEU:N    | 2.77                     | 0.47              |
| 1:B:162:ILE:CD1  | 1:B:400:LEU:N    | 2.77                     | 0.47              |
| 1:B:203:TYR:HD1  | 1:B:203:TYR:N    | 2.12                     | 0.47              |
| 1:B:227:ILE:HD12 | 1:B:258:ALA:HB1  | 1.96                     | 0.47              |
| 1:B:25:ASP:CG    | 1:B:28:LYS:HZ3   | 2.16                     | 0.47              |
| 1:B:180:GLY:HA2  | 1:B:380:LYS:HB3  | 1.96                     | 0.47              |
| 1:C:220:ILE:CD1  | 1:C:332:ILE:HD13 | 2.33                     | 0.47              |
| 1:D:200:LEU:HD12 | 1:D:275:ALA:HB1  | 1.93                     | 0.47              |
| 1:D:222:LEU:CD2  | 1:D:292:ILE:HG22 | 2.42                     | 0.47              |
| 1:E:99:ILE:CG2   | 1:E:120:ILE:HD13 | 2.44                     | 0.47              |
| 1:F:311:LYS:HD3  | 1:F:311:LYS:HA   | 1.93                     | 0.47              |
| 1:J:301:ILE:HD11 | 1:J:312:ALA:CB   | 2.32                     | 0.47              |
| 1:B:309:LEU:O    | 1:B:312:ALA:HB3  | 2.14                     | 0.47              |
| 1:D:213:VAL:O    | 1:D:324:VAL:HA   | 2.15                     | 0.47              |
| 1:D:240:VAL:HG11 | 1:D:247:LEU:CB   | 2.43                     | 0.47              |
| 1:D:278:ALA:HB2  | 1:D:289:LEU:CD1  | 2.45                     | 0.47              |
| 1:D:99:ILE:CG2   | 1:D:120:ILE:HD13 | 2.44                     | 0.47              |
| 1:E:213:VAL:CG2  | 1:E:214:GLU:N    | 2.77                     | 0.47              |
| 1:E:278:ALA:HB2  | 1:E:289:LEU:CD1  | 2.45                     | 0.47              |
| 1:F:241:ALA:CA   | 1:F:271:VAL:HG22 | 2.44                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:180:GLY:HA2  | 1:F:380:LYS:HB3  | 1.97                     | 0.47              |
| 1:G:158:VAL:HG13 | 1:G:396:VAL:HA   | 1.96                     | 0.47              |
| 1:G:222:LEU:CD2  | 1:G:292:ILE:HG22 | 2.42                     | 0.47              |
| 1:I:189:VAL:HG22 | 1:I:377:ALA:HB2  | 1.95                     | 0.47              |
| 1:K:183:LEU:HA   | 1:K:382:GLY:CA   | 2.44                     | 0.47              |
| 1:K:350:ARG:HD2  | 1:K:353:ILE:HD12 | 1.96                     | 0.47              |
| 1:K:136:VAL:O    | 1:K:410:GLY:HA3  | 2.13                     | 0.47              |
| 1:M:298:GLY:HA3  | 1:M:318:GLY:CA   | 2.44                     | 0.47              |
| 1:N:136:VAL:O    | 1:N:410:GLY:HA3  | 2.13                     | 0.47              |
| 1:A:221:LEU:HD21 | 1:A:309:LEU:HD11 | 1.95                     | 0.47              |
| 1:A:241:ALA:CA   | 1:A:271:VAL:HG22 | 2.44                     | 0.47              |
| 1:A:278:ALA:HB2  | 1:A:289:LEU:CD1  | 2.45                     | 0.47              |
| 1:A:180:GLY:HA2  | 1:A:380:LYS:HB3  | 1.96                     | 0.47              |
| 1:A:521:VAL:HG21 | 1:B:59:GLU:CB    | 2.43                     | 0.47              |
| 1:B:227:ILE:HG12 | 1:B:309:LEU:HG   | 1.95                     | 0.47              |
| 1:B:353:ILE:HD13 | 1:B:366:GLN:HG2  | 1.97                     | 0.47              |
| 1:C:227:ILE:HG12 | 1:C:309:LEU:HG   | 1.95                     | 0.47              |
| 1:C:353:ILE:HD13 | 1:C:366:GLN:HG2  | 1.97                     | 0.47              |
| 1:C:158:VAL:HG13 | 1:C:396:VAL:HA   | 1.96                     | 0.47              |
| 1:C:99:ILE:CG2   | 1:C:120:ILE:HD13 | 2.44                     | 0.47              |
| 1:D:150:ILE:CD1  | 1:D:493:ILE:CG2  | 2.91                     | 0.47              |
| 1:D:180:GLY:HA2  | 1:D:380:LYS:HB3  | 1.97                     | 0.47              |
| 1:E:241:ALA:CA   | 1:E:271:VAL:HG22 | 2.44                     | 0.47              |
| 1:E:311:LYS:HD3  | 1:E:311:LYS:HA   | 1.93                     | 0.47              |
| 1:F:222:LEU:CD2  | 1:F:292:ILE:HG22 | 2.42                     | 0.47              |
| 1:H:298:GLY:HA3  | 1:H:318:GLY:CA   | 2.44                     | 0.47              |
| 1:J:136:VAL:O    | 1:J:410:GLY:HA3  | 2.13                     | 0.47              |
| 1:L:207:LYS:CE   | 1:L:207:LYS:HA   | 2.36                     | 0.47              |
| 1:L:221:LEU:HG   | 1:L:309:LEU:HD22 | 1.96                     | 0.47              |
| 1:M:237:LEU:CD2  | 1:M:247:LEU:HD23 | 2.44                     | 0.47              |
| 1:M:314:LEU:O    | 1:M:317:LEU:HB2  | 2.14                     | 0.47              |
| 1:M:196:ASP:OD2  | 1:M:329:THR:HG22 | 2.14                     | 0.47              |
| 1:M:427:ALA:HA   | 1:M:444:LEU:HD11 | 1.95                     | 0.47              |
| 1:N:183:LEU:HA   | 1:N:382:GLY:CA   | 2.44                     | 0.47              |
| 1:N:237:LEU:CD2  | 1:N:247:LEU:HD23 | 2.44                     | 0.47              |
| 1:B:384:ALA:HA   | 1:B:385:THR:HA   | 1.68                     | 0.47              |
| 1:C:150:ILE:CD1  | 1:C:493:ILE:CA   | 2.74                     | 0.47              |
| 1:C:240:VAL:CG1  | 1:C:247:LEU:HB2  | 2.42                     | 0.47              |
| 1:C:241:ALA:CA   | 1:C:271:VAL:HG22 | 2.44                     | 0.47              |
| 1:C:180:GLY:HA2  | 1:C:380:LYS:HB3  | 1.96                     | 0.47              |
| 1:D:353:ILE:HD13 | 1:D:366:GLN:HG2  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:213:VAL:O    | 1:E:324:VAL:HA   | 2.14                     | 0.47              |
| 1:E:381:VAL:CG2  | 1:E:393:LYS:N    | 2.77                     | 0.47              |
| 1:F:223:ALA:CA   | 1:F:309:LEU:HD23 | 2.45                     | 0.47              |
| 1:G:99:ILE:CG2   | 1:G:120:ILE:HD13 | 2.44                     | 0.47              |
| 2:H:1525:PO4:P   | 4:H:1527:ATP:O1G | 2.73                     | 0.47              |
| 1:H:237:LEU:CD2  | 1:H:247:LEU:HD23 | 2.45                     | 0.47              |
| 1:J:237:LEU:CD2  | 1:J:247:LEU:HD23 | 2.45                     | 0.47              |
| 1:K:298:GLY:HA3  | 1:K:318:GLY:CA   | 2.44                     | 0.47              |
| 1:A:223:ALA:CA   | 1:A:309:LEU:HD23 | 2.45                     | 0.47              |
| 1:A:353:ILE:HD13 | 1:A:366:GLN:HG2  | 1.97                     | 0.47              |
| 1:C:213:VAL:O    | 1:C:324:VAL:HA   | 2.15                     | 0.47              |
| 1:C:222:LEU:CD2  | 1:C:292:ILE:HG22 | 2.42                     | 0.47              |
| 1:D:213:VAL:CG2  | 1:D:214:GLU:N    | 2.77                     | 0.47              |
| 1:D:221:LEU:CD1  | 1:D:309:LEU:HD21 | 2.45                     | 0.47              |
| 1:F:99:ILE:CG2   | 1:F:120:ILE:HD13 | 2.44                     | 0.47              |
| 1:G:278:ALA:HB2  | 1:G:289:LEU:CD1  | 2.45                     | 0.47              |
| 1:G:221:LEU:HD21 | 1:G:309:LEU:HD11 | 1.95                     | 0.47              |
| 1:G:180:GLY:HA2  | 1:G:380:LYS:HB3  | 1.96                     | 0.47              |
| 1:H:220:ILE:HD12 | 1:H:296:THR:HG21 | 1.96                     | 0.47              |
| 1:I:237:LEU:CD2  | 1:I:247:LEU:HD23 | 2.44                     | 0.47              |
| 1:J:350:ARG:HD2  | 1:J:353:ILE:HD12 | 1.96                     | 0.47              |
| 2:L:1525:PO4:P   | 4:L:1527:ATP:O1G | 2.73                     | 0.47              |
| 1:L:221:LEU:HD13 | 1:L:317:LEU:CD1  | 2.45                     | 0.47              |
| 1:N:221:LEU:HG   | 1:N:309:LEU:HD22 | 1.96                     | 0.47              |
| 1:B:278:ALA:HB2  | 1:B:289:LEU:CD1  | 2.45                     | 0.47              |
| 1:D:227:ILE:HG12 | 1:D:309:LEU:HG   | 1.95                     | 0.47              |
| 1:G:213:VAL:O    | 1:G:324:VAL:HA   | 2.14                     | 0.47              |
| 1:H:237:LEU:HA   | 1:H:247:LEU:HD22 | 1.97                     | 0.47              |
| 1:I:183:LEU:HA   | 1:I:382:GLY:CA   | 2.44                     | 0.47              |
| 2:K:1525:PO4:P   | 4:K:1527:ATP:O1G | 2.73                     | 0.47              |
| 1:M:203:TYR:CD1  | 1:M:267:MET:CE   | 2.97                     | 0.47              |
| 1:B:203:TYR:CD1  | 1:B:203:TYR:N    | 2.83                     | 0.47              |
| 1:B:221:LEU:CD1  | 1:B:309:LEU:HD21 | 2.45                     | 0.47              |
| 1:C:309:LEU:O    | 1:C:312:ALA:HB3  | 2.14                     | 0.47              |
| 1:F:213:VAL:CG2  | 1:F:214:GLU:N    | 2.77                     | 0.47              |
| 1:F:262:LEU:O    | 1:F:266:THR:HG23 | 2.15                     | 0.47              |
| 1:G:309:LEU:O    | 1:G:312:ALA:HB3  | 2.14                     | 0.47              |
| 2:I:1525:PO4:P   | 4:I:1527:ATP:O1G | 2.73                     | 0.47              |
| 1:I:220:ILE:HD12 | 1:I:296:THR:HG21 | 1.96                     | 0.47              |
| 1:K:227:ILE:CD1  | 1:K:233:MET:SD   | 2.92                     | 0.47              |
| 1:L:237:LEU:CD2  | 1:L:247:LEU:HD23 | 2.45                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:221:LEU:HD13 | 1:M:317:LEU:CD1  | 2.45                     | 0.47              |
| 2:N:1525:PO4:P   | 4:N:1527:ATP:O1G | 2.73                     | 0.47              |
| 1:N:205:ILE:O    | 1:N:207:LYS:CG   | 2.62                     | 0.47              |
| 1:N:34:LYS:HB2   | 1:N:457:ASN:HB3  | 1.97                     | 0.47              |
| 1:A:158:VAL:HG13 | 1:A:396:VAL:HA   | 1.96                     | 0.47              |
| 1:C:221:LEU:CD1  | 1:C:309:LEU:HD21 | 2.45                     | 0.47              |
| 1:C:192:GLY:H    | 1:C:375:GLY:HA2  | 1.80                     | 0.47              |
| 1:D:223:ALA:CA   | 1:D:309:LEU:HD23 | 2.45                     | 0.47              |
| 1:E:353:ILE:HD13 | 1:E:366:GLN:HG2  | 1.97                     | 0.47              |
| 1:F:240:VAL:HG11 | 1:F:247:LEU:CB   | 2.43                     | 0.47              |
| 1:G:227:ILE:HD12 | 1:G:258:ALA:HB1  | 1.96                     | 0.47              |
| 1:H:314:LEU:O    | 1:H:317:LEU:HB2  | 2.14                     | 0.47              |
| 1:J:203:TYR:CD1  | 1:J:267:MET:CE   | 2.97                     | 0.47              |
| 1:J:194:GLN:HG3  | 1:J:329:THR:HB   | 1.97                     | 0.47              |
| 1:L:206:ASN:HB2  | 1:L:213:VAL:HG23 | 1.96                     | 0.47              |
| 1:L:242:LYS:CB   | 1:M:257:GLU:HA   | 2.43                     | 0.47              |
| 1:N:237:LEU:HA   | 1:N:247:LEU:HD22 | 1.97                     | 0.47              |
| 1:N:50:THR:HB    | 1:N:51:LYS:HA    | 1.97                     | 0.47              |
| 1:B:213:VAL:CG2  | 1:B:214:GLU:N    | 2.77                     | 0.47              |
| 1:B:262:LEU:O    | 1:B:266:THR:HG23 | 2.15                     | 0.47              |
| 1:C:227:ILE:HD12 | 1:C:258:ALA:HB1  | 1.96                     | 0.47              |
| 1:C:278:ALA:HB2  | 1:C:289:LEU:CD1  | 2.45                     | 0.47              |
| 1:F:226:LYS:HB2  | 1:F:252:GLU:HG3  | 1.96                     | 0.47              |
| 1:G:200:LEU:HD22 | 1:G:254:VAL:HG11 | 1.96                     | 0.47              |
| 1:G:262:LEU:O    | 1:G:266:THR:HG23 | 2.15                     | 0.47              |
| 1:H:203:TYR:CE2  | 1:H:267:MET:SD   | 3.08                     | 0.47              |
| 1:I:237:LEU:HA   | 1:I:247:LEU:HD22 | 1.97                     | 0.47              |
| 1:J:236:VAL:O    | 1:J:240:VAL:HG23 | 2.13                     | 0.47              |
| 1:K:144:ILE:HG23 | 1:K:403:THR:HG21 | 1.97                     | 0.47              |
| 1:K:314:LEU:O    | 1:K:317:LEU:HB2  | 2.14                     | 0.47              |
| 1:L:144:ILE:HG23 | 1:L:403:THR:HG21 | 1.97                     | 0.47              |
| 1:A:204:PHE:CD1  | 1:A:273:VAL:O    | 2.68                     | 0.47              |
| 1:B:213:VAL:O    | 1:B:324:VAL:HA   | 2.15                     | 0.47              |
| 1:C:150:ILE:HD11 | 1:C:493:ILE:HG23 | 1.97                     | 0.47              |
| 1:D:262:LEU:O    | 1:D:266:THR:HG23 | 2.15                     | 0.47              |
| 1:F:213:VAL:O    | 1:F:324:VAL:HA   | 2.14                     | 0.47              |
| 1:F:162:ILE:CD1  | 1:F:400:LEU:N    | 2.77                     | 0.47              |
| 1:G:353:ILE:HD13 | 1:G:366:GLN:HG2  | 1.97                     | 0.47              |
| 1:I:298:GLY:HA3  | 1:I:318:GLY:CA   | 2.44                     | 0.47              |
| 1:J:220:ILE:HD12 | 1:J:296:THR:HG21 | 1.97                     | 0.47              |
| 1:J:203:TYR:CE2  | 1:J:267:MET:SD   | 3.08                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:237:LEU:HD13 | 1:K:271:VAL:HG21 | 1.97                     | 0.47              |
| 1:K:34:LYS:HB2   | 1:K:457:ASN:HB3  | 1.97                     | 0.47              |
| 1:M:237:LEU:HA   | 1:M:247:LEU:HD22 | 1.97                     | 0.47              |
| 1:B:241:ALA:CA   | 1:B:271:VAL:HG22 | 2.44                     | 0.46              |
| 1:E:226:LYS:HB2  | 1:E:252:GLU:HG3  | 1.96                     | 0.46              |
| 1:G:213:VAL:CG2  | 1:G:214:GLU:N    | 2.77                     | 0.46              |
| 1:H:182:GLY:HA3  | 1:H:383:ALA:N    | 2.11                     | 0.46              |
| 1:H:34:LYS:HB2   | 1:H:457:ASN:HB3  | 1.97                     | 0.46              |
| 1:J:144:ILE:HG23 | 1:J:403:THR:HG21 | 1.97                     | 0.46              |
| 1:K:237:LEU:CD2  | 1:K:247:LEU:HD23 | 2.44                     | 0.46              |
| 1:L:237:LEU:HD13 | 1:L:271:VAL:HG21 | 1.97                     | 0.46              |
| 1:M:34:LYS:HB2   | 1:M:457:ASN:HB3  | 1.97                     | 0.46              |
| 1:M:411:VAL:HG21 | 1:M:494:LEU:HD13 | 1.97                     | 0.46              |
| 1:M:50:THR:HB    | 1:M:51:LYS:HA    | 1.97                     | 0.46              |
| 1:A:25:ASP:CG    | 1:A:28:LYS:HZ3   | 2.19                     | 0.46              |
| 1:B:158:VAL:HG13 | 1:B:396:VAL:HA   | 1.96                     | 0.46              |
| 1:B:195:PHE:N    | 1:B:195:PHE:CD1  | 2.82                     | 0.46              |
| 1:C:226:LYS:HB2  | 1:C:252:GLU:HG3  | 1.96                     | 0.46              |
| 1:E:162:ILE:CD1  | 1:E:400:LEU:N    | 2.77                     | 0.46              |
| 1:E:206:ASN:HB3  | 1:E:208:PRO:HD2  | 1.96                     | 0.46              |
| 1:E:262:LEU:O    | 1:E:266:THR:HG23 | 2.15                     | 0.46              |
| 1:F:227:ILE:HD12 | 1:F:258:ALA:HB1  | 1.96                     | 0.46              |
| 1:F:204:PHE:CD1  | 1:F:273:VAL:O    | 2.68                     | 0.46              |
| 1:F:278:ALA:HB2  | 1:F:289:LEU:CD1  | 2.45                     | 0.46              |
| 1:I:314:LEU:O    | 1:I:317:LEU:HB2  | 2.14                     | 0.46              |
| 1:J:30:THR:C     | 1:J:35:GLY:HA3   | 2.36                     | 0.46              |
| 1:K:220:ILE:HD12 | 1:K:296:THR:HG21 | 1.96                     | 0.46              |
| 1:L:203:TYR:CD1  | 1:L:267:MET:CE   | 2.99                     | 0.46              |
| 2:M:1525:PO4:P   | 4:M:1527:ATP:O1G | 2.73                     | 0.46              |
| 1:N:220:ILE:HD12 | 1:N:296:THR:HG21 | 1.96                     | 0.46              |
| 1:N:233:MET:CE   | 1:N:249:ILE:HD11 | 2.42                     | 0.46              |
| 1:N:314:LEU:O    | 1:N:317:LEU:HB2  | 2.15                     | 0.46              |
| 1:A:353:ILE:HD13 | 1:A:366:GLN:CG   | 2.46                     | 0.46              |
| 1:C:262:LEU:O    | 1:C:266:THR:HG23 | 2.15                     | 0.46              |
| 1:D:207:LYS:N    | 1:D:208:PRO:HD2  | 2.29                     | 0.46              |
| 1:D:204:PHE:CD1  | 1:D:273:VAL:O    | 2.68                     | 0.46              |
| 1:G:207:LYS:CB   | 1:G:208:PRO:HD3  | 2.46                     | 0.46              |
| 1:H:50:THR:HB    | 1:H:51:LYS:HA    | 1.97                     | 0.46              |
| 1:I:144:ILE:HG23 | 1:I:403:THR:HG21 | 1.97                     | 0.46              |
| 1:J:314:LEU:O    | 1:J:317:LEU:HB2  | 2.14                     | 0.46              |
| 1:J:298:GLY:HA3  | 1:J:318:GLY:CA   | 2.44                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:34:LYS:HB2   | 1:J:457:ASN:HB3  | 1.97                     | 0.46              |
| 1:J:77:VAL:HG22  | 1:J:510:VAL:CG2  | 2.46                     | 0.46              |
| 1:L:220:ILE:HD12 | 1:L:296:THR:HG21 | 1.96                     | 0.46              |
| 1:M:183:LEU:HA   | 1:M:382:GLY:HA3  | 1.97                     | 0.46              |
| 1:N:183:LEU:HA   | 1:N:382:GLY:HA3  | 1.98                     | 0.46              |
| 1:B:226:LYS:HB2  | 1:B:252:GLU:HG3  | 1.96                     | 0.46              |
| 1:B:250:ILE:HD11 | 1:B:332:ILE:HD11 | 1.98                     | 0.46              |
| 1:C:240:VAL:HG11 | 1:C:247:LEU:CB   | 2.43                     | 0.46              |
| 1:C:250:ILE:HD11 | 1:C:332:ILE:HD11 | 1.98                     | 0.46              |
| 1:D:250:ILE:HD11 | 1:D:332:ILE:HD11 | 1.98                     | 0.46              |
| 1:D:311:LYS:HD3  | 1:D:311:LYS:HA   | 1.93                     | 0.46              |
| 1:E:353:ILE:HD13 | 1:E:366:GLN:CG   | 2.46                     | 0.46              |
| 1:G:226:LYS:HB2  | 1:G:252:GLU:HG3  | 1.96                     | 0.46              |
| 1:H:411:VAL:HG21 | 1:H:494:LEU:HD13 | 1.97                     | 0.46              |
| 1:I:249:ILE:HB   | 1:I:275:ALA:CB   | 2.40                     | 0.46              |
| 1:I:50:THR:HB    | 1:I:51:LYS:HA    | 1.97                     | 0.46              |
| 2:J:1525:PO4:P   | 4:J:1527:ATP:O1G | 2.73                     | 0.46              |
| 1:J:237:LEU:HD13 | 1:J:271:VAL:HG21 | 1.97                     | 0.46              |
| 1:K:203:TYR:CD1  | 1:K:267:MET:CE   | 2.97                     | 0.46              |
| 1:M:144:ILE:HG23 | 1:M:403:THR:HG21 | 1.97                     | 0.46              |
| 1:M:221:LEU:HG   | 1:M:309:LEU:HD22 | 1.96                     | 0.46              |
| 1:D:200:LEU:HD11 | 1:D:254:VAL:HA   | 1.94                     | 0.46              |
| 1:D:226:LYS:HB2  | 1:D:252:GLU:HG3  | 1.96                     | 0.46              |
| 1:G:353:ILE:HD13 | 1:G:366:GLN:CG   | 2.46                     | 0.46              |
| 1:H:237:LEU:HD13 | 1:H:271:VAL:HG21 | 1.97                     | 0.46              |
| 1:L:314:LEU:O    | 1:L:317:LEU:HB2  | 2.14                     | 0.46              |
| 1:B:111:MET:O    | 1:B:113:PRO:HD3  | 2.16                     | 0.46              |
| 1:B:353:ILE:HD13 | 1:B:366:GLN:CG   | 2.46                     | 0.46              |
| 1:E:111:MET:O    | 1:E:113:PRO:HD3  | 2.16                     | 0.46              |
| 1:F:165:ALA:CA   | 1:F:187:LEU:HD21 | 2.46                     | 0.46              |
| 1:F:353:ILE:HD13 | 1:F:366:GLN:HG2  | 1.97                     | 0.46              |
| 1:H:144:ILE:HG23 | 1:H:403:THR:HG21 | 1.97                     | 0.46              |
| 1:I:242:LYS:C    | 1:J:257:GLU:CA   | 2.78                     | 0.46              |
| 1:I:237:LEU:HD13 | 1:I:271:VAL:HG21 | 1.97                     | 0.46              |
| 1:J:237:LEU:HA   | 1:J:247:LEU:HD22 | 1.97                     | 0.46              |
| 1:J:411:VAL:HG21 | 1:J:494:LEU:HD13 | 1.97                     | 0.46              |
| 1:M:220:ILE:HD12 | 1:M:296:THR:HG21 | 1.96                     | 0.46              |
| 1:N:203:TYR:CD1  | 1:N:267:MET:CE   | 2.98                     | 0.46              |
| 1:A:262:LEU:O    | 1:A:266:THR:HG23 | 2.15                     | 0.46              |
| 1:B:223:ALA:CA   | 1:B:309:LEU:HD23 | 2.45                     | 0.46              |
| 1:B:204:PHE:CD1  | 1:B:273:VAL:O    | 2.68                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:196:ASP:OD1  | 1:C:329:THR:HG22 | 2.16                     | 0.46              |
| 1:C:204:PHE:CD1  | 1:C:273:VAL:O    | 2.69                     | 0.46              |
| 1:H:199:TYR:CB   | 1:H:325:ILE:HD11 | 2.41                     | 0.46              |
| 1:K:233:MET:HE2  | 1:K:249:ILE:HD11 | 1.93                     | 0.46              |
| 1:K:203:TYR:CE2  | 1:K:267:MET:SD   | 3.08                     | 0.46              |
| 1:L:30:THR:C     | 1:L:35:GLY:HA3   | 2.36                     | 0.46              |
| 1:L:40:LEU:HD21  | 1:L:55:SER:HB3   | 1.98                     | 0.46              |
| 1:M:353:ILE:HD11 | 1:M:369:VAL:HG21 | 1.98                     | 0.46              |
| 1:N:144:ILE:HG23 | 1:N:403:THR:HG21 | 1.97                     | 0.46              |
| 1:A:250:ILE:HD11 | 1:A:332:ILE:HD11 | 1.98                     | 0.46              |
| 1:B:240:VAL:CG1  | 1:B:247:LEU:HB2  | 2.42                     | 0.46              |
| 1:C:353:ILE:HD13 | 1:C:366:GLN:CG   | 2.46                     | 0.46              |
| 1:F:381:VAL:CG2  | 1:F:393:LYS:N    | 2.77                     | 0.46              |
| 1:G:240:VAL:HG11 | 1:G:247:LEU:CB   | 2.43                     | 0.46              |
| 1:H:30:THR:C     | 1:H:35:GLY:HA3   | 2.36                     | 0.46              |
| 1:K:233:MET:CE   | 1:K:249:ILE:HD11 | 2.42                     | 0.46              |
| 1:L:237:LEU:HA   | 1:L:247:LEU:HD22 | 1.97                     | 0.46              |
| 1:L:50:THR:HB    | 1:L:51:LYS:HA    | 1.97                     | 0.46              |
| 1:L:77:VAL:HG22  | 1:L:510:VAL:CG2  | 2.46                     | 0.46              |
| 1:M:237:LEU:HD13 | 1:M:271:VAL:HG21 | 1.97                     | 0.46              |
| 1:M:182:GLY:HA2  | 1:M:382:GLY:HA2  | 1.98                     | 0.46              |
| 1:M:40:LEU:HD21  | 1:M:55:SER:HB3   | 1.98                     | 0.46              |
| 1:N:353:ILE:HD11 | 1:N:369:VAL:HG21 | 1.98                     | 0.46              |
| 1:A:111:MET:O    | 1:A:113:PRO:HD3  | 2.16                     | 0.46              |
| 1:A:226:LYS:HB2  | 1:A:252:GLU:HG3  | 1.96                     | 0.46              |
| 1:C:278:ALA:CB   | 1:C:289:LEU:HD12 | 2.46                     | 0.46              |
| 1:D:278:ALA:HB2  | 1:D:289:LEU:HD12 | 1.98                     | 0.46              |
| 1:F:220:ILE:CD1  | 1:F:332:ILE:HD13 | 2.33                     | 0.46              |
| 1:F:353:ILE:HD13 | 1:F:366:GLN:CG   | 2.46                     | 0.46              |
| 1:K:237:LEU:HA   | 1:K:247:LEU:HD22 | 1.97                     | 0.46              |
| 1:M:196:ASP:CG   | 1:M:329:THR:HG22 | 2.35                     | 0.46              |
| 1:N:169:VAL:HG21 | 1:N:175:ILE:HG13 | 1.98                     | 0.46              |
| 1:N:298:GLY:HA3  | 1:N:318:GLY:CA   | 2.44                     | 0.46              |
| 1:C:111:MET:O    | 1:C:113:PRO:HD3  | 2.16                     | 0.46              |
| 1:D:191:GLU:HA   | 1:D:191:GLU:OE1  | 2.16                     | 0.46              |
| 1:H:169:VAL:HG21 | 1:H:175:ILE:HG13 | 1.98                     | 0.46              |
| 1:H:77:VAL:HG22  | 1:H:510:VAL:CG2  | 2.46                     | 0.46              |
| 1:J:29:VAL:O     | 1:J:35:GLY:HA2   | 2.16                     | 0.46              |
| 1:J:50:THR:HB    | 1:J:51:LYS:HA    | 1.97                     | 0.46              |
| 1:K:282:GLY:O    | 1:K:285:ARG:HB3  | 2.16                     | 0.46              |
| 1:L:182:GLY:HA2  | 1:L:382:GLY:HA2  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:411:VAL:HG21 | 1:L:494:LEU:HD13 | 1.97                     | 0.46              |
| 1:M:29:VAL:O     | 1:M:35:GLY:HA2   | 2.16                     | 0.46              |
| 1:N:77:VAL:HG22  | 1:N:510:VAL:CG2  | 2.46                     | 0.46              |
| 1:A:150:ILE:HD11 | 1:A:493:ILE:HG23 | 1.97                     | 0.45              |
| 1:B:521:VAL:O    | 1:C:41:ASP:HB3   | 2.16                     | 0.45              |
| 1:C:289:LEU:HD23 | 1:C:289:LEU:O    | 2.17                     | 0.45              |
| 1:D:353:ILE:HD13 | 1:D:366:GLN:CG   | 2.46                     | 0.45              |
| 1:E:227:ILE:HD12 | 1:E:258:ALA:HB1  | 1.96                     | 0.45              |
| 1:G:111:MET:O    | 1:G:113:PRO:HD3  | 2.16                     | 0.45              |
| 1:I:169:VAL:HG21 | 1:I:175:ILE:HG13 | 1.98                     | 0.45              |
| 1:I:227:ILE:CD1  | 1:I:233:MET:SD   | 2.92                     | 0.45              |
| 1:I:203:TYR:CD1  | 1:I:267:MET:CE   | 2.98                     | 0.45              |
| 1:I:30:THR:C     | 1:I:35:GLY:HA3   | 2.36                     | 0.45              |
| 1:K:199:TYR:CB   | 1:K:325:ILE:HD11 | 2.39                     | 0.45              |
| 1:K:40:LEU:HD21  | 1:K:55:SER:HB3   | 1.98                     | 0.45              |
| 1:L:183:LEU:HA   | 1:L:382:GLY:CA   | 2.45                     | 0.45              |
| 1:L:34:LYS:HB2   | 1:L:457:ASN:HB3  | 1.97                     | 0.45              |
| 1:N:205:ILE:C    | 1:N:207:LYS:HG2  | 2.36                     | 0.45              |
| 1:B:207:LYS:HB2  | 1:B:207:LYS:HE2  | 1.62                     | 0.45              |
| 1:C:278:ALA:HB2  | 1:C:289:LEU:HD12 | 1.98                     | 0.45              |
| 1:D:521:VAL:O    | 1:E:41:ASP:HB3   | 2.16                     | 0.45              |
| 1:E:250:ILE:HD11 | 1:E:332:ILE:HD11 | 1.98                     | 0.45              |
| 1:F:278:ALA:HB2  | 1:F:289:LEU:HD12 | 1.99                     | 0.45              |
| 1:G:223:ALA:CA   | 1:G:309:LEU:HD23 | 2.45                     | 0.45              |
| 1:I:227:ILE:HB   | 1:I:262:LEU:HD11 | 1.98                     | 0.45              |
| 1:I:40:LEU:HD21  | 1:I:55:SER:HB3   | 1.98                     | 0.45              |
| 1:J:227:ILE:HB   | 1:J:262:LEU:HD11 | 1.98                     | 0.45              |
| 1:L:227:ILE:HB   | 1:L:262:LEU:HD11 | 1.98                     | 0.45              |
| 1:N:40:LEU:HD21  | 1:N:55:SER:HB3   | 1.97                     | 0.45              |
| 1:B:278:ALA:CB   | 1:B:289:LEU:HD12 | 2.46                     | 0.45              |
| 1:D:111:MET:O    | 1:D:113:PRO:HD3  | 2.16                     | 0.45              |
| 2:D:1525:PO4:P   | 4:D:1527:ATP:PG  | 3.15                     | 0.45              |
| 1:D:190:VAL:HG21 | 1:D:333:ILE:HG22 | 1.99                     | 0.45              |
| 1:D:278:ALA:CB   | 1:D:289:LEU:HD12 | 2.46                     | 0.45              |
| 1:G:204:PHE:CD1  | 1:G:273:VAL:O    | 2.69                     | 0.45              |
| 1:G:278:ALA:HB2  | 1:G:289:LEU:HD12 | 1.98                     | 0.45              |
| 1:G:289:LEU:HD23 | 1:G:289:LEU:O    | 2.17                     | 0.45              |
| 1:H:406:ALA:HB1  | 1:H:411:VAL:HG12 | 1.99                     | 0.45              |
| 1:K:183:LEU:HA   | 1:K:382:GLY:HA3  | 1.97                     | 0.45              |
| 1:K:29:VAL:O     | 1:K:35:GLY:HA2   | 2.16                     | 0.45              |
| 1:K:30:THR:C     | 1:K:35:GLY:HA3   | 2.36                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:50:THR:HB    | 1:K:51:LYS:HA    | 1.97                     | 0.45              |
| 1:K:77:VAL:HG22  | 1:K:510:VAL:CG2  | 2.46                     | 0.45              |
| 1:L:182:GLY:HA2  | 1:L:183:LEU:HA   | 1.57                     | 0.45              |
| 1:M:77:VAL:HG22  | 1:M:510:VAL:CG2  | 2.46                     | 0.45              |
| 1:N:182:GLY:HA2  | 1:N:382:GLY:HA2  | 1.98                     | 0.45              |
| 1:C:521:VAL:O    | 1:D:41:ASP:HB3   | 2.16                     | 0.45              |
| 1:D:402:ALA:HB1  | 1:D:496:PRO:HG2  | 1.99                     | 0.45              |
| 1:E:200:LEU:HD11 | 1:E:254:VAL:HA   | 1.94                     | 0.45              |
| 1:E:223:ALA:CA   | 1:E:309:LEU:HD23 | 2.45                     | 0.45              |
| 1:F:200:LEU:HD11 | 1:F:254:VAL:CA   | 2.12                     | 0.45              |
| 1:F:200:LEU:HD11 | 1:F:254:VAL:HA   | 1.94                     | 0.45              |
| 1:F:272:LYS:H    | 1:F:272:LYS:CD   | 2.30                     | 0.45              |
| 1:F:384:ALA:HA   | 1:F:385:THR:HA   | 1.68                     | 0.45              |
| 1:G:219:PHE:HB3  | 1:G:317:LEU:HD11 | 1.98                     | 0.45              |
| 1:H:353:ILE:HD11 | 1:H:369:VAL:HG21 | 1.98                     | 0.45              |
| 1:I:29:VAL:O     | 1:I:35:GLY:HA2   | 2.16                     | 0.45              |
| 1:K:227:ILE:HB   | 1:K:262:LEU:HD11 | 1.98                     | 0.45              |
| 1:K:353:ILE:HD11 | 1:K:369:VAL:HG21 | 1.98                     | 0.45              |
| 1:L:190:VAL:HG21 | 1:L:333:ILE:HG12 | 1.98                     | 0.45              |
| 1:L:151:SER:HB3  | 1:L:399:ALA:HA   | 1.99                     | 0.45              |
| 1:M:169:VAL:HG21 | 1:M:175:ILE:HG13 | 1.98                     | 0.45              |
| 1:N:184:GLN:HG2  | 1:N:186:GLU:HG2  | 1.97                     | 0.45              |
| 1:N:227:ILE:HB   | 1:N:262:LEU:HD11 | 1.97                     | 0.45              |
| 1:N:237:LEU:HD13 | 1:N:271:VAL:HG21 | 1.97                     | 0.45              |
| 1:N:29:VAL:O     | 1:N:35:GLY:HA2   | 2.16                     | 0.45              |
| 1:A:289:LEU:HD23 | 1:A:289:LEU:O    | 2.17                     | 0.45              |
| 1:B:249:ILE:HD11 | 1:B:262:LEU:HD22 | 1.87                     | 0.45              |
| 1:A:521:VAL:O    | 1:B:41:ASP:HB3   | 2.16                     | 0.45              |
| 1:E:272:LYS:H    | 1:E:272:LYS:CD   | 2.30                     | 0.45              |
| 1:F:195:PHE:N    | 1:F:195:PHE:CD1  | 2.82                     | 0.45              |
| 1:F:207:LYS:HB2  | 1:F:207:LYS:HE3  | 1.73                     | 0.45              |
| 1:F:219:PHE:HB3  | 1:F:317:LEU:HD11 | 1.98                     | 0.45              |
| 1:H:255:GLU:CD   | 1:H:256:GLY:H    | 2.20                     | 0.45              |
| 1:H:215:LEU:HB2  | 1:H:323:VAL:HG22 | 1.99                     | 0.45              |
| 1:I:182:GLY:HA2  | 1:I:382:GLY:HA2  | 1.98                     | 0.45              |
| 1:I:34:LYS:HB2   | 1:I:457:ASN:HB3  | 1.97                     | 0.45              |
| 1:J:182:GLY:HA2  | 1:J:382:GLY:HA2  | 1.98                     | 0.45              |
| 1:J:183:LEU:HA   | 1:J:382:GLY:HA3  | 1.97                     | 0.45              |
| 1:K:151:SER:HB3  | 1:K:399:ALA:HA   | 1.99                     | 0.45              |
| 1:K:406:ALA:HB1  | 1:K:411:VAL:HG12 | 1.98                     | 0.45              |
| 1:K:411:VAL:HG21 | 1:K:494:LEU:HD13 | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:233:MET:CE   | 1:L:249:ILE:HD11 | 2.44                     | 0.45              |
| 1:C:402:ALA:HB1  | 1:C:496:PRO:HG2  | 1.99                     | 0.45              |
| 1:D:289:LEU:HD23 | 1:D:289:LEU:O    | 2.17                     | 0.45              |
| 1:E:402:ALA:HB1  | 1:E:496:PRO:HG2  | 1.99                     | 0.45              |
| 1:H:207:LYS:HE2  | 1:H:207:LYS:HA   | 1.99                     | 0.45              |
| 1:H:27:VAL:CG1   | 1:H:90:THR:HG23  | 2.47                     | 0.45              |
| 1:I:215:LEU:HB2  | 1:I:323:VAL:HG22 | 1.99                     | 0.45              |
| 1:I:77:VAL:HG22  | 1:I:510:VAL:CG2  | 2.46                     | 0.45              |
| 1:J:40:LEU:HD21  | 1:J:55:SER:HB3   | 1.98                     | 0.45              |
| 1:K:182:GLY:HA2  | 1:K:183:LEU:HA   | 1.63                     | 0.45              |
| 1:L:353:ILE:HD11 | 1:L:369:VAL:HG21 | 1.98                     | 0.45              |
| 1:L:29:VAL:O     | 1:L:35:GLY:HA2   | 2.16                     | 0.45              |
| 1:M:30:THR:C     | 1:M:35:GLY:HA3   | 2.36                     | 0.45              |
| 1:A:240:VAL:HG11 | 1:A:247:LEU:CB   | 2.43                     | 0.45              |
| 1:C:207:LYS:N    | 1:C:207:LYS:HE3  | 2.23                     | 0.45              |
| 1:D:227:ILE:HD12 | 1:D:258:ALA:HB1  | 1.96                     | 0.45              |
| 1:F:521:VAL:O    | 1:G:41:ASP:HB3   | 2.16                     | 0.45              |
| 1:H:227:ILE:HB   | 1:H:262:LEU:HD11 | 1.98                     | 0.45              |
| 1:J:169:VAL:HG21 | 1:J:175:ILE:HG13 | 1.99                     | 0.45              |
| 1:J:151:SER:HB3  | 1:J:399:ALA:HA   | 1.99                     | 0.45              |
| 1:M:203:TYR:CE2  | 1:M:267:MET:SD   | 3.09                     | 0.45              |
| 1:M:151:SER:HB3  | 1:M:399:ALA:HA   | 1.99                     | 0.45              |
| 1:A:278:ALA:CB   | 1:A:289:LEU:HD12 | 2.46                     | 0.45              |
| 1:B:402:ALA:HB1  | 1:B:496:PRO:HG2  | 1.99                     | 0.45              |
| 1:C:177:VAL:HG21 | 1:C:397:GLU:HG2  | 1.99                     | 0.45              |
| 1:D:272:LYS:CD   | 1:D:272:LYS:H    | 2.30                     | 0.45              |
| 1:E:278:ALA:CB   | 1:E:289:LEU:HD12 | 2.46                     | 0.45              |
| 1:F:111:MET:O    | 1:F:113:PRO:HD3  | 2.16                     | 0.45              |
| 1:E:521:VAL:O    | 1:F:41:ASP:HB3   | 2.16                     | 0.45              |
| 1:G:272:LYS:CD   | 1:G:272:LYS:H    | 2.30                     | 0.45              |
| 1:H:196:ASP:OD1  | 1:H:329:THR:HG22 | 2.17                     | 0.45              |
| 1:J:215:LEU:HB2  | 1:J:323:VAL:HG22 | 1.99                     | 0.45              |
| 1:J:196:ASP:HA   | 1:J:329:THR:HG22 | 1.98                     | 0.45              |
| 1:K:255:GLU:CD   | 1:K:256:GLY:H    | 2.20                     | 0.45              |
| 1:L:406:ALA:HB1  | 1:L:411:VAL:HG12 | 1.98                     | 0.45              |
| 1:A:240:VAL:CG1  | 1:A:247:LEU:HB2  | 2.42                     | 0.45              |
| 1:B:278:ALA:HB2  | 1:B:289:LEU:HD12 | 1.98                     | 0.45              |
| 2:F:1525:PO4:P   | 4:F:1527:ATP:PG  | 3.15                     | 0.45              |
| 1:H:282:GLY:O    | 1:H:285:ARG:HB3  | 2.16                     | 0.45              |
| 1:H:242:LYS:HG3  | 1:I:257:GLU:C    | 2.38                     | 0.45              |
| 1:K:177:VAL:CG2  | 1:K:379:ILE:HB   | 2.42                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:182:GLY:HA2  | 1:K:382:GLY:HA2  | 1.98                     | 0.45              |
| 1:K:19:GLY:HA2   | 1:K:62:LEU:CD1   | 2.47                     | 0.45              |
| 1:L:183:LEU:CD2  | 1:L:183:LEU:H    | 2.22                     | 0.45              |
| 1:M:227:ILE:HB   | 1:M:262:LEU:HD11 | 1.98                     | 0.45              |
| 1:F:250:ILE:HD11 | 1:F:332:ILE:HD11 | 1.98                     | 0.45              |
| 1:G:384:ALA:HA   | 1:G:385:THR:HA   | 1.68                     | 0.45              |
| 1:H:40:LEU:HD21  | 1:H:55:SER:HB3   | 1.98                     | 0.45              |
| 1:H:517:THR:HG21 | 1:H:520:MET:HG3  | 1.99                     | 0.45              |
| 1:I:183:LEU:HA   | 1:I:382:GLY:HA3  | 1.98                     | 0.45              |
| 1:I:517:THR:HG21 | 1:I:520:MET:HG3  | 1.99                     | 0.45              |
| 1:L:19:GLY:HA2   | 1:L:62:LEU:CD1   | 2.47                     | 0.45              |
| 1:M:223:ALA:HB2  | 1:M:309:LEU:CG   | 2.47                     | 0.45              |
| 1:N:215:LEU:HB2  | 1:N:323:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:41:ASP:HB3   | 1:G:521:VAL:O    | 2.16                     | 0.44              |
| 1:A:52:ASP:HB3   | 1:A:55:SER:H     | 1.82                     | 0.44              |
| 1:C:219:PHE:HB3  | 1:C:317:LEU:HD11 | 1.98                     | 0.44              |
| 1:C:461:GLU:HA   | 1:C:462:PRO:HD3  | 1.87                     | 0.44              |
| 1:E:384:ALA:HA   | 1:E:385:THR:HA   | 1.68                     | 0.44              |
| 1:G:278:ALA:CB   | 1:G:289:LEU:HD12 | 2.46                     | 0.44              |
| 1:I:203:TYR:CE2  | 1:I:267:MET:SD   | 3.09                     | 0.44              |
| 1:I:295:LEU:HD23 | 1:I:342:ILE:CD1  | 2.46                     | 0.44              |
| 1:I:353:ILE:HD11 | 1:I:369:VAL:HG21 | 1.98                     | 0.44              |
| 1:I:27:VAL:CG1   | 1:I:90:THR:HG23  | 2.47                     | 0.44              |
| 1:J:353:ILE:HD11 | 1:J:369:VAL:HG21 | 1.98                     | 0.44              |
| 1:L:295:LEU:HD23 | 1:L:342:ILE:CD1  | 2.46                     | 0.44              |
| 1:M:19:GLY:HA2   | 1:M:62:LEU:CD1   | 2.47                     | 0.44              |
| 1:B:177:VAL:HG21 | 1:B:397:GLU:HG2  | 1.99                     | 0.44              |
| 1:C:152:ALA:HB2  | 1:C:399:ALA:HB2  | 2.00                     | 0.44              |
| 1:D:219:PHE:HB3  | 1:D:317:LEU:HD11 | 1.99                     | 0.44              |
| 1:D:177:VAL:HG21 | 1:D:397:GLU:HG2  | 1.99                     | 0.44              |
| 1:E:513:LEU:HB3  | 1:F:49:ILE:HD12  | 2.00                     | 0.44              |
| 1:F:221:LEU:CD1  | 1:F:309:LEU:HD21 | 2.45                     | 0.44              |
| 1:F:291:ASP:OD1  | 1:F:349:ILE:HD11 | 2.18                     | 0.44              |
| 1:G:240:VAL:CG1  | 1:G:247:LEU:HB2  | 2.42                     | 0.44              |
| 1:G:250:ILE:HD11 | 1:G:332:ILE:HD11 | 1.98                     | 0.44              |
| 1:F:513:LEU:HB3  | 1:G:49:ILE:HD12  | 1.99                     | 0.44              |
| 1:H:19:GLY:HA2   | 1:H:62:LEU:CD1   | 2.47                     | 0.44              |
| 1:I:272:LYS:H    | 1:I:272:LYS:HD3  | 1.82                     | 0.44              |
| 1:J:517:THR:HG21 | 1:J:520:MET:HG3  | 1.99                     | 0.44              |
| 1:K:215:LEU:HB2  | 1:K:323:VAL:HG22 | 1.99                     | 0.44              |
| 1:L:223:ALA:HB2  | 1:L:309:LEU:CG   | 2.47                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:278:ALA:HB2  | 1:A:289:LEU:HD12 | 1.98                     | 0.44              |
| 1:A:402:ALA:HB1  | 1:A:496:PRO:HG2  | 1.99                     | 0.44              |
| 1:B:291:ASP:OD1  | 1:B:349:ILE:HD11 | 2.18                     | 0.44              |
| 1:B:311:LYS:HD3  | 1:B:311:LYS:HA   | 1.93                     | 0.44              |
| 1:B:152:ALA:HB2  | 1:B:399:ALA:HB2  | 2.00                     | 0.44              |
| 1:E:291:ASP:OD1  | 1:E:349:ILE:HD11 | 2.17                     | 0.44              |
| 1:F:289:LEU:HD23 | 1:F:289:LEU:O    | 2.17                     | 0.44              |
| 1:F:402:ALA:HB1  | 1:F:496:PRO:HG2  | 1.99                     | 0.44              |
| 1:G:381:VAL:CG2  | 1:G:393:LYS:N    | 2.77                     | 0.44              |
| 1:I:222:LEU:CD2  | 1:I:250:ILE:HD12 | 2.48                     | 0.44              |
| 1:J:222:LEU:CD2  | 1:J:250:ILE:HD12 | 2.47                     | 0.44              |
| 1:J:518:GLU:CB   | 1:J:519:CYS:N    | 2.74                     | 0.44              |
| 1:K:169:VAL:HG21 | 1:K:175:ILE:HG13 | 1.98                     | 0.44              |
| 1:L:203:TYR:CE2  | 1:L:267:MET:SD   | 3.09                     | 0.44              |
| 1:L:272:LYS:HD3  | 1:L:272:LYS:H    | 1.82                     | 0.44              |
| 1:M:255:GLU:CD   | 1:M:256:GLY:H    | 2.20                     | 0.44              |
| 1:N:203:TYR:CE2  | 1:N:267:MET:SD   | 3.09                     | 0.44              |
| 1:N:30:THR:C     | 1:N:35:GLY:HA3   | 2.36                     | 0.44              |
| 1:A:219:PHE:HB3  | 1:A:317:LEU:HD11 | 1.98                     | 0.44              |
| 1:B:272:LYS:H    | 1:B:272:LYS:CD   | 2.30                     | 0.44              |
| 1:D:513:LEU:HB3  | 1:E:49:ILE:HD12  | 2.00                     | 0.44              |
| 1:G:291:ASP:OD1  | 1:G:349:ILE:HD11 | 2.18                     | 0.44              |
| 1:H:295:LEU:HD23 | 1:H:342:ILE:CD1  | 2.46                     | 0.44              |
| 1:J:272:LYS:HD3  | 1:J:272:LYS:H    | 1.82                     | 0.44              |
| 1:N:255:GLU:CD   | 1:N:256:GLY:H    | 2.21                     | 0.44              |
| 1:N:223:ALA:HB2  | 1:N:309:LEU:CG   | 2.47                     | 0.44              |
| 1:N:19:GLY:HA2   | 1:N:62:LEU:CD1   | 2.47                     | 0.44              |
| 1:A:272:LYS:CD   | 1:A:272:LYS:H    | 2.30                     | 0.44              |
| 1:B:240:VAL:HG11 | 1:B:247:LEU:CB   | 2.43                     | 0.44              |
| 1:B:289:LEU:O    | 1:B:289:LEU:HD23 | 2.17                     | 0.44              |
| 1:B:194:GLN:HG2  | 1:B:329:THR:HG21 | 1.99                     | 0.44              |
| 1:E:289:LEU:O    | 1:E:289:LEU:HD23 | 2.17                     | 0.44              |
| 1:J:206:ASN:HB3  | 1:J:208:PRO:HD2  | 1.98                     | 0.44              |
| 1:M:406:ALA:HB1  | 1:M:411:VAL:HG12 | 1.98                     | 0.44              |
| 1:M:27:VAL:CG1   | 1:M:90:THR:HG23  | 2.47                     | 0.44              |
| 1:A:291:ASP:OD1  | 1:A:349:ILE:HD11 | 2.17                     | 0.44              |
| 1:A:49:ILE:HD12  | 1:G:513:LEU:HB3  | 2.00                     | 0.44              |
| 1:C:193:MET:SD   | 1:C:292:ILE:HG12 | 2.57                     | 0.44              |
| 1:H:29:VAL:O     | 1:H:35:GLY:HA2   | 2.16                     | 0.44              |
| 1:H:218:PRO:HG3  | 1:H:323:VAL:HG13 | 2.00                     | 0.44              |
| 1:I:60:ILE:HA    | 1:J:6:VAL:CG2    | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:255:GLU:CD   | 1:J:256:GLY:H    | 2.20                     | 0.44              |
| 1:M:413:ALA:HB1  | 1:M:488:MET:HB2  | 2.00                     | 0.44              |
| 1:N:215:LEU:HB3  | 1:N:246:PRO:HG2  | 2.00                     | 0.44              |
| 1:N:517:THR:HG21 | 1:N:520:MET:HG3  | 1.99                     | 0.44              |
| 1:C:200:LEU:HD11 | 1:C:254:VAL:CA   | 2.12                     | 0.44              |
| 1:G:402:ALA:HB1  | 1:G:496:PRO:HG2  | 1.99                     | 0.44              |
| 1:H:224:ASP:HB2  | 1:H:303:GLU:H    | 1.82                     | 0.44              |
| 1:H:215:LEU:HB3  | 1:H:246:PRO:HG2  | 2.00                     | 0.44              |
| 1:H:60:ILE:HA    | 1:I:6:VAL:CG2    | 2.48                     | 0.44              |
| 1:K:272:LYS:HD3  | 1:K:272:LYS:H    | 1.82                     | 0.44              |
| 1:J:60:ILE:HA    | 1:K:6:VAL:CG2    | 2.48                     | 0.44              |
| 1:L:356:ALA:HB1  | 1:L:361:ASP:HB2  | 2.00                     | 0.44              |
| 1:M:215:LEU:HB2  | 1:M:323:VAL:HG22 | 1.99                     | 0.44              |
| 1:N:413:ALA:HB1  | 1:N:488:MET:HB2  | 2.00                     | 0.44              |
| 1:A:221:LEU:CD1  | 1:A:309:LEU:HD21 | 2.45                     | 0.44              |
| 1:C:272:LYS:H    | 1:C:272:LYS:CD   | 2.30                     | 0.44              |
| 1:D:152:ALA:HB2  | 1:D:399:ALA:HB2  | 2.00                     | 0.44              |
| 1:G:278:ALA:HA   | 1:G:279:PRO:HD3  | 1.72                     | 0.44              |
| 1:I:182:GLY:HA2  | 1:I:183:LEU:HA   | 1.63                     | 0.44              |
| 1:I:356:ALA:HB1  | 1:I:361:ASP:HB2  | 2.00                     | 0.44              |
| 1:J:215:LEU:HB3  | 1:J:246:PRO:HG2  | 2.00                     | 0.44              |
| 1:J:406:ALA:HB1  | 1:J:411:VAL:HG12 | 1.99                     | 0.44              |
| 1:K:215:LEU:HB3  | 1:K:246:PRO:HG2  | 2.00                     | 0.44              |
| 1:K:356:ALA:HB1  | 1:K:361:ASP:HB2  | 2.00                     | 0.44              |
| 1:K:60:ILE:HA    | 1:L:6:VAL:CG2    | 2.48                     | 0.44              |
| 1:L:215:LEU:HB3  | 1:L:246:PRO:HG2  | 2.00                     | 0.44              |
| 1:L:240:VAL:HG21 | 1:L:317:LEU:HD22 | 2.00                     | 0.44              |
| 1:N:272:LYS:HD3  | 1:N:272:LYS:H    | 1.82                     | 0.44              |
| 1:A:152:ALA:HB2  | 1:A:399:ALA:HB2  | 2.00                     | 0.44              |
| 1:A:513:LEU:HB3  | 1:B:49:ILE:HD12  | 2.00                     | 0.44              |
| 1:B:381:VAL:CG2  | 1:B:393:LYS:N    | 2.77                     | 0.44              |
| 1:B:52:ASP:HB2   | 1:B:55:SER:HB2   | 2.00                     | 0.44              |
| 1:C:52:ASP:HB3   | 1:C:55:SER:H     | 1.82                     | 0.44              |
| 1:E:278:ALA:HB2  | 1:E:289:LEU:HD12 | 1.98                     | 0.44              |
| 1:E:219:PHE:HB3  | 1:E:317:LEU:HD11 | 1.98                     | 0.44              |
| 1:F:52:ASP:HB2   | 1:F:55:SER:HB2   | 2.00                     | 0.44              |
| 1:G:177:VAL:HG21 | 1:G:397:GLU:HG2  | 1.99                     | 0.44              |
| 1:H:237:LEU:HA   | 1:H:247:LEU:CD2  | 2.48                     | 0.44              |
| 1:I:255:GLU:CD   | 1:I:256:GLY:H    | 2.21                     | 0.44              |
| 1:I:413:ALA:HB1  | 1:I:488:MET:HB2  | 2.00                     | 0.44              |
| 1:J:62:LEU:HB2   | 1:J:68:ASN:HA    | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:215:LEU:HB2  | 1:L:323:VAL:HG22 | 1.99                     | 0.44              |
| 1:M:215:LEU:HB3  | 1:M:246:PRO:HG2  | 2.00                     | 0.44              |
| 1:M:227:ILE:CD1  | 1:M:233:MET:SD   | 2.93                     | 0.44              |
| 1:B:219:PHE:HB3  | 1:B:317:LEU:HD11 | 1.98                     | 0.43              |
| 2:C:1525:PO4:P   | 4:C:1527:ATP:PG  | 3.16                     | 0.43              |
| 1:C:513:LEU:HB3  | 1:D:49:ILE:HD12  | 2.00                     | 0.43              |
| 1:F:278:ALA:CB   | 1:F:289:LEU:HD12 | 2.47                     | 0.43              |
| 1:F:524:LEU:HG   | 1:F:525:PRO:N    | 2.33                     | 0.43              |
| 1:H:272:LYS:H    | 1:H:272:LYS:HD3  | 1.82                     | 0.43              |
| 1:H:413:ALA:HB1  | 1:H:488:MET:HB2  | 2.00                     | 0.43              |
| 1:J:19:GLY:HA2   | 1:J:62:LEU:CD1   | 2.47                     | 0.43              |
| 1:J:242:LYS:HA   | 1:J:243:ALA:HA   | 1.12                     | 0.43              |
| 1:J:356:ALA:HB1  | 1:J:361:ASP:HB2  | 2.00                     | 0.43              |
| 1:K:218:PRO:HG3  | 1:K:323:VAL:HG13 | 1.99                     | 0.43              |
| 1:N:218:PRO:HG3  | 1:N:323:VAL:HG13 | 2.00                     | 0.43              |
| 1:B:513:LEU:HB3  | 1:C:49:ILE:HD12  | 2.00                     | 0.43              |
| 1:C:291:ASP:OD1  | 1:C:349:ILE:HD11 | 2.18                     | 0.43              |
| 1:D:52:ASP:HB2   | 1:D:55:SER:HB2   | 2.00                     | 0.43              |
| 1:E:152:ALA:HB2  | 1:E:399:ALA:HB2  | 2.00                     | 0.43              |
| 1:E:524:LEU:HG   | 1:E:525:PRO:N    | 2.33                     | 0.43              |
| 1:K:240:VAL:HG21 | 1:K:317:LEU:HD22 | 2.00                     | 0.43              |
| 1:K:517:THR:HG21 | 1:K:520:MET:HG3  | 1.99                     | 0.43              |
| 1:L:190:VAL:HG21 | 1:L:333:ILE:HG23 | 1.98                     | 0.43              |
| 1:M:240:VAL:HG21 | 1:M:317:LEU:HD22 | 2.00                     | 0.43              |
| 1:D:278:ALA:HB2  | 1:D:289:LEU:CG   | 2.49                     | 0.43              |
| 1:D:291:ASP:OD1  | 1:D:349:ILE:HD11 | 2.17                     | 0.43              |
| 1:F:240:VAL:CG1  | 1:F:247:LEU:HB2  | 2.42                     | 0.43              |
| 1:F:177:VAL:HG21 | 1:F:397:GLU:HG2  | 1.99                     | 0.43              |
| 1:G:220:ILE:CD1  | 1:G:296:THR:HG21 | 2.47                     | 0.43              |
| 1:H:240:VAL:HG21 | 1:H:317:LEU:CD2  | 2.49                     | 0.43              |
| 1:H:356:ALA:HB1  | 1:H:361:ASP:HB2  | 2.00                     | 0.43              |
| 1:H:62:LEU:HB2   | 1:H:68:ASN:HA    | 2.00                     | 0.43              |
| 1:I:215:LEU:HB3  | 1:I:246:PRO:HG2  | 2.00                     | 0.43              |
| 1:I:237:LEU:HA   | 1:I:247:LEU:CD2  | 2.49                     | 0.43              |
| 1:I:218:PRO:HG3  | 1:I:323:VAL:HG13 | 2.00                     | 0.43              |
| 1:L:218:PRO:HG3  | 1:L:323:VAL:HG13 | 2.00                     | 0.43              |
| 1:L:413:ALA:HB1  | 1:L:488:MET:HB2  | 2.00                     | 0.43              |
| 1:M:356:ALA:HB1  | 1:M:361:ASP:HB2  | 2.00                     | 0.43              |
| 1:A:240:VAL:HG13 | 1:A:245:LYS:O    | 2.19                     | 0.43              |
| 1:A:278:ALA:HB2  | 1:A:289:LEU:CG   | 2.49                     | 0.43              |
| 1:A:177:VAL:HA   | 1:A:379:ILE:O    | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:524:LEU:HG   | 1:D:525:PRO:N    | 2.33                     | 0.43              |
| 1:I:19:GLY:HA2   | 1:I:62:LEU:CD1   | 2.47                     | 0.43              |
| 1:I:62:LEU:HB2   | 1:I:68:ASN:HA    | 2.00                     | 0.43              |
| 1:J:27:VAL:CG1   | 1:J:90:THR:HG23  | 2.47                     | 0.43              |
| 1:K:240:VAL:HG21 | 1:K:317:LEU:CD2  | 2.49                     | 0.43              |
| 1:K:62:LEU:HB2   | 1:K:68:ASN:HA    | 2.00                     | 0.43              |
| 1:K:77:VAL:HG22  | 1:K:510:VAL:CB   | 2.49                     | 0.43              |
| 1:L:240:VAL:HG21 | 1:L:317:LEU:CD2  | 2.49                     | 0.43              |
| 1:M:240:VAL:HG21 | 1:M:317:LEU:CD2  | 2.49                     | 0.43              |
| 1:M:60:ILE:HA    | 1:N:6:VAL:CG2    | 2.48                     | 0.43              |
| 1:N:227:ILE:CD1  | 1:N:233:MET:SD   | 2.93                     | 0.43              |
| 1:N:301:ILE:HD11 | 1:N:312:ALA:CB   | 2.32                     | 0.43              |
| 1:A:150:ILE:CD1  | 1:A:493:ILE:CA   | 2.74                     | 0.43              |
| 1:C:311:LYS:HA   | 1:C:311:LYS:HD3  | 1.93                     | 0.43              |
| 1:D:177:VAL:HA   | 1:D:379:ILE:O    | 2.18                     | 0.43              |
| 1:E:240:VAL:HG13 | 1:E:245:LYS:O    | 2.18                     | 0.43              |
| 1:F:150:ILE:CD1  | 1:F:493:ILE:CG2  | 2.91                     | 0.43              |
| 1:G:240:VAL:HG13 | 1:G:245:LYS:O    | 2.18                     | 0.43              |
| 1:G:177:VAL:HA   | 1:G:379:ILE:O    | 2.19                     | 0.43              |
| 1:G:152:ALA:HB2  | 1:G:399:ALA:HB2  | 2.00                     | 0.43              |
| 1:I:233:MET:CE   | 1:I:249:ILE:HD11 | 2.40                     | 0.43              |
| 1:J:240:VAL:HG21 | 1:J:317:LEU:CD2  | 2.49                     | 0.43              |
| 1:J:77:VAL:HG22  | 1:J:510:VAL:CB   | 2.49                     | 0.43              |
| 1:K:169:VAL:HG21 | 1:K:175:ILE:CG1  | 2.49                     | 0.43              |
| 1:K:223:ALA:HB2  | 1:K:309:LEU:CG   | 2.48                     | 0.43              |
| 1:L:60:ILE:HA    | 1:M:6:VAL:CG2    | 2.48                     | 0.43              |
| 1:N:356:ALA:HB1  | 1:N:361:ASP:HB2  | 2.00                     | 0.43              |
| 1:N:99:ILE:CG2   | 1:N:120:ILE:HD13 | 2.49                     | 0.43              |
| 1:B:240:VAL:HG13 | 1:B:245:LYS:O    | 2.18                     | 0.43              |
| 1:B:381:VAL:HG11 | 1:B:393:LYS:HB2  | 2.00                     | 0.43              |
| 1:C:197:ARG:HG3  | 1:C:198:GLY:O    | 2.18                     | 0.43              |
| 1:C:223:ALA:CA   | 1:C:309:LEU:HD23 | 2.45                     | 0.43              |
| 1:C:524:LEU:HG   | 1:C:525:PRO:N    | 2.33                     | 0.43              |
| 1:F:240:VAL:HG13 | 1:F:245:LYS:O    | 2.18                     | 0.43              |
| 1:F:381:VAL:HG11 | 1:F:393:LYS:HB2  | 2.00                     | 0.43              |
| 2:G:1525:PO4:P   | 4:G:1527:ATP:PG  | 3.16                     | 0.43              |
| 1:G:221:LEU:CD1  | 1:G:309:LEU:HD21 | 2.45                     | 0.43              |
| 1:H:223:ALA:HB2  | 1:H:309:LEU:CG   | 2.48                     | 0.43              |
| 1:H:151:SER:HB3  | 1:H:399:ALA:HA   | 1.99                     | 0.43              |
| 1:I:181:THR:HG22 | 1:I:182:GLY:O    | 2.19                     | 0.43              |
| 1:J:240:VAL:HG21 | 1:J:317:LEU:HD22 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:77:VAL:HG22  | 1:L:510:VAL:CB   | 2.49                     | 0.43              |
| 1:M:229:ASN:HB3  | 1:M:231:ARG:HG3  | 2.01                     | 0.43              |
| 1:M:272:LYS:HD3  | 1:M:272:LYS:H    | 1.82                     | 0.43              |
| 1:M:517:THR:HG21 | 1:M:520:MET:HG3  | 2.00                     | 0.43              |
| 1:M:99:ILE:CG2   | 1:M:120:ILE:HD13 | 2.49                     | 0.43              |
| 1:N:240:VAL:HG21 | 1:N:317:LEU:HD22 | 2.00                     | 0.43              |
| 2:A:1525:PO4:P   | 4:A:1527:ATP:PG  | 3.16                     | 0.43              |
| 1:B:236:VAL:HG13 | 1:B:317:LEU:HD13 | 2.01                     | 0.43              |
| 1:B:524:LEU:HG   | 1:B:525:PRO:N    | 2.33                     | 0.43              |
| 1:E:191:GLU:H    | 1:E:334:ASP:HA   | 1.84                     | 0.43              |
| 1:E:177:VAL:HA   | 1:E:379:ILE:O    | 2.19                     | 0.43              |
| 1:I:169:VAL:HG21 | 1:I:175:ILE:CG1  | 2.49                     | 0.43              |
| 1:J:218:PRO:HG3  | 1:J:323:VAL:HG13 | 2.00                     | 0.43              |
| 1:J:413:ALA:HB1  | 1:J:488:MET:HB2  | 2.00                     | 0.43              |
| 1:K:237:LEU:HA   | 1:K:247:LEU:CD2  | 2.48                     | 0.43              |
| 1:K:413:ALA:HB1  | 1:K:488:MET:HB2  | 2.00                     | 0.43              |
| 1:L:242:LYS:HG3  | 1:M:257:GLU:HB2  | 2.00                     | 0.43              |
| 1:N:169:VAL:HG21 | 1:N:175:ILE:CG1  | 2.49                     | 0.43              |
| 1:A:200:LEU:HD13 | 1:A:259:LEU:HB2  | 2.00                     | 0.43              |
| 1:A:236:VAL:HG13 | 1:A:317:LEU:HD13 | 2.01                     | 0.43              |
| 1:A:177:VAL:HG21 | 1:A:397:GLU:HG2  | 1.99                     | 0.43              |
| 1:C:144:ILE:CG2  | 1:C:163:ALA:HA   | 2.49                     | 0.43              |
| 1:D:240:VAL:HG13 | 1:D:245:LYS:O    | 2.18                     | 0.43              |
| 1:J:179:ASP:HB3  | 1:J:383:ALA:HB2  | 2.01                     | 0.43              |
| 1:J:214:GLU:CD   | 1:J:322:ARG:HE   | 2.22                     | 0.43              |
| 1:L:517:THR:HG21 | 1:L:520:MET:HG3  | 1.99                     | 0.43              |
| 1:M:222:LEU:CD2  | 1:M:250:ILE:HD12 | 2.48                     | 0.43              |
| 1:N:295:LEU:HD23 | 1:N:342:ILE:CD1  | 2.46                     | 0.43              |
| 1:H:6:VAL:CG2    | 1:N:60:ILE:HA    | 2.48                     | 0.43              |
| 1:N:62:LEU:HB2   | 1:N:68:ASN:HA    | 2.00                     | 0.43              |
| 1:A:381:VAL:CG2  | 1:A:393:LYS:N    | 2.77                     | 0.43              |
| 1:B:144:ILE:CG2  | 1:B:163:ALA:HA   | 2.49                     | 0.43              |
| 1:A:521:VAL:HG11 | 1:B:59:GLU:CG    | 2.49                     | 0.43              |
| 1:C:236:VAL:HG13 | 1:C:317:LEU:HD13 | 2.01                     | 0.43              |
| 1:C:240:VAL:HG13 | 1:C:245:LYS:O    | 2.18                     | 0.43              |
| 1:C:278:ALA:HB2  | 1:C:289:LEU:CG   | 2.49                     | 0.43              |
| 1:E:144:ILE:CG2  | 1:E:163:ALA:HA   | 2.49                     | 0.43              |
| 1:E:513:LEU:O    | 1:F:49:ILE:HD13  | 2.19                     | 0.43              |
| 1:F:152:ALA:HB2  | 1:F:399:ALA:HB2  | 2.00                     | 0.43              |
| 1:G:381:VAL:HG11 | 1:G:393:LYS:HB2  | 2.00                     | 0.43              |
| 1:G:52:ASP:HB3   | 1:G:55:SER:H     | 1.82                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:227:ILE:CD1  | 1:H:233:MET:SD   | 2.92                     | 0.43              |
| 1:I:240:VAL:HG21 | 1:I:317:LEU:CD2  | 2.49                     | 0.43              |
| 1:I:240:VAL:HG21 | 1:I:317:LEU:HD22 | 2.00                     | 0.43              |
| 1:I:77:VAL:HG22  | 1:I:510:VAL:CB   | 2.49                     | 0.43              |
| 1:L:99:ILE:CG2   | 1:L:120:ILE:HD13 | 2.49                     | 0.43              |
| 1:M:237:LEU:HA   | 1:M:247:LEU:CD2  | 2.48                     | 0.43              |
| 1:H:257:GLU:CA   | 1:N:242:LYS:C    | 2.78                     | 0.43              |
| 1:N:282:GLY:O    | 1:N:285:ARG:HB3  | 2.19                     | 0.43              |
| 1:A:513:LEU:O    | 1:B:49:ILE:HD13  | 2.19                     | 0.43              |
| 1:A:524:LEU:HG   | 1:A:525:PRO:N    | 2.33                     | 0.43              |
| 1:B:200:LEU:HD13 | 1:B:259:LEU:HB2  | 2.00                     | 0.43              |
| 1:C:191:GLU:H    | 1:C:334:ASP:HA   | 1.84                     | 0.43              |
| 1:C:381:VAL:HG11 | 1:C:393:LYS:HB2  | 2.00                     | 0.43              |
| 1:D:236:VAL:HG13 | 1:D:317:LEU:HD13 | 2.01                     | 0.43              |
| 1:E:177:VAL:HG21 | 1:E:397:GLU:HG2  | 1.99                     | 0.43              |
| 1:F:165:ALA:HA   | 1:F:187:LEU:HD21 | 2.01                     | 0.43              |
| 1:F:236:VAL:HG13 | 1:F:317:LEU:HD13 | 2.01                     | 0.43              |
| 1:F:177:VAL:HA   | 1:F:379:ILE:O    | 2.19                     | 0.43              |
| 1:F:513:LEU:O    | 1:G:49:ILE:HD13  | 2.19                     | 0.43              |
| 1:F:521:VAL:HG11 | 1:G:59:GLU:CG    | 2.49                     | 0.43              |
| 1:G:236:VAL:HG13 | 1:G:317:LEU:HD13 | 2.01                     | 0.43              |
| 1:G:524:LEU:HG   | 1:G:525:LEU:N    | 2.34                     | 0.43              |
| 1:H:518:GLU:CB   | 1:H:519:CYS:N    | 2.74                     | 0.43              |
| 1:J:237:LEU:HA   | 1:J:247:LEU:CD2  | 2.49                     | 0.43              |
| 1:K:224:ASP:HB2  | 1:K:303:GLU:H    | 1.82                     | 0.43              |
| 1:K:301:ILE:HG23 | 1:K:307:MET:HB2  | 2.01                     | 0.43              |
| 1:L:237:LEU:HA   | 1:L:247:LEU:CD2  | 2.48                     | 0.43              |
| 1:L:27:VAL:CG1   | 1:L:90:THR:HG23  | 2.47                     | 0.43              |
| 1:B:150:ILE:CD1  | 1:B:493:ILE:CG2  | 2.91                     | 0.42              |
| 2:B:1525:PO4:P   | 4:B:1527:ATP:PG  | 3.17                     | 0.42              |
| 1:B:191:GLU:H    | 1:B:334:ASP:HA   | 1.84                     | 0.42              |
| 1:B:206:ASN:CB   | 1:B:208:PRO:HD2  | 2.42                     | 0.42              |
| 1:B:278:ALA:HB2  | 1:B:289:LEU:CG   | 2.49                     | 0.42              |
| 2:E:1525:PO4:P   | 4:E:1527:ATP:PG  | 3.16                     | 0.42              |
| 1:E:200:LEU:HD13 | 1:E:259:LEU:HB2  | 2.00                     | 0.42              |
| 1:E:236:VAL:HG13 | 1:E:317:LEU:HD13 | 2.01                     | 0.42              |
| 1:E:521:VAL:HG11 | 1:F:59:GLU:CG    | 2.49                     | 0.42              |
| 1:H:222:LEU:CD2  | 1:H:250:ILE:HD12 | 2.48                     | 0.42              |
| 1:H:240:VAL:HG21 | 1:H:317:LEU:HD22 | 2.00                     | 0.42              |
| 1:I:298:GLY:CA   | 1:I:318:GLY:HA3  | 2.49                     | 0.42              |
| 1:J:99:ILE:CG2   | 1:J:120:ILE:HD13 | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:62:LEU:HB2   | 1:L:68:ASN:HA    | 2.00                     | 0.42              |
| 1:M:282:GLY:O    | 1:M:285:ARG:HB3  | 2.19                     | 0.42              |
| 1:M:218:PRO:HG3  | 1:M:323:VAL:HG13 | 2.00                     | 0.42              |
| 1:A:220:ILE:CD1  | 1:A:296:THR:HG21 | 2.47                     | 0.42              |
| 1:B:223:ALA:HB3  | 1:B:251:ALA:HA   | 2.02                     | 0.42              |
| 1:C:223:ALA:HB3  | 1:C:251:ALA:HA   | 2.02                     | 0.42              |
| 1:E:207:LYS:HB2  | 1:E:208:PRO:HD3  | 2.01                     | 0.42              |
| 1:E:381:VAL:HG11 | 1:E:393:LYS:HB2  | 2.00                     | 0.42              |
| 1:F:200:LEU:HD13 | 1:F:259:LEU:HB2  | 2.00                     | 0.42              |
| 1:F:249:ILE:HD11 | 1:F:262:LEU:HD22 | 1.87                     | 0.42              |
| 1:G:190:VAL:HB   | 1:G:334:ASP:HB2  | 2.01                     | 0.42              |
| 1:H:182:GLY:HA2  | 1:H:183:LEU:HA   | 1.66                     | 0.42              |
| 1:H:242:LYS:C    | 1:I:257:GLU:CA   | 2.78                     | 0.42              |
| 1:I:278:ALA:HA   | 1:I:279:PRO:HD3  | 1.87                     | 0.42              |
| 1:I:214:GLU:CD   | 1:I:322:ARG:HE   | 2.22                     | 0.42              |
| 1:J:169:VAL:HG21 | 1:J:175:ILE:CG1  | 2.49                     | 0.42              |
| 1:L:190:VAL:HG21 | 1:L:333:ILE:CG1  | 2.49                     | 0.42              |
| 1:L:227:ILE:HG22 | 1:L:262:LEU:HD21 | 2.01                     | 0.42              |
| 1:L:242:LYS:C    | 1:M:257:GLU:CA   | 2.78                     | 0.42              |
| 1:M:62:LEU:HB2   | 1:M:68:ASN:HA    | 2.00                     | 0.42              |
| 1:N:182:GLY:HA2  | 1:N:183:LEU:HA   | 1.63                     | 0.42              |
| 1:N:240:VAL:HG21 | 1:N:317:LEU:CD2  | 2.49                     | 0.42              |
| 1:C:278:ALA:HB2  | 1:C:289:LEU:HG   | 2.01                     | 0.42              |
| 1:C:521:VAL:HG11 | 1:D:59:GLU:CG    | 2.49                     | 0.42              |
| 1:D:200:LEU:HD13 | 1:D:259:LEU:HB2  | 2.00                     | 0.42              |
| 1:E:221:LEU:CD1  | 1:E:309:LEU:HD21 | 2.45                     | 0.42              |
| 1:F:223:ALA:HB3  | 1:F:251:ALA:HA   | 2.02                     | 0.42              |
| 1:G:278:ALA:HB2  | 1:G:289:LEU:CG   | 2.49                     | 0.42              |
| 1:G:52:ASP:HB2   | 1:G:55:SER:HB2   | 2.01                     | 0.42              |
| 1:H:169:VAL:HG21 | 1:H:175:ILE:CG1  | 2.49                     | 0.42              |
| 1:I:209:GLU:CD   | 1:I:209:GLU:H    | 2.23                     | 0.42              |
| 1:I:223:ALA:HB2  | 1:I:309:LEU:CG   | 2.48                     | 0.42              |
| 1:J:223:ALA:HB2  | 1:J:309:LEU:CG   | 2.49                     | 0.42              |
| 1:J:37:ASN:HB2   | 1:K:516:THR:O    | 2.20                     | 0.42              |
| 1:L:222:LEU:CD2  | 1:L:250:ILE:HD12 | 2.48                     | 0.42              |
| 1:M:225:LYS:CA   | 1:M:303:GLU:HB2  | 2.50                     | 0.42              |
| 1:A:190:VAL:HB   | 1:A:334:ASP:HB2  | 2.01                     | 0.42              |
| 1:A:381:VAL:HG11 | 1:A:393:LYS:HB2  | 2.00                     | 0.42              |
| 1:A:52:ASP:HB2   | 1:A:55:SER:HB2   | 2.01                     | 0.42              |
| 1:B:521:VAL:HG11 | 1:C:59:GLU:CG    | 2.49                     | 0.42              |
| 1:E:223:ALA:HB3  | 1:E:251:ALA:HA   | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:278:ALA:HB2  | 1:E:289:LEU:CG   | 2.49                     | 0.42              |
| 1:E:52:ASP:HB2   | 1:E:55:SER:HB2   | 2.01                     | 0.42              |
| 1:D:521:VAL:HG11 | 1:E:59:GLU:CG    | 2.49                     | 0.42              |
| 1:F:278:ALA:HB2  | 1:F:289:LEU:CG   | 2.49                     | 0.42              |
| 1:F:190:VAL:HB   | 1:F:334:ASP:HB2  | 2.01                     | 0.42              |
| 1:G:161:LEU:HD21 | 1:G:185:ASP:HB3  | 2.00                     | 0.42              |
| 1:G:144:ILE:CG2  | 1:G:163:ALA:HA   | 2.49                     | 0.42              |
| 1:H:100:ILE:HD11 | 1:H:514:MET:HE3  | 2.01                     | 0.42              |
| 1:I:99:ILE:CG2   | 1:I:120:ILE:HD13 | 2.49                     | 0.42              |
| 1:I:301:ILE:HG23 | 1:I:307:MET:HB2  | 2.01                     | 0.42              |
| 1:J:100:ILE:HD11 | 1:J:514:MET:HE3  | 2.02                     | 0.42              |
| 1:K:37:ASN:HB2   | 1:L:516:THR:O    | 2.20                     | 0.42              |
| 1:M:295:LEU:HD13 | 1:M:335:GLY:HA3  | 2.02                     | 0.42              |
| 1:N:222:LEU:CD2  | 1:N:250:ILE:HD12 | 2.48                     | 0.42              |
| 1:A:213:VAL:HG23 | 1:A:214:GLU:N    | 2.33                     | 0.42              |
| 1:A:215:LEU:HB3  | 1:A:246:PRO:HG2  | 2.02                     | 0.42              |
| 1:C:286:LYS:HD3  | 1:C:304:GLU:HA   | 2.01                     | 0.42              |
| 1:D:278:ALA:HB2  | 1:D:289:LEU:HG   | 2.01                     | 0.42              |
| 1:D:513:LEU:O    | 1:E:49:ILE:HD13  | 2.19                     | 0.42              |
| 1:G:249:ILE:HD11 | 1:G:262:LEU:HD22 | 1.87                     | 0.42              |
| 1:H:193:MET:HG2  | 1:H:372:LEU:HA   | 2.02                     | 0.42              |
| 1:I:151:SER:HB3  | 1:I:399:ALA:HA   | 1.99                     | 0.42              |
| 1:J:239:ALA:CB   | 1:J:314:LEU:HB3  | 2.49                     | 0.42              |
| 1:K:214:GLU:CD   | 1:K:322:ARG:HE   | 2.22                     | 0.42              |
| 1:K:99:ILE:CG2   | 1:K:120:ILE:HD13 | 2.49                     | 0.42              |
| 1:L:227:ILE:CD1  | 1:L:233:MET:SD   | 2.93                     | 0.42              |
| 1:M:169:VAL:HG21 | 1:M:175:ILE:CG1  | 2.49                     | 0.42              |
| 1:M:298:GLY:CA   | 1:M:318:GLY:HA3  | 2.49                     | 0.42              |
| 1:N:237:LEU:HA   | 1:N:247:LEU:CD2  | 2.49                     | 0.42              |
| 1:N:295:LEU:HD13 | 1:N:335:GLY:HA3  | 2.02                     | 0.42              |
| 1:A:144:ILE:CG2  | 1:A:163:ALA:HA   | 2.49                     | 0.42              |
| 1:A:223:ALA:HB3  | 1:A:251:ALA:HA   | 2.02                     | 0.42              |
| 1:A:191:GLU:H    | 1:A:334:ASP:HA   | 1.84                     | 0.42              |
| 1:A:49:ILE:HD13  | 1:G:513:LEU:O    | 2.19                     | 0.42              |
| 1:B:513:LEU:O    | 1:C:49:ILE:HD13  | 2.19                     | 0.42              |
| 1:C:52:ASP:HB2   | 1:C:55:SER:HB2   | 2.01                     | 0.42              |
| 1:D:271:VAL:O    | 1:D:273:VAL:HG23 | 2.20                     | 0.42              |
| 1:D:381:VAL:CG2  | 1:D:393:LYS:N    | 2.77                     | 0.42              |
| 1:E:207:LYS:N    | 1:E:208:PRO:HD2  | 2.34                     | 0.42              |
| 1:E:271:VAL:O    | 1:E:273:VAL:HG23 | 2.20                     | 0.42              |
| 1:G:223:ALA:HB3  | 1:G:251:ALA:HA   | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:59:GLU:CG    | 1:G:521:VAL:HG11 | 2.49                     | 0.42              |
| 1:H:295:LEU:HD13 | 1:H:335:GLY:HA3  | 2.02                     | 0.42              |
| 1:H:214:GLU:CD   | 1:H:322:ARG:HE   | 2.22                     | 0.42              |
| 1:I:227:ILE:H    | 1:I:254:VAL:HG22 | 1.85                     | 0.42              |
| 1:J:295:LEU:HD23 | 1:J:342:ILE:CD1  | 2.46                     | 0.42              |
| 1:I:37:ASN:HB2   | 1:J:516:THR:O    | 2.20                     | 0.42              |
| 1:K:295:LEU:HD13 | 1:K:335:GLY:HA3  | 2.02                     | 0.42              |
| 1:L:225:LYS:CA   | 1:L:303:GLU:HB2  | 2.50                     | 0.42              |
| 1:L:295:LEU:HD13 | 1:L:335:GLY:HA3  | 2.02                     | 0.42              |
| 1:M:227:ILE:HG22 | 1:M:262:LEU:HD21 | 2.01                     | 0.42              |
| 1:M:446:ALA:O    | 1:M:450:PRO:HD2  | 2.20                     | 0.42              |
| 1:N:193:MET:HG2  | 1:N:372:LEU:HA   | 2.02                     | 0.42              |
| 1:B:278:ALA:HB2  | 1:B:289:LEU:HG   | 2.01                     | 0.42              |
| 1:B:286:LYS:HD3  | 1:B:304:GLU:HA   | 2.01                     | 0.42              |
| 1:D:144:ILE:CG2  | 1:D:163:ALA:HA   | 2.49                     | 0.42              |
| 1:D:223:ALA:HB3  | 1:D:251:ALA:HA   | 2.02                     | 0.42              |
| 1:D:270:ILE:O    | 1:D:271:VAL:HB   | 2.20                     | 0.42              |
| 1:D:190:VAL:HB   | 1:D:334:ASP:CA   | 2.50                     | 0.42              |
| 1:D:384:ALA:HA   | 1:D:385:THR:HA   | 1.68                     | 0.42              |
| 1:D:381:VAL:HG11 | 1:D:393:LYS:HB2  | 2.00                     | 0.42              |
| 1:E:270:ILE:O    | 1:E:271:VAL:HB   | 2.20                     | 0.42              |
| 1:F:191:GLU:H    | 1:F:334:ASP:HA   | 1.84                     | 0.42              |
| 1:G:215:LEU:HB3  | 1:G:246:PRO:HG2  | 2.02                     | 0.42              |
| 1:G:191:GLU:H    | 1:G:334:ASP:HA   | 1.84                     | 0.42              |
| 1:G:150:ILE:HD11 | 1:G:493:ILE:HG23 | 1.97                     | 0.42              |
| 1:H:227:ILE:H    | 1:H:254:VAL:HG22 | 1.85                     | 0.42              |
| 1:H:82:ASN:HA    | 1:H:89:THR:HG22  | 2.02                     | 0.42              |
| 1:I:295:LEU:HD13 | 1:I:335:GLY:HA3  | 2.02                     | 0.42              |
| 1:K:27:VAL:CG1   | 1:K:90:THR:HG23  | 2.47                     | 0.42              |
| 1:L:183:LEU:HA   | 1:L:382:GLY:HA3  | 2.01                     | 0.42              |
| 1:L:209:GLU:H    | 1:L:209:GLU:CD   | 2.23                     | 0.42              |
| 1:L:82:ASN:HA    | 1:L:89:THR:HG22  | 2.02                     | 0.42              |
| 1:M:82:ASN:HA    | 1:M:89:THR:HG22  | 2.02                     | 0.42              |
| 1:N:301:ILE:HG23 | 1:N:307:MET:HB2  | 2.01                     | 0.42              |
| 1:N:239:ALA:CB   | 1:N:314:LEU:HB3  | 2.49                     | 0.42              |
| 1:N:406:ALA:HB1  | 1:N:411:VAL:CG1  | 2.49                     | 0.42              |
| 1:N:446:ALA:O    | 1:N:450:PRO:HD2  | 2.20                     | 0.42              |
| 1:C:177:VAL:HA   | 1:C:379:ILE:O    | 2.19                     | 0.42              |
| 1:C:271:VAL:O    | 1:C:273:VAL:HG23 | 2.20                     | 0.42              |
| 1:F:215:LEU:HB3  | 1:F:246:PRO:HG2  | 2.02                     | 0.42              |
| 1:F:270:ILE:O    | 1:F:271:VAL:HB   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:286:LYS:HD3  | 1:F:304:GLU:HA   | 2.01                     | 0.42              |
| 1:G:165:ALA:HB2  | 1:G:187:LEU:HD13 | 2.02                     | 0.42              |
| 1:H:225:LYS:CA   | 1:H:303:GLU:HB2  | 2.50                     | 0.42              |
| 1:H:239:ALA:CB   | 1:H:314:LEU:HB3  | 2.49                     | 0.42              |
| 1:H:446:ALA:O    | 1:H:450:PRO:HD2  | 2.20                     | 0.42              |
| 1:I:406:ALA:HB1  | 1:I:411:VAL:CG1  | 2.50                     | 0.42              |
| 1:I:406:ALA:HB1  | 1:I:411:VAL:HG12 | 2.02                     | 0.42              |
| 1:I:82:ASN:HA    | 1:I:89:THR:HG22  | 2.02                     | 0.42              |
| 1:J:295:LEU:HD13 | 1:J:335:GLY:HA3  | 2.02                     | 0.42              |
| 1:J:82:ASN:HA    | 1:J:89:THR:HG22  | 2.02                     | 0.42              |
| 1:K:222:LEU:CD2  | 1:K:250:ILE:HD12 | 2.49                     | 0.42              |
| 1:L:282:GLY:O    | 1:L:285:ARG:HB3  | 2.19                     | 0.42              |
| 1:L:214:GLU:CD   | 1:L:322:ARG:HE   | 2.22                     | 0.42              |
| 1:L:100:ILE:HD11 | 1:L:514:MET:HE3  | 2.01                     | 0.42              |
| 1:M:77:VAL:HG22  | 1:M:510:VAL:CB   | 2.49                     | 0.42              |
| 1:M:8:PHE:HA     | 1:M:9:GLY:HA3    | 1.82                     | 0.42              |
| 1:N:206:ASN:O    | 1:N:208:PRO:N    | 2.52                     | 0.42              |
| 1:N:151:SER:HB3  | 1:N:399:ALA:HA   | 1.99                     | 0.42              |
| 1:B:177:VAL:HA   | 1:B:379:ILE:O    | 2.19                     | 0.42              |
| 1:C:270:ILE:O    | 1:C:271:VAL:HB   | 2.20                     | 0.42              |
| 1:E:52:ASP:HB3   | 1:E:55:SER:H     | 1.83                     | 0.42              |
| 1:F:271:VAL:O    | 1:F:273:VAL:HG23 | 2.20                     | 0.42              |
| 1:H:227:ILE:HG22 | 1:H:262:LEU:HD21 | 2.02                     | 0.42              |
| 1:H:298:GLY:CA   | 1:H:318:GLY:HA3  | 2.49                     | 0.42              |
| 1:I:149:THR:HG22 | 1:I:154:SER:HB3  | 2.02                     | 0.42              |
| 1:J:227:ILE:HG22 | 1:J:262:LEU:HD21 | 2.02                     | 0.42              |
| 1:K:150:ILE:HD12 | 1:K:494:LEU:H    | 1.85                     | 0.42              |
| 1:K:82:ASN:HA    | 1:K:89:THR:HG22  | 2.02                     | 0.42              |
| 1:L:239:ALA:CB   | 1:L:314:LEU:HB3  | 2.49                     | 0.42              |
| 1:M:240:VAL:HB   | 1:M:247:LEU:HD22 | 2.02                     | 0.42              |
| 1:N:406:ALA:HB1  | 1:N:411:VAL:HG12 | 2.02                     | 0.42              |
| 1:N:82:ASN:HA    | 1:N:89:THR:HG22  | 2.02                     | 0.42              |
| 1:A:165:ALA:HB2  | 1:A:187:LEU:HD13 | 2.02                     | 0.42              |
| 1:B:215:LEU:HB3  | 1:B:246:PRO:HG2  | 2.02                     | 0.42              |
| 1:D:286:LYS:HD3  | 1:D:304:GLU:HA   | 2.01                     | 0.42              |
| 1:E:190:VAL:HB   | 1:E:334:ASP:HB2  | 2.01                     | 0.42              |
| 1:G:270:ILE:O    | 1:G:271:VAL:HB   | 2.20                     | 0.42              |
| 1:H:149:THR:HG22 | 1:H:154:SER:HB3  | 2.02                     | 0.42              |
| 1:H:77:VAL:HG22  | 1:H:510:VAL:CB   | 2.49                     | 0.42              |
| 1:H:99:ILE:CG2   | 1:H:120:ILE:HD13 | 2.49                     | 0.42              |
| 1:I:227:ILE:HG22 | 1:I:262:LEU:HD21 | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:240:VAL:HB   | 1:J:247:LEU:HD22 | 2.02                     | 0.42              |
| 1:K:100:ILE:HD11 | 1:K:514:MET:HE3  | 2.02                     | 0.42              |
| 1:K:227:ILE:H    | 1:K:254:VAL:HG22 | 1.85                     | 0.42              |
| 1:K:227:ILE:HG22 | 1:K:262:LEU:HD21 | 2.02                     | 0.42              |
| 1:K:309:LEU:HD23 | 1:K:309:LEU:HA   | 1.81                     | 0.42              |
| 1:L:190:VAL:HG23 | 1:L:191:GLU:O    | 2.20                     | 0.42              |
| 1:K:242:LYS:HG3  | 1:L:257:GLU:C    | 2.40                     | 0.42              |
| 1:M:153:ASN:N    | 1:M:154:SER:CA   | 2.82                     | 0.42              |
| 1:M:301:ILE:HG23 | 1:M:307:MET:HB2  | 2.01                     | 0.42              |
| 1:M:417:VAL:HG11 | 1:M:477:GLY:HA3  | 2.02                     | 0.42              |
| 1:L:37:ASN:HB2   | 1:M:516:THR:O    | 2.20                     | 0.42              |
| 1:N:204:PHE:CA   | 1:N:207:LYS:HE2  | 2.50                     | 0.42              |
| 1:N:227:ILE:HG22 | 1:N:262:LEU:HD21 | 2.02                     | 0.42              |
| 1:B:200:LEU:HD11 | 1:B:254:VAL:CA   | 2.12                     | 0.41              |
| 1:C:513:LEU:O    | 1:D:49:ILE:HD13  | 2.19                     | 0.41              |
| 1:E:215:LEU:HB3  | 1:E:246:PRO:HG2  | 2.02                     | 0.41              |
| 1:E:150:ILE:HD11 | 1:E:493:ILE:HG23 | 1.97                     | 0.41              |
| 1:F:165:ALA:HB2  | 1:F:187:LEU:CD1  | 2.50                     | 0.41              |
| 1:F:200:LEU:HD11 | 1:F:254:VAL:CG2  | 2.20                     | 0.41              |
| 1:H:37:ASN:HB2   | 1:I:516:THR:O    | 2.20                     | 0.41              |
| 1:I:161:LEU:HD22 | 1:I:379:ILE:HG23 | 2.02                     | 0.41              |
| 1:J:182:GLY:HA2  | 1:J:183:LEU:HA   | 1.63                     | 0.41              |
| 1:K:298:GLY:CA   | 1:K:318:GLY:HA3  | 2.50                     | 0.41              |
| 1:L:161:LEU:HD22 | 1:L:379:ILE:HG23 | 2.02                     | 0.41              |
| 1:M:214:GLU:CD   | 1:M:322:ARG:HE   | 2.22                     | 0.41              |
| 1:M:31:LEU:HB3   | 1:M:90:THR:HG21  | 2.03                     | 0.41              |
| 1:N:214:GLU:CD   | 1:N:322:ARG:HE   | 2.22                     | 0.41              |
| 1:A:193:MET:CE   | 1:A:292:ILE:HG23 | 2.51                     | 0.41              |
| 1:C:200:LEU:HD13 | 1:C:259:LEU:HB2  | 2.00                     | 0.41              |
| 1:F:144:ILE:CG2  | 1:F:163:ALA:HA   | 2.49                     | 0.41              |
| 1:G:286:LYS:HD3  | 1:G:304:GLU:HA   | 2.01                     | 0.41              |
| 1:I:240:VAL:HB   | 1:I:247:LEU:HD22 | 2.02                     | 0.41              |
| 1:L:417:VAL:HG11 | 1:L:477:GLY:HA3  | 2.02                     | 0.41              |
| 1:A:270:ILE:O    | 1:A:271:VAL:HB   | 2.20                     | 0.41              |
| 1:A:278:ALA:HB2  | 1:A:289:LEU:HG   | 2.02                     | 0.41              |
| 1:A:286:LYS:HD3  | 1:A:304:GLU:HA   | 2.01                     | 0.41              |
| 1:B:270:ILE:O    | 1:B:271:VAL:HB   | 2.20                     | 0.41              |
| 1:B:190:VAL:HB   | 1:B:334:ASP:HB2  | 2.01                     | 0.41              |
| 1:C:254:VAL:HG12 | 1:C:259:LEU:HB2  | 2.03                     | 0.41              |
| 1:C:381:VAL:CG2  | 1:C:393:LYS:N    | 2.77                     | 0.41              |
| 1:D:193:MET:CE   | 1:D:292:ILE:HG23 | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:286:LYS:HD3  | 1:E:304:GLU:HA   | 2.01                     | 0.41              |
| 1:E:193:MET:CE   | 1:E:292:ILE:HG23 | 2.50                     | 0.41              |
| 1:F:209:GLU:CD   | 1:F:209:GLU:H    | 2.24                     | 0.41              |
| 1:H:242:LYS:HA   | 1:H:243:ALA:HA   | 1.16                     | 0.41              |
| 1:H:182:GLY:HA2  | 1:H:382:GLY:HA2  | 2.02                     | 0.41              |
| 1:I:239:ALA:CB   | 1:I:314:LEU:HB3  | 2.49                     | 0.41              |
| 1:I:417:VAL:HG11 | 1:I:477:GLY:HA3  | 2.02                     | 0.41              |
| 1:J:233:MET:CE   | 1:J:249:ILE:HD11 | 2.40                     | 0.41              |
| 1:J:301:ILE:HG23 | 1:J:307:MET:HB2  | 2.01                     | 0.41              |
| 1:K:161:LEU:HD22 | 1:K:379:ILE:HG23 | 2.02                     | 0.41              |
| 1:K:225:LYS:CA   | 1:K:303:GLU:HB2  | 2.50                     | 0.41              |
| 1:L:227:ILE:H    | 1:L:254:VAL:HG22 | 1.85                     | 0.41              |
| 1:L:31:LEU:HB3   | 1:L:90:THR:HG21  | 2.03                     | 0.41              |
| 1:M:150:ILE:HD12 | 1:M:494:LEU:H    | 1.85                     | 0.41              |
| 1:M:295:LEU:HD23 | 1:M:342:ILE:CD1  | 2.46                     | 0.41              |
| 1:N:417:VAL:HG11 | 1:N:477:GLY:HA3  | 2.02                     | 0.41              |
| 1:B:193:MET:CE   | 1:B:292:ILE:HG23 | 2.51                     | 0.41              |
| 1:B:220:ILE:CD1  | 1:B:296:THR:HG21 | 2.47                     | 0.41              |
| 1:E:165:ALA:HB2  | 1:E:187:LEU:HD13 | 2.02                     | 0.41              |
| 1:E:278:ALA:HB2  | 1:E:289:LEU:HG   | 2.01                     | 0.41              |
| 1:F:254:VAL:HG12 | 1:F:259:LEU:HB2  | 2.03                     | 0.41              |
| 1:G:278:ALA:HB2  | 1:G:289:LEU:HG   | 2.01                     | 0.41              |
| 1:H:161:LEU:HD22 | 1:H:379:ILE:HG23 | 2.02                     | 0.41              |
| 1:H:417:VAL:HG11 | 1:H:477:GLY:HA3  | 2.03                     | 0.41              |
| 1:J:225:LYS:CA   | 1:J:303:GLU:HB2  | 2.50                     | 0.41              |
| 1:J:161:LEU:HD22 | 1:J:379:ILE:HG23 | 2.02                     | 0.41              |
| 1:L:446:ALA:O    | 1:L:450:PRO:HD2  | 2.20                     | 0.41              |
| 1:M:161:LEU:HD22 | 1:M:379:ILE:HG23 | 2.03                     | 0.41              |
| 1:M:278:ALA:HA   | 1:M:279:PRO:HD3  | 1.87                     | 0.41              |
| 1:M:100:ILE:HD11 | 1:M:514:MET:HE3  | 2.02                     | 0.41              |
| 1:N:150:ILE:HD12 | 1:N:494:LEU:H    | 1.85                     | 0.41              |
| 1:C:250:ILE:HD13 | 1:C:292:ILE:HG21 | 2.02                     | 0.41              |
| 1:D:215:LEU:HB3  | 1:D:246:PRO:HG2  | 2.02                     | 0.41              |
| 1:D:254:VAL:HG12 | 1:D:259:LEU:HB2  | 2.03                     | 0.41              |
| 1:E:197:ARG:HG3  | 1:E:198:GLY:O    | 2.20                     | 0.41              |
| 1:E:254:VAL:HG12 | 1:E:259:LEU:HB2  | 2.03                     | 0.41              |
| 1:F:278:ALA:HA   | 1:F:279:PRO:HD3  | 1.72                     | 0.41              |
| 1:I:193:MET:HG2  | 1:I:372:LEU:HA   | 2.02                     | 0.41              |
| 1:I:31:LEU:HB3   | 1:I:90:THR:HG21  | 2.02                     | 0.41              |
| 1:K:518:GLU:CB   | 1:K:519:CYS:N    | 2.74                     | 0.41              |
| 1:N:240:VAL:HB   | 1:N:247:LEU:HD22 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:171:LYS:HE3  | 1:N:408:GLU:OE1  | 2.21                     | 0.41              |
| 1:N:77:VAL:HG22  | 1:N:510:VAL:CB   | 2.49                     | 0.41              |
| 1:A:34:LYS:NZ    | 1:A:483:GLU:OE2  | 2.52                     | 0.41              |
| 1:B:271:VAL:O    | 1:B:273:VAL:HG23 | 2.20                     | 0.41              |
| 1:C:223:ALA:HB3  | 1:C:251:ALA:CA   | 2.51                     | 0.41              |
| 1:D:249:ILE:HD11 | 1:D:262:LEU:HD22 | 1.87                     | 0.41              |
| 1:D:223:ALA:HB3  | 1:D:251:ALA:CA   | 2.51                     | 0.41              |
| 1:F:278:ALA:HB2  | 1:F:289:LEU:HG   | 2.01                     | 0.41              |
| 1:G:271:VAL:O    | 1:G:273:VAL:HG23 | 2.20                     | 0.41              |
| 1:H:301:ILE:HG23 | 1:H:307:MET:HB2  | 2.01                     | 0.41              |
| 1:H:309:LEU:HD23 | 1:H:309:LEU:HA   | 1.81                     | 0.41              |
| 1:I:446:ALA:O    | 1:I:450:PRO:HD2  | 2.20                     | 0.41              |
| 1:I:150:ILE:HD12 | 1:I:494:LEU:H    | 1.85                     | 0.41              |
| 1:J:149:THR:HG22 | 1:J:154:SER:HB3  | 2.02                     | 0.41              |
| 1:K:240:VAL:HB   | 1:K:247:LEU:HD22 | 2.02                     | 0.41              |
| 1:L:240:VAL:HB   | 1:L:247:LEU:HD22 | 2.02                     | 0.41              |
| 1:L:301:ILE:HG23 | 1:L:307:MET:HB2  | 2.01                     | 0.41              |
| 1:M:193:MET:HG2  | 1:M:372:LEU:HA   | 2.02                     | 0.41              |
| 1:A:209:GLU:H    | 1:A:209:GLU:CD   | 2.24                     | 0.41              |
| 1:A:73:MET:HG2   | 1:B:46:ALA:CB    | 2.51                     | 0.41              |
| 1:B:165:ALA:HB2  | 1:B:187:LEU:HD13 | 2.02                     | 0.41              |
| 1:B:254:VAL:HG12 | 1:B:259:LEU:HB2  | 2.03                     | 0.41              |
| 1:C:165:ALA:HB2  | 1:C:187:LEU:HD13 | 2.02                     | 0.41              |
| 1:C:215:LEU:HB3  | 1:C:246:PRO:HG2  | 2.02                     | 0.41              |
| 1:D:250:ILE:HD13 | 1:D:292:ILE:HG21 | 2.02                     | 0.41              |
| 1:E:197:ARG:HA   | 1:E:197:ARG:HD3  | 2.02                     | 0.41              |
| 1:H:233:MET:CE   | 1:H:249:ILE:HD11 | 2.42                     | 0.41              |
| 1:I:8:PHE:HA     | 1:I:9:GLY:HA3    | 1.81                     | 0.41              |
| 1:J:227:ILE:H    | 1:J:254:VAL:HG22 | 1.85                     | 0.41              |
| 1:J:446:ALA:O    | 1:J:450:PRO:HD2  | 2.20                     | 0.41              |
| 1:J:31:LEU:HB3   | 1:J:90:THR:HG21  | 2.03                     | 0.41              |
| 1:K:31:LEU:HB3   | 1:K:90:THR:HG21  | 2.03                     | 0.41              |
| 1:L:321:LYS:HZ3  | 1:L:334:ASP:CG   | 2.23                     | 0.41              |
| 1:M:37:ASN:HB2   | 1:N:516:THR:O    | 2.20                     | 0.41              |
| 1:N:149:THR:HG22 | 1:N:154:SER:HB3  | 2.02                     | 0.41              |
| 1:N:227:ILE:H    | 1:N:254:VAL:HG22 | 1.85                     | 0.41              |
| 1:H:516:THR:O    | 1:N:37:ASN:HB2   | 2.20                     | 0.41              |
| 1:B:236:VAL:CG1  | 1:B:317:LEU:HD13 | 2.51                     | 0.41              |
| 1:D:165:ALA:HB2  | 1:D:187:LEU:HD13 | 2.02                     | 0.41              |
| 1:F:236:VAL:CG1  | 1:F:317:LEU:HD13 | 2.51                     | 0.41              |
| 1:G:193:MET:SD   | 1:G:295:LEU:CB   | 3.09                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:236:VAL:CG1  | 1:G:317:LEU:HD13 | 2.51                     | 0.41              |
| 1:A:46:ALA:CB    | 1:G:73:MET:HG2   | 2.51                     | 0.41              |
| 1:H:225:LYS:HA   | 1:H:303:GLU:HB2  | 2.02                     | 0.41              |
| 1:J:417:VAL:HG11 | 1:J:477:GLY:HA3  | 2.02                     | 0.41              |
| 1:M:242:LYS:C    | 1:N:257:GLU:CA   | 2.78                     | 0.41              |
| 1:M:309:LEU:HD23 | 1:M:309:LEU:HA   | 1.81                     | 0.41              |
| 1:N:225:LYS:CA   | 1:N:303:GLU:HB2  | 2.50                     | 0.41              |
| 1:B:250:ILE:HD13 | 1:B:292:ILE:HG21 | 2.02                     | 0.41              |
| 1:C:190:VAL:HB   | 1:C:334:ASP:HB2  | 2.01                     | 0.41              |
| 1:D:190:VAL:CG2  | 1:D:333:ILE:CG2  | 2.98                     | 0.41              |
| 1:H:240:VAL:HB   | 1:H:247:LEU:HD22 | 2.02                     | 0.41              |
| 1:H:150:ILE:HD12 | 1:H:494:LEU:H    | 1.85                     | 0.41              |
| 1:K:207:LYS:HB3  | 1:K:208:PRO:HD3  | 2.03                     | 0.41              |
| 1:K:239:ALA:CB   | 1:K:314:LEU:HB3  | 2.51                     | 0.41              |
| 1:K:417:VAL:HG11 | 1:K:477:GLY:HA3  | 2.03                     | 0.41              |
| 1:L:149:THR:HG22 | 1:L:154:SER:HB3  | 2.02                     | 0.41              |
| 1:L:193:MET:HG2  | 1:L:372:LEU:HA   | 2.02                     | 0.41              |
| 1:M:149:THR:HG22 | 1:M:154:SER:HB3  | 2.02                     | 0.41              |
| 1:N:161:LEU:HD22 | 1:N:379:ILE:HG23 | 2.03                     | 0.41              |
| 1:N:31:LEU:HB3   | 1:N:90:THR:HG21  | 2.03                     | 0.41              |
| 1:A:250:ILE:HD13 | 1:A:292:ILE:HG21 | 2.02                     | 0.41              |
| 1:B:144:ILE:HG23 | 1:B:403:THR:HG23 | 2.03                     | 0.41              |
| 1:C:271:VAL:HG12 | 1:C:273:VAL:HG22 | 2.02                     | 0.41              |
| 1:D:236:VAL:CG1  | 1:D:317:LEU:HD13 | 2.51                     | 0.41              |
| 1:D:73:MET:HG2   | 1:E:46:ALA:CB    | 2.51                     | 0.41              |
| 2:E:1525:PO4:P   | 4:E:1527:ATP:O3G | 2.79                     | 0.41              |
| 1:E:250:ILE:HD13 | 1:E:292:ILE:HG21 | 2.02                     | 0.41              |
| 1:E:236:VAL:CG1  | 1:E:317:LEU:HD13 | 2.51                     | 0.41              |
| 1:G:254:VAL:HG12 | 1:G:259:LEU:HB2  | 2.03                     | 0.41              |
| 1:I:225:LYS:HA   | 1:I:303:GLU:HB2  | 2.03                     | 0.41              |
| 1:I:100:ILE:HD11 | 1:I:514:MET:HE3  | 2.03                     | 0.41              |
| 1:J:150:ILE:HD12 | 1:J:494:LEU:H    | 1.85                     | 0.41              |
| 1:K:278:ALA:HB3  | 1:K:285:ARG:HG2  | 2.02                     | 0.41              |
| 1:K:225:LYS:HA   | 1:K:303:GLU:HB2  | 2.02                     | 0.41              |
| 1:L:223:ALA:HB2  | 1:L:309:LEU:HD11 | 2.03                     | 0.41              |
| 1:M:209:GLU:CD   | 1:M:209:GLU:H    | 2.24                     | 0.41              |
| 1:N:242:LYS:HA   | 1:N:243:ALA:HA   | 1.12                     | 0.41              |
| 1:N:38:VAL:HG21  | 1:N:56:VAL:HG22  | 2.03                     | 0.41              |
| 1:N:27:VAL:CG1   | 1:N:90:THR:HG23  | 2.47                     | 0.41              |
| 1:A:311:LYS:O    | 1:A:313:THR:HG23 | 2.21                     | 0.41              |
| 1:A:236:VAL:CG1  | 1:A:317:LEU:HD13 | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:250:ILE:HD13 | 1:F:292:ILE:HG21 | 2.02                     | 0.41              |
| 1:F:193:MET:CE   | 1:F:292:ILE:HG23 | 2.50                     | 0.41              |
| 1:E:73:MET:HG2   | 1:F:46:ALA:CB    | 2.51                     | 0.41              |
| 1:G:250:ILE:HD13 | 1:G:292:ILE:HG21 | 2.02                     | 0.41              |
| 1:K:356:ALA:HB2  | 1:K:365:LEU:HD12 | 2.03                     | 0.41              |
| 1:L:405:ALA:HB1  | 1:L:498:LYS:CD   | 2.51                     | 0.41              |
| 1:M:182:GLY:HA2  | 1:M:183:LEU:HA   | 1.63                     | 0.41              |
| 1:M:239:ALA:CB   | 1:M:314:LEU:HB3  | 2.50                     | 0.41              |
| 1:A:254:VAL:HG12 | 1:A:259:LEU:HB2  | 2.03                     | 0.40              |
| 1:C:236:VAL:CG1  | 1:C:317:LEU:HD13 | 2.51                     | 0.40              |
| 1:F:311:LYS:O    | 1:F:313:THR:HG23 | 2.21                     | 0.40              |
| 1:F:73:MET:HG2   | 1:G:46:ALA:CB    | 2.51                     | 0.40              |
| 1:G:200:LEU:HD13 | 1:G:254:VAL:CG1  | 2.44                     | 0.40              |
| 1:G:311:LYS:O    | 1:G:313:THR:HG23 | 2.21                     | 0.40              |
| 1:H:50:THR:HG22  | 1:H:52:ASP:O     | 2.21                     | 0.40              |
| 1:H:38:VAL:HG21  | 1:H:56:VAL:HG22  | 2.04                     | 0.40              |
| 1:I:225:LYS:CA   | 1:I:303:GLU:HB2  | 2.50                     | 0.40              |
| 1:I:50:THR:HG22  | 1:I:52:ASP:O     | 2.21                     | 0.40              |
| 1:M:38:VAL:HG21  | 1:M:56:VAL:HG22  | 2.03                     | 0.40              |
| 1:N:338:GLU:O    | 1:N:342:ILE:HG13 | 2.22                     | 0.40              |
| 1:N:356:ALA:HB2  | 1:N:365:LEU:HD12 | 2.04                     | 0.40              |
| 1:B:73:MET:HG2   | 1:C:46:ALA:CB    | 2.51                     | 0.40              |
| 1:D:201:SER:HA   | 1:D:202:PRO:HD3  | 1.98                     | 0.40              |
| 1:D:203:TYR:CD1  | 1:D:203:TYR:N    | 2.90                     | 0.40              |
| 1:D:311:LYS:O    | 1:D:313:THR:HG23 | 2.21                     | 0.40              |
| 1:E:225:LYS:HB2  | 1:E:307:MET:O    | 2.22                     | 0.40              |
| 1:G:225:LYS:HB2  | 1:G:307:MET:O    | 2.22                     | 0.40              |
| 1:J:493:ILE:HD13 | 4:J:1527:ATP:C6  | 2.57                     | 0.40              |
| 1:M:206:ASN:HB3  | 1:M:208:PRO:HD2  | 2.03                     | 0.40              |
| 1:M:223:ALA:HB2  | 1:M:309:LEU:HD11 | 2.03                     | 0.40              |
| 1:M:356:ALA:HB2  | 1:M:365:LEU:HD12 | 2.04                     | 0.40              |
| 1:A:271:VAL:O    | 1:A:273:VAL:HG23 | 2.20                     | 0.40              |
| 1:B:223:ALA:HB3  | 1:B:251:ALA:CA   | 2.51                     | 0.40              |
| 2:C:1525:PO4:P   | 4:C:1527:ATP:O3G | 2.79                     | 0.40              |
| 1:C:194:GLN:HG3  | 1:C:329:THR:HG21 | 2.03                     | 0.40              |
| 1:F:223:ALA:HB3  | 1:F:251:ALA:CA   | 2.51                     | 0.40              |
| 1:J:193:MET:HG2  | 1:J:372:LEU:HA   | 2.02                     | 0.40              |
| 1:J:207:LYS:HE2  | 1:J:207:LYS:HA   | 2.04                     | 0.40              |
| 1:J:209:GLU:CD   | 1:J:209:GLU:H    | 2.25                     | 0.40              |
| 1:K:149:THR:HG22 | 1:K:154:SER:HB3  | 2.02                     | 0.40              |
| 1:K:338:GLU:O    | 1:K:342:ILE:HG13 | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:446:ALA:O    | 1:K:450:PRO:HD2  | 2.20                     | 0.40              |
| 1:M:80:LYS:HA    | 1:M:80:LYS:HD3   | 1.98                     | 0.40              |
| 1:A:223:ALA:HB3  | 1:A:251:ALA:CA   | 2.51                     | 0.40              |
| 1:C:203:TYR:N    | 1:C:203:TYR:CD1  | 2.90                     | 0.40              |
| 1:C:311:LYS:O    | 1:C:313:THR:HG23 | 2.21                     | 0.40              |
| 1:D:223:ALA:HB1  | 1:D:227:ILE:HG12 | 2.03                     | 0.40              |
| 1:E:311:LYS:O    | 1:E:313:THR:HG23 | 2.21                     | 0.40              |
| 1:H:356:ALA:HB2  | 1:H:365:LEU:HD12 | 2.04                     | 0.40              |
| 1:J:356:ALA:HB2  | 1:J:365:LEU:HD12 | 2.04                     | 0.40              |
| 1:K:62:LEU:HD23  | 1:K:62:LEU:HA    | 2.02                     | 0.40              |
| 1:L:338:GLU:O    | 1:L:342:ILE:HG13 | 2.22                     | 0.40              |
| 1:L:150:ILE:HD12 | 1:L:494:LEU:H    | 1.85                     | 0.40              |
| 1:C:201:SER:HA   | 1:C:202:PRO:HD3  | 1.84                     | 0.40              |
| 1:C:252:GLU:HA   | 1:C:289:LEU:CD1  | 2.52                     | 0.40              |
| 1:D:225:LYS:HB2  | 1:D:307:MET:O    | 2.22                     | 0.40              |
| 1:E:203:TYR:N    | 1:E:203:TYR:CD1  | 2.90                     | 0.40              |
| 1:E:223:ALA:HB1  | 1:E:227:ILE:HG12 | 2.03                     | 0.40              |
| 1:F:225:LYS:HB2  | 1:F:307:MET:O    | 2.22                     | 0.40              |
| 1:H:169:VAL:HB   | 1:H:173:GLY:CA   | 2.51                     | 0.40              |
| 1:H:338:GLU:O    | 1:H:342:ILE:HG13 | 2.22                     | 0.40              |
| 1:H:405:ALA:HB1  | 1:H:498:LYS:CD   | 2.51                     | 0.40              |
| 1:J:278:ALA:HA   | 1:J:279:PRO:HD3  | 1.86                     | 0.40              |
| 1:J:38:VAL:HG21  | 1:J:56:VAL:HG22  | 2.04                     | 0.40              |
| 1:K:161:LEU:HD21 | 1:K:185:ASP:HB3  | 2.03                     | 0.40              |
| 1:K:213:VAL:CG1  | 1:K:325:ILE:HG12 | 2.51                     | 0.40              |
| 1:K:405:ALA:HB1  | 1:K:498:LYS:CD   | 2.52                     | 0.40              |
| 1:L:493:ILE:HD13 | 4:L:1527:ATP:C6  | 2.57                     | 0.40              |
| 1:M:206:ASN:HB2  | 1:M:213:VAL:HG23 | 2.02                     | 0.40              |
| 1:M:242:LYS:HA   | 1:M:243:ALA:HA   | 1.13                     | 0.40              |
| 1:M:227:ILE:H    | 1:M:254:VAL:HG22 | 1.85                     | 0.40              |
| 1:M:493:ILE:HD13 | 4:M:1527:ATP:C6  | 2.57                     | 0.40              |
| 1:N:493:ILE:HD13 | 4:N:1527:ATP:C6  | 2.57                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 522/548 (95%)   | 498 (95%)  | 21 (4%)  | 3 (1%)   | 27          | 70  |
| 1   | B     | 522/548 (95%)   | 497 (95%)  | 23 (4%)  | 2 (0%)   | 36          | 77  |
| 1   | C     | 522/548 (95%)   | 497 (95%)  | 22 (4%)  | 3 (1%)   | 27          | 70  |
| 1   | D     | 522/548 (95%)   | 497 (95%)  | 22 (4%)  | 3 (1%)   | 27          | 70  |
| 1   | E     | 522/548 (95%)   | 497 (95%)  | 21 (4%)  | 4 (1%)   | 21          | 65  |
| 1   | F     | 522/548 (95%)   | 497 (95%)  | 21 (4%)  | 4 (1%)   | 21          | 65  |
| 1   | G     | 522/548 (95%)   | 495 (95%)  | 24 (5%)  | 3 (1%)   | 27          | 70  |
| 1   | H     | 522/548 (95%)   | 516 (99%)  | 6 (1%)   | 0        | 100         | 100 |
| 1   | I     | 522/548 (95%)   | 516 (99%)  | 6 (1%)   | 0        | 100         | 100 |
| 1   | J     | 522/548 (95%)   | 517 (99%)  | 5 (1%)   | 0        | 100         | 100 |
| 1   | K     | 522/548 (95%)   | 517 (99%)  | 5 (1%)   | 0        | 100         | 100 |
| 1   | L     | 522/548 (95%)   | 513 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | M     | 522/548 (95%)   | 515 (99%)  | 7 (1%)   | 0        | 100         | 100 |
| 1   | N     | 522/548 (95%)   | 515 (99%)  | 5 (1%)   | 2 (0%)   | 36          | 77  |
| All | All   | 7308/7672 (95%) | 7087 (97%) | 197 (3%) | 24 (0%)  | 47          | 81  |

All (24) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 199 | TYR  |
| 1   | N     | 207 | LYS  |
| 1   | N     | 208 | PRO  |
| 1   | A     | 384 | ALA  |
| 1   | B     | 384 | ALA  |
| 1   | C     | 199 | TYR  |
| 1   | C     | 384 | ALA  |
| 1   | D     | 384 | ALA  |
| 1   | E     | 199 | TYR  |
| 1   | E     | 384 | ALA  |
| 1   | F     | 199 | TYR  |
| 1   | F     | 384 | ALA  |
| 1   | G     | 384 | ALA  |
| 1   | A     | 271 | VAL  |
| 1   | B     | 271 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 271 | VAL  |
| 1   | D     | 208 | PRO  |
| 1   | D     | 271 | VAL  |
| 1   | E     | 271 | VAL  |
| 1   | F     | 271 | VAL  |
| 1   | G     | 271 | VAL  |
| 1   | A     | 199 | TYR  |
| 1   | E     | 208 | PRO  |
| 1   | F     | 208 | PRO  |

### 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     | 402/414 (97%)   | 367 (91%)  | 35 (9%)   | 11          | 37 |
| 1   | B     | 402/414 (97%)   | 366 (91%)  | 36 (9%)   | 10          | 36 |
| 1   | C     | 402/414 (97%)   | 367 (91%)  | 35 (9%)   | 11          | 37 |
| 1   | D     | 402/414 (97%)   | 369 (92%)  | 33 (8%)   | 12          | 41 |
| 1   | E     | 402/414 (97%)   | 368 (92%)  | 34 (8%)   | 12          | 40 |
| 1   | F     | 402/414 (97%)   | 367 (91%)  | 35 (9%)   | 11          | 37 |
| 1   | G     | 402/414 (97%)   | 367 (91%)  | 35 (9%)   | 11          | 37 |
| 1   | H     | 402/414 (97%)   | 359 (89%)  | 43 (11%)  | 7           | 28 |
| 1   | I     | 402/414 (97%)   | 361 (90%)  | 41 (10%)  | 8           | 30 |
| 1   | J     | 402/414 (97%)   | 361 (90%)  | 41 (10%)  | 8           | 30 |
| 1   | K     | 402/414 (97%)   | 358 (89%)  | 44 (11%)  | 7           | 28 |
| 1   | L     | 402/414 (97%)   | 364 (90%)  | 38 (10%)  | 9           | 33 |
| 1   | M     | 402/414 (97%)   | 358 (89%)  | 44 (11%)  | 7           | 28 |
| 1   | N     | 402/414 (97%)   | 360 (90%)  | 42 (10%)  | 8           | 30 |
| All | All   | 5628/5796 (97%) | 5092 (90%) | 536 (10%) | 13          | 33 |

All (536) residues with a non-rotameric sidechain are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | ASN  |
| 1   | A     | 18  | ARG  |
| 1   | A     | 25  | ASP  |
| 1   | A     | 34  | LYS  |
| 1   | A     | 36  | ARG  |
| 1   | A     | 37  | ASN  |
| 1   | A     | 171 | LYS  |
| 1   | A     | 172 | GLU  |
| 1   | A     | 177 | VAL  |
| 1   | A     | 183 | LEU  |
| 1   | A     | 190 | VAL  |
| 1   | A     | 196 | ASP  |
| 1   | A     | 197 | ARG  |
| 1   | A     | 199 | TYR  |
| 1   | A     | 207 | LYS  |
| 1   | A     | 213 | VAL  |
| 1   | A     | 226 | LYS  |
| 1   | A     | 242 | LYS  |
| 1   | A     | 252 | GLU  |
| 1   | A     | 272 | LYS  |
| 1   | A     | 295 | LEU  |
| 1   | A     | 300 | VAL  |
| 1   | A     | 309 | LEU  |
| 1   | A     | 311 | LYS  |
| 1   | A     | 316 | ASP  |
| 1   | A     | 325 | ILE  |
| 1   | A     | 326 | ASN  |
| 1   | A     | 327 | LYS  |
| 1   | A     | 334 | ASP  |
| 1   | A     | 404 | ARG  |
| 1   | A     | 428 | ASP  |
| 1   | A     | 435 | ASP  |
| 1   | A     | 453 | GLN  |
| 1   | A     | 484 | GLU  |
| 1   | A     | 522 | THR  |
| 1   | B     | 10  | ASN  |
| 1   | B     | 18  | ARG  |
| 1   | B     | 25  | ASP  |
| 1   | B     | 34  | LYS  |
| 1   | B     | 36  | ARG  |
| 1   | B     | 37  | ASN  |
| 1   | B     | 171 | LYS  |
| 1   | B     | 172 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 177 | VAL  |
| 1   | B     | 183 | LEU  |
| 1   | B     | 190 | VAL  |
| 1   | B     | 195 | PHE  |
| 1   | B     | 197 | ARG  |
| 1   | B     | 199 | TYR  |
| 1   | B     | 207 | LYS  |
| 1   | B     | 210 | THR  |
| 1   | B     | 213 | VAL  |
| 1   | B     | 226 | LYS  |
| 1   | B     | 242 | LYS  |
| 1   | B     | 252 | GLU  |
| 1   | B     | 272 | LYS  |
| 1   | B     | 295 | LEU  |
| 1   | B     | 300 | VAL  |
| 1   | B     | 309 | LEU  |
| 1   | B     | 311 | LYS  |
| 1   | B     | 316 | ASP  |
| 1   | B     | 325 | ILE  |
| 1   | B     | 326 | ASN  |
| 1   | B     | 327 | LYS  |
| 1   | B     | 334 | ASP  |
| 1   | B     | 404 | ARG  |
| 1   | B     | 428 | ASP  |
| 1   | B     | 435 | ASP  |
| 1   | B     | 453 | GLN  |
| 1   | B     | 484 | GLU  |
| 1   | B     | 522 | THR  |
| 1   | C     | 10  | ASN  |
| 1   | C     | 18  | ARG  |
| 1   | C     | 25  | ASP  |
| 1   | C     | 34  | LYS  |
| 1   | C     | 36  | ARG  |
| 1   | C     | 37  | ASN  |
| 1   | C     | 171 | LYS  |
| 1   | C     | 172 | GLU  |
| 1   | C     | 177 | VAL  |
| 1   | C     | 183 | LEU  |
| 1   | C     | 190 | VAL  |
| 1   | C     | 193 | MET  |
| 1   | C     | 197 | ARG  |
| 1   | C     | 199 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 207 | LYS  |
| 1   | C     | 213 | VAL  |
| 1   | C     | 226 | LYS  |
| 1   | C     | 242 | LYS  |
| 1   | C     | 252 | GLU  |
| 1   | C     | 272 | LYS  |
| 1   | C     | 295 | LEU  |
| 1   | C     | 300 | VAL  |
| 1   | C     | 309 | LEU  |
| 1   | C     | 311 | LYS  |
| 1   | C     | 316 | ASP  |
| 1   | C     | 325 | ILE  |
| 1   | C     | 326 | ASN  |
| 1   | C     | 327 | LYS  |
| 1   | C     | 334 | ASP  |
| 1   | C     | 404 | ARG  |
| 1   | C     | 428 | ASP  |
| 1   | C     | 435 | ASP  |
| 1   | C     | 453 | GLN  |
| 1   | C     | 484 | GLU  |
| 1   | C     | 522 | THR  |
| 1   | D     | 10  | ASN  |
| 1   | D     | 18  | ARG  |
| 1   | D     | 25  | ASP  |
| 1   | D     | 34  | LYS  |
| 1   | D     | 36  | ARG  |
| 1   | D     | 37  | ASN  |
| 1   | D     | 153 | ASN  |
| 1   | D     | 171 | LYS  |
| 1   | D     | 172 | GLU  |
| 1   | D     | 177 | VAL  |
| 1   | D     | 183 | LEU  |
| 1   | D     | 190 | VAL  |
| 1   | D     | 197 | ARG  |
| 1   | D     | 213 | VAL  |
| 1   | D     | 226 | LYS  |
| 1   | D     | 242 | LYS  |
| 1   | D     | 252 | GLU  |
| 1   | D     | 272 | LYS  |
| 1   | D     | 295 | LEU  |
| 1   | D     | 300 | VAL  |
| 1   | D     | 309 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 311 | LYS  |
| 1   | D     | 316 | ASP  |
| 1   | D     | 325 | ILE  |
| 1   | D     | 326 | ASN  |
| 1   | D     | 327 | LYS  |
| 1   | D     | 334 | ASP  |
| 1   | D     | 404 | ARG  |
| 1   | D     | 428 | ASP  |
| 1   | D     | 435 | ASP  |
| 1   | D     | 453 | GLN  |
| 1   | D     | 484 | GLU  |
| 1   | D     | 522 | THR  |
| 1   | E     | 10  | ASN  |
| 1   | E     | 18  | ARG  |
| 1   | E     | 25  | ASP  |
| 1   | E     | 34  | LYS  |
| 1   | E     | 36  | ARG  |
| 1   | E     | 37  | ASN  |
| 1   | E     | 171 | LYS  |
| 1   | E     | 172 | GLU  |
| 1   | E     | 177 | VAL  |
| 1   | E     | 183 | LEU  |
| 1   | E     | 190 | VAL  |
| 1   | E     | 197 | ARG  |
| 1   | E     | 199 | TYR  |
| 1   | E     | 207 | LYS  |
| 1   | E     | 213 | VAL  |
| 1   | E     | 226 | LYS  |
| 1   | E     | 242 | LYS  |
| 1   | E     | 252 | GLU  |
| 1   | E     | 272 | LYS  |
| 1   | E     | 295 | LEU  |
| 1   | E     | 300 | VAL  |
| 1   | E     | 309 | LEU  |
| 1   | E     | 311 | LYS  |
| 1   | E     | 316 | ASP  |
| 1   | E     | 325 | ILE  |
| 1   | E     | 326 | ASN  |
| 1   | E     | 327 | LYS  |
| 1   | E     | 334 | ASP  |
| 1   | E     | 404 | ARG  |
| 1   | E     | 428 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 435 | ASP  |
| 1   | E     | 453 | GLN  |
| 1   | E     | 484 | GLU  |
| 1   | E     | 522 | THR  |
| 1   | F     | 10  | ASN  |
| 1   | F     | 18  | ARG  |
| 1   | F     | 25  | ASP  |
| 1   | F     | 34  | LYS  |
| 1   | F     | 36  | ARG  |
| 1   | F     | 37  | ASN  |
| 1   | F     | 153 | ASN  |
| 1   | F     | 171 | LYS  |
| 1   | F     | 172 | GLU  |
| 1   | F     | 177 | VAL  |
| 1   | F     | 183 | LEU  |
| 1   | F     | 190 | VAL  |
| 1   | F     | 197 | ARG  |
| 1   | F     | 199 | TYR  |
| 1   | F     | 207 | LYS  |
| 1   | F     | 213 | VAL  |
| 1   | F     | 226 | LYS  |
| 1   | F     | 242 | LYS  |
| 1   | F     | 252 | GLU  |
| 1   | F     | 272 | LYS  |
| 1   | F     | 295 | LEU  |
| 1   | F     | 300 | VAL  |
| 1   | F     | 309 | LEU  |
| 1   | F     | 311 | LYS  |
| 1   | F     | 316 | ASP  |
| 1   | F     | 325 | ILE  |
| 1   | F     | 326 | ASN  |
| 1   | F     | 327 | LYS  |
| 1   | F     | 334 | ASP  |
| 1   | F     | 404 | ARG  |
| 1   | F     | 428 | ASP  |
| 1   | F     | 435 | ASP  |
| 1   | F     | 453 | GLN  |
| 1   | F     | 484 | GLU  |
| 1   | F     | 522 | THR  |
| 1   | G     | 10  | ASN  |
| 1   | G     | 18  | ARG  |
| 1   | G     | 25  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 34  | LYS  |
| 1   | G     | 36  | ARG  |
| 1   | G     | 37  | ASN  |
| 1   | G     | 171 | LYS  |
| 1   | G     | 172 | GLU  |
| 1   | G     | 177 | VAL  |
| 1   | G     | 183 | LEU  |
| 1   | G     | 190 | VAL  |
| 1   | G     | 197 | ARG  |
| 1   | G     | 199 | TYR  |
| 1   | G     | 201 | SER  |
| 1   | G     | 207 | LYS  |
| 1   | G     | 213 | VAL  |
| 1   | G     | 226 | LYS  |
| 1   | G     | 242 | LYS  |
| 1   | G     | 252 | GLU  |
| 1   | G     | 272 | LYS  |
| 1   | G     | 295 | LEU  |
| 1   | G     | 300 | VAL  |
| 1   | G     | 309 | LEU  |
| 1   | G     | 311 | LYS  |
| 1   | G     | 316 | ASP  |
| 1   | G     | 325 | ILE  |
| 1   | G     | 326 | ASN  |
| 1   | G     | 327 | LYS  |
| 1   | G     | 334 | ASP  |
| 1   | G     | 404 | ARG  |
| 1   | G     | 428 | ASP  |
| 1   | G     | 435 | ASP  |
| 1   | G     | 453 | GLN  |
| 1   | G     | 484 | GLU  |
| 1   | G     | 522 | THR  |
| 1   | H     | 18  | ARG  |
| 1   | H     | 31  | LEU  |
| 1   | H     | 36  | ARG  |
| 1   | H     | 37  | ASN  |
| 1   | H     | 48  | THR  |
| 1   | H     | 54  | VAL  |
| 1   | H     | 63  | GLU  |
| 1   | H     | 155 | ASP  |
| 1   | H     | 166 | MET  |
| 1   | H     | 183 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 188 | ASP  |
| 1   | H     | 191 | GLU  |
| 1   | H     | 193 | MET  |
| 1   | H     | 195 | PHE  |
| 1   | H     | 197 | ARG  |
| 1   | H     | 207 | LYS  |
| 1   | H     | 213 | VAL  |
| 1   | H     | 225 | LYS  |
| 1   | H     | 226 | LYS  |
| 1   | H     | 229 | ASN  |
| 1   | H     | 231 | ARG  |
| 1   | H     | 236 | VAL  |
| 1   | H     | 238 | GLU  |
| 1   | H     | 253 | ASP  |
| 1   | H     | 257 | GLU  |
| 1   | H     | 272 | LYS  |
| 1   | H     | 289 | LEU  |
| 1   | H     | 290 | GLN  |
| 1   | H     | 321 | LYS  |
| 1   | H     | 325 | ILE  |
| 1   | H     | 343 | GLN  |
| 1   | H     | 358 | SER  |
| 1   | H     | 389 | MET  |
| 1   | H     | 391 | GLU  |
| 1   | H     | 404 | ARG  |
| 1   | H     | 408 | GLU  |
| 1   | H     | 430 | ARG  |
| 1   | H     | 435 | ASP  |
| 1   | H     | 453 | GLN  |
| 1   | H     | 460 | GLU  |
| 1   | H     | 484 | GLU  |
| 1   | H     | 518 | GLU  |
| 1   | H     | 523 | ASP  |
| 1   | I     | 18  | ARG  |
| 1   | I     | 31  | LEU  |
| 1   | I     | 36  | ARG  |
| 1   | I     | 37  | ASN  |
| 1   | I     | 48  | THR  |
| 1   | I     | 54  | VAL  |
| 1   | I     | 63  | GLU  |
| 1   | I     | 155 | ASP  |
| 1   | I     | 166 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 188 | ASP  |
| 1   | I     | 191 | GLU  |
| 1   | I     | 193 | MET  |
| 1   | I     | 195 | PHE  |
| 1   | I     | 196 | ASP  |
| 1   | I     | 197 | ARG  |
| 1   | I     | 199 | TYR  |
| 1   | I     | 207 | LYS  |
| 1   | I     | 213 | VAL  |
| 1   | I     | 225 | LYS  |
| 1   | I     | 226 | LYS  |
| 1   | I     | 236 | VAL  |
| 1   | I     | 238 | GLU  |
| 1   | I     | 253 | ASP  |
| 1   | I     | 257 | GLU  |
| 1   | I     | 272 | LYS  |
| 1   | I     | 289 | LEU  |
| 1   | I     | 321 | LYS  |
| 1   | I     | 325 | ILE  |
| 1   | I     | 343 | GLN  |
| 1   | I     | 358 | SER  |
| 1   | I     | 389 | MET  |
| 1   | I     | 391 | GLU  |
| 1   | I     | 404 | ARG  |
| 1   | I     | 408 | GLU  |
| 1   | I     | 430 | ARG  |
| 1   | I     | 435 | ASP  |
| 1   | I     | 453 | GLN  |
| 1   | I     | 460 | GLU  |
| 1   | I     | 484 | GLU  |
| 1   | I     | 518 | GLU  |
| 1   | I     | 523 | ASP  |
| 1   | J     | 18  | ARG  |
| 1   | J     | 31  | LEU  |
| 1   | J     | 36  | ARG  |
| 1   | J     | 37  | ASN  |
| 1   | J     | 48  | THR  |
| 1   | J     | 54  | VAL  |
| 1   | J     | 63  | GLU  |
| 1   | J     | 155 | ASP  |
| 1   | J     | 166 | MET  |
| 1   | J     | 188 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 191 | GLU  |
| 1   | J     | 193 | MET  |
| 1   | J     | 195 | PHE  |
| 1   | J     | 197 | ARG  |
| 1   | J     | 199 | TYR  |
| 1   | J     | 207 | LYS  |
| 1   | J     | 213 | VAL  |
| 1   | J     | 225 | LYS  |
| 1   | J     | 226 | LYS  |
| 1   | J     | 229 | ASN  |
| 1   | J     | 236 | VAL  |
| 1   | J     | 238 | GLU  |
| 1   | J     | 253 | ASP  |
| 1   | J     | 257 | GLU  |
| 1   | J     | 272 | LYS  |
| 1   | J     | 289 | LEU  |
| 1   | J     | 321 | LYS  |
| 1   | J     | 325 | ILE  |
| 1   | J     | 343 | GLN  |
| 1   | J     | 358 | SER  |
| 1   | J     | 389 | MET  |
| 1   | J     | 391 | GLU  |
| 1   | J     | 404 | ARG  |
| 1   | J     | 408 | GLU  |
| 1   | J     | 430 | ARG  |
| 1   | J     | 435 | ASP  |
| 1   | J     | 453 | GLN  |
| 1   | J     | 460 | GLU  |
| 1   | J     | 484 | GLU  |
| 1   | J     | 518 | GLU  |
| 1   | J     | 523 | ASP  |
| 1   | K     | 18  | ARG  |
| 1   | K     | 31  | LEU  |
| 1   | K     | 36  | ARG  |
| 1   | K     | 37  | ASN  |
| 1   | K     | 48  | THR  |
| 1   | K     | 54  | VAL  |
| 1   | K     | 63  | GLU  |
| 1   | K     | 155 | ASP  |
| 1   | K     | 166 | MET  |
| 1   | K     | 185 | ASP  |
| 1   | K     | 188 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 191 | GLU  |
| 1   | K     | 193 | MET  |
| 1   | K     | 195 | PHE  |
| 1   | K     | 197 | ARG  |
| 1   | K     | 199 | TYR  |
| 1   | K     | 207 | LYS  |
| 1   | K     | 213 | VAL  |
| 1   | K     | 225 | LYS  |
| 1   | K     | 226 | LYS  |
| 1   | K     | 229 | ASN  |
| 1   | K     | 231 | ARG  |
| 1   | K     | 236 | VAL  |
| 1   | K     | 238 | GLU  |
| 1   | K     | 253 | ASP  |
| 1   | K     | 257 | GLU  |
| 1   | K     | 272 | LYS  |
| 1   | K     | 289 | LEU  |
| 1   | K     | 290 | GLN  |
| 1   | K     | 321 | LYS  |
| 1   | K     | 325 | ILE  |
| 1   | K     | 343 | GLN  |
| 1   | K     | 358 | SER  |
| 1   | K     | 389 | MET  |
| 1   | K     | 391 | GLU  |
| 1   | K     | 404 | ARG  |
| 1   | K     | 408 | GLU  |
| 1   | K     | 430 | ARG  |
| 1   | K     | 435 | ASP  |
| 1   | K     | 453 | GLN  |
| 1   | K     | 460 | GLU  |
| 1   | K     | 484 | GLU  |
| 1   | K     | 518 | GLU  |
| 1   | K     | 523 | ASP  |
| 1   | L     | 18  | ARG  |
| 1   | L     | 31  | LEU  |
| 1   | L     | 36  | ARG  |
| 1   | L     | 37  | ASN  |
| 1   | L     | 48  | THR  |
| 1   | L     | 54  | VAL  |
| 1   | L     | 63  | GLU  |
| 1   | L     | 155 | ASP  |
| 1   | L     | 166 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 174 | VAL  |
| 1   | L     | 188 | ASP  |
| 1   | L     | 193 | MET  |
| 1   | L     | 195 | PHE  |
| 1   | L     | 197 | ARG  |
| 1   | L     | 199 | TYR  |
| 1   | L     | 207 | LYS  |
| 1   | L     | 213 | VAL  |
| 1   | L     | 225 | LYS  |
| 1   | L     | 226 | LYS  |
| 1   | L     | 236 | VAL  |
| 1   | L     | 253 | ASP  |
| 1   | L     | 272 | LYS  |
| 1   | L     | 289 | LEU  |
| 1   | L     | 321 | LYS  |
| 1   | L     | 325 | ILE  |
| 1   | L     | 343 | GLN  |
| 1   | L     | 358 | SER  |
| 1   | L     | 389 | MET  |
| 1   | L     | 391 | GLU  |
| 1   | L     | 404 | ARG  |
| 1   | L     | 408 | GLU  |
| 1   | L     | 430 | ARG  |
| 1   | L     | 435 | ASP  |
| 1   | L     | 453 | GLN  |
| 1   | L     | 460 | GLU  |
| 1   | L     | 484 | GLU  |
| 1   | L     | 518 | GLU  |
| 1   | L     | 523 | ASP  |
| 1   | M     | 18  | ARG  |
| 1   | M     | 31  | LEU  |
| 1   | M     | 36  | ARG  |
| 1   | M     | 37  | ASN  |
| 1   | M     | 48  | THR  |
| 1   | M     | 54  | VAL  |
| 1   | M     | 63  | GLU  |
| 1   | M     | 155 | ASP  |
| 1   | M     | 166 | MET  |
| 1   | M     | 172 | GLU  |
| 1   | M     | 188 | ASP  |
| 1   | M     | 191 | GLU  |
| 1   | M     | 193 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 195 | PHE  |
| 1   | M     | 197 | ARG  |
| 1   | M     | 199 | TYR  |
| 1   | M     | 207 | LYS  |
| 1   | M     | 213 | VAL  |
| 1   | M     | 225 | LYS  |
| 1   | M     | 226 | LYS  |
| 1   | M     | 228 | SER  |
| 1   | M     | 229 | ASN  |
| 1   | M     | 231 | ARG  |
| 1   | M     | 232 | GLU  |
| 1   | M     | 236 | VAL  |
| 1   | M     | 253 | ASP  |
| 1   | M     | 257 | GLU  |
| 1   | M     | 272 | LYS  |
| 1   | M     | 289 | LEU  |
| 1   | M     | 321 | LYS  |
| 1   | M     | 325 | ILE  |
| 1   | M     | 343 | GLN  |
| 1   | M     | 358 | SER  |
| 1   | M     | 389 | MET  |
| 1   | M     | 391 | GLU  |
| 1   | M     | 404 | ARG  |
| 1   | M     | 408 | GLU  |
| 1   | M     | 430 | ARG  |
| 1   | M     | 435 | ASP  |
| 1   | M     | 453 | GLN  |
| 1   | M     | 460 | GLU  |
| 1   | M     | 484 | GLU  |
| 1   | M     | 518 | GLU  |
| 1   | M     | 523 | ASP  |
| 1   | N     | 18  | ARG  |
| 1   | N     | 31  | LEU  |
| 1   | N     | 36  | ARG  |
| 1   | N     | 37  | ASN  |
| 1   | N     | 48  | THR  |
| 1   | N     | 54  | VAL  |
| 1   | N     | 63  | GLU  |
| 1   | N     | 155 | ASP  |
| 1   | N     | 166 | MET  |
| 1   | N     | 171 | LYS  |
| 1   | N     | 188 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 191 | GLU  |
| 1   | N     | 193 | MET  |
| 1   | N     | 195 | PHE  |
| 1   | N     | 197 | ARG  |
| 1   | N     | 199 | TYR  |
| 1   | N     | 207 | LYS  |
| 1   | N     | 213 | VAL  |
| 1   | N     | 225 | LYS  |
| 1   | N     | 226 | LYS  |
| 1   | N     | 231 | ARG  |
| 1   | N     | 236 | VAL  |
| 1   | N     | 238 | GLU  |
| 1   | N     | 253 | ASP  |
| 1   | N     | 257 | GLU  |
| 1   | N     | 272 | LYS  |
| 1   | N     | 289 | LEU  |
| 1   | N     | 321 | LYS  |
| 1   | N     | 325 | ILE  |
| 1   | N     | 343 | GLN  |
| 1   | N     | 358 | SER  |
| 1   | N     | 389 | MET  |
| 1   | N     | 391 | GLU  |
| 1   | N     | 404 | ARG  |
| 1   | N     | 408 | GLU  |
| 1   | N     | 430 | ARG  |
| 1   | N     | 435 | ASP  |
| 1   | N     | 453 | GLN  |
| 1   | N     | 460 | GLU  |
| 1   | N     | 484 | GLU  |
| 1   | N     | 518 | GLU  |
| 1   | N     | 523 | ASP  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 475 | ASN  |
| 1   | B     | 351 | GLN  |
| 1   | B     | 475 | ASN  |
| 1   | C     | 351 | GLN  |
| 1   | C     | 475 | ASN  |
| 1   | D     | 351 | GLN  |
| 1   | D     | 475 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 475 | ASN  |
| 1   | F     | 475 | ASN  |
| 1   | G     | 351 | GLN  |
| 1   | G     | 475 | ASN  |
| 1   | H     | 401 | HIS  |
| 1   | I     | 401 | HIS  |
| 1   | J     | 401 | HIS  |
| 1   | K     | 401 | HIS  |
| 1   | L     | 401 | HIS  |
| 1   | M     | 401 | HIS  |
| 1   | N     | 401 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 14 are monoatomic and 14 are modelled with single atom - leaving 14 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | ATP  | A     | 1527 | 3    | 27,33,33     | 0.72 | 0           | 27,52,52    | 1.77 | 3 (11%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | ATP  | B     | 1527 | 3    | 27,33,33     | 0.66 | 0        | 27,52,52    | 1.65 | 3 (11%)  |
| 4   | ATP  | C     | 1527 | 3    | 27,33,33     | 0.72 | 0        | 27,52,52    | 1.77 | 3 (11%)  |
| 4   | ATP  | D     | 1527 | 3    | 27,33,33     | 0.67 | 0        | 27,52,52    | 1.61 | 3 (11%)  |
| 4   | ATP  | E     | 1527 | 3    | 27,33,33     | 0.72 | 0        | 27,52,52    | 1.77 | 3 (11%)  |
| 4   | ATP  | F     | 1527 | 3    | 27,33,33     | 0.67 | 0        | 27,52,52    | 1.61 | 3 (11%)  |
| 4   | ATP  | G     | 1527 | 3    | 27,33,33     | 0.72 | 0        | 27,52,52    | 1.77 | 3 (11%)  |
| 4   | ATP  | H     | 1527 | 3    | 27,33,33     | 0.76 | 0        | 27,52,52    | 1.70 | 3 (11%)  |
| 4   | ATP  | I     | 1527 | 3    | 27,33,33     | 0.77 | 0        | 27,52,52    | 1.70 | 4 (14%)  |
| 4   | ATP  | J     | 1527 | 3    | 27,33,33     | 0.77 | 0        | 27,52,52    | 1.70 | 3 (11%)  |
| 4   | ATP  | K     | 1527 | 3    | 27,33,33     | 0.76 | 0        | 27,52,52    | 1.70 | 3 (11%)  |
| 4   | ATP  | L     | 1527 | 3    | 27,33,33     | 0.76 | 0        | 27,52,52    | 1.70 | 3 (11%)  |
| 4   | ATP  | M     | 1527 | 3    | 27,33,33     | 0.77 | 0        | 27,52,52    | 1.70 | 4 (14%)  |
| 4   | ATP  | N     | 1527 | 3    | 27,33,33     | 0.76 | 0        | 27,52,52    | 1.69 | 3 (11%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 4   | ATP  | A     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | B     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | C     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | D     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | E     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | F     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | G     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | H     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | I     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | J     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | K     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | L     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | M     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | N     | 1527 | 3    | -       | 0/18/38/38 | 0/3/3/3 |

There are no bond length outliers.

All (44) bond angle outliers are listed below:



| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | E     | 1527 | ATP  | PB-O3B-PG   | -5.86 | 112.94      | 132.63   |
| 4   | C     | 1527 | ATP  | PB-O3B-PG   | -5.85 | 112.95      | 132.63   |
| 4   | A     | 1527 | ATP  | PB-O3B-PG   | -5.85 | 112.96      | 132.63   |
| 4   | G     | 1527 | ATP  | PB-O3B-PG   | -5.85 | 112.96      | 132.63   |
| 4   | M     | 1527 | ATP  | PA-O3A-PB   | -5.47 | 114.23      | 132.63   |
| 4   | H     | 1527 | ATP  | PA-O3A-PB   | -5.47 | 114.25      | 132.63   |
| 4   | I     | 1527 | ATP  | PA-O3A-PB   | -5.47 | 114.25      | 132.63   |
| 4   | K     | 1527 | ATP  | PA-O3A-PB   | -5.47 | 114.26      | 132.63   |
| 4   | J     | 1527 | ATP  | PA-O3A-PB   | -5.46 | 114.28      | 132.63   |
| 4   | L     | 1527 | ATP  | PA-O3A-PB   | -5.46 | 114.29      | 132.63   |
| 4   | N     | 1527 | ATP  | PA-O3A-PB   | -5.45 | 114.30      | 132.63   |
| 4   | B     | 1527 | ATP  | PB-O3B-PG   | -5.22 | 115.09      | 132.63   |
| 4   | F     | 1527 | ATP  | PB-O3B-PG   | -5.11 | 115.47      | 132.63   |
| 4   | D     | 1527 | ATP  | PB-O3B-PG   | -5.10 | 115.48      | 132.63   |
| 4   | A     | 1527 | ATP  | PA-O3A-PB   | -5.01 | 115.80      | 132.63   |
| 4   | E     | 1527 | ATP  | PA-O3A-PB   | -5.01 | 115.80      | 132.63   |
| 4   | G     | 1527 | ATP  | PA-O3A-PB   | -5.00 | 115.81      | 132.63   |
| 4   | C     | 1527 | ATP  | PA-O3A-PB   | -5.00 | 115.83      | 132.63   |
| 4   | B     | 1527 | ATP  | PA-O3A-PB   | -4.99 | 115.85      | 132.63   |
| 4   | D     | 1527 | ATP  | PA-O3A-PB   | -4.69 | 116.87      | 132.63   |
| 4   | F     | 1527 | ATP  | PA-O3A-PB   | -4.67 | 116.92      | 132.63   |
| 4   | H     | 1527 | ATP  | PB-O3B-PG   | -4.31 | 118.13      | 132.63   |
| 4   | L     | 1527 | ATP  | PB-O3B-PG   | -4.31 | 118.14      | 132.63   |
| 4   | K     | 1527 | ATP  | PB-O3B-PG   | -4.31 | 118.15      | 132.63   |
| 4   | N     | 1527 | ATP  | PB-O3B-PG   | -4.31 | 118.16      | 132.63   |
| 4   | M     | 1527 | ATP  | PB-O3B-PG   | -4.30 | 118.16      | 132.63   |
| 4   | J     | 1527 | ATP  | PB-O3B-PG   | -4.30 | 118.17      | 132.63   |
| 4   | I     | 1527 | ATP  | PB-O3B-PG   | -4.30 | 118.17      | 132.63   |
| 4   | I     | 1527 | ATP  | C4-C5-N7    | 2.00  | 111.35      | 109.41   |
| 4   | M     | 1527 | ATP  | C4-C5-N7    | 2.01  | 111.35      | 109.41   |
| 4   | E     | 1527 | ATP  | C4-C5-N7    | 2.07  | 111.41      | 109.41   |
| 4   | A     | 1527 | ATP  | C4-C5-N7    | 2.07  | 111.41      | 109.41   |
| 4   | C     | 1527 | ATP  | C4-C5-N7    | 2.08  | 111.42      | 109.41   |
| 4   | G     | 1527 | ATP  | C4-C5-N7    | 2.09  | 111.43      | 109.41   |
| 4   | J     | 1527 | ATP  | O3G-PG-O2G  | 2.10  | 115.89      | 107.59   |
| 4   | K     | 1527 | ATP  | O3G-PG-O2G  | 2.10  | 115.90      | 107.59   |
| 4   | M     | 1527 | ATP  | O3G-PG-O2G  | 2.10  | 115.91      | 107.59   |
| 4   | N     | 1527 | ATP  | O3G-PG-O2G  | 2.10  | 115.91      | 107.59   |
| 4   | I     | 1527 | ATP  | O3G-PG-O2G  | 2.11  | 115.92      | 107.59   |
| 4   | L     | 1527 | ATP  | O3G-PG-O2G  | 2.11  | 115.93      | 107.59   |
| 4   | H     | 1527 | ATP  | O3G-PG-O2G  | 2.11  | 115.93      | 107.59   |
| 4   | B     | 1527 | ATP  | O5'-C5'-C4' | 2.13  | 116.39      | 109.00   |
| 4   | D     | 1527 | ATP  | O5'-C5'-C4' | 2.14  | 116.45      | 109.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 4   | F     | 1527 | ATP  | O5'-C5'-C4' | 2.15 | 116.48      | 109.00   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 48 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | A     | 1527 | ATP  | 2       | 0            |
| 4   | B     | 1527 | ATP  | 2       | 0            |
| 4   | C     | 1527 | ATP  | 3       | 0            |
| 4   | D     | 1527 | ATP  | 2       | 0            |
| 4   | E     | 1527 | ATP  | 3       | 0            |
| 4   | F     | 1527 | ATP  | 2       | 0            |
| 4   | G     | 1527 | ATP  | 2       | 0            |
| 4   | H     | 1527 | ATP  | 4       | 0            |
| 4   | I     | 1527 | ATP  | 4       | 0            |
| 4   | J     | 1527 | ATP  | 5       | 0            |
| 4   | K     | 1527 | ATP  | 4       | 0            |
| 4   | L     | 1527 | ATP  | 5       | 0            |
| 4   | M     | 1527 | ATP  | 5       | 0            |
| 4   | N     | 1527 | ATP  | 5       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | G     | 5                |
| 1   | D     | 5                |
| 1   | E     | 5                |
| 1   | B     | 5                |
| 1   | C     | 5                |
| 1   | F     | 5                |
| 1   | A     | 4                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 52:ASP    | C      | 53:GLY    | N      | 1.20         |
| 1     | B     | 52:ASP    | C      | 53:GLY    | N      | 1.20         |
| 1     | C     | 52:ASP    | C      | 53:GLY    | N      | 1.20         |
| 1     | D     | 52:ASP    | C      | 53:GLY    | N      | 1.20         |
| 1     | E     | 52:ASP    | C      | 53:GLY    | N      | 1.20         |
| 1     | F     | 52:ASP    | C      | 53:GLY    | N      | 1.20         |
| 1     | G     | 52:ASP    | C      | 53:GLY    | N      | 1.20         |
| 1     | A     | 518:GLU   | C      | 519:CYS   | N      | 1.19         |
| 1     | B     | 518:GLU   | C      | 519:CYS   | N      | 1.19         |
| 1     | C     | 518:GLU   | C      | 519:CYS   | N      | 1.19         |
| 1     | D     | 513:LEU   | C      | 514:MET   | N      | 1.19         |
| 1     | D     | 518:GLU   | C      | 519:CYS   | N      | 1.19         |
| 1     | E     | 518:GLU   | C      | 519:CYS   | N      | 1.19         |
| 1     | F     | 518:GLU   | C      | 519:CYS   | N      | 1.19         |
| 1     | G     | 518:GLU   | C      | 519:CYS   | N      | 1.19         |
| 1     | A     | 513:LEU   | C      | 514:MET   | N      | 1.18         |
| 1     | B     | 513:LEU   | C      | 514:MET   | N      | 1.18         |
| 1     | C     | 513:LEU   | C      | 514:MET   | N      | 1.18         |
| 1     | E     | 513:LEU   | C      | 514:MET   | N      | 1.18         |
| 1     | F     | 513:LEU   | C      | 514:MET   | N      | 1.18         |
| 1     | G     | 513:LEU   | C      | 514:MET   | N      | 1.18         |
| 1     | B     | 213:VAL   | C      | 214:GLU   | N      | 1.08         |
| 1     | C     | 213:VAL   | C      | 214:GLU   | N      | 1.08         |
| 1     | D     | 213:VAL   | C      | 214:GLU   | N      | 1.08         |
| 1     | E     | 213:VAL   | C      | 214:GLU   | N      | 1.08         |
| 1     | F     | 213:VAL   | C      | 214:GLU   | N      | 1.08         |
| 1     | G     | 213:VAL   | C      | 214:GLU   | N      | 1.08         |
| 1     | A     | 7:LYS     | C      | 8:PHE     | N      | 1.07         |
| 1     | B     | 7:LYS     | C      | 8:PHE     | N      | 1.07         |
| 1     | C     | 7:LYS     | C      | 8:PHE     | N      | 1.07         |
| 1     | D     | 7:LYS     | C      | 8:PHE     | N      | 1.07         |
| 1     | E     | 7:LYS     | C      | 8:PHE     | N      | 1.07         |
| 1     | F     | 7:LYS     | C      | 8:PHE     | N      | 1.07         |
| 1     | G     | 7:LYS     | C      | 8:PHE     | N      | 1.07         |