



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:08 AM UTC

PDB ID : 1Q57 / pdb\_00001q57  
Title : The Crystal Structure of the Bifunctional Primase-Helicase of Bacteriophage T7  
Authors : Toth, E.A.; Li, Y.; Sawaya, M.R.; Cheng, Y.; Ellenberger, T.  
Deposited on : 2003-08-06  
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

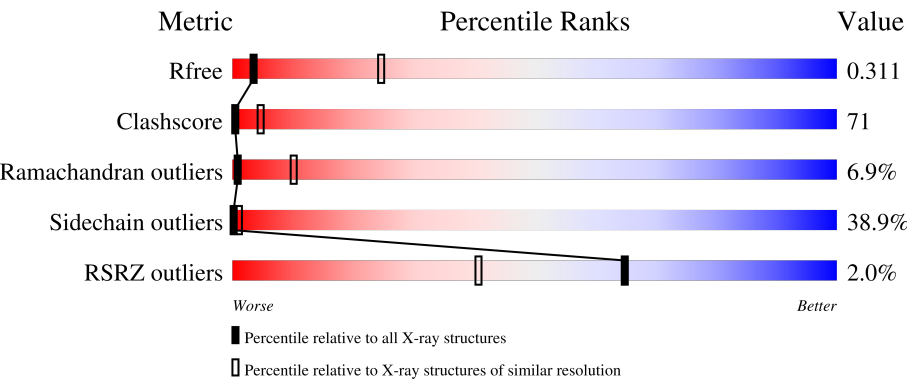
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1070 (3.50-3.42)                                      |
| Clashscore            | 190562                      | 1128 (3.50-3.42)                                      |
| Ramachandran outliers | 187476                      | 1101 (3.50-3.42)                                      |
| Sidechain outliers    | 187428                      | 1102 (3.50-3.42)                                      |
| RSRZ outliers         | 180081                      | 1070 (3.50-3.42)                                      |

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

| Mol | Chain | Length | Quality of chain                             |
|-----|-------|--------|----------------------------------------------|
| 1   | A     | 503    | <div><div>22%44%25%5%</div><div></div></div> |
| 1   | B     | 503    | <div><div>22%46%23%</div><div></div></div>   |
| 1   | C     | 503    | <div><div>22%46%24%</div><div></div></div>   |
| 1   | D     | 503    | <div><div>23%45%24%</div><div></div></div>   |
| 1   | E     | 503    | <div><div>22%46%25%</div><div></div></div>   |

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| Mol | Chain | Length | Quality of chain                                                                                       |
|-----|-------|--------|--------------------------------------------------------------------------------------------------------|
| 1   | F     | 503    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>4%22%45%24%5%•</div></div> |
| 1   | G     | 503    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%23%46%23%••</div></div>  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26208 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA primase/helicase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 483      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3744  | 2341 | 657 | 721 | 25 |         |         |       |
| 1   | B     | 483      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3744  | 2341 | 657 | 721 | 25 |         |         |       |
| 1   | C     | 483      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3744  | 2341 | 657 | 721 | 25 |         |         |       |
| 1   | D     | 483      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3744  | 2341 | 657 | 721 | 25 |         |         |       |
| 1   | E     | 483      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3744  | 2341 | 657 | 721 | 25 |         |         |       |
| 1   | F     | 483      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3744  | 2341 | 657 | 721 | 25 |         |         |       |
| 1   | G     | 483      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3744  | 2341 | 657 | 721 | 25 |         |         |       |

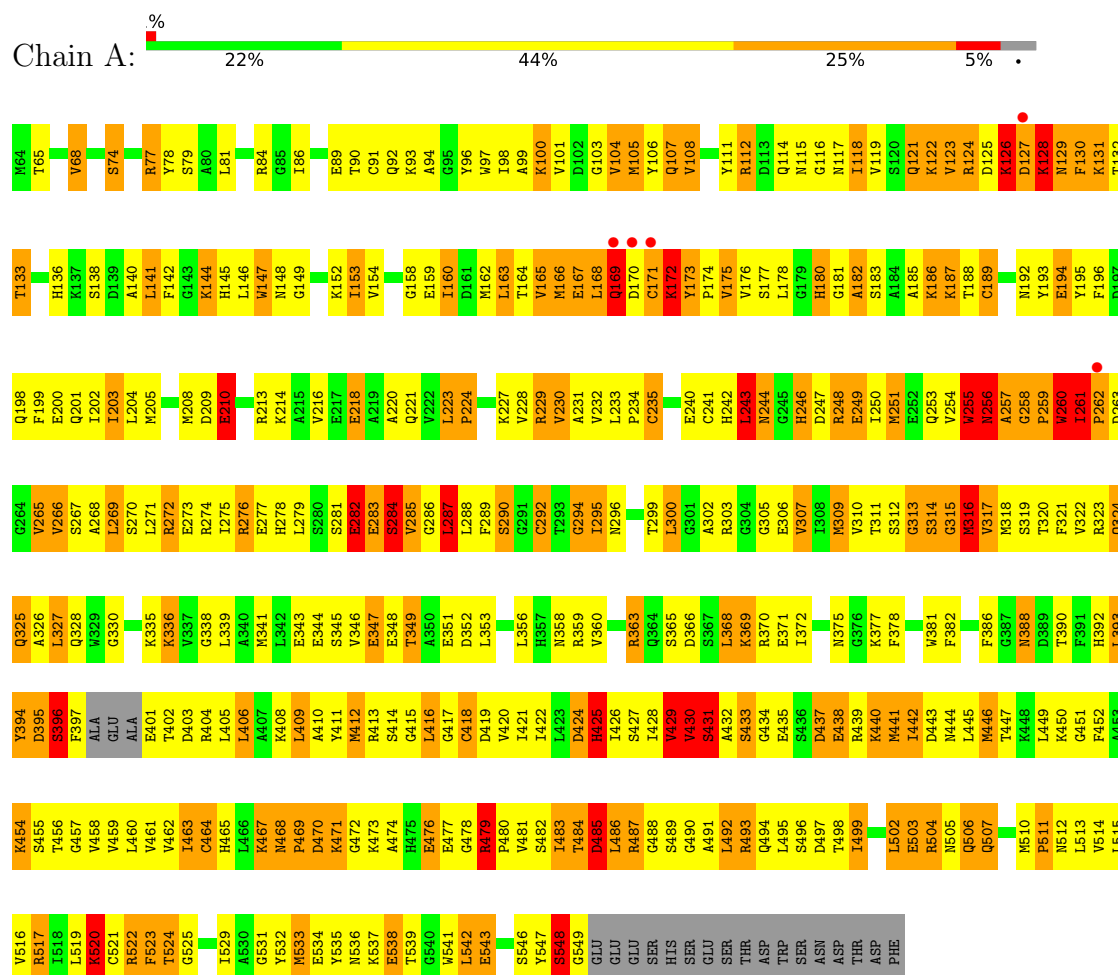
There are 14 discrepancies between the modelled and reference sequences:

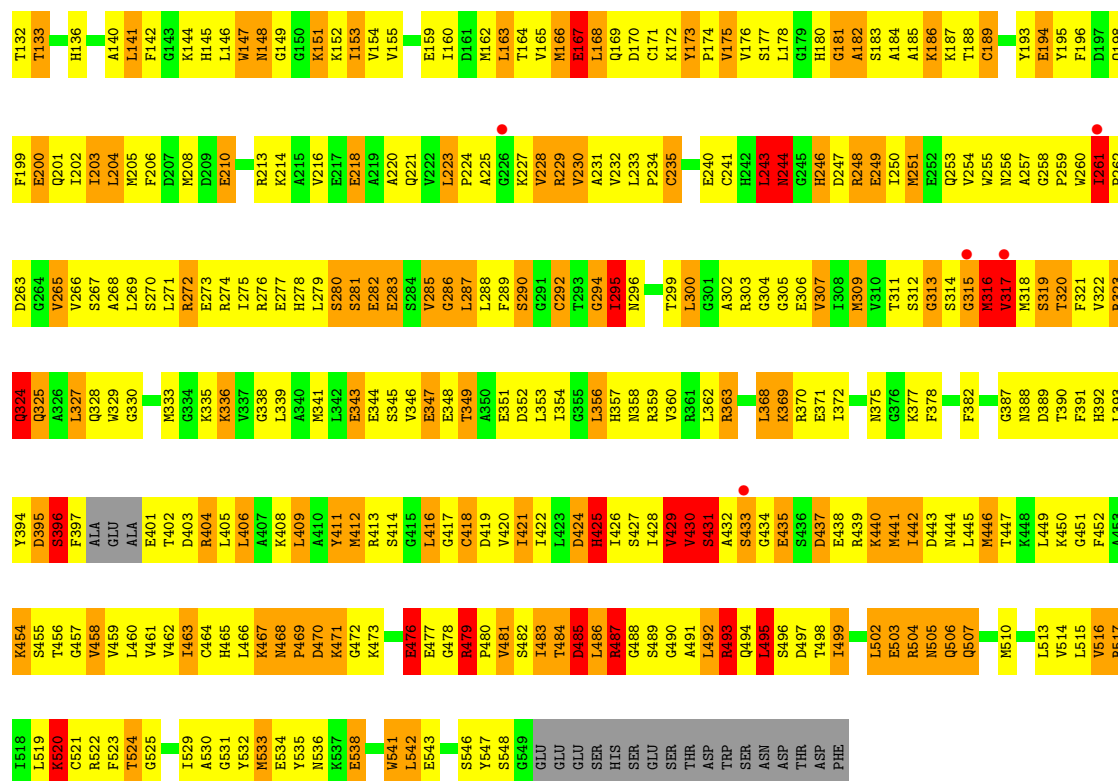
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 317     | VAL      | GLY    | engineered mutation | UNP P03692 |
| A     | 318     | MET      | LYS    | engineered mutation | UNP P03692 |
| B     | 317     | VAL      | GLY    | engineered mutation | UNP P03692 |
| B     | 318     | MET      | LYS    | engineered mutation | UNP P03692 |
| C     | 317     | VAL      | GLY    | engineered mutation | UNP P03692 |
| C     | 318     | MET      | LYS    | engineered mutation | UNP P03692 |
| D     | 317     | VAL      | GLY    | engineered mutation | UNP P03692 |
| D     | 318     | MET      | LYS    | engineered mutation | UNP P03692 |
| E     | 317     | VAL      | GLY    | engineered mutation | UNP P03692 |
| E     | 318     | MET      | LYS    | engineered mutation | UNP P03692 |
| F     | 317     | VAL      | GLY    | engineered mutation | UNP P03692 |
| F     | 318     | MET      | LYS    | engineered mutation | UNP P03692 |
| G     | 317     | VAL      | GLY    | engineered mutation | UNP P03692 |
| G     | 318     | MET      | LYS    | engineered mutation | UNP P03692 |

### 3 Residue-property plots

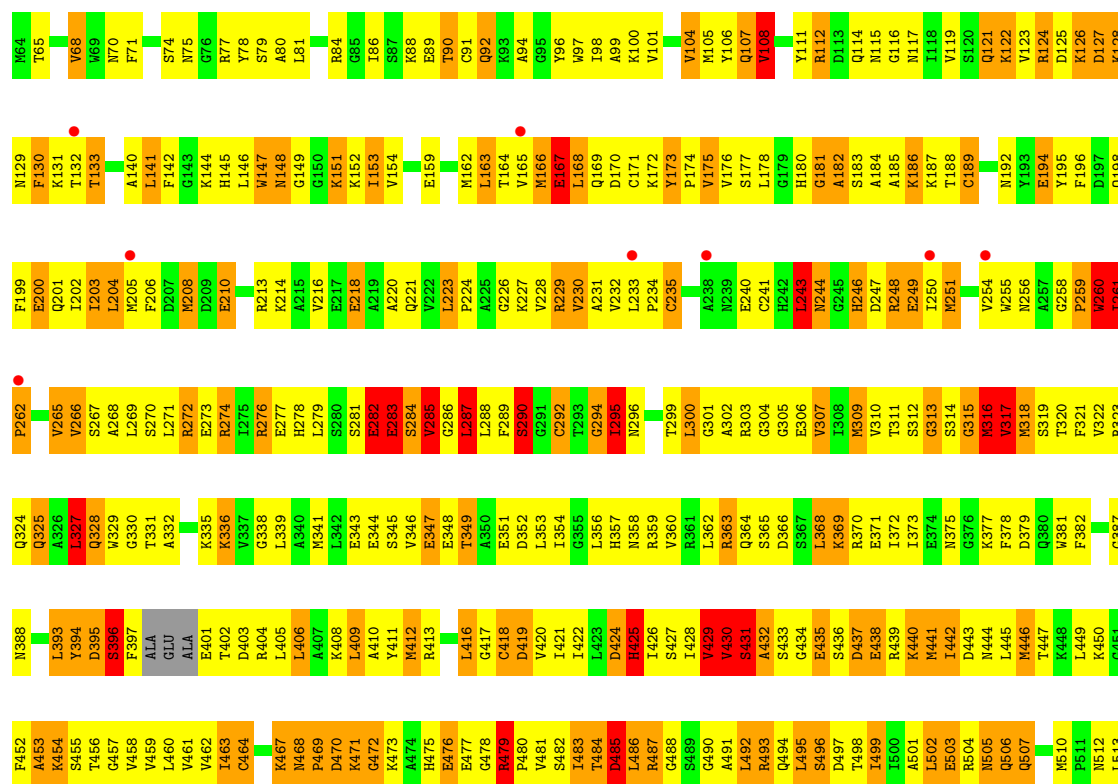
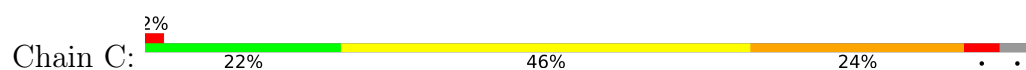
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

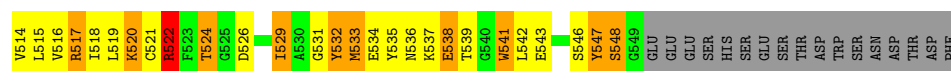
#### • Molecule 1: DNA primase/helicase



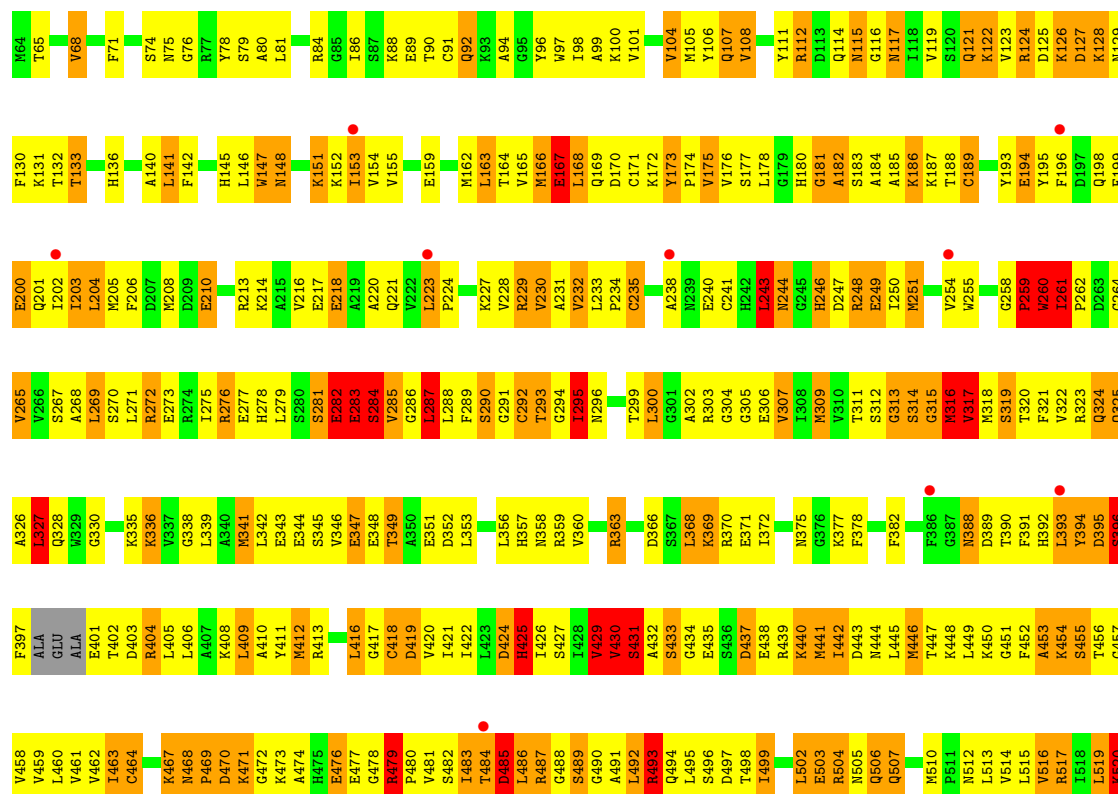
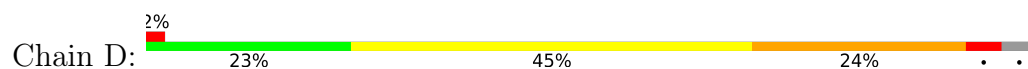


• Molecule 1: DNA primase/helicase

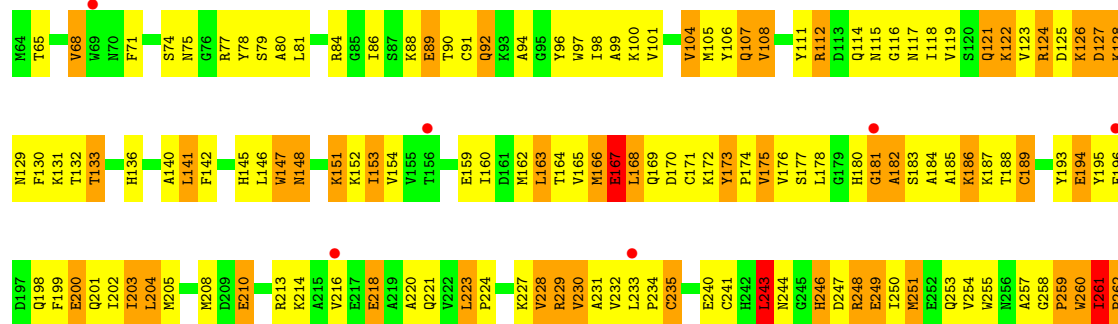
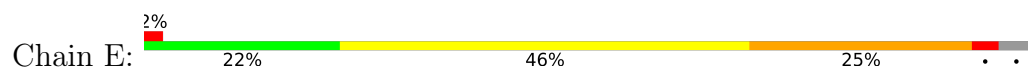


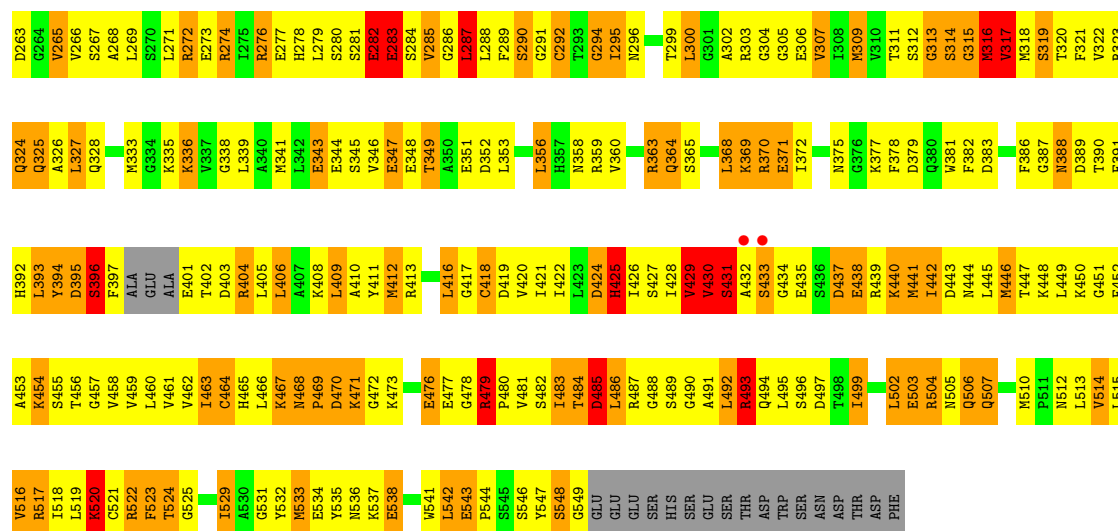


• Molecule 1: DNA primase/helicase

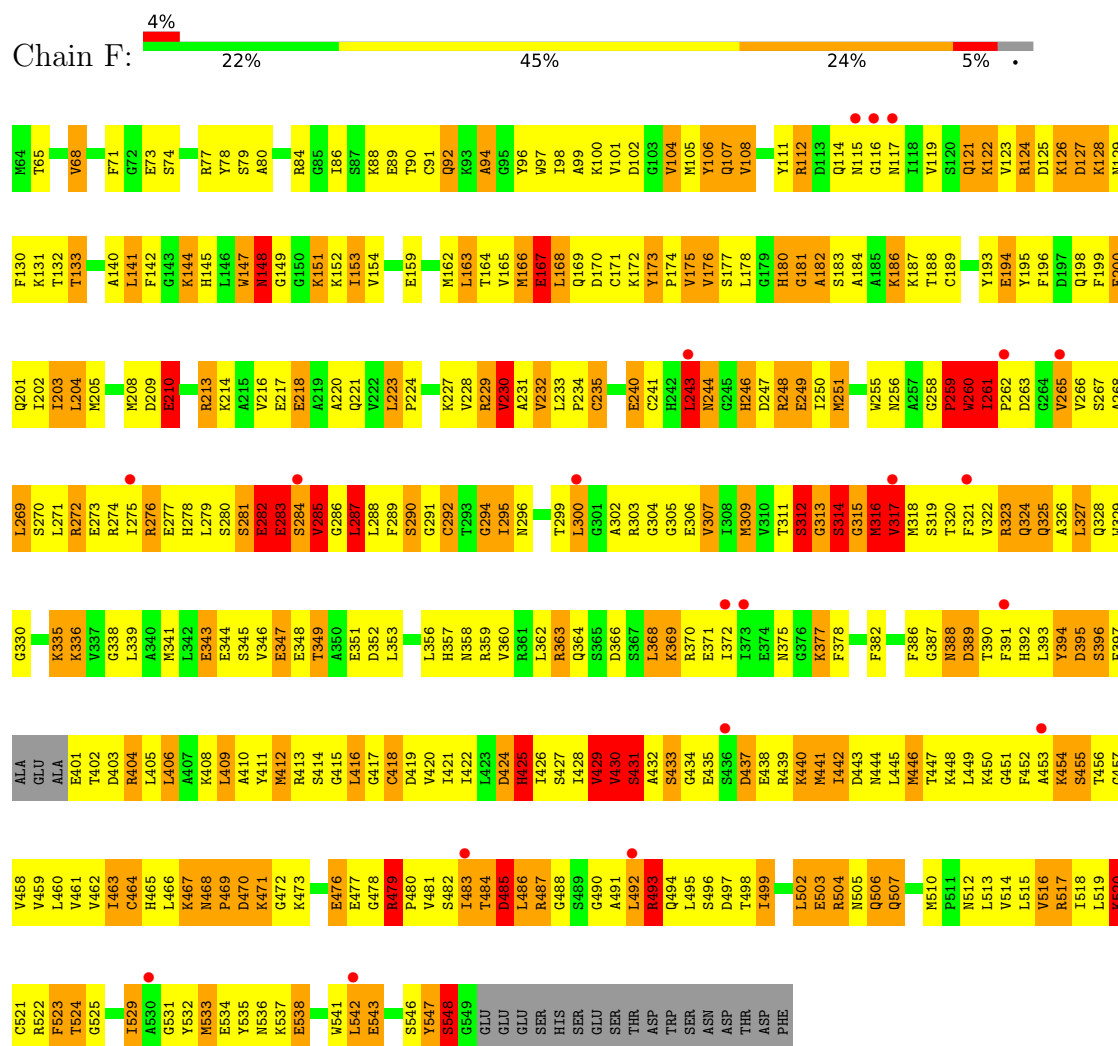


• Molecule 1: DNA primase/helicase



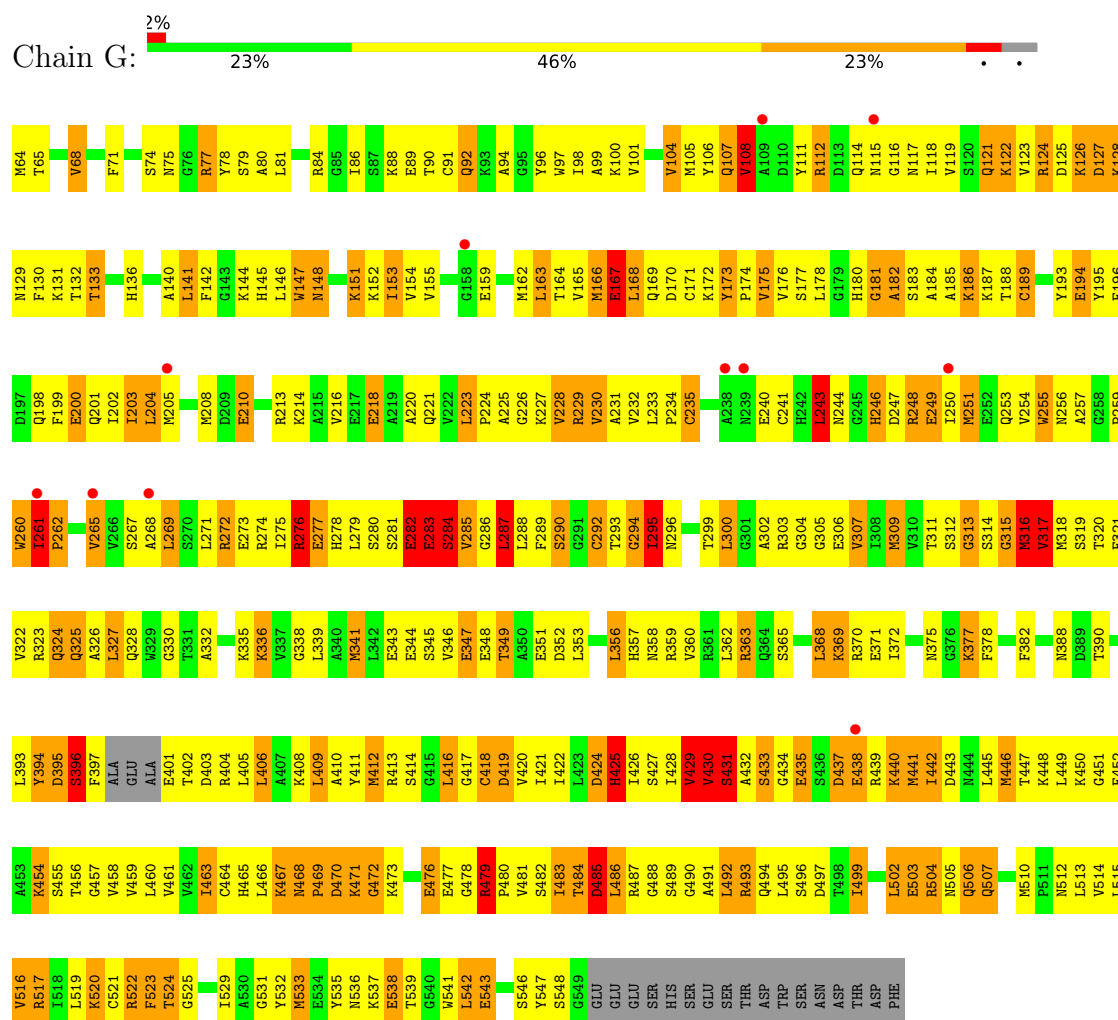


• Molecule 1: DNA primase/helicase



• Molecule 1: DNA primase/helicase





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 117.18Å 171.57Å 118.58Å<br>90.00° 99.86° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 20.00 – 3.45<br>20.00 – 3.45                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.7 (20.00-3.45)<br>99.1 (20.00-3.45)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.04                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.91 (at 3.49Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.1.80                                               | Depositor        |
| R, $R_{free}$                                                           | 0.299 , 0.326<br>0.284 , 0.311                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3055 reflections (5.04%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 127.0                                                       | Xtriage          |
| Anisotropy                                                              | 0.322                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 177.0                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.001 for l,-k,h                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 26208                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 138.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 1.16         | 8/3806 (0.2%)   | 1.42        | 50/5124 (1.0%)   |
| 1   | B     | 1.09         | 15/3806 (0.4%)  | 1.32        | 35/5124 (0.7%)   |
| 1   | C     | 1.07         | 16/3806 (0.4%)  | 1.35        | 36/5124 (0.7%)   |
| 1   | D     | 0.98         | 7/3806 (0.2%)   | 1.32        | 36/5124 (0.7%)   |
| 1   | E     | 0.94         | 6/3806 (0.2%)   | 1.27        | 31/5124 (0.6%)   |
| 1   | F     | 1.05         | 8/3806 (0.2%)   | 1.34        | 38/5124 (0.7%)   |
| 1   | G     | 0.94         | 9/3806 (0.2%)   | 1.30        | 42/5124 (0.8%)   |
| All | All   | 1.03         | 69/26642 (0.3%) | 1.33        | 268/35868 (0.7%) |

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                   | 4                   |
| 1   | B     | 0                   | 3                   |
| 1   | C     | 0                   | 5                   |
| 1   | D     | 0                   | 4                   |
| 1   | E     | 0                   | 4                   |
| 1   | F     | 0                   | 5                   |
| 1   | G     | 0                   | 4                   |
| All | All   | 0                   | 29                  |

All (69) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 261 | ILE  | CA-C  | 9.88 | 1.63        | 1.52     |
| 1   | B     | 429 | VAL  | CA-C  | 7.69 | 1.62        | 1.52     |
| 1   | E     | 429 | VAL  | CA-C  | 7.67 | 1.62        | 1.52     |
| 1   | G     | 261 | ILE  | N-CA  | 7.64 | 1.55        | 1.46     |
| 1   | D     | 429 | VAL  | CA-C  | 7.63 | 1.62        | 1.52     |
| 1   | G     | 261 | ILE  | CA-C  | 7.57 | 1.60        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 429 | VAL  | CA-C  | 7.51  | 1.62        | 1.52     |
| 1   | C     | 429 | VAL  | CA-C  | 7.50  | 1.62        | 1.52     |
| 1   | D     | 259 | PRO  | N-CA  | 7.49  | 1.56        | 1.47     |
| 1   | A     | 429 | VAL  | CA-C  | 7.44  | 1.62        | 1.52     |
| 1   | G     | 429 | VAL  | CA-C  | 7.31  | 1.62        | 1.52     |
| 1   | C     | 173 | TYR  | C-N   | -7.25 | 1.25        | 1.33     |
| 1   | B     | 429 | VAL  | C-N   | 6.99  | 1.43        | 1.33     |
| 1   | C     | 429 | VAL  | C-N   | 6.89  | 1.43        | 1.33     |
| 1   | G     | 429 | VAL  | C-N   | 6.88  | 1.43        | 1.33     |
| 1   | E     | 429 | VAL  | C-N   | 6.76  | 1.42        | 1.33     |
| 1   | A     | 429 | VAL  | C-N   | 6.75  | 1.42        | 1.33     |
| 1   | D     | 429 | VAL  | C-N   | 6.75  | 1.42        | 1.33     |
| 1   | F     | 429 | VAL  | C-N   | 6.71  | 1.42        | 1.33     |
| 1   | G     | 430 | VAL  | N-CA  | 6.53  | 1.54        | 1.46     |
| 1   | C     | 430 | VAL  | N-CA  | 6.46  | 1.54        | 1.46     |
| 1   | E     | 430 | VAL  | N-CA  | 6.37  | 1.54        | 1.46     |
| 1   | B     | 430 | VAL  | N-CA  | 6.34  | 1.54        | 1.46     |
| 1   | F     | 430 | VAL  | N-CA  | 6.25  | 1.54        | 1.46     |
| 1   | A     | 430 | VAL  | N-CA  | 6.22  | 1.54        | 1.46     |
| 1   | G     | 431 | SER  | N-CA  | 6.15  | 1.54        | 1.46     |
| 1   | D     | 430 | VAL  | N-CA  | 6.11  | 1.53        | 1.46     |
| 1   | C     | 310 | VAL  | CA-CB | -6.10 | 1.46        | 1.54     |
| 1   | D     | 431 | SER  | N-CA  | 6.10  | 1.54        | 1.46     |
| 1   | C     | 318 | MET  | SD-CE | -6.09 | 1.64        | 1.79     |
| 1   | A     | 431 | SER  | N-CA  | 6.05  | 1.53        | 1.46     |
| 1   | F     | 94  | ALA  | CA-CB | -6.02 | 1.43        | 1.53     |
| 1   | F     | 148 | ASN  | CA-C  | -5.94 | 1.46        | 1.53     |
| 1   | G     | 284 | SER  | N-CA  | -5.93 | 1.40        | 1.46     |
| 1   | B     | 421 | ILE  | CA-CB | -5.89 | 1.46        | 1.54     |
| 1   | F     | 431 | SER  | N-CA  | 5.86  | 1.53        | 1.46     |
| 1   | E     | 431 | SER  | N-CA  | 5.85  | 1.53        | 1.46     |
| 1   | B     | 433 | SER  | N-CA  | 5.82  | 1.54        | 1.46     |
| 1   | B     | 431 | SER  | N-CA  | 5.78  | 1.53        | 1.46     |
| 1   | B     | 414 | SER  | CA-C  | -5.68 | 1.45        | 1.52     |
| 1   | E     | 433 | SER  | N-CA  | 5.65  | 1.53        | 1.46     |
| 1   | G     | 433 | SER  | N-CA  | 5.64  | 1.53        | 1.46     |
| 1   | D     | 433 | SER  | N-CA  | 5.63  | 1.53        | 1.46     |
| 1   | G     | 430 | VAL  | C-N   | 5.60  | 1.41        | 1.33     |
| 1   | F     | 433 | SER  | N-CA  | 5.60  | 1.53        | 1.46     |
| 1   | A     | 433 | SER  | N-CA  | 5.57  | 1.53        | 1.46     |
| 1   | C     | 433 | SER  | N-CA  | 5.55  | 1.53        | 1.46     |
| 1   | B     | 487 | ARG  | CA-C  | 5.50  | 1.60        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 431 | SER  | N-CA  | 5.48  | 1.53        | 1.46     |
| 1   | B     | 430 | VAL  | C-N   | 5.48  | 1.41        | 1.33     |
| 1   | B     | 324 | GLN  | N-CA  | -5.45 | 1.40        | 1.46     |
| 1   | C     | 522 | ARG  | CA-C  | -5.34 | 1.46        | 1.52     |
| 1   | D     | 430 | VAL  | C-N   | 5.34  | 1.41        | 1.33     |
| 1   | A     | 430 | VAL  | C-N   | 5.33  | 1.41        | 1.33     |
| 1   | B     | 458 | VAL  | CA-CB | -5.33 | 1.48        | 1.54     |
| 1   | E     | 430 | VAL  | C-N   | 5.27  | 1.41        | 1.33     |
| 1   | B     | 281 | SER  | C-N   | 5.26  | 1.40        | 1.33     |
| 1   | F     | 430 | VAL  | C-N   | 5.24  | 1.41        | 1.33     |
| 1   | B     | 281 | SER  | C-O   | 5.23  | 1.30        | 1.24     |
| 1   | C     | 301 | GLY  | C-O   | 5.20  | 1.29        | 1.23     |
| 1   | C     | 261 | ILE  | CA-C  | 5.20  | 1.58        | 1.52     |
| 1   | C     | 329 | TRP  | N-CA  | 5.18  | 1.52        | 1.46     |
| 1   | C     | 430 | VAL  | C-N   | 5.11  | 1.40        | 1.33     |
| 1   | A     | 310 | VAL  | CA-CB | -5.11 | 1.48        | 1.54     |
| 1   | C     | 261 | ILE  | CA-CB | 5.08  | 1.60        | 1.54     |
| 1   | B     | 530 | ALA  | CA-CB | -5.07 | 1.45        | 1.53     |
| 1   | B     | 411 | TYR  | C-O   | -5.07 | 1.17        | 1.24     |
| 1   | C     | 501 | ALA  | CA-CB | -5.05 | 1.44        | 1.53     |
| 1   | C     | 290 | SER  | CA-CB | 5.02  | 1.61        | 1.53     |

All (268) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 172 | LYS  | N-CA-C  | 17.34  | 136.17      | 113.97   |
| 1   | F     | 260 | TRP  | N-CA-C  | 14.90  | 128.90      | 107.88   |
| 1   | D     | 259 | PRO  | CA-N-CD | -13.62 | 92.93       | 112.00   |
| 1   | D     | 167 | GLU  | O-C-N   | 12.97  | 136.67      | 121.76   |
| 1   | B     | 173 | TYR  | CA-C-N  | -12.24 | 104.55      | 119.84   |
| 1   | B     | 173 | TYR  | C-N-CA  | -12.24 | 104.55      | 119.84   |
| 1   | B     | 430 | VAL  | CA-C-N  | 12.14  | 144.72      | 121.54   |
| 1   | B     | 430 | VAL  | C-N-CA  | 12.14  | 144.72      | 121.54   |
| 1   | D     | 430 | VAL  | CA-C-N  | 12.09  | 144.63      | 121.54   |
| 1   | D     | 430 | VAL  | C-N-CA  | 12.09  | 144.63      | 121.54   |
| 1   | E     | 167 | GLU  | O-C-N   | 12.07  | 135.64      | 121.76   |
| 1   | G     | 430 | VAL  | CA-C-N  | 12.04  | 144.53      | 121.54   |
| 1   | G     | 430 | VAL  | C-N-CA  | 12.04  | 144.53      | 121.54   |
| 1   | A     | 430 | VAL  | CA-C-N  | 11.96  | 144.39      | 121.54   |
| 1   | A     | 430 | VAL  | C-N-CA  | 11.96  | 144.39      | 121.54   |
| 1   | E     | 430 | VAL  | CA-C-N  | 11.93  | 144.33      | 121.54   |
| 1   | E     | 430 | VAL  | C-N-CA  | 11.93  | 144.33      | 121.54   |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | F     | 430 | VAL  | CA-C-N  | 11.90  | 144.26      | 121.54   |
| 1   | F     | 430 | VAL  | C-N-CA  | 11.90  | 144.26      | 121.54   |
| 1   | B     | 167 | GLU  | O-C-N   | 11.82  | 135.35      | 121.76   |
| 1   | A     | 262 | PRO  | N-CD-CG | -11.76 | 85.56       | 103.20   |
| 1   | G     | 173 | TYR  | CA-C-N  | -11.75 | 105.15      | 119.84   |
| 1   | G     | 173 | TYR  | C-N-CA  | -11.75 | 105.15      | 119.84   |
| 1   | C     | 167 | GLU  | O-C-N   | 11.75  | 135.27      | 121.76   |
| 1   | G     | 167 | GLU  | O-C-N   | 11.73  | 135.26      | 121.76   |
| 1   | C     | 316 | MET  | N-CA-C  | -11.71 | 97.56       | 112.90   |
| 1   | C     | 430 | VAL  | CA-C-N  | 11.71  | 143.90      | 121.54   |
| 1   | C     | 430 | VAL  | C-N-CA  | 11.71  | 143.90      | 121.54   |
| 1   | E     | 173 | TYR  | CA-C-N  | -11.45 | 105.53      | 119.84   |
| 1   | E     | 173 | TYR  | C-N-CA  | -11.45 | 105.53      | 119.84   |
| 1   | G     | 261 | ILE  | CA-C-N  | 11.37  | 134.05      | 119.84   |
| 1   | G     | 261 | ILE  | C-N-CA  | 11.37  | 134.05      | 119.84   |
| 1   | D     | 261 | ILE  | CA-C-N  | 10.88  | 133.44      | 119.84   |
| 1   | D     | 261 | ILE  | C-N-CA  | 10.88  | 133.44      | 119.84   |
| 1   | E     | 430 | VAL  | N-CA-C  | 10.88  | 131.96      | 109.34   |
| 1   | A     | 430 | VAL  | N-CA-C  | 10.78  | 131.77      | 109.34   |
| 1   | E     | 283 | GLU  | N-CA-C  | 10.77  | 125.78      | 109.41   |
| 1   | C     | 430 | VAL  | N-CA-C  | 10.72  | 131.65      | 109.34   |
| 1   | D     | 430 | VAL  | N-CA-C  | 10.71  | 131.62      | 109.34   |
| 1   | B     | 430 | VAL  | N-CA-C  | 10.70  | 131.59      | 109.34   |
| 1   | G     | 430 | VAL  | N-CA-C  | 10.68  | 131.54      | 109.34   |
| 1   | F     | 430 | VAL  | N-CA-C  | 10.66  | 131.51      | 109.34   |
| 1   | F     | 167 | GLU  | O-C-N   | 10.44  | 133.77      | 121.76   |
| 1   | A     | 173 | TYR  | N-CA-CB | -10.34 | 91.88       | 110.39   |
| 1   | F     | 256 | ASN  | N-CA-C  | 10.16  | 125.27      | 111.24   |
| 1   | D     | 167 | GLU  | CA-C-N  | -10.08 | 102.28      | 121.54   |
| 1   | D     | 167 | GLU  | C-N-CA  | -10.08 | 102.28      | 121.54   |
| 1   | D     | 433 | SER  | N-CA-C  | 10.08  | 124.76      | 108.63   |
| 1   | F     | 433 | SER  | N-CA-C  | 9.99   | 124.61      | 108.63   |
| 1   | C     | 433 | SER  | N-CA-C  | 9.95   | 124.55      | 108.63   |
| 1   | E     | 433 | SER  | N-CA-C  | 9.93   | 124.52      | 108.63   |
| 1   | G     | 167 | GLU  | CA-C-N  | -9.90  | 102.63      | 121.54   |
| 1   | G     | 167 | GLU  | C-N-CA  | -9.90  | 102.63      | 121.54   |
| 1   | D     | 316 | MET  | N-CA-C  | -9.89  | 99.94       | 112.90   |
| 1   | B     | 433 | SER  | N-CA-C  | 9.87   | 124.43      | 108.63   |
| 1   | B     | 167 | GLU  | CA-C-N  | -9.86  | 102.71      | 121.54   |
| 1   | B     | 167 | GLU  | C-N-CA  | -9.86  | 102.71      | 121.54   |
| 1   | D     | 173 | TYR  | CA-C-N  | -9.86  | 107.52      | 119.84   |
| 1   | D     | 173 | TYR  | C-N-CA  | -9.86  | 107.52      | 119.84   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | G     | 433 | SER  | N-CA-C     | 9.86  | 124.40      | 108.63   |
| 1   | C     | 167 | GLU  | CA-C-N     | -9.83 | 102.77      | 121.54   |
| 1   | C     | 167 | GLU  | C-N-CA     | -9.83 | 102.77      | 121.54   |
| 1   | G     | 261 | ILE  | N-CA-C     | 9.80  | 130.05      | 108.88   |
| 1   | A     | 433 | SER  | N-CA-C     | 9.79  | 124.30      | 108.63   |
| 1   | E     | 167 | GLU  | CA-C-N     | -9.71 | 102.99      | 121.54   |
| 1   | E     | 167 | GLU  | C-N-CA     | -9.71 | 102.99      | 121.54   |
| 1   | F     | 167 | GLU  | CA-C-N     | -9.51 | 103.39      | 121.54   |
| 1   | F     | 167 | GLU  | C-N-CA     | -9.51 | 103.39      | 121.54   |
| 1   | C     | 328 | GLN  | OE1-CD-NE2 | -9.48 | 113.11      | 122.60   |
| 1   | C     | 173 | TYR  | CA-C-N     | -9.45 | 107.49      | 120.25   |
| 1   | C     | 173 | TYR  | C-N-CA     | -9.45 | 107.49      | 120.25   |
| 1   | A     | 261 | ILE  | CA-C-N     | 9.06  | 131.17      | 119.84   |
| 1   | A     | 261 | ILE  | C-N-CA     | 9.06  | 131.17      | 119.84   |
| 1   | F     | 316 | MET  | N-CA-C     | -8.99 | 101.12      | 112.90   |
| 1   | F     | 261 | ILE  | CA-C-N     | -8.80 | 108.84      | 119.84   |
| 1   | F     | 261 | ILE  | C-N-CA     | -8.80 | 108.84      | 119.84   |
| 1   | E     | 316 | MET  | N-CA-C     | -8.79 | 100.23      | 112.45   |
| 1   | B     | 256 | ASN  | N-CA-C     | 8.34  | 122.81      | 112.47   |
| 1   | D     | 173 | TYR  | O-C-N      | -8.22 | 111.86      | 121.32   |
| 1   | B     | 424 | ASP  | O-C-N      | 8.13  | 133.63      | 122.41   |
| 1   | E     | 173 | TYR  | O-C-N      | -8.07 | 112.04      | 121.32   |
| 1   | G     | 173 | TYR  | O-C-N      | -8.02 | 112.10      | 121.32   |
| 1   | D     | 259 | PRO  | N-CA-CB    | 8.00  | 111.65      | 103.25   |
| 1   | A     | 424 | ASP  | O-C-N      | 7.97  | 132.81      | 122.68   |
| 1   | A     | 511 | PRO  | CA-N-CD    | -7.97 | 100.84      | 112.00   |
| 1   | D     | 425 | HIS  | CB-CA-C    | 7.93  | 126.20      | 110.42   |
| 1   | E     | 429 | VAL  | CA-C-N     | 7.89  | 136.18      | 121.97   |
| 1   | E     | 429 | VAL  | C-N-CA     | 7.89  | 136.18      | 121.97   |
| 1   | E     | 364 | GLN  | OE1-CD-NE2 | -7.88 | 114.72      | 122.60   |
| 1   | C     | 332 | ALA  | N-CA-C     | -7.80 | 102.47      | 110.97   |
| 1   | F     | 282 | GLU  | N-CA-C     | 7.77  | 122.69      | 110.17   |
| 1   | G     | 429 | VAL  | CA-C-N     | 7.77  | 135.96      | 121.97   |
| 1   | G     | 429 | VAL  | C-N-CA     | 7.77  | 135.96      | 121.97   |
| 1   | C     | 429 | VAL  | CA-C-N     | 7.74  | 135.90      | 121.97   |
| 1   | C     | 429 | VAL  | C-N-CA     | 7.74  | 135.90      | 121.97   |
| 1   | F     | 429 | VAL  | CA-C-N     | 7.71  | 135.85      | 121.97   |
| 1   | F     | 429 | VAL  | C-N-CA     | 7.71  | 135.85      | 121.97   |
| 1   | C     | 173 | TYR  | O-C-N      | -7.66 | 112.51      | 121.32   |
| 1   | G     | 316 | MET  | N-CA-C     | -7.62 | 101.86      | 112.45   |
| 1   | A     | 429 | VAL  | CA-C-N     | 7.60  | 135.65      | 121.97   |
| 1   | A     | 429 | VAL  | C-N-CA     | 7.60  | 135.65      | 121.97   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 316 | MET  | N-CA-C     | -7.60 | 102.95      | 112.90   |
| 1   | B     | 425 | HIS  | N-CA-CB    | -7.56 | 97.71       | 110.49   |
| 1   | B     | 430 | VAL  | O-C-N      | 7.56  | 132.02      | 122.57   |
| 1   | D     | 429 | VAL  | CA-C-N     | 7.54  | 135.54      | 121.97   |
| 1   | D     | 429 | VAL  | C-N-CA     | 7.54  | 135.54      | 121.97   |
| 1   | A     | 261 | ILE  | N-CA-C     | 7.53  | 125.15      | 108.88   |
| 1   | B     | 429 | VAL  | CA-C-N     | 7.49  | 135.44      | 121.97   |
| 1   | B     | 429 | VAL  | C-N-CA     | 7.49  | 135.44      | 121.97   |
| 1   | G     | 276 | ARG  | O-C-N      | -7.47 | 114.32      | 122.09   |
| 1   | F     | 173 | TYR  | O-C-N      | -7.44 | 112.76      | 121.32   |
| 1   | C     | 424 | ASP  | O-C-N      | 7.38  | 132.05      | 122.68   |
| 1   | G     | 430 | VAL  | O-C-N      | 7.36  | 131.78      | 122.57   |
| 1   | C     | 430 | VAL  | O-C-N      | 7.32  | 131.72      | 122.57   |
| 1   | B     | 173 | TYR  | O-C-N      | -7.29 | 112.94      | 121.32   |
| 1   | D     | 430 | VAL  | O-C-N      | 7.26  | 131.64      | 122.57   |
| 1   | B     | 425 | HIS  | CB-CA-C    | 7.25  | 124.86      | 110.42   |
| 1   | E     | 430 | VAL  | O-C-N      | 7.22  | 131.60      | 122.57   |
| 1   | A     | 430 | VAL  | O-C-N      | 7.22  | 131.59      | 122.57   |
| 1   | C     | 294 | GLY  | N-CA-C     | -7.22 | 96.08       | 113.18   |
| 1   | A     | 92  | GLN  | OE1-CD-NE2 | -7.21 | 115.39      | 122.60   |
| 1   | B     | 316 | MET  | N-CA-C     | -7.12 | 103.58      | 112.90   |
| 1   | F     | 430 | VAL  | O-C-N      | 7.05  | 131.38      | 122.57   |
| 1   | A     | 468 | ASN  | N-CA-C     | 6.96  | 120.77      | 109.15   |
| 1   | A     | 130 | PHE  | N-CA-C     | 6.94  | 119.04      | 109.18   |
| 1   | A     | 260 | TRP  | CA-CB-CG   | 6.90  | 126.70      | 113.60   |
| 1   | A     | 261 | ILE  | C-N-CD     | -6.89 | 96.75       | 125.00   |
| 1   | G     | 431 | SER  | N-CA-C     | 6.87  | 125.42      | 110.80   |
| 1   | C     | 541 | TRP  | N-CA-C     | 6.84  | 121.19      | 110.32   |
| 1   | E     | 431 | SER  | N-CA-C     | 6.84  | 125.36      | 110.80   |
| 1   | D     | 431 | SER  | N-CA-C     | 6.79  | 125.27      | 110.80   |
| 1   | B     | 281 | SER  | N-CA-C     | 6.77  | 122.47      | 111.37   |
| 1   | A     | 431 | SER  | N-CA-C     | 6.75  | 125.17      | 110.80   |
| 1   | F     | 431 | SER  | N-CA-C     | 6.74  | 125.16      | 110.80   |
| 1   | C     | 431 | SER  | N-CA-C     | 6.70  | 125.08      | 110.80   |
| 1   | C     | 522 | ARG  | N-CA-C     | -6.67 | 103.70      | 110.97   |
| 1   | E     | 424 | ASP  | O-C-N      | 6.62  | 131.09      | 122.68   |
| 1   | G     | 347 | GLU  | N-CA-C     | -6.61 | 104.00      | 111.14   |
| 1   | B     | 431 | SER  | N-CA-C     | 6.58  | 124.82      | 110.80   |
| 1   | G     | 283 | GLU  | N-CA-C     | 6.56  | 119.86      | 109.50   |
| 1   | B     | 283 | GLU  | N-CA-C     | 6.53  | 119.37      | 108.73   |
| 1   | F     | 173 | TYR  | CA-C-N     | -6.50 | 111.47      | 120.25   |
| 1   | F     | 173 | TYR  | C-N-CA     | -6.50 | 111.47      | 120.25   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | G     | 261 | ILE  | O-C-N    | 6.45  | 128.46      | 121.10   |
| 1   | B     | 320 | THR  | N-CA-C   | -6.34 | 102.91      | 112.04   |
| 1   | B     | 468 | ASN  | N-CA-C   | 6.33  | 120.75      | 108.85   |
| 1   | B     | 280 | SER  | N-CA-C   | 6.29  | 118.01      | 111.03   |
| 1   | C     | 256 | ASN  | N-CA-C   | 6.27  | 119.89      | 111.24   |
| 1   | G     | 468 | ASN  | N-CA-C   | 6.26  | 119.61      | 109.15   |
| 1   | D     | 282 | GLU  | N-CA-C   | 6.24  | 120.22      | 110.17   |
| 1   | C     | 365 | SER  | N-CA-C   | 6.22  | 118.43      | 107.61   |
| 1   | D     | 424 | ASP  | O-C-N    | 6.19  | 130.55      | 122.68   |
| 1   | F     | 424 | ASP  | O-C-N    | 6.16  | 130.50      | 122.68   |
| 1   | A     | 224 | PRO  | CA-C-O   | -6.15 | 114.82      | 121.27   |
| 1   | C     | 425 | HIS  | N-CA-CB  | -6.13 | 100.14      | 110.49   |
| 1   | D     | 281 | SER  | N-CA-C   | 6.12  | 117.64      | 110.97   |
| 1   | C     | 425 | HIS  | CB-CA-C  | 6.02  | 122.40      | 110.42   |
| 1   | F     | 335 | LYS  | N-CA-C   | 6.01  | 118.72      | 110.24   |
| 1   | G     | 425 | HIS  | CB-CA-C  | 6.00  | 122.36      | 110.42   |
| 1   | A     | 256 | ASN  | CA-CB-CG | -5.99 | 106.61      | 112.60   |
| 1   | G     | 262 | PRO  | N-CD-CG  | -5.94 | 94.29       | 103.20   |
| 1   | G     | 396 | SER  | N-CA-C   | 5.91  | 123.38      | 110.80   |
| 1   | F     | 266 | VAL  | CB-CA-C  | -5.83 | 101.72      | 111.29   |
| 1   | G     | 261 | ILE  | C-N-CD   | -5.82 | 101.15      | 125.00   |
| 1   | E     | 468 | ASN  | N-CA-C   | 5.80  | 119.76      | 108.85   |
| 1   | E     | 260 | TRP  | N-CA-C   | 5.80  | 117.06      | 108.60   |
| 1   | A     | 282 | GLU  | N-CA-C   | 5.78  | 119.48      | 110.17   |
| 1   | D     | 260 | TRP  | N-CA-C   | 5.78  | 123.12      | 110.80   |
| 1   | A     | 256 | ASN  | N-CA-C   | 5.77  | 123.09      | 110.80   |
| 1   | E     | 294 | GLY  | N-CA-C   | -5.75 | 99.56       | 113.18   |
| 1   | C     | 282 | GLU  | N-CA-C   | 5.73  | 119.40      | 110.17   |
| 1   | B     | 294 | GLY  | N-CA-C   | -5.71 | 99.64       | 113.18   |
| 1   | A     | 425 | HIS  | CA-C-N   | 5.68  | 128.24      | 120.46   |
| 1   | A     | 425 | HIS  | C-N-CA   | 5.68  | 128.24      | 120.46   |
| 1   | G     | 424 | ASP  | O-C-N    | 5.68  | 130.18      | 122.57   |
| 1   | E     | 431 | SER  | CA-C-N   | 5.66  | 132.35      | 121.54   |
| 1   | E     | 431 | SER  | C-N-CA   | 5.66  | 132.35      | 121.54   |
| 1   | A     | 284 | SER  | N-CA-C   | 5.66  | 122.86      | 110.80   |
| 1   | A     | 431 | SER  | CA-C-N   | 5.66  | 132.34      | 121.54   |
| 1   | A     | 431 | SER  | C-N-CA   | 5.66  | 132.34      | 121.54   |
| 1   | A     | 425 | HIS  | CB-CA-C  | 5.63  | 121.63      | 110.42   |
| 1   | E     | 425 | HIS  | N-CA-CB  | -5.62 | 100.99      | 110.49   |
| 1   | F     | 468 | ASN  | N-CA-C   | 5.61  | 119.39      | 108.85   |
| 1   | A     | 129 | ASN  | N-CA-C   | 5.60  | 118.08      | 110.35   |
| 1   | F     | 259 | PRO  | CA-C-N   | -5.58 | 112.53      | 122.45   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | F     | 259 | PRO  | C-N-CA  | -5.58 | 112.53      | 122.45   |
| 1   | B     | 476 | GLU  | N-CA-C  | -5.56 | 106.45      | 113.18   |
| 1   | B     | 431 | SER  | CA-C-N  | 5.55  | 132.14      | 121.54   |
| 1   | B     | 431 | SER  | C-N-CA  | 5.55  | 132.14      | 121.54   |
| 1   | F     | 431 | SER  | CA-C-N  | 5.55  | 132.13      | 121.54   |
| 1   | F     | 431 | SER  | C-N-CA  | 5.55  | 132.13      | 121.54   |
| 1   | G     | 365 | SER  | N-CA-C  | 5.54  | 116.62      | 107.20   |
| 1   | G     | 282 | GLU  | N-CA-C  | 5.52  | 119.06      | 110.17   |
| 1   | A     | 283 | GLU  | CA-C-N  | 5.52  | 132.09      | 121.54   |
| 1   | A     | 283 | GLU  | C-N-CA  | 5.52  | 132.09      | 121.54   |
| 1   | C     | 431 | SER  | CA-C-N  | 5.52  | 132.09      | 121.54   |
| 1   | C     | 431 | SER  | C-N-CA  | 5.52  | 132.09      | 121.54   |
| 1   | G     | 468 | ASN  | CA-C-N  | 5.51  | 126.72      | 119.84   |
| 1   | G     | 468 | ASN  | C-N-CA  | 5.51  | 126.72      | 119.84   |
| 1   | E     | 365 | SER  | N-CA-C  | 5.46  | 116.47      | 107.20   |
| 1   | A     | 92  | GLN  | N-CA-C  | 5.45  | 117.22      | 111.28   |
| 1   | D     | 431 | SER  | CA-C-N  | 5.45  | 131.95      | 121.54   |
| 1   | D     | 431 | SER  | C-N-CA  | 5.45  | 131.95      | 121.54   |
| 1   | G     | 431 | SER  | CA-C-N  | 5.44  | 131.93      | 121.54   |
| 1   | G     | 431 | SER  | C-N-CA  | 5.44  | 131.93      | 121.54   |
| 1   | C     | 468 | ASN  | N-CA-C  | 5.44  | 119.08      | 108.85   |
| 1   | F     | 180 | HIS  | N-CA-C  | -5.43 | 104.92      | 113.02   |
| 1   | A     | 396 | SER  | N-CA-C  | 5.40  | 122.31      | 110.80   |
| 1   | C     | 396 | SER  | N-CA-C  | 5.40  | 122.30      | 110.80   |
| 1   | A     | 172 | LYS  | CB-CA-C | -5.40 | 100.01      | 109.07   |
| 1   | F     | 468 | ASN  | CA-C-N  | 5.38  | 126.57      | 119.84   |
| 1   | F     | 468 | ASN  | C-N-CA  | 5.38  | 126.57      | 119.84   |
| 1   | G     | 294 | GLY  | N-CA-C  | -5.38 | 100.42      | 113.18   |
| 1   | D     | 425 | HIS  | N-CA-CB | -5.37 | 101.41      | 110.49   |
| 1   | E     | 381 | TRP  | N-CA-C  | -5.36 | 105.52      | 111.36   |
| 1   | A     | 165 | VAL  | N-CA-C  | -5.35 | 104.36      | 111.05   |
| 1   | C     | 130 | PHE  | N-CA-C  | 5.35  | 116.40      | 108.86   |
| 1   | A     | 260 | TRP  | N-CA-C  | 5.35  | 122.19      | 110.80   |
| 1   | A     | 468 | ASN  | CA-C-N  | 5.34  | 126.52      | 119.84   |
| 1   | A     | 468 | ASN  | C-N-CA  | 5.34  | 126.52      | 119.84   |
| 1   | D     | 259 | PRO  | CB-CA-C | -5.32 | 102.78      | 111.56   |
| 1   | B     | 266 | VAL  | CB-CA-C | -5.32 | 102.57      | 111.29   |
| 1   | D     | 283 | GLU  | CA-C-N  | 5.29  | 131.63      | 121.54   |
| 1   | D     | 283 | GLU  | C-N-CA  | 5.29  | 131.63      | 121.54   |
| 1   | E     | 544 | PRO  | CA-C-O  | -5.28 | 115.22      | 121.67   |
| 1   | D     | 468 | ASN  | CA-C-N  | 5.26  | 126.42      | 119.84   |
| 1   | D     | 468 | ASN  | C-N-CA  | 5.26  | 126.42      | 119.84   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 365 | SER  | N-CA-C    | 5.26  | 116.14      | 107.20   |
| 1   | F     | 281 | SER  | N-CA-C    | 5.25  | 116.69      | 110.97   |
| 1   | A     | 266 | VAL  | CB-CA-C   | -5.24 | 102.70      | 111.29   |
| 1   | A     | 158 | GLY  | N-CA-C    | 5.24  | 118.79      | 111.14   |
| 1   | G     | 283 | GLU  | CA-C-O    | 5.23  | 127.23      | 121.11   |
| 1   | B     | 541 | TRP  | N-CA-C    | 5.23  | 118.64      | 110.32   |
| 1   | A     | 294 | GLY  | N-CA-C    | -5.22 | 100.81      | 113.18   |
| 1   | B     | 435 | GLU  | N-CA-C    | 5.21  | 117.90      | 109.40   |
| 1   | C     | 435 | GLU  | N-CA-C    | 5.21  | 117.89      | 109.40   |
| 1   | E     | 282 | GLU  | N-CA-C    | 5.21  | 118.55      | 110.17   |
| 1   | G     | 276 | ARG  | CA-C-N    | -5.21 | 112.78      | 120.28   |
| 1   | G     | 276 | ARG  | C-N-CA    | -5.21 | 112.78      | 120.28   |
| 1   | E     | 514 | VAL  | N-CA-C    | 5.20  | 115.61      | 108.12   |
| 1   | F     | 240 | GLU  | N-CA-C    | -5.20 | 105.73      | 111.71   |
| 1   | F     | 294 | GLY  | N-CA-C    | -5.20 | 100.86      | 113.18   |
| 1   | C     | 310 | VAL  | CB-CA-C   | -5.19 | 104.48      | 110.91   |
| 1   | F     | 176 | VAL  | N-CA-C    | -5.17 | 100.32      | 108.90   |
| 1   | B     | 430 | VAL  | CA-C-O    | 5.17  | 127.24      | 120.78   |
| 1   | C     | 260 | TRP  | N-CA-C    | 5.16  | 121.79      | 110.80   |
| 1   | A     | 169 | GLN  | N-CA-C    | -5.15 | 99.83       | 110.80   |
| 1   | A     | 92  | GLN  | CG-CD-NE2 | 5.14  | 124.11      | 116.40   |
| 1   | E     | 430 | VAL  | CA-C-O    | 5.13  | 127.19      | 120.78   |
| 1   | D     | 396 | SER  | N-CA-C    | 5.11  | 121.68      | 110.80   |
| 1   | C     | 108 | VAL  | N-CA-C    | 5.09  | 115.18      | 107.80   |
| 1   | G     | 332 | ALA  | N-CA-C    | -5.09 | 105.42      | 110.97   |
| 1   | D     | 519 | LEU  | N-CA-C    | -5.08 | 107.08      | 113.28   |
| 1   | D     | 430 | VAL  | CA-C-O    | 5.07  | 127.12      | 120.78   |
| 1   | F     | 430 | VAL  | CA-C-O    | 5.07  | 127.11      | 120.78   |
| 1   | C     | 430 | VAL  | CA-C-O    | 5.05  | 127.09      | 120.78   |
| 1   | B     | 468 | ASN  | CA-C-N    | 5.04  | 126.14      | 119.84   |
| 1   | B     | 468 | ASN  | C-N-CA    | 5.04  | 126.14      | 119.84   |
| 1   | G     | 261 | ILE  | CA-C-O    | 5.04  | 126.70      | 119.95   |
| 1   | G     | 435 | GLU  | N-CA-C    | 5.03  | 117.60      | 109.40   |
| 1   | A     | 255 | TRP  | N-CA-CB   | 5.03  | 117.46      | 109.71   |
| 1   | G     | 108 | VAL  | N-CA-C    | 5.03  | 115.09      | 107.80   |
| 1   | B     | 396 | SER  | N-CA-C    | 5.03  | 121.51      | 110.80   |
| 1   | A     | 180 | HIS  | N-CA-C    | -5.02 | 105.54      | 113.02   |
| 1   | D     | 293 | THR  | N-CA-C    | -5.02 | 102.86      | 110.24   |
| 1   | F     | 230 | VAL  | N-CA-C    | 5.01  | 115.80      | 108.58   |
| 1   | F     | 425 | HIS  | N-CA-CB   | -5.00 | 102.03      | 110.49   |
| 1   | E     | 396 | SER  | N-CA-C    | 5.00  | 121.46      | 110.80   |

There are no chirality outliers.

All (29) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 260 | TRP  | Mainchain |
| 1   | A     | 261 | ILE  | Peptide   |
| 1   | A     | 282 | GLU  | Peptide   |
| 1   | A     | 396 | SER  | Peptide   |
| 1   | B     | 167 | GLU  | Mainchain |
| 1   | B     | 173 | TYR  | Mainchain |
| 1   | B     | 396 | SER  | Peptide   |
| 1   | C     | 167 | GLU  | Mainchain |
| 1   | C     | 173 | TYR  | Mainchain |
| 1   | C     | 282 | GLU  | Peptide   |
| 1   | C     | 283 | GLU  | Peptide   |
| 1   | C     | 396 | SER  | Peptide   |
| 1   | D     | 167 | GLU  | Mainchain |
| 1   | D     | 173 | TYR  | Mainchain |
| 1   | D     | 282 | GLU  | Peptide   |
| 1   | D     | 396 | SER  | Peptide   |
| 1   | E     | 167 | GLU  | Mainchain |
| 1   | E     | 173 | TYR  | Mainchain |
| 1   | E     | 282 | GLU  | Peptide   |
| 1   | E     | 396 | SER  | Peptide   |
| 1   | F     | 167 | GLU  | Mainchain |
| 1   | F     | 173 | TYR  | Mainchain |
| 1   | F     | 282 | GLU  | Peptide   |
| 1   | F     | 283 | GLU  | Peptide   |
| 1   | F     | 396 | SER  | Peptide   |
| 1   | G     | 167 | GLU  | Mainchain |
| 1   | G     | 173 | TYR  | Mainchain |
| 1   | G     | 282 | GLU  | Peptide   |
| 1   | G     | 396 | SER  | Peptide   |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3744  | 0        | 3697     | 581     | 0            |
| 1   | B     | 3744  | 0        | 3697     | 515     | 0            |
| 1   | C     | 3744  | 0        | 3697     | 580     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | D     | 3744  | 0        | 3697     | 553     | 0            |
| 1   | E     | 3744  | 0        | 3697     | 557     | 0            |
| 1   | F     | 3744  | 0        | 3697     | 554     | 0            |
| 1   | G     | 3744  | 0        | 3697     | 531     | 0            |
| All | All   | 26208 | 0        | 25879    | 3706    | 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 71.

All (3706) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:276:ARG:HH11 | 1:G:276:ARG:CB   | 1.16                     | 1.55              |
| 1:B:248:ARG:HH11 | 1:B:248:ARG:CB   | 1.19                     | 1.51              |
| 1:F:260:TRP:HB2  | 1:F:262:PRO:CD   | 1.49                     | 1.40              |
| 1:G:276:ARG:HB3  | 1:G:276:ARG:NH1  | 1.31                     | 1.40              |
| 1:F:260:TRP:CB   | 1:F:262:PRO:HD2  | 1.56                     | 1.35              |
| 1:B:441:MET:HE2  | 1:B:441:MET:O    | 1.27                     | 1.34              |
| 1:B:244:ASN:HD22 | 1:B:244:ASN:C    | 1.31                     | 1.34              |
| 1:B:248:ARG:NH1  | 1:B:248:ARG:HB3  | 1.38                     | 1.33              |
| 1:G:220:ALA:CB   | 1:G:261:ILE:HG21 | 1.63                     | 1.27              |
| 1:D:483:ILE:O    | 1:D:486:LEU:HB2  | 1.34                     | 1.25              |
| 1:A:260:TRP:O    | 1:A:261:ILE:HG22 | 1.38                     | 1.23              |
| 1:D:366:ASP:HB2  | 1:E:284:SER:OG   | 1.37                     | 1.22              |
| 1:C:290:SER:H    | 1:C:325:GLN:NE2  | 1.37                     | 1.22              |
| 1:B:483:ILE:O    | 1:B:486:LEU:HB2  | 1.38                     | 1.20              |
| 1:C:260:TRP:HB2  | 1:C:262:PRO:HD2  | 1.23                     | 1.19              |
| 1:F:483:ILE:O    | 1:F:486:LEU:HB2  | 1.41                     | 1.18              |
| 1:E:261:ILE:H    | 1:E:262:PRO:CD   | 1.55                     | 1.18              |
| 1:A:315:GLY:HA2  | 1:A:317:VAL:CG2  | 1.74                     | 1.18              |
| 1:E:220:ALA:CB   | 1:E:261:ILE:HG21 | 1.74                     | 1.17              |
| 1:F:127:ASP:O    | 1:F:128:LYS:HB2  | 1.38                     | 1.16              |
| 1:B:483:ILE:H    | 1:B:483:ILE:HD12 | 1.04                     | 1.16              |
| 1:D:220:ALA:HB3  | 1:D:261:ILE:CG2  | 1.73                     | 1.16              |
| 1:A:440:LYS:HZ3  | 1:A:441:MET:HA   | 1.05                     | 1.16              |
| 1:D:339:LEU:HB3  | 1:D:341:MET:CE   | 1.75                     | 1.15              |
| 1:E:440:LYS:HZ3  | 1:E:441:MET:HA   | 1.05                     | 1.15              |
| 1:A:412:MET:HE2  | 1:A:421:ILE:CD1  | 1.76                     | 1.15              |
| 1:D:290:SER:H    | 1:D:325:GLN:NE2  | 1.43                     | 1.15              |
| 1:G:483:ILE:O    | 1:G:486:LEU:HB2  | 1.45                     | 1.15              |
| 1:G:483:ILE:H    | 1:G:483:ILE:HD12 | 1.07                     | 1.15              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:440:LYS:NZ   | 1:E:441:MET:HA   | 1.63                     | 1.14              |
| 1:C:261:ILE:H    | 1:C:262:PRO:CD   | 1.55                     | 1.14              |
| 1:D:127:ASP:O    | 1:D:128:LYS:HB2  | 1.34                     | 1.14              |
| 1:E:483:ILE:O    | 1:E:486:LEU:HB2  | 1.46                     | 1.14              |
| 1:A:220:ALA:CB   | 1:A:261:ILE:HD12 | 1.78                     | 1.14              |
| 1:C:412:MET:HA   | 1:C:416:LEU:HD12 | 1.30                     | 1.13              |
| 1:B:127:ASP:O    | 1:B:128:LYS:HB2  | 1.43                     | 1.13              |
| 1:F:483:ILE:HD12 | 1:F:483:ILE:H    | 1.13                     | 1.12              |
| 1:A:290:SER:H    | 1:A:325:GLN:NE2  | 1.46                     | 1.12              |
| 1:A:315:GLY:CA   | 1:A:317:VAL:HG23 | 1.79                     | 1.12              |
| 1:A:126:LYS:HZ2  | 1:A:127:ASP:CA   | 1.63                     | 1.11              |
| 1:C:440:LYS:NZ   | 1:C:441:MET:HA   | 1.65                     | 1.11              |
| 1:E:412:MET:HE2  | 1:E:421:ILE:CD1  | 1.80                     | 1.11              |
| 1:F:440:LYS:HZ3  | 1:F:441:MET:HA   | 1.03                     | 1.11              |
| 1:B:283:GLU:CG   | 1:B:286:GLY:HA2  | 1.80                     | 1.11              |
| 1:D:261:ILE:N    | 1:D:262:PRO:HD2  | 1.48                     | 1.11              |
| 1:C:127:ASP:O    | 1:C:128:LYS:HB2  | 1.39                     | 1.11              |
| 1:C:339:LEU:HB3  | 1:C:341:MET:CE   | 1.82                     | 1.10              |
| 1:A:483:ILE:O    | 1:A:486:LEU:HB2  | 1.50                     | 1.10              |
| 1:E:504:ARG:HD3  | 1:E:506:GLN:HG2  | 1.22                     | 1.10              |
| 1:F:504:ARG:HD3  | 1:F:506:GLN:HG2  | 1.23                     | 1.10              |
| 1:C:261:ILE:H    | 1:C:262:PRO:HD2  | 1.15                     | 1.10              |
| 1:C:440:LYS:HZ3  | 1:C:441:MET:HA   | 1.05                     | 1.10              |
| 1:E:220:ALA:HB3  | 1:E:261:ILE:HG21 | 1.22                     | 1.10              |
| 1:G:220:ALA:HB3  | 1:G:261:ILE:HG21 | 1.12                     | 1.10              |
| 1:G:504:ARG:HD3  | 1:G:506:GLN:HG2  | 1.23                     | 1.09              |
| 1:B:244:ASN:O    | 1:B:244:ASN:ND2  | 1.83                     | 1.09              |
| 1:B:283:GLU:HG3  | 1:B:286:GLY:HA2  | 1.24                     | 1.09              |
| 1:D:483:ILE:H    | 1:D:483:ILE:HD12 | 1.15                     | 1.09              |
| 1:A:260:TRP:O    | 1:A:261:ILE:CG2  | 2.00                     | 1.09              |
| 1:B:504:ARG:HD3  | 1:B:506:GLN:HG2  | 1.32                     | 1.09              |
| 1:D:261:ILE:N    | 1:D:262:PRO:CD   | 2.12                     | 1.09              |
| 1:B:283:GLU:HG3  | 1:B:286:GLY:CA   | 1.83                     | 1.09              |
| 1:E:127:ASP:O    | 1:E:128:LYS:HB2  | 1.32                     | 1.09              |
| 1:G:290:SER:H    | 1:G:325:GLN:NE2  | 1.48                     | 1.09              |
| 1:C:483:ILE:H    | 1:C:483:ILE:HD12 | 1.14                     | 1.08              |
| 1:E:370:ARG:NH1  | 1:E:371:GLU:HG2  | 1.67                     | 1.08              |
| 1:D:220:ALA:CB   | 1:D:261:ILE:HG21 | 1.82                     | 1.08              |
| 1:D:447:THR:HG22 | 1:D:495:LEU:HD21 | 1.29                     | 1.08              |
| 1:B:248:ARG:CB   | 1:B:248:ARG:NH1  | 2.03                     | 1.08              |
| 1:A:220:ALA:HB3  | 1:A:261:ILE:HD12 | 1.32                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:454:LYS:NZ   | 1:G:344:GLU:HA   | 1.68                     | 1.07              |
| 1:E:441:MET:HE2  | 1:E:444:ASN:HB3  | 1.37                     | 1.07              |
| 1:B:483:ILE:HD12 | 1:B:483:ILE:N    | 1.62                     | 1.07              |
| 1:F:283:GLU:OE2  | 1:F:286:GLY:HA2  | 1.55                     | 1.07              |
| 1:E:253:GLN:HA   | 1:E:257:ALA:HB2  | 1.37                     | 1.07              |
| 1:F:440:LYS:NZ   | 1:F:441:MET:HA   | 1.69                     | 1.07              |
| 1:F:447:THR:HG22 | 1:F:495:LEU:HD21 | 1.35                     | 1.06              |
| 1:A:315:GLY:HA2  | 1:A:317:VAL:HG23 | 1.12                     | 1.06              |
| 1:B:290:SER:H    | 1:B:325:GLN:NE2  | 1.53                     | 1.06              |
| 1:C:441:MET:HE2  | 1:C:441:MET:O    | 1.56                     | 1.06              |
| 1:B:339:LEU:HB3  | 1:B:341:MET:CE   | 1.85                     | 1.05              |
| 1:A:127:ASP:O    | 1:A:128:LYS:HB2  | 1.26                     | 1.05              |
| 1:C:483:ILE:HD12 | 1:C:483:ILE:N    | 1.71                     | 1.05              |
| 1:D:321:PHE:CD2  | 1:D:533:MET:HE1  | 1.90                     | 1.05              |
| 1:D:440:LYS:HZ3  | 1:D:441:MET:HA   | 1.16                     | 1.05              |
| 1:E:412:MET:HA   | 1:E:416:LEU:HD12 | 1.35                     | 1.05              |
| 1:F:290:SER:H    | 1:F:325:GLN:NE2  | 1.52                     | 1.05              |
| 1:C:504:ARG:HD3  | 1:C:506:GLN:HG2  | 1.35                     | 1.05              |
| 1:E:483:ILE:H    | 1:E:483:ILE:HD12 | 1.19                     | 1.04              |
| 1:G:358:ASN:O    | 1:G:360:VAL:HG13 | 1.57                     | 1.04              |
| 1:A:126:LYS:NZ   | 1:A:127:ASP:HA   | 1.72                     | 1.04              |
| 1:A:504:ARG:HD3  | 1:A:506:GLN:HG2  | 1.40                     | 1.04              |
| 1:C:412:MET:HE2  | 1:C:421:ILE:CD1  | 1.88                     | 1.04              |
| 1:G:483:ILE:HD12 | 1:G:483:ILE:N    | 1.72                     | 1.04              |
| 1:B:412:MET:HA   | 1:B:416:LEU:HD12 | 1.37                     | 1.04              |
| 1:D:440:LYS:NZ   | 1:D:441:MET:HA   | 1.71                     | 1.04              |
| 1:D:412:MET:HA   | 1:D:416:LEU:HD12 | 1.34                     | 1.04              |
| 1:B:229:ARG:NH2  | 1:B:259:PRO:HB3  | 1.73                     | 1.04              |
| 1:B:447:THR:HG22 | 1:B:495:LEU:HD21 | 1.36                     | 1.04              |
| 1:A:339:LEU:HB3  | 1:A:341:MET:CE   | 1.86                     | 1.03              |
| 1:A:412:MET:HA   | 1:A:416:LEU:HD12 | 1.40                     | 1.03              |
| 1:E:290:SER:H    | 1:E:325:GLN:NE2  | 1.54                     | 1.03              |
| 1:F:412:MET:HA   | 1:F:416:LEU:HD12 | 1.36                     | 1.03              |
| 1:D:401:GLU:HG3  | 1:D:431:SER:O    | 1.57                     | 1.03              |
| 1:G:447:THR:HG22 | 1:G:495:LEU:HD21 | 1.37                     | 1.03              |
| 1:G:440:LYS:HZ3  | 1:G:441:MET:HA   | 1.13                     | 1.03              |
| 1:A:126:LYS:HZ2  | 1:A:127:ASP:HA   | 1.20                     | 1.03              |
| 1:C:450:LYS:CE   | 1:C:454:LYS:HD3  | 1.88                     | 1.03              |
| 1:G:440:LYS:NZ   | 1:G:441:MET:HA   | 1.74                     | 1.03              |
| 1:C:312:SER:HB2  | 1:C:502:LEU:O    | 1.60                     | 1.02              |
| 1:C:450:LYS:HE2  | 1:C:454:LYS:HD3  | 1.38                     | 1.02              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:483:ILE:H    | 1:B:483:ILE:CD1  | 1.72                     | 1.02              |
| 1:B:440:LYS:NZ   | 1:B:441:MET:HA   | 1.73                     | 1.02              |
| 1:A:483:ILE:HD12 | 1:A:483:ILE:H    | 1.18                     | 1.02              |
| 1:E:450:LYS:HE2  | 1:E:454:LYS:HD3  | 1.40                     | 1.02              |
| 1:B:440:LYS:HZ3  | 1:B:441:MET:HA   | 1.23                     | 1.01              |
| 1:C:483:ILE:O    | 1:C:486:LEU:HB2  | 1.58                     | 1.01              |
| 1:F:339:LEU:HB3  | 1:F:341:MET:CE   | 1.89                     | 1.01              |
| 1:A:440:LYS:NZ   | 1:A:441:MET:HA   | 1.76                     | 1.01              |
| 1:E:339:LEU:HB3  | 1:E:341:MET:CE   | 1.90                     | 1.01              |
| 1:B:321:PHE:CD2  | 1:B:533:MET:HE1  | 1.96                     | 1.01              |
| 1:E:261:ILE:H    | 1:E:262:PRO:HD3  | 1.25                     | 1.01              |
| 1:A:450:LYS:HE2  | 1:A:454:LYS:HD3  | 1.43                     | 1.00              |
| 1:B:450:LYS:CE   | 1:B:454:LYS:HD3  | 1.91                     | 1.00              |
| 1:B:450:LYS:HE2  | 1:B:454:LYS:HD3  | 1.43                     | 1.00              |
| 1:A:172:LYS:O    | 1:A:172:LYS:CG   | 2.06                     | 1.00              |
| 1:E:450:LYS:CE   | 1:E:454:LYS:HD3  | 1.91                     | 1.00              |
| 1:F:321:PHE:CD2  | 1:F:533:MET:HE1  | 1.97                     | 0.99              |
| 1:D:409:LEU:HD23 | 1:D:421:ILE:HG21 | 1.44                     | 0.99              |
| 1:D:412:MET:HE2  | 1:D:421:ILE:CD1  | 1.92                     | 0.99              |
| 1:C:447:THR:HG22 | 1:C:495:LEU:HD21 | 1.44                     | 0.99              |
| 1:D:260:TRP:HB2  | 1:D:262:PRO:CG   | 1.92                     | 0.99              |
| 1:A:447:THR:HG22 | 1:A:495:LEU:HD21 | 1.40                     | 0.98              |
| 1:F:409:LEU:HD23 | 1:F:421:ILE:HG21 | 1.42                     | 0.98              |
| 1:F:112:ARG:HB3  | 1:F:117:ASN:O    | 1.63                     | 0.98              |
| 1:A:441:MET:HE2  | 1:A:444:ASN:HB3  | 1.45                     | 0.98              |
| 1:F:441:MET:HE2  | 1:F:444:ASN:HB3  | 1.45                     | 0.98              |
| 1:A:450:LYS:CE   | 1:A:454:LYS:HD3  | 1.92                     | 0.98              |
| 1:E:483:ILE:HD12 | 1:E:483:ILE:N    | 1.77                     | 0.98              |
| 1:A:259:PRO:O    | 1:A:260:TRP:HB3  | 1.64                     | 0.98              |
| 1:F:483:ILE:HD12 | 1:F:483:ILE:N    | 1.76                     | 0.98              |
| 1:G:412:MET:HA   | 1:G:416:LEU:HD12 | 1.41                     | 0.98              |
| 1:G:127:ASP:O    | 1:G:128:LYS:HB2  | 1.59                     | 0.98              |
| 1:F:412:MET:HE2  | 1:F:421:ILE:CD1  | 1.94                     | 0.97              |
| 1:G:483:ILE:H    | 1:G:483:ILE:CD1  | 1.78                     | 0.97              |
| 1:G:450:LYS:HE2  | 1:G:454:LYS:HD3  | 1.44                     | 0.97              |
| 1:D:260:TRP:C    | 1:D:262:PRO:HD2  | 1.89                     | 0.97              |
| 1:D:499:ILE:HG22 | 1:D:519:LEU:HB2  | 1.47                     | 0.97              |
| 1:C:409:LEU:HD23 | 1:C:421:ILE:HG21 | 1.45                     | 0.97              |
| 1:D:504:ARG:HD3  | 1:D:506:GLN:HG2  | 1.44                     | 0.97              |
| 1:E:447:THR:HG22 | 1:E:495:LEU:HD21 | 1.43                     | 0.97              |
| 1:E:321:PHE:CD2  | 1:E:533:MET:HE1  | 2.00                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:412:MET:HE2  | 1:G:421:ILE:CD1  | 1.94                     | 0.97              |
| 1:C:483:ILE:H    | 1:C:483:ILE:CD1  | 1.78                     | 0.97              |
| 1:A:321:PHE:CD2  | 1:A:533:MET:HE1  | 2.00                     | 0.96              |
| 1:A:510:MET:HE2  | 1:A:513:LEU:HD22 | 1.45                     | 0.96              |
| 1:C:260:TRP:O    | 1:C:261:ILE:HG23 | 1.63                     | 0.96              |
| 1:G:492:LEU:H    | 1:G:492:LEU:HD12 | 1.29                     | 0.96              |
| 1:C:510:MET:CE   | 1:C:547:TYR:HE1  | 1.79                     | 0.96              |
| 1:E:370:ARG:HD2  | 1:E:371:GLU:N    | 1.81                     | 0.96              |
| 1:G:499:ILE:HG22 | 1:G:519:LEU:HB2  | 1.48                     | 0.96              |
| 1:D:510:MET:CE   | 1:D:547:TYR:HE1  | 1.79                     | 0.95              |
| 1:D:483:ILE:HD12 | 1:D:483:ILE:N    | 1.77                     | 0.95              |
| 1:G:248:ARG:HB3  | 1:G:248:ARG:HH11 | 1.31                     | 0.95              |
| 1:A:172:LYS:O    | 1:A:172:LYS:HG3  | 1.11                     | 0.95              |
| 1:G:450:LYS:CE   | 1:G:454:LYS:HD3  | 1.96                     | 0.95              |
| 1:E:412:MET:HA   | 1:E:416:LEU:CD1  | 1.95                     | 0.95              |
| 1:D:492:LEU:HD12 | 1:D:492:LEU:H    | 1.32                     | 0.95              |
| 1:E:186:LYS:HD3  | 1:E:218:GLU:HG3  | 1.48                     | 0.95              |
| 1:C:248:ARG:HB3  | 1:C:248:ARG:HH11 | 1.29                     | 0.95              |
| 1:A:126:LYS:HE3  | 1:A:127:ASP:OD1  | 1.66                     | 0.95              |
| 1:A:126:LYS:HG2  | 1:A:127:ASP:N    | 1.77                     | 0.95              |
| 1:A:127:ASP:O    | 1:A:128:LYS:CB   | 2.15                     | 0.95              |
| 1:C:412:MET:HA   | 1:C:416:LEU:CD1  | 1.97                     | 0.94              |
| 1:F:248:ARG:HB3  | 1:F:248:ARG:HH11 | 1.29                     | 0.94              |
| 1:G:276:ARG:CB   | 1:G:276:ARG:NH1  | 2.02                     | 0.94              |
| 1:D:441:MET:HE2  | 1:D:444:ASN:HB3  | 1.45                     | 0.94              |
| 1:F:107:GLN:HB2  | 1:F:124:ARG:HG3  | 1.50                     | 0.94              |
| 1:D:186:LYS:HD3  | 1:D:218:GLU:HG3  | 1.49                     | 0.94              |
| 1:D:366:ASP:HB2  | 1:E:284:SER:CB   | 1.97                     | 0.94              |
| 1:B:229:ARG:HB3  | 1:B:259:PRO:HA   | 1.49                     | 0.94              |
| 1:F:412:MET:HA   | 1:F:416:LEU:CD1  | 1.96                     | 0.94              |
| 1:F:483:ILE:H    | 1:F:483:ILE:CD1  | 1.81                     | 0.94              |
| 1:F:499:ILE:HG22 | 1:F:519:LEU:HB2  | 1.45                     | 0.94              |
| 1:D:97:TRP:CZ3   | 1:D:99:ALA:HB2   | 2.03                     | 0.94              |
| 1:D:510:MET:HE2  | 1:D:513:LEU:HD22 | 1.50                     | 0.94              |
| 1:A:483:ILE:HD12 | 1:A:483:ILE:N    | 1.83                     | 0.93              |
| 1:D:321:PHE:HD2  | 1:D:533:MET:HE1  | 1.28                     | 0.93              |
| 1:A:312:SER:HB2  | 1:A:502:LEU:O    | 1.67                     | 0.93              |
| 1:B:244:ASN:C    | 1:B:244:ASN:ND2  | 2.14                     | 0.93              |
| 1:F:450:LYS:HE2  | 1:F:454:LYS:HD3  | 1.51                     | 0.93              |
| 1:F:309:MET:HB3  | 1:F:499:ILE:HD12 | 1.48                     | 0.93              |
| 1:G:276:ARG:HH11 | 1:G:276:ARG:CG   | 1.82                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:186:LYS:HD3  | 1:B:218:GLU:HG3  | 1.48                     | 0.93              |
| 1:E:216:VAL:HG11 | 1:E:230:VAL:CG2  | 1.99                     | 0.93              |
| 1:G:261:ILE:O    | 1:G:261:ILE:HG22 | 1.69                     | 0.93              |
| 1:A:510:MET:HE2  | 1:A:513:LEU:CD2  | 1.99                     | 0.93              |
| 1:E:409:LEU:HD23 | 1:E:421:ILE:HG21 | 1.49                     | 0.93              |
| 1:C:186:LYS:HD3  | 1:C:218:GLU:HG3  | 1.50                     | 0.93              |
| 1:G:220:ALA:HB3  | 1:G:261:ILE:CG2  | 1.99                     | 0.92              |
| 1:G:321:PHE:CD2  | 1:G:533:MET:HE1  | 2.03                     | 0.92              |
| 1:B:339:LEU:HB3  | 1:B:341:MET:HE1  | 1.50                     | 0.92              |
| 1:F:186:LYS:HD3  | 1:F:218:GLU:HG3  | 1.50                     | 0.92              |
| 1:D:312:SER:HB2  | 1:D:502:LEU:O    | 1.70                     | 0.92              |
| 1:G:290:SER:H    | 1:G:325:GLN:HE21 | 1.16                     | 0.92              |
| 1:C:97:TRP:CZ3   | 1:C:99:ALA:HB2   | 2.05                     | 0.92              |
| 1:E:248:ARG:HB3  | 1:E:248:ARG:HH11 | 1.34                     | 0.91              |
| 1:A:412:MET:HE2  | 1:A:421:ILE:HD12 | 1.50                     | 0.91              |
| 1:G:186:LYS:HD3  | 1:G:218:GLU:HG3  | 1.50                     | 0.91              |
| 1:D:248:ARG:HH11 | 1:D:248:ARG:HB3  | 1.35                     | 0.91              |
| 1:B:492:LEU:H    | 1:B:492:LEU:HD12 | 1.33                     | 0.91              |
| 1:D:290:SER:H    | 1:D:325:GLN:HE21 | 1.14                     | 0.91              |
| 1:F:312:SER:HB2  | 1:F:502:LEU:O    | 1.71                     | 0.91              |
| 1:A:344:GLU:HG3  | 1:A:349:THR:HG22 | 1.53                     | 0.91              |
| 1:D:216:VAL:HG11 | 1:D:230:VAL:CG2  | 2.01                     | 0.91              |
| 1:B:228:VAL:HB   | 1:B:261:ILE:HD11 | 1.52                     | 0.91              |
| 1:B:344:GLU:HG3  | 1:B:349:THR:HG22 | 1.51                     | 0.91              |
| 1:E:483:ILE:H    | 1:E:483:ILE:CD1  | 1.83                     | 0.91              |
| 1:C:208:MET:HE2  | 1:C:233:LEU:H    | 1.36                     | 0.90              |
| 1:D:166:MET:HE2  | 1:D:171:CYS:SG   | 2.11                     | 0.90              |
| 1:E:499:ILE:HG22 | 1:E:519:LEU:HB2  | 1.53                     | 0.90              |
| 1:B:510:MET:CE   | 1:B:547:TYR:HE1  | 1.84                     | 0.90              |
| 1:D:412:MET:HA   | 1:D:416:LEU:CD1  | 2.00                     | 0.90              |
| 1:E:289:PHE:H    | 1:E:296:ASN:HD21 | 1.19                     | 0.90              |
| 1:B:282:GLU:OE2  | 1:B:282:GLU:HA   | 1.69                     | 0.90              |
| 1:C:321:PHE:CD2  | 1:C:533:MET:HE1  | 2.07                     | 0.90              |
| 1:D:152:LYS:HD3  | 1:D:203:ILE:HD11 | 1.53                     | 0.90              |
| 1:D:259:PRO:O    | 1:D:260:TRP:HB3  | 1.68                     | 0.90              |
| 1:F:450:LYS:CE   | 1:F:454:LYS:HD3  | 2.01                     | 0.90              |
| 1:C:290:SER:H    | 1:C:325:GLN:HE21 | 1.10                     | 0.90              |
| 1:D:289:PHE:H    | 1:D:296:ASN:HD21 | 1.15                     | 0.90              |
| 1:D:510:MET:CE   | 1:D:547:TYR:CE1  | 2.54                     | 0.90              |
| 1:D:483:ILE:H    | 1:D:483:ILE:CD1  | 1.84                     | 0.90              |
| 1:E:290:SER:H    | 1:E:325:GLN:HE21 | 1.20                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:469:PRO:O    | 1:E:470:ASP:HB2  | 1.71                     | 0.90              |
| 1:F:344:GLU:HG3  | 1:F:349:THR:HG22 | 1.51                     | 0.90              |
| 1:G:312:SER:HB2  | 1:G:502:LEU:O    | 1.72                     | 0.90              |
| 1:A:510:MET:CE   | 1:A:547:TYR:CE1  | 2.55                     | 0.90              |
| 1:C:261:ILE:N    | 1:C:262:PRO:HD2  | 1.84                     | 0.90              |
| 1:C:469:PRO:O    | 1:C:470:ASP:HB2  | 1.71                     | 0.90              |
| 1:D:260:TRP:HB2  | 1:D:262:PRO:HG3  | 1.49                     | 0.90              |
| 1:A:186:LYS:HD3  | 1:A:218:GLU:HG3  | 1.52                     | 0.89              |
| 1:A:499:ILE:HG22 | 1:A:519:LEU:HB2  | 1.53                     | 0.89              |
| 1:E:97:TRP:CZ3   | 1:E:99:ALA:HB2   | 2.08                     | 0.89              |
| 1:B:409:LEU:HD23 | 1:B:421:ILE:HG21 | 1.53                     | 0.89              |
| 1:E:127:ASP:O    | 1:E:128:LYS:CB   | 2.19                     | 0.89              |
| 1:E:261:ILE:N    | 1:E:262:PRO:CD   | 2.31                     | 0.89              |
| 1:A:97:TRP:CZ3   | 1:A:99:ALA:HB2   | 2.07                     | 0.89              |
| 1:F:546:SER:O    | 1:F:547:TYR:HB2  | 1.70                     | 0.89              |
| 1:G:220:ALA:HB1  | 1:G:261:ILE:HG21 | 1.54                     | 0.89              |
| 1:G:409:LEU:HD23 | 1:G:421:ILE:HG21 | 1.52                     | 0.89              |
| 1:A:409:LEU:HD23 | 1:A:421:ILE:HG21 | 1.55                     | 0.89              |
| 1:C:107:GLN:HB2  | 1:C:124:ARG:HG3  | 1.53                     | 0.89              |
| 1:C:344:GLU:HG3  | 1:C:349:THR:HG22 | 1.53                     | 0.89              |
| 1:G:339:LEU:HB3  | 1:G:341:MET:HE2  | 1.53                     | 0.89              |
| 1:G:510:MET:CE   | 1:G:547:TYR:HE1  | 1.86                     | 0.89              |
| 1:E:168:LEU:HD21 | 1:E:247:ASP:OD2  | 1.72                     | 0.89              |
| 1:G:401:GLU:HG3  | 1:G:431:SER:O    | 1.73                     | 0.88              |
| 1:C:510:MET:CE   | 1:C:547:TYR:CE1  | 2.56                     | 0.88              |
| 1:B:499:ILE:HG22 | 1:B:519:LEU:HB2  | 1.53                     | 0.88              |
| 1:A:248:ARG:HB3  | 1:A:248:ARG:HH11 | 1.38                     | 0.88              |
| 1:E:107:GLN:HB2  | 1:E:124:ARG:HG3  | 1.56                     | 0.88              |
| 1:A:412:MET:HA   | 1:A:416:LEU:CD1  | 2.03                     | 0.88              |
| 1:F:217:GLU:OE2  | 1:F:261:ILE:HG22 | 1.72                     | 0.88              |
| 1:C:168:LEU:HD21 | 1:C:247:ASP:OD2  | 1.73                     | 0.88              |
| 1:C:260:TRP:HB2  | 1:C:262:PRO:CD   | 2.04                     | 0.88              |
| 1:E:490:GLY:HA2  | 1:E:493:ARG:HG3  | 1.56                     | 0.88              |
| 1:C:290:SER:N    | 1:C:325:GLN:NE2  | 2.22                     | 0.88              |
| 1:B:168:LEU:HD21 | 1:B:247:ASP:OD2  | 1.73                     | 0.87              |
| 1:G:108:VAL:HG13 | 1:G:123:VAL:HG22 | 1.56                     | 0.87              |
| 1:B:510:MET:CE   | 1:B:547:TYR:CE1  | 2.57                     | 0.87              |
| 1:G:152:LYS:HD3  | 1:G:203:ILE:HD11 | 1.57                     | 0.87              |
| 1:A:469:PRO:O    | 1:A:470:ASP:HB2  | 1.73                     | 0.87              |
| 1:E:370:ARG:HH11 | 1:E:371:GLU:HG2  | 1.34                     | 0.87              |
| 1:B:107:GLN:HB2  | 1:B:124:ARG:HG3  | 1.55                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:199:PHE:O    | 1:D:227:LYS:HE2  | 1.75                     | 0.87              |
| 1:F:168:LEU:HD21 | 1:F:247:ASP:OD2  | 1.75                     | 0.87              |
| 1:B:316:MET:HE1  | 1:B:535:TYR:CE2  | 2.10                     | 0.87              |
| 1:C:289:PHE:H    | 1:C:296:ASN:HD21 | 1.21                     | 0.87              |
| 1:E:108:VAL:HG13 | 1:E:123:VAL:HG22 | 1.57                     | 0.87              |
| 1:A:483:ILE:H    | 1:A:483:ILE:CD1  | 1.88                     | 0.86              |
| 1:F:178:LEU:HB3  | 1:F:181:GLY:HA2  | 1.57                     | 0.86              |
| 1:A:510:MET:CE   | 1:A:547:TYR:HE1  | 1.88                     | 0.86              |
| 1:E:318:MET:HE1  | 1:E:465:HIS:CD2  | 2.10                     | 0.86              |
| 1:G:168:LEU:HD21 | 1:G:247:ASP:OD2  | 1.74                     | 0.86              |
| 1:A:366:ASP:HB2  | 1:C:285:VAL:CG2  | 2.05                     | 0.86              |
| 1:B:412:MET:HA   | 1:B:416:LEU:CD1  | 2.04                     | 0.86              |
| 1:D:108:VAL:HG13 | 1:D:123:VAL:HG22 | 1.57                     | 0.86              |
| 1:G:276:ARG:HH11 | 1:G:276:ARG:HB3  | 0.69                     | 0.86              |
| 1:D:450:LYS:HE2  | 1:D:454:LYS:HD3  | 1.58                     | 0.86              |
| 1:F:107:GLN:CB   | 1:F:124:ARG:HG3  | 2.06                     | 0.86              |
| 1:A:290:SER:H    | 1:A:325:GLN:HE21 | 1.17                     | 0.86              |
| 1:D:107:GLN:HB2  | 1:D:124:ARG:HG3  | 1.56                     | 0.86              |
| 1:D:166:MET:CE   | 1:D:171:CYS:SG   | 2.64                     | 0.86              |
| 1:G:216:VAL:HG11 | 1:G:230:VAL:CG2  | 2.06                     | 0.86              |
| 1:B:321:PHE:HD2  | 1:B:533:MET:HE1  | 1.40                     | 0.85              |
| 1:E:315:GLY:HA2  | 1:E:317:VAL:HG23 | 1.58                     | 0.85              |
| 1:G:107:GLN:HB2  | 1:G:124:ARG:HG3  | 1.56                     | 0.85              |
| 1:G:504:ARG:CD   | 1:G:506:GLN:HG2  | 2.06                     | 0.85              |
| 1:A:260:TRP:C    | 1:A:261:ILE:HG22 | 1.98                     | 0.85              |
| 1:C:127:ASP:O    | 1:C:128:LYS:CB   | 2.24                     | 0.85              |
| 1:D:339:LEU:HB3  | 1:D:341:MET:HE1  | 1.56                     | 0.85              |
| 1:G:412:MET:HA   | 1:G:416:LEU:CD1  | 2.04                     | 0.85              |
| 1:G:97:TRP:CZ3   | 1:G:99:ALA:HB2   | 2.12                     | 0.85              |
| 1:B:283:GLU:CD   | 1:B:286:GLY:HA2  | 2.01                     | 0.85              |
| 1:C:166:MET:CE   | 1:C:171:CYS:SG   | 2.65                     | 0.85              |
| 1:C:499:ILE:HG22 | 1:C:519:LEU:HB2  | 1.59                     | 0.85              |
| 1:C:510:MET:HE2  | 1:C:513:LEU:HD22 | 1.57                     | 0.85              |
| 1:C:510:MET:HE3  | 1:C:547:TYR:HE1  | 1.39                     | 0.85              |
| 1:E:108:VAL:HG12 | 1:E:121:GLN:HG2  | 1.59                     | 0.85              |
| 1:E:312:SER:HB2  | 1:E:502:LEU:O    | 1.77                     | 0.85              |
| 1:C:108:VAL:HG13 | 1:C:123:VAL:HG22 | 1.59                     | 0.85              |
| 1:E:482:SER:H    | 1:E:485:ASP:HB2  | 1.41                     | 0.85              |
| 1:B:108:VAL:HG13 | 1:B:123:VAL:HG22 | 1.56                     | 0.84              |
| 1:D:220:ALA:HB3  | 1:D:261:ILE:HG21 | 0.88                     | 0.84              |
| 1:G:510:MET:CE   | 1:G:547:TYR:CE1  | 2.60                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:490:GLY:HA2  | 1:B:493:ARG:HG3  | 1.58                     | 0.84              |
| 1:B:510:MET:HE2  | 1:B:513:LEU:HD22 | 1.60                     | 0.84              |
| 1:E:413:ARG:HE   | 1:E:458:VAL:HB   | 1.43                     | 0.84              |
| 1:D:168:LEU:HD21 | 1:D:247:ASP:OD2  | 1.75                     | 0.84              |
| 1:F:425:HIS:CE1  | 1:F:427:SER:HB2  | 2.13                     | 0.84              |
| 1:A:510:MET:HE3  | 1:A:547:TYR:HE1  | 1.39                     | 0.84              |
| 1:D:344:GLU:HG3  | 1:D:349:THR:HG22 | 1.58                     | 0.84              |
| 1:A:482:SER:H    | 1:A:485:ASP:HB2  | 1.41                     | 0.84              |
| 1:B:141:LEU:HD13 | 1:B:176:VAL:HG21 | 1.60                     | 0.84              |
| 1:B:152:LYS:HD3  | 1:B:203:ILE:HD11 | 1.58                     | 0.84              |
| 1:C:369:LYS:HG2  | 1:D:279:LEU:HD23 | 1.58                     | 0.84              |
| 1:E:370:ARG:CD   | 1:E:371:GLU:N    | 2.41                     | 0.84              |
| 1:G:166:MET:CE   | 1:G:171:CYS:SG   | 2.66                     | 0.84              |
| 1:B:289:PHE:H    | 1:B:296:ASN:HD21 | 1.25                     | 0.84              |
| 1:D:442:ILE:HD11 | 1:D:492:LEU:HD21 | 1.60                     | 0.84              |
| 1:F:152:LYS:HD3  | 1:F:203:ILE:HD11 | 1.59                     | 0.84              |
| 1:F:107:GLN:HB2  | 1:F:124:ARG:CG   | 2.08                     | 0.83              |
| 1:F:178:LEU:CB   | 1:F:181:GLY:HA2  | 2.08                     | 0.83              |
| 1:G:309:MET:HB3  | 1:G:499:ILE:HD12 | 1.61                     | 0.83              |
| 1:G:199:PHE:O    | 1:G:227:LYS:HE2  | 1.77                     | 0.83              |
| 1:G:166:MET:HE2  | 1:G:171:CYS:SG   | 2.18                     | 0.83              |
| 1:G:510:MET:HE3  | 1:G:547:TYR:HE1  | 1.43                     | 0.83              |
| 1:G:482:SER:H    | 1:G:485:ASP:HB2  | 1.44                     | 0.83              |
| 1:A:492:LEU:HD12 | 1:A:492:LEU:H    | 1.41                     | 0.83              |
| 1:E:492:LEU:H    | 1:E:492:LEU:HD12 | 1.43                     | 0.83              |
| 1:E:510:MET:CE   | 1:E:547:TYR:HE1  | 1.91                     | 0.83              |
| 1:F:321:PHE:HD2  | 1:F:533:MET:HE1  | 1.38                     | 0.83              |
| 1:C:216:VAL:HG11 | 1:C:230:VAL:CG2  | 2.09                     | 0.83              |
| 1:D:409:LEU:CD2  | 1:D:421:ILE:HG21 | 2.09                     | 0.83              |
| 1:C:141:LEU:HD13 | 1:C:176:VAL:HG21 | 1.60                     | 0.83              |
| 1:E:283:GLU:HG2  | 1:E:284:SER:N    | 1.89                     | 0.83              |
| 1:B:309:MET:HB3  | 1:B:499:ILE:HD12 | 1.59                     | 0.83              |
| 1:C:166:MET:HE2  | 1:C:171:CYS:SG   | 2.18                     | 0.83              |
| 1:F:290:SER:H    | 1:F:325:GLN:HE21 | 1.22                     | 0.83              |
| 1:B:469:PRO:O    | 1:B:470:ASP:HB2  | 1.78                     | 0.82              |
| 1:D:510:MET:HE3  | 1:D:547:TYR:HE1  | 1.44                     | 0.82              |
| 1:G:321:PHE:HD2  | 1:G:533:MET:HE1  | 1.40                     | 0.82              |
| 1:B:441:MET:O    | 1:B:441:MET:CE   | 2.21                     | 0.82              |
| 1:D:309:MET:HB3  | 1:D:499:ILE:HD12 | 1.59                     | 0.82              |
| 1:A:220:ALA:CB   | 1:A:261:ILE:HG21 | 2.08                     | 0.82              |
| 1:B:427:SER:HB3  | 1:B:487:ARG:HH12 | 1.43                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:290:SER:N    | 1:D:325:GLN:NE2  | 2.25                     | 0.82              |
| 1:G:290:SER:N    | 1:G:325:GLN:NE2  | 2.28                     | 0.82              |
| 1:D:289:PHE:N    | 1:D:296:ASN:HD21 | 1.76                     | 0.82              |
| 1:B:253:GLN:HA   | 1:B:257:ALA:HB2  | 1.62                     | 0.82              |
| 1:B:316:MET:HE1  | 1:B:535:TYR:CZ   | 2.15                     | 0.82              |
| 1:C:178:LEU:CB   | 1:C:181:GLY:HA2  | 2.09                     | 0.82              |
| 1:C:208:MET:HE2  | 1:C:233:LEU:N    | 1.95                     | 0.82              |
| 1:D:338:GLY:HA3  | 1:D:412:MET:CE   | 2.10                     | 0.82              |
| 1:D:490:GLY:HA2  | 1:D:493:ARG:HG3  | 1.59                     | 0.82              |
| 1:G:178:LEU:CB   | 1:G:181:GLY:HA2  | 2.09                     | 0.82              |
| 1:A:178:LEU:CB   | 1:A:181:GLY:HA2  | 2.09                     | 0.81              |
| 1:E:405:LEU:HG   | 1:E:409:LEU:HD12 | 1.62                     | 0.81              |
| 1:C:405:LEU:HG   | 1:C:409:LEU:HD12 | 1.62                     | 0.81              |
| 1:F:469:PRO:O    | 1:F:470:ASP:HB2  | 1.80                     | 0.81              |
| 1:G:315:GLY:HA2  | 1:G:317:VAL:HG23 | 1.62                     | 0.81              |
| 1:A:126:LYS:CE   | 1:A:127:ASP:OD1  | 2.28                     | 0.81              |
| 1:A:311:THR:HA   | 1:A:318:MET:HE2  | 1.62                     | 0.81              |
| 1:C:482:SER:H    | 1:C:485:ASP:HB2  | 1.46                     | 0.81              |
| 1:E:141:LEU:HD13 | 1:E:176:VAL:HG21 | 1.60                     | 0.81              |
| 1:F:425:HIS:HE1  | 1:F:427:SER:CB   | 1.93                     | 0.81              |
| 1:F:482:SER:H    | 1:F:485:ASP:HB2  | 1.45                     | 0.81              |
| 1:A:168:LEU:O    | 1:A:169:GLN:HB2  | 1.78                     | 0.81              |
| 1:B:97:TRP:CZ3   | 1:B:99:ALA:HB2   | 2.15                     | 0.81              |
| 1:G:339:LEU:HB3  | 1:G:341:MET:CE   | 2.10                     | 0.81              |
| 1:A:311:THR:C    | 1:A:318:MET:HE2  | 2.06                     | 0.81              |
| 1:A:347:GLU:OE1  | 1:C:274:ARG:HD2  | 1.81                     | 0.81              |
| 1:C:152:LYS:HD3  | 1:C:203:ILE:HD11 | 1.63                     | 0.81              |
| 1:G:344:GLU:HG3  | 1:G:349:THR:HG22 | 1.60                     | 0.81              |
| 1:A:253:GLN:CA   | 1:A:257:ALA:HB2  | 2.11                     | 0.81              |
| 1:F:492:LEU:H    | 1:F:492:LEU:HD12 | 1.43                     | 0.81              |
| 1:D:469:PRO:O    | 1:D:470:ASP:HB2  | 1.80                     | 0.81              |
| 1:E:321:PHE:HD2  | 1:E:533:MET:HE1  | 1.46                     | 0.81              |
| 1:A:292:CYS:O    | 1:A:295:ILE:HG12 | 1.80                     | 0.81              |
| 1:E:510:MET:CE   | 1:E:547:TYR:CE1  | 2.63                     | 0.81              |
| 1:F:425:HIS:CE1  | 1:F:427:SER:OG   | 2.33                     | 0.81              |
| 1:G:515:LEU:HD21 | 1:G:529:ILE:CD1  | 2.10                     | 0.81              |
| 1:A:107:GLN:HB2  | 1:A:124:ARG:HG3  | 1.61                     | 0.81              |
| 1:C:309:MET:HB3  | 1:C:499:ILE:HD12 | 1.62                     | 0.81              |
| 1:A:208:MET:HE2  | 1:A:233:LEU:H    | 1.44                     | 0.81              |
| 1:A:141:LEU:HD11 | 1:A:196:PHE:CZ   | 2.15                     | 0.80              |
| 1:A:229:ARG:CB   | 1:A:258:GLY:O    | 2.29                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:290:SER:N    | 1:A:325:GLN:NE2  | 2.28                     | 0.80              |
| 1:D:178:LEU:CB   | 1:D:181:GLY:HA2  | 2.11                     | 0.80              |
| 1:D:260:TRP:HB2  | 1:D:262:PRO:CD   | 2.10                     | 0.80              |
| 1:A:251:MET:HA   | 1:A:251:MET:HE3  | 1.63                     | 0.80              |
| 1:C:108:VAL:HG12 | 1:C:121:GLN:HG2  | 1.62                     | 0.80              |
| 1:C:473:LYS:HE2  | 1:C:479:ARG:HA   | 1.62                     | 0.80              |
| 1:E:152:LYS:HD3  | 1:E:203:ILE:HD11 | 1.63                     | 0.80              |
| 1:E:344:GLU:HG3  | 1:E:349:THR:HG22 | 1.62                     | 0.80              |
| 1:F:108:VAL:HG13 | 1:F:123:VAL:HG22 | 1.63                     | 0.80              |
| 1:A:229:ARG:HB2  | 1:A:258:GLY:O    | 1.81                     | 0.80              |
| 1:B:510:MET:HE3  | 1:B:547:TYR:HE1  | 1.45                     | 0.80              |
| 1:E:220:ALA:HB1  | 1:E:261:ILE:HD13 | 1.63                     | 0.80              |
| 1:B:216:VAL:HG11 | 1:B:230:VAL:CG2  | 2.11                     | 0.80              |
| 1:D:413:ARG:HE   | 1:D:458:VAL:HB   | 1.47                     | 0.80              |
| 1:D:473:LYS:HG3  | 1:D:479:ARG:HB2  | 1.64                     | 0.80              |
| 1:E:515:LEU:HD21 | 1:E:529:ILE:CD1  | 2.12                     | 0.80              |
| 1:F:251:MET:HA   | 1:F:251:MET:HE3  | 1.62                     | 0.80              |
| 1:A:369:LYS:HG2  | 1:C:279:LEU:CD2  | 2.12                     | 0.80              |
| 1:C:199:PHE:O    | 1:C:227:LYS:HE2  | 1.81                     | 0.80              |
| 1:E:412:MET:HE2  | 1:E:421:ILE:HD13 | 1.63                     | 0.80              |
| 1:B:108:VAL:HG12 | 1:B:121:GLN:HG2  | 1.64                     | 0.79              |
| 1:C:121:GLN:HB2  | 1:C:133:THR:OG1  | 1.82                     | 0.79              |
| 1:F:283:GLU:OE2  | 1:F:286:GLY:CA   | 2.29                     | 0.79              |
| 1:F:425:HIS:CE1  | 1:F:427:SER:CB   | 2.65                     | 0.79              |
| 1:A:141:LEU:HD13 | 1:A:176:VAL:HG21 | 1.63                     | 0.79              |
| 1:D:141:LEU:HD11 | 1:D:196:PHE:CZ   | 2.16                     | 0.79              |
| 1:D:450:LYS:CE   | 1:D:454:LYS:HD3  | 2.12                     | 0.79              |
| 1:E:166:MET:HE2  | 1:E:171:CYS:SG   | 2.21                     | 0.79              |
| 1:E:412:MET:HE2  | 1:E:421:ILE:HD12 | 1.63                     | 0.79              |
| 1:A:427:SER:HB3  | 1:A:487:ARG:HH12 | 1.48                     | 0.79              |
| 1:C:141:LEU:HD11 | 1:C:196:PHE:CZ   | 2.18                     | 0.79              |
| 1:C:492:LEU:H    | 1:C:492:LEU:HD12 | 1.46                     | 0.79              |
| 1:A:121:GLN:HB2  | 1:A:133:THR:OG1  | 1.82                     | 0.79              |
| 1:A:261:ILE:HG12 | 1:A:261:ILE:O    | 1.83                     | 0.79              |
| 1:E:178:LEU:CB   | 1:E:181:GLY:HA2  | 2.13                     | 0.79              |
| 1:A:413:ARG:HE   | 1:A:458:VAL:HB   | 1.48                     | 0.79              |
| 1:E:411:TYR:HE1  | 1:F:265:VAL:HG11 | 1.47                     | 0.79              |
| 1:A:199:PHE:O    | 1:A:227:LYS:HE2  | 1.83                     | 0.79              |
| 1:E:510:MET:HE3  | 1:E:547:TYR:HE1  | 1.48                     | 0.79              |
| 1:D:515:LEU:HD21 | 1:D:529:ILE:CD1  | 2.13                     | 0.79              |
| 1:F:166:MET:CE   | 1:F:171:CYS:SG   | 2.71                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:152:LYS:HG3  | 1:A:201:GLN:HG2  | 1.65                     | 0.79              |
| 1:A:473:LYS:HG3  | 1:A:479:ARG:HB2  | 1.65                     | 0.79              |
| 1:C:168:LEU:CD2  | 1:C:247:ASP:OD2  | 2.31                     | 0.79              |
| 1:C:510:MET:HE2  | 1:C:513:LEU:CD2  | 2.13                     | 0.79              |
| 1:E:108:VAL:CG1  | 1:E:121:GLN:HG2  | 2.13                     | 0.79              |
| 1:E:168:LEU:CD2  | 1:E:247:ASP:OD2  | 2.30                     | 0.79              |
| 1:F:473:LYS:HE2  | 1:F:479:ARG:HA   | 1.64                     | 0.79              |
| 1:G:405:LEU:HG   | 1:G:409:LEU:HD12 | 1.65                     | 0.79              |
| 1:A:220:ALA:HB1  | 1:A:261:ILE:HD12 | 1.65                     | 0.78              |
| 1:D:483:ILE:O    | 1:D:486:LEU:CB   | 2.25                     | 0.78              |
| 1:F:316:MET:HE1  | 1:F:535:TYR:CE2  | 2.18                     | 0.78              |
| 1:F:292:CYS:O    | 1:F:295:ILE:HG12 | 1.82                     | 0.78              |
| 1:B:166:MET:HE2  | 1:B:171:CYS:SG   | 2.22                     | 0.78              |
| 1:C:107:GLN:HB2  | 1:C:124:ARG:CG   | 2.13                     | 0.78              |
| 1:C:488:GLY:HA3  | 1:C:492:LEU:HD11 | 1.66                     | 0.78              |
| 1:D:405:LEU:HG   | 1:D:409:LEU:HD12 | 1.64                     | 0.78              |
| 1:E:166:MET:CE   | 1:E:171:CYS:SG   | 2.71                     | 0.78              |
| 1:E:442:ILE:HD11 | 1:E:492:LEU:HD21 | 1.63                     | 0.78              |
| 1:G:425:HIS:CE1  | 1:G:427:SER:OG   | 2.35                     | 0.78              |
| 1:A:395:ASP:HB3  | 1:C:266:VAL:HG21 | 1.64                     | 0.78              |
| 1:B:442:ILE:CD1  | 1:B:492:LEU:HD11 | 2.12                     | 0.78              |
| 1:C:108:VAL:CG1  | 1:C:121:GLN:HG2  | 2.13                     | 0.78              |
| 1:E:216:VAL:HG11 | 1:E:230:VAL:HG21 | 1.64                     | 0.78              |
| 1:G:425:HIS:HE1  | 1:G:427:SER:OG   | 1.65                     | 0.78              |
| 1:A:321:PHE:HD2  | 1:A:533:MET:HE1  | 1.47                     | 0.78              |
| 1:A:446:MET:HE2  | 1:A:492:LEU:HB3  | 1.66                     | 0.78              |
| 1:C:107:GLN:CB   | 1:C:124:ARG:HG3  | 2.12                     | 0.78              |
| 1:E:292:CYS:O    | 1:E:295:ILE:HG12 | 1.83                     | 0.78              |
| 1:G:141:LEU:HD13 | 1:G:176:VAL:HG21 | 1.63                     | 0.78              |
| 1:A:178:LEU:HB3  | 1:A:181:GLY:HA2  | 1.64                     | 0.78              |
| 1:A:490:GLY:HA2  | 1:A:493:ARG:HG3  | 1.63                     | 0.78              |
| 1:G:473:LYS:HG3  | 1:G:479:ARG:HB2  | 1.65                     | 0.78              |
| 1:C:368:LEU:O    | 1:C:368:LEU:HD22 | 1.84                     | 0.78              |
| 1:F:168:LEU:CD2  | 1:F:247:ASP:OD2  | 2.32                     | 0.78              |
| 1:G:316:MET:HE1  | 1:G:535:TYR:CE2  | 2.19                     | 0.78              |
| 1:A:154:VAL:HB   | 1:A:175:VAL:HG13 | 1.65                     | 0.78              |
| 1:D:153:ILE:HG13 | 1:D:174:PRO:HB2  | 1.66                     | 0.78              |
| 1:E:473:LYS:HG3  | 1:E:479:ARG:HB2  | 1.66                     | 0.78              |
| 1:F:378:PHE:CE2  | 1:G:276:ARG:HD3  | 2.19                     | 0.78              |
| 1:E:303:ARG:O    | 1:E:306:GLU:HG3  | 1.83                     | 0.78              |
| 1:G:168:LEU:CD2  | 1:G:247:ASP:OD2  | 2.32                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:253:GLN:HA   | 1:A:257:ALA:HB2  | 1.67                     | 0.77              |
| 1:B:152:LYS:HG3  | 1:B:201:GLN:HG2  | 1.65                     | 0.77              |
| 1:D:338:GLY:HA3  | 1:D:412:MET:HE1  | 1.66                     | 0.77              |
| 1:A:401:GLU:HG2  | 1:A:402:THR:N    | 1.99                     | 0.77              |
| 1:A:414:SER:HB3  | 1:C:226:GLY:H    | 1.50                     | 0.77              |
| 1:B:208:MET:HE2  | 1:B:233:LEU:H    | 1.48                     | 0.77              |
| 1:A:126:LYS:CG   | 1:A:127:ASP:N    | 2.44                     | 0.77              |
| 1:A:405:LEU:HG   | 1:A:409:LEU:HD12 | 1.65                     | 0.77              |
| 1:E:290:SER:N    | 1:E:325:GLN:NE2  | 2.32                     | 0.77              |
| 1:F:121:GLN:HB3  | 1:F:133:THR:HG23 | 1.65                     | 0.77              |
| 1:F:504:ARG:HH21 | 1:F:506:GLN:HB3  | 1.47                     | 0.77              |
| 1:G:108:VAL:HG12 | 1:G:121:GLN:HG2  | 1.65                     | 0.77              |
| 1:B:168:LEU:CD2  | 1:B:247:ASP:OD2  | 2.32                     | 0.77              |
| 1:D:259:PRO:O    | 1:D:260:TRP:CB   | 2.33                     | 0.77              |
| 1:F:220:ALA:CB   | 1:F:261:ILE:HG12 | 2.15                     | 0.77              |
| 1:A:312:SER:N    | 1:A:318:MET:HE2  | 1.99                     | 0.77              |
| 1:A:339:LEU:HB3  | 1:A:341:MET:HE1  | 1.65                     | 0.77              |
| 1:B:166:MET:CE   | 1:B:171:CYS:SG   | 2.73                     | 0.77              |
| 1:D:283:GLU:OE2  | 1:D:286:GLY:HA2  | 1.84                     | 0.77              |
| 1:A:425:HIS:CE1  | 1:A:427:SER:OG   | 2.37                     | 0.77              |
| 1:B:290:SER:H    | 1:B:325:GLN:HE21 | 1.32                     | 0.77              |
| 1:C:409:LEU:CD2  | 1:C:421:ILE:HG21 | 2.15                     | 0.77              |
| 1:G:178:LEU:HB3  | 1:G:181:GLY:HA2  | 1.65                     | 0.77              |
| 1:G:469:PRO:O    | 1:G:470:ASP:HB2  | 1.85                     | 0.77              |
| 1:C:205:MET:HA   | 1:C:231:ALA:HB3  | 1.66                     | 0.77              |
| 1:D:412:MET:HE2  | 1:D:421:ILE:HD12 | 1.65                     | 0.77              |
| 1:G:141:LEU:HD11 | 1:G:196:PHE:CZ   | 2.20                     | 0.77              |
| 1:G:316:MET:HE1  | 1:G:535:TYR:CZ   | 2.20                     | 0.77              |
| 1:G:339:LEU:HD22 | 1:G:341:MET:HE1  | 1.65                     | 0.77              |
| 1:B:199:PHE:O    | 1:B:227:LYS:HE2  | 1.83                     | 0.77              |
| 1:G:152:LYS:HG3  | 1:G:201:GLN:HG2  | 1.66                     | 0.77              |
| 1:A:442:ILE:HD11 | 1:A:492:LEU:HD21 | 1.66                     | 0.77              |
| 1:B:482:SER:H    | 1:B:485:ASP:HB2  | 1.47                     | 0.77              |
| 1:D:127:ASP:O    | 1:D:128:LYS:CB   | 2.23                     | 0.77              |
| 1:D:482:SER:H    | 1:D:485:ASP:HB2  | 1.48                     | 0.77              |
| 1:C:473:LYS:HG3  | 1:C:479:ARG:HB2  | 1.66                     | 0.77              |
| 1:E:318:MET:HE1  | 1:E:465:HIS:HD2  | 1.49                     | 0.77              |
| 1:A:208:MET:HE2  | 1:A:233:LEU:N    | 1.99                     | 0.76              |
| 1:D:427:SER:HB3  | 1:D:487:ARG:HH12 | 1.48                     | 0.76              |
| 1:F:251:MET:HA   | 1:F:251:MET:CE   | 2.16                     | 0.76              |
| 1:A:311:THR:CA   | 1:A:318:MET:HE2  | 2.15                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:178:LEU:CB   | 1:B:181:GLY:HA2  | 2.14                     | 0.76              |
| 1:D:499:ILE:CG2  | 1:D:519:LEU:HB2  | 2.16                     | 0.76              |
| 1:F:409:LEU:CD2  | 1:F:421:ILE:HG21 | 2.15                     | 0.76              |
| 1:B:248:ARG:HH11 | 1:B:248:ARG:HB3  | 0.59                     | 0.76              |
| 1:B:292:CYS:O    | 1:B:295:ILE:HG12 | 1.85                     | 0.76              |
| 1:B:442:ILE:HD12 | 1:B:488:GLY:HA2  | 1.67                     | 0.76              |
| 1:E:208:MET:HE2  | 1:E:233:LEU:H    | 1.50                     | 0.76              |
| 1:F:358:ASN:O    | 1:F:360:VAL:HG13 | 1.86                     | 0.76              |
| 1:F:504:ARG:NH2  | 1:F:506:GLN:HB3  | 1.99                     | 0.76              |
| 1:G:409:LEU:CD2  | 1:G:421:ILE:HG21 | 2.15                     | 0.76              |
| 1:B:290:SER:N    | 1:B:325:GLN:NE2  | 2.33                     | 0.76              |
| 1:B:473:LYS:HE2  | 1:B:479:ARG:HA   | 1.68                     | 0.76              |
| 1:C:339:LEU:HB3  | 1:C:341:MET:HE1  | 1.67                     | 0.76              |
| 1:F:112:ARG:HG3  | 1:F:145:HIS:CD2  | 2.20                     | 0.76              |
| 1:F:510:MET:HE2  | 1:F:513:LEU:HD22 | 1.66                     | 0.76              |
| 1:A:257:ALA:O    | 1:A:258:GLY:O    | 2.04                     | 0.76              |
| 1:A:442:ILE:CD1  | 1:A:492:LEU:HD11 | 2.16                     | 0.76              |
| 1:B:107:GLN:CB   | 1:B:124:ARG:HG3  | 2.14                     | 0.76              |
| 1:B:441:MET:HE2  | 1:B:441:MET:C    | 2.11                     | 0.76              |
| 1:F:315:GLY:HA2  | 1:F:317:VAL:HG23 | 1.66                     | 0.76              |
| 1:E:482:SER:OG   | 1:E:484:THR:HG23 | 1.85                     | 0.76              |
| 1:F:217:GLU:OE2  | 1:F:261:ILE:CG2  | 2.33                     | 0.76              |
| 1:D:152:LYS:HG3  | 1:D:201:GLN:HG2  | 1.68                     | 0.76              |
| 1:D:510:MET:HE2  | 1:D:513:LEU:CD2  | 2.16                     | 0.76              |
| 1:G:246:HIS:HB2  | 1:G:249:GLU:HB2  | 1.68                     | 0.76              |
| 1:B:483:ILE:O    | 1:B:486:LEU:CB   | 2.29                     | 0.75              |
| 1:D:168:LEU:CD2  | 1:D:247:ASP:OD2  | 2.33                     | 0.75              |
| 1:D:473:LYS:HE2  | 1:D:479:ARG:HA   | 1.68                     | 0.75              |
| 1:G:490:GLY:HA2  | 1:G:493:ARG:HG3  | 1.67                     | 0.75              |
| 1:D:220:ALA:CB   | 1:D:261:ILE:CG2  | 2.53                     | 0.75              |
| 1:F:311:THR:O    | 1:F:312:SER:HB3  | 1.86                     | 0.75              |
| 1:B:283:GLU:OE2  | 1:B:286:GLY:HA2  | 1.86                     | 0.75              |
| 1:B:358:ASN:O    | 1:B:360:VAL:HG13 | 1.85                     | 0.75              |
| 1:C:482:SER:OG   | 1:C:484:THR:HG23 | 1.87                     | 0.75              |
| 1:E:261:ILE:H    | 1:E:262:PRO:HD2  | 1.47                     | 0.75              |
| 1:F:412:MET:HE2  | 1:F:421:ILE:HD12 | 1.69                     | 0.75              |
| 1:F:473:LYS:HG3  | 1:F:479:ARG:HB2  | 1.66                     | 0.75              |
| 1:G:504:ARG:HH21 | 1:G:506:GLN:HB3  | 1.52                     | 0.75              |
| 1:E:358:ASN:O    | 1:E:360:VAL:HG13 | 1.87                     | 0.75              |
| 1:F:415:GLY:HA2  | 1:G:226:GLY:N    | 2.01                     | 0.75              |
| 1:G:442:ILE:CD1  | 1:G:492:LEU:HD11 | 2.17                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:482:SER:OG   | 1:G:484:THR:HG23 | 1.87                     | 0.75              |
| 1:E:229:ARG:NH2  | 1:E:259:PRO:HG3  | 2.02                     | 0.75              |
| 1:F:208:MET:HE2  | 1:F:233:LEU:H    | 1.50                     | 0.75              |
| 1:F:425:HIS:HE1  | 1:F:427:SER:OG   | 1.66                     | 0.75              |
| 1:G:205:MET:HA   | 1:G:231:ALA:HB3  | 1.68                     | 0.75              |
| 1:A:369:LYS:HG2  | 1:C:279:LEU:HD23 | 1.66                     | 0.75              |
| 1:B:121:GLN:HB2  | 1:B:133:THR:OG1  | 1.86                     | 0.75              |
| 1:C:442:ILE:CD1  | 1:C:492:LEU:HD11 | 2.15                     | 0.75              |
| 1:B:121:GLN:HB3  | 1:B:133:THR:HG23 | 1.69                     | 0.75              |
| 1:B:141:LEU:HD11 | 1:B:196:PHE:CZ   | 2.21                     | 0.75              |
| 1:C:295:ILE:O    | 1:C:299:THR:HG23 | 1.87                     | 0.75              |
| 1:D:194:GLU:CD   | 1:D:194:GLU:H    | 1.92                     | 0.75              |
| 1:D:303:ARG:O    | 1:D:306:GLU:HG3  | 1.86                     | 0.75              |
| 1:B:315:GLY:HA2  | 1:B:317:VAL:HG23 | 1.69                     | 0.75              |
| 1:F:216:VAL:HG11 | 1:F:230:VAL:CG2  | 2.17                     | 0.75              |
| 1:F:368:LEU:HD22 | 1:F:368:LEU:O    | 1.87                     | 0.75              |
| 1:C:412:MET:HE2  | 1:C:421:ILE:HD13 | 1.69                     | 0.74              |
| 1:G:289:PHE:H    | 1:G:296:ASN:HD21 | 1.34                     | 0.74              |
| 1:A:68:VAL:HG12  | 1:A:121:GLN:OE1  | 1.86                     | 0.74              |
| 1:F:152:LYS:HG3  | 1:F:201:GLN:HG2  | 1.69                     | 0.74              |
| 1:B:127:ASP:O    | 1:B:128:LYS:CB   | 2.30                     | 0.74              |
| 1:B:482:SER:OG   | 1:B:484:THR:HG23 | 1.86                     | 0.74              |
| 1:C:442:ILE:HD12 | 1:C:488:GLY:HA2  | 1.69                     | 0.74              |
| 1:E:246:HIS:HB2  | 1:E:249:GLU:HB2  | 1.69                     | 0.74              |
| 1:G:121:GLN:HB2  | 1:G:133:THR:OG1  | 1.87                     | 0.74              |
| 1:A:126:LYS:HZ2  | 1:A:127:ASP:N    | 1.85                     | 0.74              |
| 1:B:312:SER:N    | 1:B:318:MET:HE2  | 2.03                     | 0.74              |
| 1:C:229:ARG:NH2  | 1:C:259:PRO:HB3  | 2.03                     | 0.74              |
| 1:E:258:GLY:HA3  | 1:E:260:TRP:HZ3  | 1.52                     | 0.74              |
| 1:G:483:ILE:O    | 1:G:486:LEU:CB   | 2.32                     | 0.74              |
| 1:G:510:MET:HE2  | 1:G:513:LEU:HD22 | 1.69                     | 0.74              |
| 1:B:220:ALA:HB1  | 1:B:261:ILE:HD12 | 1.69                     | 0.74              |
| 1:E:178:LEU:HB3  | 1:E:181:GLY:HA2  | 1.69                     | 0.74              |
| 1:A:168:LEU:HD12 | 1:A:251:MET:HE1  | 1.69                     | 0.74              |
| 1:E:112:ARG:HG3  | 1:E:145:HIS:CD2  | 2.23                     | 0.74              |
| 1:F:405:LEU:HG   | 1:F:409:LEU:HD12 | 1.68                     | 0.74              |
| 1:G:167:GLU:C    | 1:G:169:GLN:N    | 2.46                     | 0.74              |
| 1:G:260:TRP:O    | 1:G:262:PRO:HD2  | 1.87                     | 0.74              |
| 1:A:261:ILE:O    | 1:A:261:ILE:CG1  | 2.34                     | 0.74              |
| 1:B:108:VAL:CG1  | 1:B:121:GLN:HG2  | 2.18                     | 0.74              |
| 1:B:368:LEU:O    | 1:B:368:LEU:HD22 | 1.88                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:205:MET:HA   | 1:D:231:ALA:HB3  | 1.70                     | 0.74              |
| 1:E:473:LYS:HE2  | 1:E:479:ARG:HA   | 1.70                     | 0.74              |
| 1:G:107:GLN:CB   | 1:G:124:ARG:HG3  | 2.18                     | 0.74              |
| 1:G:208:MET:HE2  | 1:G:233:LEU:H    | 1.52                     | 0.74              |
| 1:D:178:LEU:HB3  | 1:D:181:GLY:HA2  | 1.70                     | 0.74              |
| 1:E:107:GLN:CB   | 1:E:124:ARG:HG3  | 2.17                     | 0.74              |
| 1:F:372:ILE:HA   | 1:F:375:ASN:OD1  | 1.87                     | 0.74              |
| 1:F:499:ILE:CG2  | 1:F:519:LEU:HB2  | 2.18                     | 0.74              |
| 1:C:446:MET:HE2  | 1:C:492:LEU:HB3  | 1.69                     | 0.74              |
| 1:D:141:LEU:HD13 | 1:D:176:VAL:HG21 | 1.69                     | 0.74              |
| 1:E:420:VAL:HG22 | 1:E:459:VAL:HB   | 1.68                     | 0.73              |
| 1:B:289:PHE:N    | 1:B:296:ASN:HD21 | 1.86                     | 0.73              |
| 1:B:450:LYS:CE   | 1:B:454:LYS:CD   | 2.66                     | 0.73              |
| 1:C:316:MET:HE1  | 1:C:535:TYR:CE2  | 2.23                     | 0.73              |
| 1:C:413:ARG:HE   | 1:C:458:VAL:HB   | 1.53                     | 0.73              |
| 1:E:322:VAL:HG21 | 1:E:463:ILE:HD11 | 1.70                     | 0.73              |
| 1:E:411:TYR:CE1  | 1:F:262:PRO:HB3  | 2.23                     | 0.73              |
| 1:C:372:ILE:HA   | 1:C:375:ASN:OD1  | 1.89                     | 0.73              |
| 1:D:311:THR:O    | 1:D:312:SER:HB3  | 1.88                     | 0.73              |
| 1:E:261:ILE:N    | 1:E:262:PRO:HD2  | 2.02                     | 0.73              |
| 1:F:366:ASP:HB2  | 1:G:284:SER:CB   | 2.17                     | 0.73              |
| 1:A:425:HIS:CE1  | 1:A:465:HIS:CG   | 2.76                     | 0.73              |
| 1:B:229:ARG:HH21 | 1:B:259:PRO:HB3  | 1.52                     | 0.73              |
| 1:C:229:ARG:CZ   | 1:C:259:PRO:HB3  | 2.18                     | 0.73              |
| 1:C:412:MET:HE2  | 1:C:421:ILE:HD12 | 1.69                     | 0.73              |
| 1:F:389:ASP:HA   | 1:G:269:LEU:CD2  | 2.17                     | 0.73              |
| 1:A:289:PHE:H    | 1:A:296:ASN:HD21 | 1.35                     | 0.73              |
| 1:A:368:LEU:O    | 1:A:368:LEU:HD22 | 1.88                     | 0.73              |
| 1:B:186:LYS:HD3  | 1:B:218:GLU:CG   | 2.19                     | 0.73              |
| 1:C:152:LYS:HG3  | 1:C:201:GLN:HG2  | 1.71                     | 0.73              |
| 1:C:369:LYS:HG2  | 1:D:279:LEU:CD2  | 2.17                     | 0.73              |
| 1:E:199:PHE:O    | 1:E:227:LYS:HE2  | 1.89                     | 0.73              |
| 1:E:409:LEU:CD2  | 1:E:421:ILE:HG21 | 2.17                     | 0.73              |
| 1:A:256:ASN:OD1  | 1:A:257:ALA:N    | 2.21                     | 0.73              |
| 1:B:208:MET:HE2  | 1:B:233:LEU:N    | 2.03                     | 0.73              |
| 1:F:295:ILE:O    | 1:F:299:THR:HG23 | 1.87                     | 0.73              |
| 1:C:321:PHE:HD2  | 1:C:533:MET:HE1  | 1.52                     | 0.73              |
| 1:E:368:LEU:HD22 | 1:E:372:ILE:HG23 | 1.68                     | 0.73              |
| 1:G:111:TYR:CE2  | 1:G:142:PHE:HB2  | 2.23                     | 0.73              |
| 1:C:515:LEU:HD21 | 1:C:529:ILE:CD1  | 2.19                     | 0.73              |
| 1:D:108:VAL:HG12 | 1:D:121:GLN:HG2  | 1.68                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:208:MET:HE2  | 1:D:233:LEU:H    | 1.54                     | 0.73              |
| 1:E:510:MET:HE2  | 1:E:513:LEU:HD22 | 1.71                     | 0.73              |
| 1:F:515:LEU:HD21 | 1:F:529:ILE:CD1  | 2.18                     | 0.73              |
| 1:F:316:MET:HE1  | 1:F:535:TYR:CZ   | 2.24                     | 0.73              |
| 1:F:504:ARG:CD   | 1:F:506:GLN:HG2  | 2.11                     | 0.73              |
| 1:G:427:SER:HB3  | 1:G:487:ARG:HH12 | 1.53                     | 0.73              |
| 1:A:112:ARG:HG3  | 1:A:145:HIS:CD2  | 2.23                     | 0.73              |
| 1:E:121:GLN:HB2  | 1:E:133:THR:OG1  | 1.88                     | 0.73              |
| 1:F:248:ARG:HB3  | 1:F:248:ARG:NH1  | 2.04                     | 0.73              |
| 1:G:413:ARG:HE   | 1:G:458:VAL:HB   | 1.53                     | 0.73              |
| 1:A:104:VAL:HG12 | 1:A:106:TYR:CE1  | 2.24                     | 0.72              |
| 1:A:358:ASN:O    | 1:A:360:VAL:HG13 | 1.88                     | 0.72              |
| 1:D:167:GLU:C    | 1:D:169:GLN:N    | 2.44                     | 0.72              |
| 1:D:217:GLU:OE2  | 1:D:261:ILE:HA   | 1.89                     | 0.72              |
| 1:D:312:SER:N    | 1:D:318:MET:HE2  | 2.04                     | 0.72              |
| 1:A:488:GLY:HA3  | 1:A:492:LEU:HD11 | 1.71                     | 0.72              |
| 1:B:488:GLY:HA3  | 1:B:492:LEU:HD11 | 1.71                     | 0.72              |
| 1:E:152:LYS:HG3  | 1:E:201:GLN:HG2  | 1.70                     | 0.72              |
| 1:F:290:SER:N    | 1:F:325:GLN:NE2  | 2.32                     | 0.72              |
| 1:B:412:MET:HE2  | 1:B:421:ILE:CD1  | 2.19                     | 0.72              |
| 1:C:167:GLU:C    | 1:C:169:GLN:N    | 2.48                     | 0.72              |
| 1:C:248:ARG:HB3  | 1:C:248:ARG:NH1  | 2.04                     | 0.72              |
| 1:E:442:ILE:CD1  | 1:E:492:LEU:HD11 | 2.19                     | 0.72              |
| 1:B:248:ARG:HH11 | 1:B:248:ARG:HB2  | 1.45                     | 0.72              |
| 1:B:205:MET:HA   | 1:B:231:ALA:HB3  | 1.71                     | 0.72              |
| 1:C:208:MET:CE   | 1:C:232:VAL:HA   | 2.18                     | 0.72              |
| 1:D:358:ASN:O    | 1:D:360:VAL:HG13 | 1.89                     | 0.72              |
| 1:E:167:GLU:C    | 1:E:169:GLN:N    | 2.47                     | 0.72              |
| 1:F:167:GLU:C    | 1:F:169:GLN:N    | 2.46                     | 0.72              |
| 1:F:208:MET:HE2  | 1:F:233:LEU:N    | 2.04                     | 0.72              |
| 1:C:246:HIS:HB2  | 1:C:249:GLU:HB2  | 1.71                     | 0.72              |
| 1:D:154:VAL:HB   | 1:D:175:VAL:HG13 | 1.71                     | 0.72              |
| 1:E:289:PHE:N    | 1:E:296:ASN:HD21 | 1.87                     | 0.72              |
| 1:F:389:ASP:HA   | 1:G:269:LEU:HD23 | 1.70                     | 0.72              |
| 1:G:208:MET:HE2  | 1:G:233:LEU:N    | 2.04                     | 0.72              |
| 1:A:253:GLN:O    | 1:A:257:ALA:HB2  | 1.90                     | 0.72              |
| 1:C:261:ILE:N    | 1:C:262:PRO:CD   | 2.35                     | 0.72              |
| 1:C:268:ALA:HA   | 1:C:271:LEU:CD1  | 2.19                     | 0.72              |
| 1:C:441:MET:O    | 1:C:441:MET:CE   | 2.36                     | 0.72              |
| 1:C:490:GLY:HA2  | 1:C:493:ARG:HG3  | 1.70                     | 0.72              |
| 1:E:488:GLY:HA3  | 1:E:492:LEU:HD11 | 1.72                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:409:LEU:CD2  | 1:A:421:ILE:HG21 | 2.20                     | 0.72              |
| 1:B:467:LYS:HE3  | 1:B:486:LEU:O    | 1.90                     | 0.72              |
| 1:D:121:GLN:HB2  | 1:D:133:THR:OG1  | 1.90                     | 0.72              |
| 1:E:141:LEU:HD11 | 1:E:196:PHE:CZ   | 2.25                     | 0.72              |
| 1:E:208:MET:HE2  | 1:E:233:LEU:N    | 2.05                     | 0.72              |
| 1:E:425:HIS:CE1  | 1:E:427:SER:OG   | 2.43                     | 0.72              |
| 1:F:108:VAL:HG12 | 1:F:121:GLN:HG2  | 1.71                     | 0.72              |
| 1:F:268:ALA:HA   | 1:F:271:LEU:CD1  | 2.19                     | 0.72              |
| 1:A:467:LYS:HE3  | 1:A:486:LEU:O    | 1.89                     | 0.72              |
| 1:B:260:TRP:O    | 1:B:261:ILE:HG12 | 1.90                     | 0.72              |
| 1:B:447:THR:HG22 | 1:B:495:LEU:CD2  | 2.18                     | 0.72              |
| 1:C:290:SER:H    | 1:C:325:GLN:HE22 | 1.33                     | 0.72              |
| 1:C:536:ASN:HD22 | 1:C:538:GLU:H    | 1.36                     | 0.72              |
| 1:D:142:PHE:CE2  | 1:D:162:MET:HE3  | 2.25                     | 0.72              |
| 1:D:351:GLU:OE1  | 1:E:278:HIS:CD2  | 2.43                     | 0.72              |
| 1:D:488:GLY:HA3  | 1:D:492:LEU:HD11 | 1.71                     | 0.72              |
| 1:G:499:ILE:CG2  | 1:G:519:LEU:HB2  | 2.19                     | 0.72              |
| 1:B:112:ARG:HG3  | 1:B:145:HIS:CD2  | 2.25                     | 0.71              |
| 1:B:167:GLU:C    | 1:B:169:GLN:N    | 2.46                     | 0.71              |
| 1:C:294:GLY:O    | 1:C:295:ILE:C    | 2.29                     | 0.71              |
| 1:E:104:VAL:HG12 | 1:E:106:TYR:CE1  | 2.24                     | 0.71              |
| 1:F:442:ILE:HD11 | 1:F:492:LEU:HD21 | 1.71                     | 0.71              |
| 1:F:483:ILE:O    | 1:F:486:LEU:CB   | 2.32                     | 0.71              |
| 1:A:366:ASP:HB2  | 1:C:285:VAL:HG23 | 1.72                     | 0.71              |
| 1:C:178:LEU:HB3  | 1:C:181:GLY:HA2  | 1.71                     | 0.71              |
| 1:C:521:CYS:SG   | 1:C:524:THR:HG23 | 2.30                     | 0.71              |
| 1:F:104:VAL:HG12 | 1:F:106:TYR:CE1  | 2.24                     | 0.71              |
| 1:A:442:ILE:HD12 | 1:A:488:GLY:HA2  | 1.72                     | 0.71              |
| 1:G:104:VAL:HG12 | 1:G:106:TYR:CE1  | 2.24                     | 0.71              |
| 1:G:292:CYS:O    | 1:G:295:ILE:HG12 | 1.91                     | 0.71              |
| 1:C:194:GLU:H    | 1:C:194:GLU:CD   | 1.95                     | 0.71              |
| 1:G:504:ARG:NH2  | 1:G:506:GLN:HB3  | 2.03                     | 0.71              |
| 1:A:372:ILE:HA   | 1:A:375:ASN:OD1  | 1.90                     | 0.71              |
| 1:C:504:ARG:CD   | 1:C:506:GLN:HG2  | 2.18                     | 0.71              |
| 1:D:246:HIS:HB2  | 1:D:249:GLU:HB2  | 1.73                     | 0.71              |
| 1:A:251:MET:HA   | 1:A:251:MET:CE   | 2.20                     | 0.71              |
| 1:D:208:MET:HE2  | 1:D:233:LEU:N    | 2.05                     | 0.71              |
| 1:F:482:SER:OG   | 1:F:484:THR:HG23 | 1.91                     | 0.71              |
| 1:B:107:GLN:HB2  | 1:B:124:ARG:CG   | 2.20                     | 0.71              |
| 1:B:178:LEU:HB3  | 1:B:181:GLY:HA2  | 1.71                     | 0.71              |
| 1:B:260:TRP:C    | 1:B:261:ILE:HG12 | 2.14                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:504:ARG:CD   | 1:E:506:GLN:HG2  | 2.12                     | 0.71              |
| 1:F:229:ARG:HB2  | 1:F:258:GLY:O    | 1.90                     | 0.71              |
| 1:F:366:ASP:HB2  | 1:G:284:SER:HB2  | 1.70                     | 0.71              |
| 1:F:122:LYS:HE2  | 1:F:159:GLU:OE1  | 1.90                     | 0.71              |
| 1:A:86:ILE:HG21  | 1:A:163:LEU:HD12 | 1.73                     | 0.71              |
| 1:B:246:HIS:HB2  | 1:B:249:GLU:HB2  | 1.71                     | 0.71              |
| 1:B:473:LYS:HG3  | 1:B:479:ARG:HB2  | 1.72                     | 0.71              |
| 1:C:121:GLN:HB3  | 1:C:133:THR:HG23 | 1.73                     | 0.71              |
| 1:C:441:MET:CE   | 1:C:444:ASN:HB3  | 2.20                     | 0.71              |
| 1:E:467:LYS:HE3  | 1:E:486:LEU:O    | 1.89                     | 0.71              |
| 1:F:289:PHE:H    | 1:F:296:ASN:HD21 | 1.39                     | 0.71              |
| 1:G:312:SER:N    | 1:G:318:MET:HE2  | 2.06                     | 0.71              |
| 1:G:412:MET:HE2  | 1:G:421:ILE:HD12 | 1.70                     | 0.71              |
| 1:C:186:LYS:HD3  | 1:C:218:GLU:CG   | 2.20                     | 0.71              |
| 1:D:292:CYS:O    | 1:D:295:ILE:HG12 | 1.91                     | 0.71              |
| 1:D:369:LYS:HG2  | 1:E:279:LEU:CD2  | 2.21                     | 0.71              |
| 1:F:229:ARG:CB   | 1:F:258:GLY:O    | 2.39                     | 0.71              |
| 1:G:248:ARG:HB3  | 1:G:248:ARG:NH1  | 2.04                     | 0.71              |
| 1:A:246:HIS:HB2  | 1:A:249:GLU:HB2  | 1.73                     | 0.70              |
| 1:G:154:VAL:HB   | 1:G:175:VAL:HG13 | 1.73                     | 0.70              |
| 1:G:228:VAL:HB   | 1:G:261:ILE:CD1  | 2.21                     | 0.70              |
| 1:B:442:ILE:HD12 | 1:B:488:GLY:CA   | 2.21                     | 0.70              |
| 1:D:447:THR:CG2  | 1:D:495:LEU:HD21 | 2.17                     | 0.70              |
| 1:G:268:ALA:HA   | 1:G:271:LEU:CD1  | 2.21                     | 0.70              |
| 1:G:220:ALA:CB   | 1:G:261:ILE:CG2  | 2.58                     | 0.70              |
| 1:B:499:ILE:CG2  | 1:B:519:LEU:HB2  | 2.21                     | 0.70              |
| 1:C:111:TYR:CE2  | 1:C:142:PHE:HB2  | 2.26                     | 0.70              |
| 1:C:289:PHE:N    | 1:C:296:ASN:HD21 | 1.86                     | 0.70              |
| 1:D:107:GLN:CB   | 1:D:124:ARG:HG3  | 2.20                     | 0.70              |
| 1:D:121:GLN:HB3  | 1:D:133:THR:HG23 | 1.73                     | 0.70              |
| 1:E:490:GLY:CA   | 1:E:493:ARG:HG3  | 2.21                     | 0.70              |
| 1:B:442:ILE:HD11 | 1:B:492:LEU:HD21 | 1.74                     | 0.70              |
| 1:E:229:ARG:HA   | 1:E:259:PRO:HA   | 1.74                     | 0.70              |
| 1:F:446:MET:HE2  | 1:F:492:LEU:HB3  | 1.73                     | 0.70              |
| 1:A:424:ASP:OD2  | 1:A:425:HIS:HB2  | 1.92                     | 0.70              |
| 1:B:154:VAL:HB   | 1:B:175:VAL:HG13 | 1.73                     | 0.70              |
| 1:C:112:ARG:HG3  | 1:C:145:HIS:CD2  | 2.25                     | 0.70              |
| 1:D:216:VAL:HG11 | 1:D:230:VAL:HG21 | 1.72                     | 0.70              |
| 1:F:424:ASP:OD2  | 1:F:425:HIS:HB2  | 1.90                     | 0.70              |
| 1:G:368:LEU:O    | 1:G:368:LEU:HD22 | 1.92                     | 0.70              |
| 1:G:510:MET:HE2  | 1:G:513:LEU:CD2  | 2.22                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:124:ARG:HD3  | 1:A:125:ASP:C    | 2.16                     | 0.70              |
| 1:B:208:MET:CE   | 1:B:232:VAL:HA   | 2.22                     | 0.70              |
| 1:B:484:THR:C    | 1:B:486:LEU:H    | 1.96                     | 0.70              |
| 1:C:420:VAL:HG22 | 1:C:459:VAL:HB   | 1.74                     | 0.70              |
| 1:C:476:GLU:CD   | 1:C:476:GLU:H    | 1.98                     | 0.70              |
| 1:D:79:SER:H     | 1:D:98:ILE:HD13  | 1.56                     | 0.70              |
| 1:D:504:ARG:NH2  | 1:D:506:GLN:HB3  | 2.06                     | 0.70              |
| 1:E:316:MET:HE1  | 1:E:535:TYR:CE2  | 2.27                     | 0.70              |
| 1:F:259:PRO:O    | 1:F:260:TRP:HB3  | 1.89                     | 0.70              |
| 1:G:166:MET:CE   | 1:G:171:CYS:CB   | 2.69                     | 0.70              |
| 1:G:473:LYS:HE2  | 1:G:479:ARG:HA   | 1.74                     | 0.70              |
| 1:A:216:VAL:HG11 | 1:A:230:VAL:CG2  | 2.22                     | 0.70              |
| 1:B:194:GLU:CD   | 1:B:194:GLU:H    | 1.97                     | 0.70              |
| 1:B:510:MET:HE2  | 1:B:513:LEU:CD2  | 2.22                     | 0.70              |
| 1:B:536:ASN:HD22 | 1:B:538:GLU:H    | 1.40                     | 0.70              |
| 1:C:441:MET:HE2  | 1:C:444:ASN:HB3  | 1.73                     | 0.70              |
| 1:D:111:TYR:CE2  | 1:D:142:PHE:HB2  | 2.26                     | 0.70              |
| 1:G:467:LYS:HE3  | 1:G:486:LEU:O    | 1.91                     | 0.70              |
| 1:B:405:LEU:HG   | 1:B:409:LEU:HD12 | 1.74                     | 0.70              |
| 1:F:130:PHE:HB2  | 1:G:64:MET:CA    | 2.21                     | 0.70              |
| 1:F:339:LEU:HB3  | 1:F:341:MET:HE1  | 1.73                     | 0.70              |
| 1:A:208:MET:CE   | 1:A:232:VAL:HA   | 2.22                     | 0.70              |
| 1:B:278:HIS:CD2  | 1:G:351:GLU:OE1  | 2.45                     | 0.70              |
| 1:D:490:GLY:CA   | 1:D:493:ARG:HG3  | 2.22                     | 0.70              |
| 1:E:347:GLU:O    | 1:E:351:GLU:HG3  | 1.92                     | 0.70              |
| 1:E:413:ARG:O    | 1:E:417:GLY:HA2  | 1.91                     | 0.70              |
| 1:A:312:SER:N    | 1:A:318:MET:CE   | 2.54                     | 0.69              |
| 1:A:515:LEU:HD21 | 1:A:529:ILE:CD1  | 2.22                     | 0.69              |
| 1:B:454:LYS:HZ1  | 1:G:344:GLU:HA   | 1.58                     | 0.69              |
| 1:E:107:GLN:HB2  | 1:E:124:ARG:CG   | 2.21                     | 0.69              |
| 1:F:97:TRP:CZ3   | 1:F:99:ALA:HB2   | 2.26                     | 0.69              |
| 1:F:141:LEU:HD13 | 1:F:176:VAL:HG21 | 1.73                     | 0.69              |
| 1:F:378:PHE:CD2  | 1:G:276:ARG:CD   | 2.75                     | 0.69              |
| 1:A:268:ALA:HA   | 1:A:271:LEU:CD1  | 2.22                     | 0.69              |
| 1:F:96:TYR:HE2   | 1:F:107:GLN:HE21 | 1.39                     | 0.69              |
| 1:F:488:GLY:HA3  | 1:F:492:LEU:HD11 | 1.72                     | 0.69              |
| 1:D:186:LYS:HD3  | 1:D:218:GLU:CG   | 2.23                     | 0.69              |
| 1:E:392:HIS:ND1  | 1:F:267:SER:CB   | 2.56                     | 0.69              |
| 1:F:141:LEU:HD11 | 1:F:196:PHE:CZ   | 2.27                     | 0.69              |
| 1:A:473:LYS:HE2  | 1:A:479:ARG:HA   | 1.73                     | 0.69              |
| 1:A:499:ILE:CG2  | 1:A:519:LEU:HB2  | 2.23                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:338:GLY:HA3  | 1:B:412:MET:CE   | 2.23                     | 0.69              |
| 1:E:499:ILE:CG2  | 1:E:519:LEU:HB2  | 2.21                     | 0.69              |
| 1:F:476:GLU:H    | 1:F:476:GLU:CD   | 2.00                     | 0.69              |
| 1:G:112:ARG:HG3  | 1:G:145:HIS:CD2  | 2.27                     | 0.69              |
| 1:A:194:GLU:H    | 1:A:194:GLU:CD   | 1.99                     | 0.69              |
| 1:D:315:GLY:HA2  | 1:D:317:VAL:HG23 | 1.73                     | 0.69              |
| 1:G:424:ASP:OD2  | 1:G:425:HIS:HB2  | 1.92                     | 0.69              |
| 1:B:394:TYR:HE1  | 1:B:396:SER:HB2  | 1.57                     | 0.69              |
| 1:D:347:GLU:OE1  | 1:E:274:ARG:HD2  | 1.93                     | 0.69              |
| 1:E:427:SER:HB3  | 1:E:487:ARG:HH12 | 1.56                     | 0.69              |
| 1:F:108:VAL:CG1  | 1:F:121:GLN:HG2  | 2.22                     | 0.69              |
| 1:C:288:LEU:N    | 1:C:288:LEU:HD12 | 2.08                     | 0.69              |
| 1:C:412:MET:CA   | 1:C:416:LEU:HD12 | 2.18                     | 0.69              |
| 1:D:338:GLY:CA   | 1:D:412:MET:HE1  | 2.23                     | 0.69              |
| 1:E:141:LEU:HD13 | 1:E:176:VAL:CG2  | 2.22                     | 0.69              |
| 1:F:220:ALA:HB1  | 1:F:261:ILE:HG12 | 1.73                     | 0.69              |
| 1:F:412:MET:CA   | 1:F:416:LEU:HD12 | 2.19                     | 0.69              |
| 1:G:108:VAL:CG1  | 1:G:121:GLN:HG2  | 2.22                     | 0.69              |
| 1:B:490:GLY:CA   | 1:B:493:ARG:HG3  | 2.23                     | 0.69              |
| 1:C:178:LEU:HB2  | 1:C:181:GLY:HA2  | 1.74                     | 0.69              |
| 1:D:536:ASN:HD22 | 1:D:538:GLU:H    | 1.40                     | 0.69              |
| 1:E:372:ILE:HA   | 1:E:375:ASN:OD1  | 1.91                     | 0.69              |
| 1:F:112:ARG:CB   | 1:F:117:ASN:O    | 2.38                     | 0.69              |
| 1:G:166:MET:HE1  | 1:G:171:CYS:HB3  | 1.75                     | 0.69              |
| 1:G:338:GLY:HA3  | 1:G:412:MET:CE   | 2.23                     | 0.69              |
| 1:A:480:PRO:HA   | 1:A:503:GLU:CD   | 2.18                     | 0.69              |
| 1:B:86:ILE:HG21  | 1:B:163:LEU:HD12 | 1.73                     | 0.69              |
| 1:C:305:GLY:O    | 1:C:454:LYS:HD2  | 1.93                     | 0.69              |
| 1:F:166:MET:HE3  | 1:F:171:CYS:SG   | 2.33                     | 0.69              |
| 1:A:111:TYR:CE2  | 1:A:142:PHE:HB2  | 2.28                     | 0.69              |
| 1:A:205:MET:HA   | 1:A:231:ALA:HB3  | 1.73                     | 0.69              |
| 1:A:309:MET:HB3  | 1:A:499:ILE:HD12 | 1.75                     | 0.69              |
| 1:A:311:THR:O    | 1:A:312:SER:HB3  | 1.92                     | 0.69              |
| 1:A:450:LYS:CE   | 1:A:454:LYS:CD   | 2.71                     | 0.69              |
| 1:B:79:SER:H     | 1:B:98:ILE:HD13  | 1.58                     | 0.69              |
| 1:C:104:VAL:HG12 | 1:C:106:TYR:CE1  | 2.28                     | 0.69              |
| 1:C:425:HIS:CE1  | 1:C:427:SER:OG   | 2.46                     | 0.69              |
| 1:E:248:ARG:HB3  | 1:E:248:ARG:NH1  | 2.07                     | 0.69              |
| 1:F:86:ILE:HG21  | 1:F:163:LEU:HD12 | 1.75                     | 0.69              |
| 1:F:154:VAL:HB   | 1:F:175:VAL:HG13 | 1.75                     | 0.69              |
| 1:B:504:ARG:HH21 | 1:B:506:GLN:HB3  | 1.58                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:186:LYS:HD3  | 1:E:218:GLU:CG   | 2.22                     | 0.68              |
| 1:G:295:ILE:O    | 1:G:299:THR:HG23 | 1.92                     | 0.68              |
| 1:C:339:LEU:HB3  | 1:C:341:MET:HE3  | 1.70                     | 0.68              |
| 1:D:108:VAL:CG1  | 1:D:121:GLN:HG2  | 2.22                     | 0.68              |
| 1:F:309:MET:HB3  | 1:F:499:ILE:CD1  | 2.21                     | 0.68              |
| 1:B:413:ARG:HE   | 1:B:458:VAL:HB   | 1.58                     | 0.68              |
| 1:B:504:ARG:NH2  | 1:B:506:GLN:HB3  | 2.08                     | 0.68              |
| 1:C:141:LEU:HD13 | 1:C:176:VAL:CG2  | 2.23                     | 0.68              |
| 1:G:311:THR:O    | 1:G:312:SER:HB3  | 1.92                     | 0.68              |
| 1:A:108:VAL:HG13 | 1:A:123:VAL:HG22 | 1.76                     | 0.68              |
| 1:A:124:ARG:CZ   | 1:A:126:LYS:HA   | 2.23                     | 0.68              |
| 1:A:275:ILE:HD12 | 1:B:382:PHE:HE1  | 1.57                     | 0.68              |
| 1:A:496:SER:O    | 1:A:520:LYS:HE2  | 1.93                     | 0.68              |
| 1:B:96:TYR:HE2   | 1:B:107:GLN:HE21 | 1.39                     | 0.68              |
| 1:F:283:GLU:CD   | 1:F:286:GLY:HA2  | 2.18                     | 0.68              |
| 1:A:186:LYS:HD3  | 1:A:218:GLU:CG   | 2.22                     | 0.68              |
| 1:B:283:GLU:CG   | 1:B:286:GLY:CA   | 2.56                     | 0.68              |
| 1:B:372:ILE:HA   | 1:B:375:ASN:OD1  | 1.94                     | 0.68              |
| 1:C:290:SER:N    | 1:C:325:GLN:HE21 | 1.87                     | 0.68              |
| 1:E:351:GLU:OE1  | 1:F:278:HIS:CD2  | 2.46                     | 0.68              |
| 1:E:446:MET:HE2  | 1:E:492:LEU:HB3  | 1.76                     | 0.68              |
| 1:F:394:TYR:HE1  | 1:F:396:SER:HB2  | 1.59                     | 0.68              |
| 1:G:107:GLN:HB2  | 1:G:124:ARG:CG   | 2.24                     | 0.68              |
| 1:G:186:LYS:HD3  | 1:G:218:GLU:CG   | 2.24                     | 0.68              |
| 1:G:368:LEU:HD22 | 1:G:372:ILE:HG23 | 1.75                     | 0.68              |
| 1:A:394:TYR:HE1  | 1:A:396:SER:HB2  | 1.58                     | 0.68              |
| 1:B:504:ARG:CD   | 1:B:506:GLN:HG2  | 2.16                     | 0.68              |
| 1:C:368:LEU:HD22 | 1:C:372:ILE:HG23 | 1.76                     | 0.68              |
| 1:C:424:ASP:OD2  | 1:C:425:HIS:HB2  | 1.94                     | 0.68              |
| 1:E:208:MET:CE   | 1:E:232:VAL:HA   | 2.23                     | 0.68              |
| 1:F:427:SER:HB3  | 1:F:487:ARG:HH12 | 1.58                     | 0.68              |
| 1:G:141:LEU:HD13 | 1:G:176:VAL:CG2  | 2.24                     | 0.68              |
| 1:B:141:LEU:HD13 | 1:B:176:VAL:CG2  | 2.22                     | 0.68              |
| 1:G:78:TYR:CD2   | 1:G:92:GLN:HG2   | 2.28                     | 0.68              |
| 1:A:74:SER:HB2   | 1:A:99:ALA:HB1   | 1.76                     | 0.68              |
| 1:C:166:MET:CE   | 1:C:171:CYS:CB   | 2.72                     | 0.68              |
| 1:D:104:VAL:HG12 | 1:D:106:TYR:CE1  | 2.29                     | 0.68              |
| 1:D:504:ARG:HH21 | 1:D:506:GLN:HB3  | 1.56                     | 0.68              |
| 1:E:394:TYR:HE1  | 1:E:396:SER:HB2  | 1.59                     | 0.68              |
| 1:E:401:GLU:HG2  | 1:E:402:THR:N    | 2.08                     | 0.68              |
| 1:F:260:TRP:HB2  | 1:F:262:PRO:HD2  | 0.71                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:208:MET:CE   | 1:G:232:VAL:HA   | 2.24                     | 0.68              |
| 1:G:488:GLY:HA3  | 1:G:492:LEU:HD11 | 1.76                     | 0.68              |
| 1:E:309:MET:HB3  | 1:E:499:ILE:HD12 | 1.75                     | 0.68              |
| 1:E:339:LEU:HB3  | 1:E:341:MET:HE2  | 1.74                     | 0.68              |
| 1:A:169:GLN:HE22 | 1:A:254:VAL:HG11 | 1.58                     | 0.68              |
| 1:C:292:CYS:O    | 1:C:295:ILE:HG12 | 1.93                     | 0.68              |
| 1:E:202:ILE:HD13 | 1:E:223:LEU:HD22 | 1.76                     | 0.68              |
| 1:F:260:TRP:CG   | 1:F:262:PRO:HD2  | 2.27                     | 0.68              |
| 1:F:413:ARG:HE   | 1:F:458:VAL:HB   | 1.58                     | 0.68              |
| 1:G:312:SER:O    | 1:G:313:GLY:O    | 2.12                     | 0.68              |
| 1:A:504:ARG:CD   | 1:A:506:GLN:HG2  | 2.22                     | 0.67              |
| 1:C:78:TYR:CE1   | 1:C:97:TRP:HB3   | 2.29                     | 0.67              |
| 1:D:295:ILE:O    | 1:D:299:THR:HG23 | 1.93                     | 0.67              |
| 1:E:412:MET:CA   | 1:E:416:LEU:HD12 | 2.19                     | 0.67              |
| 1:F:307:VAL:O    | 1:F:307:VAL:HG12 | 1.95                     | 0.67              |
| 1:D:368:LEU:O    | 1:D:368:LEU:HD22 | 1.94                     | 0.67              |
| 1:F:153:ILE:HG13 | 1:F:174:PRO:HB2  | 1.77                     | 0.67              |
| 1:A:108:VAL:HG12 | 1:A:121:GLN:HG2  | 1.74                     | 0.67              |
| 1:D:290:SER:N    | 1:D:325:GLN:HE21 | 1.90                     | 0.67              |
| 1:E:370:ARG:HD2  | 1:E:371:GLU:H    | 1.53                     | 0.67              |
| 1:F:490:GLY:HA2  | 1:F:493:ARG:HG3  | 1.76                     | 0.67              |
| 1:G:84:ARG:HA    | 1:G:243:LEU:HD21 | 1.77                     | 0.67              |
| 1:C:96:TYR:HE2   | 1:C:107:GLN:HE21 | 1.43                     | 0.67              |
| 1:F:127:ASP:O    | 1:F:128:LYS:CB   | 2.26                     | 0.67              |
| 1:F:194:GLU:H    | 1:F:194:GLU:CD   | 2.01                     | 0.67              |
| 1:G:121:GLN:HB3  | 1:G:133:THR:HG23 | 1.74                     | 0.67              |
| 1:A:126:LYS:NZ   | 1:A:127:ASP:CA   | 2.40                     | 0.67              |
| 1:A:261:ILE:O    | 1:A:261:ILE:CD1  | 2.43                     | 0.67              |
| 1:D:230:VAL:HG11 | 1:D:260:TRP:HE1  | 1.59                     | 0.67              |
| 1:E:311:THR:O    | 1:E:312:SER:HB3  | 1.94                     | 0.67              |
| 1:F:389:ASP:H    | 1:G:269:LEU:HD21 | 1.59                     | 0.67              |
| 1:G:68:VAL:HG12  | 1:G:121:GLN:OE1  | 1.95                     | 0.67              |
| 1:G:86:ILE:HG21  | 1:G:163:LEU:HD12 | 1.75                     | 0.67              |
| 1:G:303:ARG:O    | 1:G:306:GLU:HG3  | 1.93                     | 0.67              |
| 1:G:420:VAL:HG22 | 1:G:459:VAL:HB   | 1.77                     | 0.67              |
| 1:B:352:ASP:CG   | 1:B:363:ARG:HD3  | 2.20                     | 0.67              |
| 1:C:306:GLU:HA   | 1:C:497:ASP:OD2  | 1.95                     | 0.67              |
| 1:D:86:ILE:HG21  | 1:D:163:LEU:HD12 | 1.76                     | 0.67              |
| 1:G:287:LEU:HD11 | 1:G:335:LYS:HG3  | 1.77                     | 0.67              |
| 1:C:425:HIS:HE1  | 1:C:427:SER:OG   | 1.76                     | 0.67              |
| 1:D:107:GLN:HB2  | 1:D:124:ARG:CG   | 2.25                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:121:GLN:HB3  | 1:E:133:THR:HG23 | 1.75                     | 0.67              |
| 1:E:276:ARG:HG2  | 1:E:276:ARG:HH11 | 1.58                     | 0.67              |
| 1:E:442:ILE:HD12 | 1:E:488:GLY:HA2  | 1.76                     | 0.67              |
| 1:F:382:PHE:HE1  | 1:G:275:ILE:HD12 | 1.59                     | 0.67              |
| 1:C:220:ALA:HB1  | 1:C:261:ILE:HD12 | 1.76                     | 0.67              |
| 1:C:316:MET:HE1  | 1:C:535:TYR:CZ   | 2.30                     | 0.67              |
| 1:F:442:ILE:CD1  | 1:F:492:LEU:HD11 | 2.25                     | 0.67              |
| 1:A:316:MET:HE1  | 1:A:535:TYR:CZ   | 2.30                     | 0.67              |
| 1:C:315:GLY:HA2  | 1:C:317:VAL:HG23 | 1.76                     | 0.67              |
| 1:D:316:MET:HE1  | 1:D:535:TYR:CE2  | 2.30                     | 0.67              |
| 1:F:199:PHE:O    | 1:F:227:LYS:HE2  | 1.95                     | 0.67              |
| 1:F:394:TYR:CE2  | 1:F:405:LEU:HD12 | 2.29                     | 0.67              |
| 1:C:338:GLY:HA3  | 1:C:412:MET:CE   | 2.24                     | 0.67              |
| 1:D:78:TYR:CD2   | 1:D:92:GLN:HG2   | 2.30                     | 0.67              |
| 1:E:338:GLY:HA3  | 1:E:412:MET:CE   | 2.25                     | 0.67              |
| 1:A:107:GLN:CB   | 1:A:124:ARG:HG3  | 2.25                     | 0.66              |
| 1:B:229:ARG:HB2  | 1:B:258:GLY:O    | 1.95                     | 0.66              |
| 1:E:205:MET:HA   | 1:E:231:ALA:HB3  | 1.77                     | 0.66              |
| 1:E:321:PHE:CE2  | 1:E:533:MET:HE1  | 2.30                     | 0.66              |
| 1:A:169:GLN:O    | 1:A:170:ASP:HB2  | 1.94                     | 0.66              |
| 1:B:439:ARG:O    | 1:B:442:ILE:HG22 | 1.94                     | 0.66              |
| 1:F:246:HIS:HB2  | 1:F:249:GLU:HB2  | 1.76                     | 0.66              |
| 1:G:305:GLY:O    | 1:G:454:LYS:HD2  | 1.95                     | 0.66              |
| 1:G:338:GLY:HA3  | 1:G:412:MET:HE1  | 1.77                     | 0.66              |
| 1:A:260:TRP:O    | 1:A:261:ILE:HG23 | 1.94                     | 0.66              |
| 1:B:450:LYS:HE2  | 1:B:454:LYS:CD   | 2.23                     | 0.66              |
| 1:C:344:GLU:OE1  | 1:C:349:THR:HB   | 1.94                     | 0.66              |
| 1:D:289:PHE:H    | 1:D:296:ASN:ND2  | 1.90                     | 0.66              |
| 1:D:447:THR:HG22 | 1:D:495:LEU:CD2  | 2.16                     | 0.66              |
| 1:D:476:GLU:H    | 1:D:476:GLU:CD   | 2.03                     | 0.66              |
| 1:E:194:GLU:CD   | 1:E:194:GLU:H    | 2.02                     | 0.66              |
| 1:A:142:PHE:CE2  | 1:A:162:MET:HE3  | 2.30                     | 0.66              |
| 1:B:78:TYR:CE1   | 1:B:97:TRP:HB3   | 2.31                     | 0.66              |
| 1:B:283:GLU:HG3  | 1:B:286:GLY:N    | 2.11                     | 0.66              |
| 1:E:425:HIS:HE1  | 1:E:427:SER:OG   | 1.76                     | 0.66              |
| 1:G:515:LEU:HD21 | 1:G:529:ILE:HD11 | 1.78                     | 0.66              |
| 1:A:261:ILE:O    | 1:A:261:ILE:HD13 | 1.95                     | 0.66              |
| 1:C:467:LYS:HE3  | 1:C:486:LEU:O    | 1.95                     | 0.66              |
| 1:D:268:ALA:HA   | 1:D:271:LEU:CD1  | 2.24                     | 0.66              |
| 1:F:338:GLY:HA3  | 1:F:412:MET:CE   | 2.25                     | 0.66              |
| 1:G:289:PHE:N    | 1:G:296:ASN:HD21 | 1.92                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:504:ARG:HD3  | 1:G:506:GLN:CG   | 2.15                     | 0.66              |
| 1:A:394:TYR:CD1  | 1:A:394:TYR:C    | 2.74                     | 0.66              |
| 1:A:401:GLU:HG2  | 1:A:402:THR:H    | 1.59                     | 0.66              |
| 1:E:387:GLY:HA2  | 1:F:269:LEU:HD11 | 1.77                     | 0.66              |
| 1:F:420:VAL:HG22 | 1:F:459:VAL:HB   | 1.78                     | 0.66              |
| 1:A:256:ASN:OD1  | 1:A:256:ASN:C    | 2.36                     | 0.66              |
| 1:D:307:VAL:HG12 | 1:D:307:VAL:O    | 1.95                     | 0.66              |
| 1:E:295:ILE:O    | 1:E:299:THR:HG23 | 1.95                     | 0.66              |
| 1:A:79:SER:H     | 1:A:98:ILE:HD13  | 1.61                     | 0.66              |
| 1:C:208:MET:HE1  | 1:C:232:VAL:HA   | 1.76                     | 0.66              |
| 1:C:311:THR:O    | 1:C:312:SER:HB3  | 1.94                     | 0.66              |
| 1:D:216:VAL:HG11 | 1:D:230:VAL:HG22 | 1.77                     | 0.66              |
| 1:D:439:ARG:O    | 1:D:442:ILE:HG22 | 1.95                     | 0.66              |
| 1:E:305:GLY:O    | 1:E:454:LYS:HD2  | 1.95                     | 0.66              |
| 1:E:411:TYR:CE1  | 1:F:265:VAL:HG11 | 2.29                     | 0.66              |
| 1:C:394:TYR:CE2  | 1:C:405:LEU:HD12 | 2.30                     | 0.66              |
| 1:F:162:MET:SD   | 1:F:166:MET:HG3  | 2.36                     | 0.66              |
| 1:A:251:MET:HE3  | 1:A:251:MET:CA   | 2.26                     | 0.66              |
| 1:B:409:LEU:CD2  | 1:B:421:ILE:HG21 | 2.23                     | 0.65              |
| 1:C:531:GLY:C    | 1:C:532:TYR:CD1  | 2.74                     | 0.65              |
| 1:D:147:TRP:CG   | 1:D:174:PRO:HB3  | 2.31                     | 0.65              |
| 1:D:261:ILE:H    | 1:D:262:PRO:CD   | 2.08                     | 0.65              |
| 1:F:439:ARG:O    | 1:F:442:ILE:HG22 | 1.95                     | 0.65              |
| 1:G:394:TYR:HE1  | 1:G:396:SER:HB2  | 1.60                     | 0.65              |
| 1:A:496:SER:HB2  | 1:A:499:ILE:HD11 | 1.78                     | 0.65              |
| 1:B:420:VAL:HG22 | 1:B:459:VAL:HB   | 1.78                     | 0.65              |
| 1:B:427:SER:HB3  | 1:B:487:ARG:NH1  | 2.10                     | 0.65              |
| 1:C:94:ALA:HB1   | 1:C:162:MET:HE1  | 1.78                     | 0.65              |
| 1:C:442:ILE:HD12 | 1:C:488:GLY:CA   | 2.27                     | 0.65              |
| 1:C:499:ILE:CG2  | 1:C:519:LEU:HB2  | 2.25                     | 0.65              |
| 1:D:339:LEU:HB3  | 1:D:341:MET:HE3  | 1.75                     | 0.65              |
| 1:E:223:LEU:HD23 | 1:E:224:PRO:HD2  | 1.77                     | 0.65              |
| 1:G:346:VAL:HB   | 1:G:395:ASP:HB2  | 1.78                     | 0.65              |
| 1:A:289:PHE:N    | 1:A:296:ASN:HD21 | 1.94                     | 0.65              |
| 1:D:78:TYR:CE1   | 1:D:97:TRP:HB3   | 2.32                     | 0.65              |
| 1:D:248:ARG:HB3  | 1:D:248:ARG:NH1  | 2.08                     | 0.65              |
| 1:D:316:MET:HE1  | 1:D:535:TYR:CZ   | 2.31                     | 0.65              |
| 1:E:322:VAL:CG2  | 1:E:463:ILE:HD11 | 2.27                     | 0.65              |
| 1:A:316:MET:HE1  | 1:A:535:TYR:CE2  | 2.32                     | 0.65              |
| 1:B:424:ASP:OD2  | 1:B:425:HIS:HB2  | 1.96                     | 0.65              |
| 1:D:152:LYS:HD3  | 1:D:203:ILE:CD1  | 2.24                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:178:LEU:HB2  | 1:D:181:GLY:HA2  | 1.78                     | 0.65              |
| 1:G:484:THR:C    | 1:G:486:LEU:H    | 2.04                     | 0.65              |
| 1:B:454:LYS:HZ2  | 1:G:344:GLU:HA   | 1.55                     | 0.65              |
| 1:C:124:ARG:HD3  | 1:C:125:ASP:C    | 2.22                     | 0.65              |
| 1:D:208:MET:CE   | 1:D:232:VAL:HA   | 2.27                     | 0.65              |
| 1:D:424:ASP:OD2  | 1:D:425:HIS:HB2  | 1.96                     | 0.65              |
| 1:E:111:TYR:CE2  | 1:E:142:PHE:HB2  | 2.31                     | 0.65              |
| 1:F:107:GLN:CB   | 1:F:124:ARG:CG   | 2.71                     | 0.65              |
| 1:F:111:TYR:CE2  | 1:F:142:PHE:HB2  | 2.32                     | 0.65              |
| 1:A:295:ILE:O    | 1:A:299:THR:HG23 | 1.96                     | 0.65              |
| 1:C:358:ASN:O    | 1:C:360:VAL:HG13 | 1.96                     | 0.65              |
| 1:C:490:GLY:CA   | 1:C:493:ARG:HG3  | 2.27                     | 0.65              |
| 1:E:478:GLY:HA3  | 1:E:505:ASN:HB2  | 1.79                     | 0.65              |
| 1:G:79:SER:H     | 1:G:98:ILE:HD13  | 1.60                     | 0.65              |
| 1:E:86:ILE:HG21  | 1:E:163:LEU:HD12 | 1.77                     | 0.65              |
| 1:E:389:ASP:HA   | 1:F:269:LEU:HD23 | 1.77                     | 0.65              |
| 1:F:260:TRP:HB2  | 1:F:262:PRO:HD3  | 1.69                     | 0.65              |
| 1:B:104:VAL:HG12 | 1:B:106:TYR:CE1  | 2.32                     | 0.65              |
| 1:B:142:PHE:CE2  | 1:B:162:MET:HE3  | 2.32                     | 0.65              |
| 1:B:312:SER:O    | 1:B:313:GLY:O    | 2.15                     | 0.65              |
| 1:D:517:ARG:HB3  | 1:D:519:LEU:CD1  | 2.27                     | 0.65              |
| 1:G:96:TYR:HE2   | 1:G:107:GLN:HE21 | 1.43                     | 0.65              |
| 1:G:442:ILE:HD11 | 1:G:492:LEU:HD21 | 1.78                     | 0.65              |
| 1:G:446:MET:HE2  | 1:G:492:LEU:HB3  | 1.77                     | 0.65              |
| 1:D:394:TYR:HE1  | 1:D:396:SER:HB2  | 1.61                     | 0.65              |
| 1:F:510:MET:HE2  | 1:F:513:LEU:CD2  | 2.27                     | 0.65              |
| 1:A:108:VAL:CG1  | 1:A:121:GLN:HG2  | 2.26                     | 0.65              |
| 1:D:166:MET:CE   | 1:D:171:CYS:CB   | 2.75                     | 0.65              |
| 1:D:366:ASP:HB2  | 1:E:284:SER:HG   | 1.59                     | 0.65              |
| 1:E:216:VAL:CG1  | 1:E:230:VAL:CG2  | 2.74                     | 0.65              |
| 1:A:414:SER:CB   | 1:C:226:GLY:H    | 2.10                     | 0.64              |
| 1:C:78:TYR:CD2   | 1:C:92:GLN:HG2   | 2.31                     | 0.64              |
| 1:C:425:HIS:CE1  | 1:C:427:SER:HB2  | 2.32                     | 0.64              |
| 1:F:251:MET:HE3  | 1:F:251:MET:CA   | 2.27                     | 0.64              |
| 1:F:260:TRP:C    | 1:F:261:ILE:HG13 | 2.23                     | 0.64              |
| 1:F:476:GLU:HB3  | 1:F:506:GLN:OE1  | 1.97                     | 0.64              |
| 1:A:294:GLY:O    | 1:A:295:ILE:C    | 2.39                     | 0.64              |
| 1:A:412:MET:CA   | 1:A:416:LEU:HD12 | 2.24                     | 0.64              |
| 1:A:442:ILE:HD12 | 1:A:488:GLY:CA   | 2.27                     | 0.64              |
| 1:B:68:VAL:HG12  | 1:B:121:GLN:OE1  | 1.97                     | 0.64              |
| 1:B:248:ARG:NH1  | 1:B:248:ARG:HB2  | 2.04                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:344:GLU:CG   | 1:D:349:THR:HG22 | 2.25                     | 0.64              |
| 1:E:154:VAL:HB   | 1:E:175:VAL:HG13 | 1.79                     | 0.64              |
| 1:F:289:PHE:N    | 1:F:296:ASN:HD21 | 1.93                     | 0.64              |
| 1:G:166:MET:CE   | 1:G:171:CYS:HB3  | 2.27                     | 0.64              |
| 1:G:194:GLU:CD   | 1:G:194:GLU:H    | 2.04                     | 0.64              |
| 1:G:442:ILE:HD12 | 1:G:488:GLY:HA2  | 1.79                     | 0.64              |
| 1:A:107:GLN:HB2  | 1:A:124:ARG:CG   | 2.28                     | 0.64              |
| 1:A:414:SER:HB3  | 1:C:226:GLY:N    | 2.11                     | 0.64              |
| 1:B:262:PRO:HB2  | 1:B:265:VAL:HG12 | 1.77                     | 0.64              |
| 1:B:338:GLY:HA3  | 1:B:412:MET:HE1  | 1.80                     | 0.64              |
| 1:C:427:SER:HB3  | 1:C:487:ARG:HH12 | 1.62                     | 0.64              |
| 1:G:490:GLY:CA   | 1:G:493:ARG:HG3  | 2.27                     | 0.64              |
| 1:C:344:GLU:HA   | 1:D:454:LYS:NZ   | 2.12                     | 0.64              |
| 1:C:401:GLU:HB3  | 1:C:404:ARG:HB3  | 1.80                     | 0.64              |
| 1:D:312:SER:CB   | 1:D:502:LEU:O    | 2.44                     | 0.64              |
| 1:E:504:ARG:HH21 | 1:E:506:GLN:HB3  | 1.63                     | 0.64              |
| 1:A:510:MET:HE1  | 1:A:547:TYR:CE1  | 2.33                     | 0.64              |
| 1:D:452:PHE:O    | 1:D:456:THR:HG23 | 1.97                     | 0.64              |
| 1:E:439:ARG:O    | 1:E:442:ILE:HG22 | 1.97                     | 0.64              |
| 1:F:121:GLN:HB2  | 1:F:133:THR:OG1  | 1.96                     | 0.64              |
| 1:F:121:GLN:CB   | 1:F:133:THR:HG23 | 2.27                     | 0.64              |
| 1:F:496:SER:O    | 1:F:520:LYS:HE2  | 1.98                     | 0.64              |
| 1:A:78:TYR:CE1   | 1:A:97:TRP:HB3   | 2.33                     | 0.64              |
| 1:A:303:ARG:O    | 1:A:306:GLU:HG3  | 1.97                     | 0.64              |
| 1:A:510:MET:HE1  | 1:A:547:TYR:OH   | 1.98                     | 0.64              |
| 1:B:111:TYR:CE2  | 1:B:142:PHE:HB2  | 2.32                     | 0.64              |
| 1:B:515:LEU:HD21 | 1:B:529:ILE:CD1  | 2.28                     | 0.64              |
| 1:C:79:SER:H     | 1:C:98:ILE:HD13  | 1.62                     | 0.64              |
| 1:C:216:VAL:HG11 | 1:C:230:VAL:HG22 | 1.80                     | 0.64              |
| 1:A:278:HIS:CD2  | 1:B:351:GLU:OE1  | 2.51                     | 0.64              |
| 1:C:154:VAL:HB   | 1:C:175:VAL:HG13 | 1.79                     | 0.64              |
| 1:C:166:MET:HE1  | 1:C:171:CYS:HB3  | 1.80                     | 0.64              |
| 1:D:74:SER:HB2   | 1:D:99:ALA:HB1   | 1.80                     | 0.64              |
| 1:A:94:ALA:HB1   | 1:A:162:MET:HE1  | 1.80                     | 0.64              |
| 1:A:536:ASN:HD22 | 1:A:538:GLU:H    | 1.45                     | 0.64              |
| 1:D:476:GLU:HB3  | 1:D:506:GLN:OE1  | 1.97                     | 0.64              |
| 1:F:303:ARG:O    | 1:F:306:GLU:HG3  | 1.97                     | 0.64              |
| 1:A:130:PHE:O    | 1:A:131:LYS:HG3  | 1.98                     | 0.64              |
| 1:A:145:HIS:CE1  | 1:A:146:LEU:HD23 | 2.33                     | 0.64              |
| 1:A:248:ARG:HB3  | 1:A:248:ARG:NH1  | 2.10                     | 0.64              |
| 1:A:490:GLY:CA   | 1:A:493:ARG:HG3  | 2.27                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:496:SER:O    | 1:D:520:LYS:HE2  | 1.98                     | 0.64              |
| 1:E:78:TYR:CD2   | 1:E:92:GLN:HG2   | 2.32                     | 0.64              |
| 1:E:338:GLY:HA3  | 1:E:412:MET:HE1  | 1.80                     | 0.64              |
| 1:G:356:LEU:HD12 | 1:G:541:TRP:NE1  | 2.13                     | 0.64              |
| 1:C:504:ARG:HH21 | 1:C:506:GLN:HB3  | 1.63                     | 0.64              |
| 1:E:84:ARG:HA    | 1:E:243:LEU:HD21 | 1.80                     | 0.64              |
| 1:E:124:ARG:HD3  | 1:E:125:ASP:C    | 2.23                     | 0.64              |
| 1:E:389:ASP:H    | 1:F:269:LEU:HD21 | 1.63                     | 0.64              |
| 1:E:504:ARG:NH2  | 1:E:506:GLN:HB3  | 2.13                     | 0.64              |
| 1:F:79:SER:H     | 1:F:98:ILE:HD13  | 1.63                     | 0.64              |
| 1:F:84:ARG:HA    | 1:F:243:LEU:HD21 | 1.80                     | 0.64              |
| 1:A:476:GLU:H    | 1:A:476:GLU:CD   | 2.06                     | 0.63              |
| 1:A:517:ARG:HB3  | 1:A:519:LEU:CD1  | 2.28                     | 0.63              |
| 1:B:94:ALA:HB1   | 1:B:162:MET:HE1  | 1.80                     | 0.63              |
| 1:F:261:ILE:H    | 1:F:262:PRO:CD   | 2.11                     | 0.63              |
| 1:G:166:MET:HE3  | 1:G:171:CYS:HA   | 1.79                     | 0.63              |
| 1:B:356:LEU:HD12 | 1:B:541:TRP:NE1  | 2.13                     | 0.63              |
| 1:B:480:PRO:HA   | 1:B:503:GLU:OE1  | 1.99                     | 0.63              |
| 1:C:287:LEU:HD11 | 1:C:335:LYS:HG3  | 1.79                     | 0.63              |
| 1:C:312:SER:N    | 1:C:318:MET:HE2  | 2.13                     | 0.63              |
| 1:D:84:ARG:HA    | 1:D:243:LEU:HD21 | 1.80                     | 0.63              |
| 1:E:424:ASP:OD2  | 1:E:425:HIS:HB2  | 1.98                     | 0.63              |
| 1:G:152:LYS:HD3  | 1:G:203:ILE:CD1  | 2.28                     | 0.63              |
| 1:B:166:MET:CE   | 1:B:171:CYS:CB   | 2.77                     | 0.63              |
| 1:C:303:ARG:O    | 1:C:306:GLU:HG3  | 1.97                     | 0.63              |
| 1:B:346:VAL:HB   | 1:B:395:ASP:HB2  | 1.80                     | 0.63              |
| 1:B:480:PRO:HA   | 1:B:503:GLU:CD   | 2.24                     | 0.63              |
| 1:D:216:VAL:CG1  | 1:D:230:VAL:CG2  | 2.77                     | 0.63              |
| 1:D:394:TYR:CD1  | 1:D:394:TYR:C    | 2.76                     | 0.63              |
| 1:G:216:VAL:HG11 | 1:G:230:VAL:HG22 | 1.81                     | 0.63              |
| 1:G:413:ARG:O    | 1:G:417:GLY:HA2  | 1.99                     | 0.63              |
| 1:A:253:GLN:C    | 1:A:257:ALA:HB2  | 2.23                     | 0.63              |
| 1:A:504:ARG:HH21 | 1:A:506:GLN:HG2  | 1.64                     | 0.63              |
| 1:F:124:ARG:HD3  | 1:F:125:ASP:C    | 2.23                     | 0.63              |
| 1:F:216:VAL:HG11 | 1:F:230:VAL:HG21 | 1.80                     | 0.63              |
| 1:G:152:LYS:HG3  | 1:G:201:GLN:CG   | 2.29                     | 0.63              |
| 1:B:147:TRP:CG   | 1:B:174:PRO:HB3  | 2.34                     | 0.63              |
| 1:C:121:GLN:HB2  | 1:C:133:THR:HG1  | 1.62                     | 0.63              |
| 1:D:141:LEU:HD13 | 1:D:176:VAL:CG2  | 2.28                     | 0.63              |
| 1:F:480:PRO:HA   | 1:F:503:GLU:CD   | 2.22                     | 0.63              |
| 1:B:285:VAL:HG22 | 1:B:300:LEU:HD11 | 1.81                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:411:TYR:OH   | 1:D:260:TRP:CB   | 2.46                     | 0.63              |
| 1:G:290:SER:N    | 1:G:325:GLN:HE21 | 1.91                     | 0.63              |
| 1:C:251:MET:HA   | 1:C:251:MET:CE   | 2.29                     | 0.63              |
| 1:A:269:LEU:HD11 | 1:B:387:GLY:HA2  | 1.80                     | 0.63              |
| 1:B:321:PHE:CE2  | 1:B:533:MET:HE1  | 2.33                     | 0.63              |
| 1:C:496:SER:O    | 1:C:520:LYS:HE2  | 1.98                     | 0.63              |
| 1:D:369:LYS:HG2  | 1:E:279:LEU:HD22 | 1.81                     | 0.63              |
| 1:F:394:TYR:CD1  | 1:F:394:TYR:C    | 2.77                     | 0.63              |
| 1:G:124:ARG:HD3  | 1:G:125:ASP:C    | 2.24                     | 0.63              |
| 1:A:181:GLY:O    | 1:A:182:ALA:C    | 2.40                     | 0.62              |
| 1:A:253:GLN:O    | 1:A:257:ALA:CB   | 2.47                     | 0.62              |
| 1:E:229:ARG:HB3  | 1:E:259:PRO:HB3  | 1.80                     | 0.62              |
| 1:F:486:LEU:HB3  | 1:F:493:ARG:HD2  | 1.80                     | 0.62              |
| 1:G:283:GLU:O    | 1:G:303:ARG:HG2  | 1.98                     | 0.62              |
| 1:A:141:LEU:HD11 | 1:A:196:PHE:HZ   | 1.64                     | 0.62              |
| 1:A:220:ALA:HB3  | 1:A:261:ILE:HG21 | 1.80                     | 0.62              |
| 1:F:517:ARG:HB3  | 1:F:519:LEU:CD1  | 2.29                     | 0.62              |
| 1:A:412:MET:HE2  | 1:A:421:ILE:HD13 | 1.77                     | 0.62              |
| 1:D:486:LEU:HB3  | 1:D:493:ARG:HD2  | 1.81                     | 0.62              |
| 1:F:338:GLY:HA3  | 1:F:412:MET:HE1  | 1.81                     | 0.62              |
| 1:E:166:MET:CE   | 1:E:171:CYS:CB   | 2.77                     | 0.62              |
| 1:F:504:ARG:HH21 | 1:F:506:GLN:CB   | 2.13                     | 0.62              |
| 1:A:290:SER:N    | 1:A:325:GLN:HE21 | 1.92                     | 0.62              |
| 1:A:521:CYS:SG   | 1:A:524:THR:HG23 | 2.39                     | 0.62              |
| 1:B:312:SER:HB2  | 1:B:502:LEU:O    | 1.99                     | 0.62              |
| 1:C:111:TYR:CZ   | 1:C:142:PHE:HB2  | 2.35                     | 0.62              |
| 1:C:152:LYS:HG3  | 1:C:201:GLN:CG   | 2.29                     | 0.62              |
| 1:D:152:LYS:HG3  | 1:D:201:GLN:CG   | 2.28                     | 0.62              |
| 1:E:394:TYR:C    | 1:E:394:TYR:CD1  | 2.77                     | 0.62              |
| 1:E:411:TYR:OH   | 1:F:262:PRO:HG3  | 1.99                     | 0.62              |
| 1:F:290:SER:N    | 1:F:325:GLN:HE21 | 1.96                     | 0.62              |
| 1:F:346:VAL:HB   | 1:F:395:ASP:HB2  | 1.80                     | 0.62              |
| 1:C:421:ILE:HB   | 1:C:460:LEU:HD12 | 1.81                     | 0.62              |
| 1:G:216:VAL:HG11 | 1:G:230:VAL:HG21 | 1.79                     | 0.62              |
| 1:G:344:GLU:CG   | 1:G:349:THR:HG22 | 2.28                     | 0.62              |
| 1:A:482:SER:OG   | 1:A:484:THR:HG23 | 2.00                     | 0.62              |
| 1:B:152:LYS:HG3  | 1:B:201:GLN:CG   | 2.29                     | 0.62              |
| 1:B:295:ILE:O    | 1:B:299:THR:HG23 | 2.00                     | 0.62              |
| 1:D:68:VAL:HG12  | 1:D:121:GLN:OE1  | 2.00                     | 0.62              |
| 1:E:262:PRO:HB2  | 1:E:265:VAL:HG12 | 1.81                     | 0.62              |
| 1:F:401:GLU:HG3  | 1:F:431:SER:O    | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:346:VAL:HB   | 1:D:395:ASP:HB2  | 1.82                     | 0.62              |
| 1:D:504:ARG:CD   | 1:D:506:GLN:HG2  | 2.26                     | 0.62              |
| 1:E:307:VAL:O    | 1:E:307:VAL:HG12 | 1.99                     | 0.62              |
| 1:F:68:VAL:HG12  | 1:F:121:GLN:OE1  | 1.99                     | 0.62              |
| 1:G:283:GLU:HG2  | 1:G:284:SER:N    | 2.10                     | 0.62              |
| 1:G:496:SER:HB2  | 1:G:499:ILE:HD11 | 1.79                     | 0.62              |
| 1:A:318:MET:SD   | 1:A:463:ILE:CD1  | 2.88                     | 0.62              |
| 1:B:484:THR:C    | 1:B:486:LEU:N    | 2.56                     | 0.62              |
| 1:C:345:SER:O    | 1:C:349:THR:CG2  | 2.48                     | 0.62              |
| 1:D:112:ARG:HG3  | 1:D:145:HIS:CD2  | 2.34                     | 0.62              |
| 1:D:480:PRO:HA   | 1:D:503:GLU:CD   | 2.24                     | 0.62              |
| 1:E:96:TYR:HE2   | 1:E:107:GLN:HE21 | 1.47                     | 0.62              |
| 1:E:478:GLY:CA   | 1:E:505:ASN:HB2  | 2.30                     | 0.62              |
| 1:G:178:LEU:HB2  | 1:G:181:GLY:HA2  | 1.80                     | 0.62              |
| 1:G:322:VAL:HG21 | 1:G:463:ILE:HD11 | 1.80                     | 0.62              |
| 1:B:309:MET:HB3  | 1:B:499:ILE:CD1  | 2.30                     | 0.62              |
| 1:C:251:MET:CA   | 1:C:251:MET:HE3  | 2.30                     | 0.62              |
| 1:C:312:SER:CB   | 1:C:502:LEU:O    | 2.42                     | 0.62              |
| 1:D:347:GLU:CD   | 1:E:274:ARG:HD2  | 2.24                     | 0.62              |
| 1:B:78:TYR:CD2   | 1:B:92:GLN:HG2   | 2.34                     | 0.61              |
| 1:B:253:GLN:CA   | 1:B:257:ALA:HB2  | 2.30                     | 0.61              |
| 1:B:471:LYS:HB3  | 1:B:479:ARG:NH1  | 2.15                     | 0.61              |
| 1:D:482:SER:OG   | 1:D:484:THR:HG23 | 1.99                     | 0.61              |
| 1:E:339:LEU:HB3  | 1:E:341:MET:HE1  | 1.78                     | 0.61              |
| 1:F:205:MET:HA   | 1:F:231:ALA:HB3  | 1.81                     | 0.61              |
| 1:F:208:MET:CE   | 1:F:232:VAL:HA   | 2.30                     | 0.61              |
| 1:G:223:LEU:HD23 | 1:G:224:PRO:HD2  | 1.81                     | 0.61              |
| 1:A:312:SER:H    | 1:A:318:MET:CE   | 2.12                     | 0.61              |
| 1:A:504:ARG:NH2  | 1:A:506:GLN:HB3  | 2.15                     | 0.61              |
| 1:B:303:ARG:O    | 1:B:306:GLU:HG3  | 1.99                     | 0.61              |
| 1:B:322:VAL:HG21 | 1:B:463:ILE:HD11 | 1.80                     | 0.61              |
| 1:B:368:LEU:HD22 | 1:B:372:ILE:HG23 | 1.82                     | 0.61              |
| 1:C:480:PRO:HA   | 1:C:503:GLU:CD   | 2.24                     | 0.61              |
| 1:D:447:THR:HA   | 1:D:495:LEU:HD23 | 1.82                     | 0.61              |
| 1:E:79:SER:H     | 1:E:98:ILE:HD13  | 1.64                     | 0.61              |
| 1:G:504:ARG:HH21 | 1:G:506:GLN:CB   | 2.12                     | 0.61              |
| 1:A:152:LYS:HG3  | 1:A:201:GLN:CG   | 2.30                     | 0.61              |
| 1:A:394:TYR:CE2  | 1:A:408:LYS:HD2  | 2.36                     | 0.61              |
| 1:A:412:MET:CE   | 1:A:421:ILE:CD1  | 2.67                     | 0.61              |
| 1:B:186:LYS:CD   | 1:B:218:GLU:HG3  | 2.27                     | 0.61              |
| 1:C:309:MET:HB3  | 1:C:499:ILE:CD1  | 2.30                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:344:GLU:HB2  | 1:C:348:GLU:OE2  | 2.00                     | 0.61              |
| 1:C:536:ASN:HD22 | 1:C:536:ASN:C    | 2.06                     | 0.61              |
| 1:D:142:PHE:CD2  | 1:D:162:MET:HE3  | 2.36                     | 0.61              |
| 1:D:217:GLU:HA   | 1:D:261:ILE:HG22 | 1.82                     | 0.61              |
| 1:D:412:MET:CA   | 1:D:416:LEU:HD12 | 2.21                     | 0.61              |
| 1:D:484:THR:C    | 1:D:486:LEU:H    | 2.07                     | 0.61              |
| 1:E:440:LYS:HE2  | 1:E:440:LYS:O    | 1.99                     | 0.61              |
| 1:G:401:GLU:HG2  | 1:G:402:THR:H    | 1.64                     | 0.61              |
| 1:D:372:ILE:HA   | 1:D:375:ASN:OD1  | 1.99                     | 0.61              |
| 1:A:84:ARG:HA    | 1:A:243:LEU:HD21 | 1.81                     | 0.61              |
| 1:A:322:VAL:HG21 | 1:A:463:ILE:HD11 | 1.82                     | 0.61              |
| 1:A:439:ARG:O    | 1:A:442:ILE:HG22 | 1.99                     | 0.61              |
| 1:B:309:MET:HE2  | 1:B:462:VAL:HG12 | 1.83                     | 0.61              |
| 1:C:84:ARG:HA    | 1:C:243:LEU:HD21 | 1.83                     | 0.61              |
| 1:C:259:PRO:O    | 1:C:260:TRP:HB3  | 1.99                     | 0.61              |
| 1:C:442:ILE:HD11 | 1:C:492:LEU:HD11 | 1.82                     | 0.61              |
| 1:C:450:LYS:CE   | 1:C:454:LYS:CD   | 2.73                     | 0.61              |
| 1:D:305:GLY:O    | 1:D:454:LYS:HD2  | 2.01                     | 0.61              |
| 1:E:78:TYR:CE1   | 1:E:97:TRP:HB3   | 2.36                     | 0.61              |
| 1:E:142:PHE:CE2  | 1:E:162:MET:HE3  | 2.36                     | 0.61              |
| 1:E:442:ILE:HD12 | 1:E:488:GLY:CA   | 2.31                     | 0.61              |
| 1:E:450:LYS:CE   | 1:E:454:LYS:CD   | 2.72                     | 0.61              |
| 1:E:480:PRO:HA   | 1:E:503:GLU:CD   | 2.26                     | 0.61              |
| 1:F:406:LEU:HD21 | 1:F:449:LEU:HD23 | 1.81                     | 0.61              |
| 1:G:127:ASP:O    | 1:G:128:LYS:CB   | 2.39                     | 0.61              |
| 1:G:406:LEU:HD21 | 1:G:449:LEU:HD23 | 1.82                     | 0.61              |
| 1:A:305:GLY:O    | 1:A:454:LYS:HD2  | 2.00                     | 0.61              |
| 1:B:202:ILE:HD13 | 1:B:223:LEU:HD22 | 1.81                     | 0.61              |
| 1:B:394:TYR:CE2  | 1:B:405:LEU:HD12 | 2.35                     | 0.61              |
| 1:E:147:TRP:CG   | 1:E:174:PRO:HB3  | 2.36                     | 0.61              |
| 1:E:258:GLY:HA3  | 1:E:260:TRP:CZ3  | 2.35                     | 0.61              |
| 1:E:287:LEU:HD11 | 1:E:335:LYS:HG3  | 1.82                     | 0.61              |
| 1:E:345:SER:O    | 1:E:349:THR:CG2  | 2.49                     | 0.61              |
| 1:E:521:CYS:SG   | 1:E:524:THR:HG23 | 2.40                     | 0.61              |
| 1:F:148:ASN:HD22 | 1:F:198:GLN:HE22 | 1.46                     | 0.61              |
| 1:G:324:GLN:HE22 | 1:G:542:LEU:H    | 1.47                     | 0.61              |
| 1:B:195:TYR:O    | 1:B:198:GLN:HB2  | 2.01                     | 0.61              |
| 1:B:372:ILE:HG13 | 1:B:378:PHE:HB2  | 1.81                     | 0.61              |
| 1:E:153:ILE:HG13 | 1:E:174:PRO:HB2  | 1.81                     | 0.61              |
| 1:E:370:ARG:HH11 | 1:E:371:GLU:CG   | 2.09                     | 0.61              |
| 1:F:112:ARG:HD2  | 1:F:145:HIS:CE1  | 2.35                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:312:SER:N    | 1:F:318:MET:HE2  | 2.15                     | 0.61              |
| 1:F:442:ILE:HD12 | 1:F:488:GLY:HA2  | 1.80                     | 0.61              |
| 1:G:78:TYR:CE1   | 1:G:97:TRP:HB3   | 2.34                     | 0.61              |
| 1:G:478:GLY:HA3  | 1:G:505:ASN:HB2  | 1.81                     | 0.61              |
| 1:D:202:ILE:HD13 | 1:D:223:LEU:HD22 | 1.82                     | 0.61              |
| 1:E:220:ALA:HB3  | 1:E:261:ILE:CG2  | 2.14                     | 0.61              |
| 1:F:321:PHE:CE2  | 1:F:533:MET:HE1  | 2.36                     | 0.61              |
| 1:G:439:ARG:O    | 1:G:442:ILE:HG22 | 2.00                     | 0.61              |
| 1:B:216:VAL:HG11 | 1:B:230:VAL:HG21 | 1.81                     | 0.61              |
| 1:C:394:TYR:C    | 1:C:394:TYR:CD1  | 2.78                     | 0.61              |
| 1:C:425:HIS:CE1  | 1:C:427:SER:CB   | 2.84                     | 0.61              |
| 1:F:181:GLY:O    | 1:F:182:ALA:C    | 2.43                     | 0.61              |
| 1:F:229:ARG:HB3  | 1:F:259:PRO:HA   | 1.82                     | 0.61              |
| 1:A:338:GLY:HA3  | 1:A:412:MET:CE   | 2.30                     | 0.61              |
| 1:C:484:THR:C    | 1:C:486:LEU:H    | 2.09                     | 0.61              |
| 1:D:339:LEU:HB3  | 1:D:341:MET:HE2  | 1.79                     | 0.61              |
| 1:E:68:VAL:HG12  | 1:E:121:GLN:OE1  | 2.01                     | 0.61              |
| 1:A:482:SER:N    | 1:A:485:ASP:HB2  | 2.15                     | 0.60              |
| 1:A:178:LEU:HB2  | 1:A:181:GLY:HA2  | 1.82                     | 0.60              |
| 1:B:251:MET:HA   | 1:B:251:MET:CE   | 2.31                     | 0.60              |
| 1:C:166:MET:CE   | 1:C:171:CYS:HB3  | 2.31                     | 0.60              |
| 1:C:251:MET:HA   | 1:C:251:MET:HE3  | 1.82                     | 0.60              |
| 1:C:401:GLU:CG   | 1:C:402:THR:H    | 2.14                     | 0.60              |
| 1:D:96:TYR:HE2   | 1:D:107:GLN:HE21 | 1.46                     | 0.60              |
| 1:E:94:ALA:HB1   | 1:E:162:MET:HE1  | 1.83                     | 0.60              |
| 1:F:378:PHE:CE2  | 1:G:276:ARG:CD   | 2.83                     | 0.60              |
| 1:A:220:ALA:CB   | 1:A:261:ILE:CG2  | 2.77                     | 0.60              |
| 1:C:166:MET:HE3  | 1:C:171:CYS:HA   | 1.82                     | 0.60              |
| 1:C:413:ARG:O    | 1:C:417:GLY:HA2  | 2.01                     | 0.60              |
| 1:C:536:ASN:HD21 | 1:C:538:GLU:CB   | 2.14                     | 0.60              |
| 1:G:261:ILE:O    | 1:G:261:ILE:CG2  | 2.46                     | 0.60              |
| 1:A:344:GLU:HB2  | 1:A:348:GLU:OE2  | 2.02                     | 0.60              |
| 1:B:124:ARG:HD3  | 1:B:125:ASP:C    | 2.27                     | 0.60              |
| 1:C:437:ASP:OD1  | 1:C:439:ARG:HB2  | 2.01                     | 0.60              |
| 1:C:478:GLY:HA3  | 1:C:505:ASN:HB2  | 1.81                     | 0.60              |
| 1:D:121:GLN:CB   | 1:D:133:THR:HG23 | 2.31                     | 0.60              |
| 1:D:413:ARG:NE   | 1:D:458:VAL:HB   | 2.16                     | 0.60              |
| 1:F:276:ARG:HG2  | 1:F:276:ARG:HH11 | 1.66                     | 0.60              |
| 1:G:517:ARG:HB3  | 1:G:519:LEU:CD1  | 2.32                     | 0.60              |
| 1:B:141:LEU:HD11 | 1:B:196:PHE:HZ   | 1.65                     | 0.60              |
| 1:E:208:MET:HE1  | 1:E:232:VAL:HA   | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:421:ILE:HB   | 1:F:460:LEU:HD12 | 1.83                     | 0.60              |
| 1:G:401:GLU:HG2  | 1:G:402:THR:N    | 2.16                     | 0.60              |
| 1:A:208:MET:HE1  | 1:A:232:VAL:HA   | 1.81                     | 0.60              |
| 1:B:121:GLN:CB   | 1:B:133:THR:HG23 | 2.31                     | 0.60              |
| 1:B:208:MET:HE1  | 1:B:232:VAL:HA   | 1.83                     | 0.60              |
| 1:C:504:ARG:NH2  | 1:C:506:GLN:HB3  | 2.17                     | 0.60              |
| 1:B:477:GLU:HG3  | 1:B:507:GLN:NE2  | 2.15                     | 0.60              |
| 1:D:145:HIS:CE1  | 1:D:146:LEU:HD23 | 2.37                     | 0.60              |
| 1:D:442:ILE:CD1  | 1:D:492:LEU:HD11 | 2.31                     | 0.60              |
| 1:E:486:LEU:HB3  | 1:E:493:ARG:HD2  | 1.84                     | 0.60              |
| 1:E:502:LEU:HD12 | 1:E:502:LEU:N    | 2.16                     | 0.60              |
| 1:A:446:MET:HE2  | 1:A:492:LEU:HA   | 1.82                     | 0.60              |
| 1:F:486:LEU:HD12 | 1:F:493:ARG:CD   | 2.32                     | 0.60              |
| 1:G:111:TYR:CZ   | 1:G:142:PHE:HB2  | 2.36                     | 0.60              |
| 1:G:268:ALA:HA   | 1:G:271:LEU:HD13 | 1.82                     | 0.60              |
| 1:B:478:GLY:HA3  | 1:B:505:ASN:HB2  | 1.83                     | 0.60              |
| 1:C:477:GLU:HG3  | 1:C:507:GLN:NE2  | 2.17                     | 0.60              |
| 1:F:223:LEU:HD23 | 1:F:224:PRO:HD2  | 1.83                     | 0.60              |
| 1:D:510:MET:HE1  | 1:D:547:TYR:CE1  | 2.37                     | 0.60              |
| 1:F:352:ASP:CG   | 1:F:363:ARG:HD3  | 2.26                     | 0.60              |
| 1:G:307:VAL:HG12 | 1:G:307:VAL:O    | 2.01                     | 0.60              |
| 1:A:141:LEU:HD13 | 1:A:176:VAL:CG2  | 2.32                     | 0.59              |
| 1:A:229:ARG:HB3  | 1:A:258:GLY:O    | 2.01                     | 0.59              |
| 1:A:287:LEU:HD11 | 1:A:335:LYS:HG3  | 1.83                     | 0.59              |
| 1:A:306:GLU:HA   | 1:A:497:ASP:OD2  | 2.02                     | 0.59              |
| 1:A:480:PRO:HA   | 1:A:503:GLU:OE1  | 2.01                     | 0.59              |
| 1:A:482:SER:H    | 1:A:485:ASP:CB   | 2.14                     | 0.59              |
| 1:D:287:LEU:HD11 | 1:D:335:LYS:HG3  | 1.84                     | 0.59              |
| 1:D:352:ASP:CG   | 1:D:363:ARG:HD3  | 2.26                     | 0.59              |
| 1:D:478:GLY:HA3  | 1:D:505:ASN:HB2  | 1.85                     | 0.59              |
| 1:G:303:ARG:CZ   | 1:G:523:PHE:CD1  | 2.85                     | 0.59              |
| 1:G:326:ALA:HB2  | 1:G:422:ILE:HD12 | 1.84                     | 0.59              |
| 1:G:372:ILE:HA   | 1:G:375:ASN:OD1  | 2.01                     | 0.59              |
| 1:C:442:ILE:HD11 | 1:C:492:LEU:HD21 | 1.83                     | 0.59              |
| 1:D:141:LEU:HD11 | 1:D:196:PHE:HZ   | 1.63                     | 0.59              |
| 1:E:484:THR:C    | 1:E:486:LEU:H    | 2.10                     | 0.59              |
| 1:G:352:ASP:CG   | 1:G:363:ARG:HD3  | 2.27                     | 0.59              |
| 1:A:96:TYR:HE2   | 1:A:107:GLN:HE21 | 1.49                     | 0.59              |
| 1:A:410:ALA:HA   | 1:A:452:PHE:CE1  | 2.38                     | 0.59              |
| 1:A:446:MET:HE2  | 1:A:492:LEU:CB   | 2.32                     | 0.59              |
| 1:B:152:LYS:HD3  | 1:B:203:ILE:CD1  | 2.30                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:484:THR:O    | 1:B:486:LEU:N    | 2.35                     | 0.59              |
| 1:C:352:ASP:CG   | 1:C:363:ARG:HD3  | 2.27                     | 0.59              |
| 1:E:178:LEU:HB2  | 1:E:181:GLY:HA2  | 1.83                     | 0.59              |
| 1:E:440:LYS:HE2  | 1:E:440:LYS:C    | 2.27                     | 0.59              |
| 1:F:368:LEU:HD22 | 1:F:372:ILE:HG23 | 1.85                     | 0.59              |
| 1:B:442:ILE:HD11 | 1:B:492:LEU:HD11 | 1.83                     | 0.59              |
| 1:C:107:GLN:CB   | 1:C:124:ARG:CG   | 2.78                     | 0.59              |
| 1:C:162:MET:SD   | 1:C:166:MET:HG3  | 2.42                     | 0.59              |
| 1:C:473:LYS:HE2  | 1:C:479:ARG:CA   | 2.31                     | 0.59              |
| 1:C:473:LYS:CG   | 1:C:479:ARG:HB2  | 2.32                     | 0.59              |
| 1:D:521:CYS:O    | 1:D:525:GLY:N    | 2.33                     | 0.59              |
| 1:A:352:ASP:CG   | 1:A:363:ARG:HD3  | 2.27                     | 0.59              |
| 1:B:486:LEU:HB3  | 1:B:493:ARG:HD2  | 1.84                     | 0.59              |
| 1:C:216:VAL:HG11 | 1:C:230:VAL:HG21 | 1.83                     | 0.59              |
| 1:C:366:ASP:HB2  | 1:D:284:SER:OG   | 2.03                     | 0.59              |
| 1:D:424:ASP:O    | 1:D:425:HIS:HB3  | 2.01                     | 0.59              |
| 1:D:440:LYS:C    | 1:D:440:LYS:HE2  | 2.28                     | 0.59              |
| 1:E:251:MET:HA   | 1:E:251:MET:CE   | 2.33                     | 0.59              |
| 1:F:366:ASP:CB   | 1:G:284:SER:OG   | 2.50                     | 0.59              |
| 1:F:546:SER:O    | 1:F:547:TYR:CB   | 2.42                     | 0.59              |
| 1:G:412:MET:HE2  | 1:G:421:ILE:HD13 | 1.84                     | 0.59              |
| 1:A:288:LEU:N    | 1:A:288:LEU:HD12 | 2.18                     | 0.59              |
| 1:B:440:LYS:HE2  | 1:B:440:LYS:O    | 2.02                     | 0.59              |
| 1:C:260:TRP:C    | 1:C:261:ILE:HD13 | 2.27                     | 0.59              |
| 1:D:290:SER:H    | 1:D:325:GLN:HE22 | 1.44                     | 0.59              |
| 1:D:291:GLY:O    | 1:D:292:CYS:HB2  | 2.03                     | 0.59              |
| 1:E:476:GLU:CD   | 1:E:476:GLU:H    | 2.09                     | 0.59              |
| 1:G:202:ILE:HD13 | 1:G:223:LEU:HD22 | 1.83                     | 0.59              |
| 1:A:168:LEU:HD22 | 1:A:247:ASP:OD2  | 2.03                     | 0.59              |
| 1:A:216:VAL:HG11 | 1:A:230:VAL:HG21 | 1.83                     | 0.59              |
| 1:A:344:GLU:CG   | 1:A:349:THR:HG22 | 2.30                     | 0.59              |
| 1:B:397:PHE:CD1  | 1:B:397:PHE:C    | 2.80                     | 0.59              |
| 1:C:74:SER:HB2   | 1:C:99:ALA:HB1   | 1.83                     | 0.59              |
| 1:C:152:LYS:HD3  | 1:C:203:ILE:CD1  | 2.30                     | 0.59              |
| 1:C:283:GLU:CD   | 1:C:286:GLY:HA2  | 2.27                     | 0.59              |
| 1:C:440:LYS:HE2  | 1:C:440:LYS:O    | 2.02                     | 0.59              |
| 1:D:366:ASP:CB   | 1:E:284:SER:OG   | 2.31                     | 0.59              |
| 1:E:186:LYS:CD   | 1:E:218:GLU:HG3  | 2.28                     | 0.59              |
| 1:E:306:GLU:HA   | 1:E:497:ASP:OD2  | 2.02                     | 0.59              |
| 1:E:383:ASP:OD1  | 1:F:272:ARG:NH2  | 2.34                     | 0.59              |
| 1:F:382:PHE:CE1  | 1:G:272:ARG:HA   | 2.38                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:84:ARG:HA    | 1:B:243:LEU:HD21 | 1.84                     | 0.59              |
| 1:B:288:LEU:HD12 | 1:B:288:LEU:N    | 2.18                     | 0.59              |
| 1:B:521:CYS:SG   | 1:B:524:THR:HG23 | 2.43                     | 0.59              |
| 1:C:141:LEU:HD11 | 1:C:196:PHE:HZ   | 1.65                     | 0.59              |
| 1:D:442:ILE:HD11 | 1:D:492:LEU:CD2  | 2.31                     | 0.59              |
| 1:D:480:PRO:HA   | 1:D:503:GLU:OE1  | 2.03                     | 0.59              |
| 1:E:229:ARG:CZ   | 1:E:259:PRO:HB3  | 2.32                     | 0.59              |
| 1:G:220:ALA:CB   | 1:G:261:ILE:HD13 | 2.32                     | 0.59              |
| 1:B:251:MET:HA   | 1:B:251:MET:HE3  | 1.85                     | 0.59              |
| 1:B:285:VAL:O    | 1:B:285:VAL:HG12 | 2.03                     | 0.59              |
| 1:B:471:LYS:HB3  | 1:B:479:ARG:HH11 | 1.68                     | 0.59              |
| 1:C:223:LEU:HD23 | 1:C:224:PRO:HD2  | 1.84                     | 0.59              |
| 1:E:394:TYR:CE2  | 1:E:405:LEU:HD12 | 2.38                     | 0.59              |
| 1:G:480:PRO:HA   | 1:G:503:GLU:CD   | 2.28                     | 0.59              |
| 1:A:166:MET:HG2  | 1:A:175:VAL:CG2  | 2.33                     | 0.59              |
| 1:B:251:MET:HE3  | 1:B:251:MET:CA   | 2.33                     | 0.59              |
| 1:E:389:ASP:H    | 1:F:269:LEU:CD2  | 2.16                     | 0.59              |
| 1:F:450:LYS:CE   | 1:F:454:LYS:CD   | 2.79                     | 0.59              |
| 1:A:394:TYR:CE2  | 1:A:405:LEU:HD12 | 2.39                     | 0.58              |
| 1:A:421:ILE:HB   | 1:A:460:LEU:HD12 | 1.84                     | 0.58              |
| 1:B:178:LEU:HB2  | 1:B:181:GLY:HA2  | 1.83                     | 0.58              |
| 1:C:261:ILE:H    | 1:C:262:PRO:HD3  | 1.59                     | 0.58              |
| 1:D:251:MET:CE   | 1:D:251:MET:HA   | 2.33                     | 0.58              |
| 1:G:141:LEU:HD11 | 1:G:196:PHE:HZ   | 1.68                     | 0.58              |
| 1:A:480:PRO:HA   | 1:A:503:GLU:OE2  | 2.03                     | 0.58              |
| 1:C:86:ILE:HG21  | 1:C:163:LEU:HD12 | 1.83                     | 0.58              |
| 1:C:229:ARG:HA   | 1:C:259:PRO:HA   | 1.84                     | 0.58              |
| 1:C:517:ARG:HB3  | 1:C:519:LEU:CD1  | 2.33                     | 0.58              |
| 1:D:515:LEU:HD21 | 1:D:529:ILE:HD11 | 1.85                     | 0.58              |
| 1:F:294:GLY:O    | 1:F:295:ILE:C    | 2.42                     | 0.58              |
| 1:F:366:ASP:HB2  | 1:G:284:SER:OG   | 2.03                     | 0.58              |
| 1:F:413:ARG:HH21 | 1:F:458:VAL:N    | 2.01                     | 0.58              |
| 1:G:142:PHE:CE2  | 1:G:162:MET:HE3  | 2.37                     | 0.58              |
| 1:G:442:ILE:HD12 | 1:G:488:GLY:CA   | 2.32                     | 0.58              |
| 1:A:366:ASP:CB   | 1:C:285:VAL:CG2  | 2.79                     | 0.58              |
| 1:C:496:SER:HB2  | 1:C:499:ILE:HD11 | 1.84                     | 0.58              |
| 1:D:124:ARG:HD3  | 1:D:125:ASP:C    | 2.28                     | 0.58              |
| 1:D:186:LYS:CD   | 1:D:218:GLU:HG3  | 2.29                     | 0.58              |
| 1:D:440:LYS:CE   | 1:D:441:MET:HA   | 2.33                     | 0.58              |
| 1:D:467:LYS:HE3  | 1:D:486:LEU:O    | 2.03                     | 0.58              |
| 1:E:425:HIS:CE1  | 1:E:427:SER:CB   | 2.86                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:356:LEU:HD12 | 1:F:541:TRP:NE1  | 2.18                     | 0.58              |
| 1:F:413:ARG:O    | 1:F:417:GLY:HA2  | 2.02                     | 0.58              |
| 1:B:229:ARG:CB   | 1:B:259:PRO:HA   | 2.29                     | 0.58              |
| 1:D:309:MET:HB3  | 1:D:499:ILE:CD1  | 2.33                     | 0.58              |
| 1:E:166:MET:HE1  | 1:E:171:CYS:HB3  | 1.86                     | 0.58              |
| 1:G:94:ALA:HB1   | 1:G:162:MET:HE1  | 1.85                     | 0.58              |
| 1:G:121:GLN:CB   | 1:G:133:THR:HG23 | 2.34                     | 0.58              |
| 1:A:121:GLN:HB3  | 1:A:133:THR:HG23 | 1.85                     | 0.58              |
| 1:A:347:GLU:CD   | 1:C:274:ARG:HD2  | 2.28                     | 0.58              |
| 1:A:369:LYS:HG2  | 1:C:279:LEU:HD22 | 1.85                     | 0.58              |
| 1:A:401:GLU:HG3  | 1:A:431:SER:O    | 2.04                     | 0.58              |
| 1:B:166:MET:CE   | 1:B:171:CYS:HB3  | 2.33                     | 0.58              |
| 1:C:230:VAL:N    | 1:C:258:GLY:O    | 2.35                     | 0.58              |
| 1:C:480:PRO:HA   | 1:C:503:GLU:OE1  | 2.03                     | 0.58              |
| 1:C:536:ASN:ND2  | 1:C:538:GLU:H    | 2.01                     | 0.58              |
| 1:D:294:GLY:O    | 1:D:295:ILE:C    | 2.44                     | 0.58              |
| 1:E:152:LYS:HD3  | 1:E:203:ILE:CD1  | 2.31                     | 0.58              |
| 1:E:227:LYS:O    | 1:E:229:ARG:HD2  | 2.03                     | 0.58              |
| 1:E:471:LYS:HB3  | 1:E:479:ARG:NH1  | 2.18                     | 0.58              |
| 1:F:124:ARG:CZ   | 1:F:126:LYS:HA   | 2.34                     | 0.58              |
| 1:F:261:ILE:O    | 1:F:263:ASP:N    | 2.36                     | 0.58              |
| 1:F:322:VAL:CG1  | 1:F:422:ILE:HG21 | 2.33                     | 0.58              |
| 1:F:344:GLU:CG   | 1:F:349:THR:HG22 | 2.28                     | 0.58              |
| 1:G:262:PRO:HB2  | 1:G:265:VAL:HG12 | 1.85                     | 0.58              |
| 1:B:208:MET:HE2  | 1:B:232:VAL:HA   | 1.85                     | 0.58              |
| 1:B:397:PHE:C    | 1:B:397:PHE:HD1  | 2.11                     | 0.58              |
| 1:D:94:ALA:HB1   | 1:D:162:MET:HE1  | 1.84                     | 0.58              |
| 1:E:496:SER:O    | 1:E:520:LYS:HE2  | 2.04                     | 0.58              |
| 1:E:510:MET:HE2  | 1:E:513:LEU:CD2  | 2.33                     | 0.58              |
| 1:F:141:LEU:HD11 | 1:F:196:PHE:HZ   | 1.69                     | 0.58              |
| 1:A:195:TYR:O    | 1:A:198:GLN:HB2  | 2.03                     | 0.58              |
| 1:A:452:PHE:O    | 1:A:456:THR:HG23 | 2.04                     | 0.58              |
| 1:B:166:MET:HG2  | 1:B:175:VAL:HG23 | 1.85                     | 0.58              |
| 1:C:202:ILE:HD13 | 1:C:223:LEU:HD22 | 1.84                     | 0.58              |
| 1:C:492:LEU:H    | 1:C:492:LEU:CD1  | 2.17                     | 0.58              |
| 1:C:520:LYS:HG3  | 1:C:521:CYS:N    | 2.14                     | 0.58              |
| 1:C:536:ASN:ND2  | 1:C:538:GLU:CB   | 2.67                     | 0.58              |
| 1:D:322:VAL:CG2  | 1:D:463:ILE:HD11 | 2.34                     | 0.58              |
| 1:F:86:ILE:HD12  | 1:F:163:LEU:HB3  | 1.85                     | 0.58              |
| 1:F:452:PHE:O    | 1:F:456:THR:HG23 | 2.03                     | 0.58              |
| 1:F:478:GLY:HA3  | 1:F:505:ASN:HB2  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:494:GLN:HE21 | 1:G:428:ILE:HG13 | 1.69                     | 0.58              |
| 1:C:142:PHE:CE2  | 1:C:162:MET:HE3  | 2.38                     | 0.58              |
| 1:D:145:HIS:CE1  | 1:D:146:LEU:CD2  | 2.87                     | 0.58              |
| 1:D:413:ARG:HH21 | 1:D:458:VAL:N    | 2.01                     | 0.58              |
| 1:D:499:ILE:CG2  | 1:D:519:LEU:CB   | 2.82                     | 0.58              |
| 1:E:152:LYS:HG3  | 1:E:201:GLN:CG   | 2.34                     | 0.58              |
| 1:E:202:ILE:HD13 | 1:E:223:LEU:CD2  | 2.33                     | 0.58              |
| 1:E:268:ALA:HA   | 1:E:271:LEU:CD1  | 2.34                     | 0.58              |
| 1:E:382:PHE:HE1  | 1:F:275:ILE:HD12 | 1.69                     | 0.58              |
| 1:F:490:GLY:CA   | 1:F:493:ARG:HG3  | 2.34                     | 0.58              |
| 1:G:394:TYR:CD1  | 1:G:394:TYR:C    | 2.82                     | 0.58              |
| 1:A:145:HIS:CE1  | 1:A:146:LEU:CD2  | 2.86                     | 0.58              |
| 1:A:168:LEU:HB2  | 1:A:251:MET:HE1  | 1.85                     | 0.58              |
| 1:B:268:ALA:HA   | 1:B:271:LEU:CD1  | 2.34                     | 0.58              |
| 1:B:285:VAL:CG1  | 1:B:288:LEU:HD21 | 2.34                     | 0.58              |
| 1:B:322:VAL:CG2  | 1:B:463:ILE:HD11 | 2.33                     | 0.58              |
| 1:B:494:GLN:NE2  | 1:G:428:ILE:HG13 | 2.19                     | 0.58              |
| 1:D:321:PHE:CE2  | 1:D:533:MET:HE1  | 2.35                     | 0.58              |
| 1:D:368:LEU:HD22 | 1:D:372:ILE:HG23 | 1.85                     | 0.58              |
| 1:D:492:LEU:HD12 | 1:D:492:LEU:N    | 2.12                     | 0.58              |
| 1:E:425:HIS:CE1  | 1:E:427:SER:HB2  | 2.38                     | 0.58              |
| 1:E:442:ILE:HD11 | 1:E:492:LEU:CD2  | 2.34                     | 0.58              |
| 1:F:142:PHE:CE2  | 1:F:162:MET:HE3  | 2.38                     | 0.58              |
| 1:F:378:PHE:HE2  | 1:G:276:ARG:HD3  | 1.66                     | 0.58              |
| 1:A:91:CYS:HB3   | 1:A:96:TYR:O     | 2.04                     | 0.58              |
| 1:C:405:LEU:HG   | 1:C:409:LEU:CD1  | 2.32                     | 0.58              |
| 1:D:369:LYS:HG2  | 1:E:279:LEU:HD23 | 1.85                     | 0.58              |
| 1:D:446:MET:HE2  | 1:D:492:LEU:HB3  | 1.84                     | 0.58              |
| 1:D:484:THR:C    | 1:D:486:LEU:N    | 2.59                     | 0.58              |
| 1:F:78:TYR:CE1   | 1:F:97:TRP:HB3   | 2.39                     | 0.58              |
| 1:F:467:LYS:HE3  | 1:F:486:LEU:O    | 2.04                     | 0.58              |
| 1:A:510:MET:HB3  | 1:A:513:LEU:HB2  | 1.86                     | 0.57              |
| 1:C:440:LYS:HE2  | 1:C:440:LYS:C    | 2.28                     | 0.57              |
| 1:F:339:LEU:HB3  | 1:F:341:MET:HE2  | 1.85                     | 0.57              |
| 1:F:442:ILE:HD12 | 1:F:488:GLY:CA   | 2.34                     | 0.57              |
| 1:F:446:MET:HE2  | 1:F:492:LEU:HA   | 1.86                     | 0.57              |
| 1:F:496:SER:HB2  | 1:F:499:ILE:HD11 | 1.86                     | 0.57              |
| 1:A:279:LEU:HD23 | 1:B:369:LYS:HG2  | 1.87                     | 0.57              |
| 1:A:504:ARG:HH21 | 1:A:506:GLN:HB3  | 1.69                     | 0.57              |
| 1:B:427:SER:CB   | 1:B:487:ARG:HH12 | 2.15                     | 0.57              |
| 1:F:166:MET:HG2  | 1:F:175:VAL:CG2  | 2.34                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:346:VAL:CG2  | 1:C:271:LEU:HD21 | 2.34                     | 0.57              |
| 1:A:368:LEU:HD22 | 1:A:372:ILE:HG23 | 1.86                     | 0.57              |
| 1:A:413:ARG:NE   | 1:A:458:VAL:HB   | 2.18                     | 0.57              |
| 1:B:153:ILE:HG13 | 1:B:174:PRO:HB2  | 1.86                     | 0.57              |
| 1:C:314:SER:O    | 1:C:315:GLY:C    | 2.47                     | 0.57              |
| 1:C:344:GLU:CG   | 1:C:349:THR:HG22 | 2.30                     | 0.57              |
| 1:F:195:TYR:O    | 1:F:198:GLN:HB2  | 2.04                     | 0.57              |
| 1:G:208:MET:HE1  | 1:G:232:VAL:HA   | 1.84                     | 0.57              |
| 1:G:322:VAL:CG2  | 1:G:463:ILE:HD11 | 2.33                     | 0.57              |
| 1:A:290:SER:H    | 1:A:325:GLN:HE22 | 1.46                     | 0.57              |
| 1:A:401:GLU:HB3  | 1:A:404:ARG:HB3  | 1.87                     | 0.57              |
| 1:B:294:GLY:O    | 1:B:295:ILE:C    | 2.46                     | 0.57              |
| 1:C:346:VAL:HB   | 1:C:395:ASP:HB2  | 1.87                     | 0.57              |
| 1:C:351:GLU:OE1  | 1:D:278:HIS:CD2  | 2.58                     | 0.57              |
| 1:D:440:LYS:HE2  | 1:D:440:LYS:O    | 2.04                     | 0.57              |
| 1:E:166:MET:CE   | 1:E:171:CYS:HB3  | 2.35                     | 0.57              |
| 1:F:499:ILE:CG2  | 1:F:519:LEU:CB   | 2.81                     | 0.57              |
| 1:A:154:VAL:HG21 | 1:A:254:VAL:HG22 | 1.86                     | 0.57              |
| 1:B:151:LYS:HG2  | 1:B:200:GLU:OE2  | 2.05                     | 0.57              |
| 1:B:166:MET:HE3  | 1:B:171:CYS:HA   | 1.87                     | 0.57              |
| 1:C:186:LYS:CD   | 1:C:218:GLU:HG3  | 2.29                     | 0.57              |
| 1:A:312:SER:CB   | 1:A:502:LEU:O    | 2.47                     | 0.57              |
| 1:A:347:GLU:CD   | 1:C:274:ARG:HG2  | 2.30                     | 0.57              |
| 1:D:322:VAL:HG21 | 1:D:463:ILE:HD11 | 1.86                     | 0.57              |
| 1:D:421:ILE:HB   | 1:D:460:LEU:HD12 | 1.87                     | 0.57              |
| 1:D:477:GLU:HG3  | 1:D:507:GLN:NE2  | 2.18                     | 0.57              |
| 1:E:283:GLU:CG   | 1:E:284:SER:N    | 2.64                     | 0.57              |
| 1:E:437:ASP:OD1  | 1:E:439:ARG:HB2  | 2.04                     | 0.57              |
| 1:E:484:THR:C    | 1:E:486:LEU:N    | 2.62                     | 0.57              |
| 1:G:312:SER:CB   | 1:G:502:LEU:O    | 2.50                     | 0.57              |
| 1:G:476:GLU:H    | 1:G:476:GLU:CD   | 2.11                     | 0.57              |
| 1:A:122:LYS:HE2  | 1:A:159:GLU:OE1  | 2.04                     | 0.57              |
| 1:A:414:SER:HB3  | 1:C:226:GLY:CA   | 2.34                     | 0.57              |
| 1:B:166:MET:HG2  | 1:B:175:VAL:CG2  | 2.35                     | 0.57              |
| 1:B:510:MET:HE1  | 1:B:547:TYR:CE1  | 2.38                     | 0.57              |
| 1:C:208:MET:HE2  | 1:C:232:VAL:HA   | 1.85                     | 0.57              |
| 1:C:229:ARG:NH2  | 1:C:259:PRO:CB   | 2.68                     | 0.57              |
| 1:C:289:PHE:H    | 1:C:296:ASN:ND2  | 1.99                     | 0.57              |
| 1:E:141:LEU:CD1  | 1:E:176:VAL:HG21 | 2.34                     | 0.57              |
| 1:E:401:GLU:CG   | 1:E:402:THR:N    | 2.66                     | 0.57              |
| 1:E:413:ARG:NE   | 1:E:458:VAL:HB   | 2.15                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:94:ALA:HB1   | 1:F:162:MET:HE1  | 1.86                     | 0.57              |
| 1:F:412:MET:HE2  | 1:F:421:ILE:HD13 | 1.82                     | 0.57              |
| 1:G:153:ILE:HG13 | 1:G:174:PRO:HB2  | 1.86                     | 0.57              |
| 1:G:216:VAL:CG1  | 1:G:230:VAL:CG2  | 2.82                     | 0.57              |
| 1:B:287:LEU:HD11 | 1:B:335:LYS:HG3  | 1.87                     | 0.57              |
| 1:E:386:PHE:O    | 1:F:269:LEU:HD21 | 2.04                     | 0.57              |
| 1:E:480:PRO:HA   | 1:E:503:GLU:OE1  | 2.05                     | 0.57              |
| 1:F:437:ASP:OD1  | 1:F:439:ARG:HB2  | 2.04                     | 0.57              |
| 1:F:447:THR:HG22 | 1:F:495:LEU:CD2  | 2.22                     | 0.57              |
| 1:G:294:GLY:O    | 1:G:295:ILE:C    | 2.46                     | 0.57              |
| 1:A:446:MET:CE   | 1:A:492:LEU:HA   | 2.35                     | 0.57              |
| 1:A:478:GLY:HA3  | 1:A:505:ASN:HB2  | 1.85                     | 0.57              |
| 1:D:208:MET:HE1  | 1:D:232:VAL:HA   | 1.87                     | 0.57              |
| 1:D:413:ARG:O    | 1:D:417:GLY:HA2  | 2.05                     | 0.57              |
| 1:D:473:LYS:CG   | 1:D:479:ARG:HB2  | 2.32                     | 0.57              |
| 1:E:141:LEU:HD11 | 1:E:196:PHE:HZ   | 1.69                     | 0.57              |
| 1:F:536:ASN:HD22 | 1:F:538:GLU:H    | 1.53                     | 0.57              |
| 1:G:74:SER:HB2   | 1:G:99:ALA:HB1   | 1.87                     | 0.57              |
| 1:G:401:GLU:CG   | 1:G:431:SER:O    | 2.50                     | 0.57              |
| 1:A:346:VAL:HB   | 1:A:395:ASP:HB2  | 1.87                     | 0.57              |
| 1:B:74:SER:HB3   | 1:B:101:VAL:HG22 | 1.87                     | 0.57              |
| 1:B:241:CYS:HB2  | 1:B:250:ILE:HD11 | 1.85                     | 0.57              |
| 1:D:427:SER:HB3  | 1:D:487:ARG:NH1  | 2.19                     | 0.57              |
| 1:E:251:MET:HA   | 1:E:251:MET:HE3  | 1.86                     | 0.57              |
| 1:G:251:MET:CE   | 1:G:251:MET:HA   | 2.35                     | 0.57              |
| 1:A:402:THR:HG23 | 1:A:403:ASP:H    | 1.70                     | 0.56              |
| 1:A:413:ARG:O    | 1:A:417:GLY:HA2  | 2.05                     | 0.56              |
| 1:B:223:LEU:HD23 | 1:B:224:PRO:HD2  | 1.86                     | 0.56              |
| 1:B:452:PHE:O    | 1:B:456:THR:HG23 | 2.04                     | 0.56              |
| 1:E:338:GLY:CA   | 1:E:412:MET:HE1  | 2.35                     | 0.56              |
| 1:E:471:LYS:HB3  | 1:E:479:ARG:HH11 | 1.69                     | 0.56              |
| 1:F:486:LEU:HD12 | 1:F:493:ARG:CG   | 2.35                     | 0.56              |
| 1:A:259:PRO:O    | 1:A:259:PRO:CD   | 2.53                     | 0.56              |
| 1:B:438:GLU:O    | 1:B:442:ILE:HG22 | 2.05                     | 0.56              |
| 1:C:532:TYR:CD1  | 1:C:532:TYR:N    | 2.73                     | 0.56              |
| 1:E:122:LYS:HE2  | 1:E:159:GLU:OE1  | 2.05                     | 0.56              |
| 1:E:251:MET:HE3  | 1:E:251:MET:CA   | 2.35                     | 0.56              |
| 1:E:424:ASP:O    | 1:E:425:HIS:HB3  | 2.05                     | 0.56              |
| 1:E:486:LEU:HD13 | 1:E:487:ARG:O    | 2.05                     | 0.56              |
| 1:E:510:MET:HE1  | 1:E:547:TYR:OH   | 2.04                     | 0.56              |
| 1:F:186:LYS:HD3  | 1:F:218:GLU:CG   | 2.30                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:208:MET:HE1  | 1:F:232:VAL:HG22 | 1.87                     | 0.56              |
| 1:F:369:LYS:HG2  | 1:G:279:LEU:HD23 | 1.88                     | 0.56              |
| 1:G:74:SER:HB3   | 1:G:101:VAL:HG22 | 1.87                     | 0.56              |
| 1:G:186:LYS:CD   | 1:G:218:GLU:HG3  | 2.30                     | 0.56              |
| 1:G:438:GLU:O    | 1:G:442:ILE:HG22 | 2.05                     | 0.56              |
| 1:A:307:VAL:O    | 1:A:307:VAL:HG12 | 2.05                     | 0.56              |
| 1:A:313:GLY:O    | 1:A:315:GLY:N    | 2.38                     | 0.56              |
| 1:A:477:GLU:HG3  | 1:A:507:GLN:NE2  | 2.21                     | 0.56              |
| 1:A:496:SER:CB   | 1:A:499:ILE:HD11 | 2.34                     | 0.56              |
| 1:B:74:SER:HB2   | 1:B:99:ALA:HB1   | 1.87                     | 0.56              |
| 1:C:322:VAL:CG1  | 1:C:422:ILE:HG21 | 2.35                     | 0.56              |
| 1:C:424:ASP:O    | 1:C:425:HIS:HB3  | 2.06                     | 0.56              |
| 1:C:473:LYS:CE   | 1:C:479:ARG:HA   | 2.34                     | 0.56              |
| 1:E:216:VAL:HG11 | 1:E:230:VAL:HG22 | 1.83                     | 0.56              |
| 1:E:368:LEU:HD22 | 1:E:368:LEU:O    | 2.05                     | 0.56              |
| 1:E:483:ILE:O    | 1:E:486:LEU:CB   | 2.38                     | 0.56              |
| 1:E:515:LEU:HD21 | 1:E:529:ILE:HD11 | 1.86                     | 0.56              |
| 1:F:482:SER:N    | 1:F:485:ASP:HB2  | 2.19                     | 0.56              |
| 1:G:151:LYS:HG2  | 1:G:200:GLU:OE2  | 2.05                     | 0.56              |
| 1:G:447:THR:HA   | 1:G:495:LEU:HD23 | 1.87                     | 0.56              |
| 1:G:477:GLU:HG3  | 1:G:507:GLN:NE2  | 2.19                     | 0.56              |
| 1:G:499:ILE:CG2  | 1:G:519:LEU:CB   | 2.83                     | 0.56              |
| 1:A:166:MET:HG2  | 1:A:175:VAL:HG23 | 1.88                     | 0.56              |
| 1:A:345:SER:O    | 1:A:349:THR:HG23 | 2.05                     | 0.56              |
| 1:A:442:ILE:HD11 | 1:A:492:LEU:HD11 | 1.88                     | 0.56              |
| 1:D:442:ILE:HD12 | 1:D:488:GLY:HA2  | 1.88                     | 0.56              |
| 1:E:121:GLN:CB   | 1:E:133:THR:HG23 | 2.36                     | 0.56              |
| 1:E:233:LEU:HD22 | 1:E:241:CYS:SG   | 2.45                     | 0.56              |
| 1:E:276:ARG:HH11 | 1:E:276:ARG:CG   | 2.18                     | 0.56              |
| 1:E:401:GLU:HB3  | 1:E:404:ARG:HB3  | 1.86                     | 0.56              |
| 1:E:405:LEU:HG   | 1:E:409:LEU:CD1  | 2.33                     | 0.56              |
| 1:F:473:LYS:CG   | 1:F:479:ARG:HB2  | 2.33                     | 0.56              |
| 1:G:484:THR:C    | 1:G:486:LEU:N    | 2.58                     | 0.56              |
| 1:A:486:LEU:HB3  | 1:A:493:ARG:HD2  | 1.86                     | 0.56              |
| 1:B:216:VAL:HG11 | 1:B:230:VAL:HG22 | 1.85                     | 0.56              |
| 1:B:394:TYR:CD1  | 1:B:394:TYR:C    | 2.83                     | 0.56              |
| 1:C:154:VAL:HG21 | 1:C:254:VAL:HG22 | 1.87                     | 0.56              |
| 1:C:338:GLY:HA3  | 1:C:412:MET:HE1  | 1.86                     | 0.56              |
| 1:C:364:GLN:HA   | 1:D:523:PHE:CZ   | 2.40                     | 0.56              |
| 1:D:194:GLU:CD   | 1:D:194:GLU:N    | 2.64                     | 0.56              |
| 1:E:229:ARG:NH2  | 1:E:259:PRO:CG   | 2.68                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:369:LYS:CG   | 1:C:279:LEU:CD2  | 2.83                     | 0.56              |
| 1:B:229:ARG:CZ   | 1:B:259:PRO:HB3  | 2.35                     | 0.56              |
| 1:C:68:VAL:HG12  | 1:C:121:GLN:OE1  | 2.04                     | 0.56              |
| 1:C:229:ARG:NE   | 1:C:259:PRO:HB3  | 2.20                     | 0.56              |
| 1:C:328:GLN:HA   | 1:C:331:THR:OG1  | 2.05                     | 0.56              |
| 1:D:262:PRO:HB2  | 1:D:265:VAL:HG12 | 1.86                     | 0.56              |
| 1:E:166:MET:HE3  | 1:E:171:CYS:HA   | 1.88                     | 0.56              |
| 1:E:322:VAL:HG21 | 1:E:463:ILE:CD1  | 2.35                     | 0.56              |
| 1:E:336:LYS:HB3  | 1:E:418:CYS:HB3  | 1.88                     | 0.56              |
| 1:G:486:LEU:HB3  | 1:G:493:ARG:HD2  | 1.87                     | 0.56              |
| 1:C:546:SER:O    | 1:C:547:TYR:HB2  | 2.05                     | 0.56              |
| 1:D:205:MET:HG3  | 1:D:231:ALA:CB   | 2.35                     | 0.56              |
| 1:F:178:LEU:HB2  | 1:F:181:GLY:HA2  | 1.87                     | 0.56              |
| 1:F:268:ALA:HA   | 1:F:271:LEU:HD12 | 1.88                     | 0.56              |
| 1:F:484:THR:C    | 1:F:486:LEU:H    | 2.13                     | 0.56              |
| 1:B:343:GLU:OE1  | 1:B:343:GLU:HA   | 2.06                     | 0.56              |
| 1:C:151:LYS:HG2  | 1:C:200:GLU:OE2  | 2.05                     | 0.56              |
| 1:C:488:GLY:HA3  | 1:C:492:LEU:CD1  | 2.36                     | 0.56              |
| 1:E:359:ARG:HD3  | 1:E:541:TRP:NE1  | 2.20                     | 0.56              |
| 1:F:152:LYS:HD3  | 1:F:203:ILE:CD1  | 2.33                     | 0.56              |
| 1:F:515:LEU:HD21 | 1:F:529:ILE:HD11 | 1.87                     | 0.56              |
| 1:G:336:LYS:HB3  | 1:G:418:CYS:HA   | 1.87                     | 0.56              |
| 1:G:473:LYS:CG   | 1:G:479:ARG:HB2  | 2.34                     | 0.56              |
| 1:A:338:GLY:HA3  | 1:A:412:MET:HE1  | 1.87                     | 0.56              |
| 1:A:473:LYS:CG   | 1:A:479:ARG:HB2  | 2.35                     | 0.56              |
| 1:A:499:ILE:CG2  | 1:A:519:LEU:CB   | 2.84                     | 0.56              |
| 1:B:424:ASP:O    | 1:B:425:HIS:HB3  | 2.06                     | 0.56              |
| 1:B:446:MET:HE2  | 1:B:492:LEU:HA   | 1.88                     | 0.56              |
| 1:C:369:LYS:CG   | 1:D:279:LEU:CD2  | 2.84                     | 0.56              |
| 1:C:478:GLY:CA   | 1:C:505:ASN:HB2  | 2.34                     | 0.56              |
| 1:D:347:GLU:OE2  | 1:E:274:ARG:HD2  | 2.06                     | 0.56              |
| 1:E:74:SER:HB2   | 1:E:99:ALA:HB1   | 1.88                     | 0.56              |
| 1:E:477:GLU:HG3  | 1:E:507:GLN:NE2  | 2.20                     | 0.56              |
| 1:F:471:LYS:HB3  | 1:F:479:ARG:NH1  | 2.21                     | 0.56              |
| 1:A:442:ILE:HD11 | 1:A:492:LEU:CD2  | 2.35                     | 0.56              |
| 1:B:440:LYS:HE2  | 1:B:440:LYS:C    | 2.30                     | 0.56              |
| 1:C:382:PHE:HE1  | 1:D:275:ILE:HD12 | 1.71                     | 0.56              |
| 1:C:413:ARG:HH21 | 1:C:458:VAL:N    | 2.03                     | 0.56              |
| 1:E:316:MET:HE1  | 1:E:535:TYR:CZ   | 2.40                     | 0.56              |
| 1:E:428:ILE:H    | 1:E:428:ILE:HD12 | 1.71                     | 0.56              |
| 1:A:427:SER:HB3  | 1:A:487:ARG:NH1  | 2.18                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:195:TYR:O    | 1:D:198:GLN:HB2  | 2.05                     | 0.55              |
| 1:D:369:LYS:CG   | 1:E:279:LEU:HD22 | 2.35                     | 0.55              |
| 1:D:412:MET:HE2  | 1:D:421:ILE:HD13 | 1.85                     | 0.55              |
| 1:E:394:TYR:HE1  | 1:E:396:SER:CB   | 2.19                     | 0.55              |
| 1:F:152:LYS:HG3  | 1:F:201:GLN:CG   | 2.34                     | 0.55              |
| 1:G:515:LEU:HD21 | 1:G:529:ILE:HD12 | 1.89                     | 0.55              |
| 1:A:268:ALA:HA   | 1:A:271:LEU:HD13 | 1.87                     | 0.55              |
| 1:A:351:GLU:HB2  | 1:A:363:ARG:HD2  | 1.88                     | 0.55              |
| 1:B:166:MET:HE1  | 1:B:171:CYS:HB3  | 1.88                     | 0.55              |
| 1:B:338:GLY:CA   | 1:B:412:MET:HE1  | 2.36                     | 0.55              |
| 1:C:321:PHE:CE2  | 1:C:533:MET:HE1  | 2.40                     | 0.55              |
| 1:C:439:ARG:O    | 1:C:442:ILE:HG22 | 2.06                     | 0.55              |
| 1:D:276:ARG:HG2  | 1:D:276:ARG:HH11 | 1.69                     | 0.55              |
| 1:E:312:SER:CB   | 1:E:502:LEU:O    | 2.53                     | 0.55              |
| 1:E:473:LYS:CG   | 1:E:479:ARG:HB2  | 2.35                     | 0.55              |
| 1:E:504:ARG:HH21 | 1:E:506:GLN:CB   | 2.19                     | 0.55              |
| 1:F:74:SER:HB3   | 1:F:101:VAL:HG22 | 1.88                     | 0.55              |
| 1:F:389:ASP:CA   | 1:G:269:LEU:HD23 | 2.36                     | 0.55              |
| 1:A:229:ARG:HB3  | 1:A:259:PRO:HA   | 1.88                     | 0.55              |
| 1:A:429:VAL:HG23 | 1:A:430:VAL:H    | 1.71                     | 0.55              |
| 1:A:521:CYS:O    | 1:A:525:GLY:N    | 2.34                     | 0.55              |
| 1:C:322:VAL:CG2  | 1:C:463:ILE:HD11 | 2.37                     | 0.55              |
| 1:C:438:GLU:O    | 1:C:442:ILE:HG22 | 2.06                     | 0.55              |
| 1:C:471:LYS:HB3  | 1:C:479:ARG:NH1  | 2.21                     | 0.55              |
| 1:D:429:VAL:HG23 | 1:D:430:VAL:H    | 1.71                     | 0.55              |
| 1:F:141:LEU:HD13 | 1:F:176:VAL:CG2  | 2.35                     | 0.55              |
| 1:G:482:SER:N    | 1:G:485:ASP:HB2  | 2.19                     | 0.55              |
| 1:A:208:MET:HE2  | 1:A:232:VAL:HA   | 1.87                     | 0.55              |
| 1:A:318:MET:SD   | 1:A:463:ILE:HD12 | 2.46                     | 0.55              |
| 1:B:345:SER:O    | 1:B:349:THR:HG23 | 2.06                     | 0.55              |
| 1:B:351:GLU:HB2  | 1:B:363:ARG:HD2  | 1.89                     | 0.55              |
| 1:C:366:ASP:CA   | 1:D:284:SER:OG   | 2.55                     | 0.55              |
| 1:D:471:LYS:HB3  | 1:D:479:ARG:NH1  | 2.22                     | 0.55              |
| 1:E:195:TYR:O    | 1:E:198:GLN:HB2  | 2.06                     | 0.55              |
| 1:F:262:PRO:HB2  | 1:F:265:VAL:HG12 | 1.88                     | 0.55              |
| 1:F:480:PRO:HA   | 1:F:503:GLU:OE1  | 2.05                     | 0.55              |
| 1:A:510:MET:HE3  | 1:A:547:TYR:CE1  | 2.26                     | 0.55              |
| 1:C:536:ASN:C    | 1:C:538:GLU:H    | 2.13                     | 0.55              |
| 1:D:261:ILE:N    | 1:D:262:PRO:HD3  | 2.17                     | 0.55              |
| 1:D:536:ASN:ND2  | 1:D:538:GLU:H    | 2.04                     | 0.55              |
| 1:E:499:ILE:CG2  | 1:E:519:LEU:CB   | 2.84                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:478:GLY:CA   | 1:F:505:ASN:HB2  | 2.37                     | 0.55              |
| 1:A:359:ARG:HD3  | 1:A:541:TRP:NE1  | 2.22                     | 0.55              |
| 1:A:405:LEU:HG   | 1:A:409:LEU:CD1  | 2.34                     | 0.55              |
| 1:B:111:TYR:CZ   | 1:B:142:PHE:HB2  | 2.42                     | 0.55              |
| 1:B:316:MET:CE   | 1:B:535:TYR:CE2  | 2.88                     | 0.55              |
| 1:C:216:VAL:CG1  | 1:C:230:VAL:CG2  | 2.84                     | 0.55              |
| 1:E:205:MET:HG3  | 1:E:231:ALA:CB   | 2.36                     | 0.55              |
| 1:E:290:SER:N    | 1:E:325:GLN:HE21 | 1.97                     | 0.55              |
| 1:E:316:MET:HE2  | 1:E:320:THR:OG1  | 2.07                     | 0.55              |
| 1:F:477:GLU:HG3  | 1:F:507:GLN:NE2  | 2.21                     | 0.55              |
| 1:G:147:TRP:CG   | 1:G:174:PRO:HB3  | 2.42                     | 0.55              |
| 1:G:442:ILE:HD11 | 1:G:492:LEU:HD11 | 1.89                     | 0.55              |
| 1:A:243:LEU:O    | 1:A:244:ASN:O    | 2.25                     | 0.55              |
| 1:A:454:LYS:HE3  | 1:A:522:ARG:HH22 | 1.72                     | 0.55              |
| 1:B:122:LYS:HE2  | 1:B:159:GLU:OE1  | 2.07                     | 0.55              |
| 1:B:312:SER:CB   | 1:B:502:LEU:O    | 2.55                     | 0.55              |
| 1:B:412:MET:CA   | 1:B:416:LEU:HD12 | 2.24                     | 0.55              |
| 1:C:515:LEU:HD21 | 1:C:529:ILE:HD11 | 1.89                     | 0.55              |
| 1:D:74:SER:HB3   | 1:D:101:VAL:HG22 | 1.89                     | 0.55              |
| 1:D:229:ARG:CB   | 1:D:258:GLY:O    | 2.55                     | 0.55              |
| 1:D:496:SER:HB2  | 1:D:499:ILE:HD11 | 1.87                     | 0.55              |
| 1:E:154:VAL:HG21 | 1:E:254:VAL:HG22 | 1.88                     | 0.55              |
| 1:F:392:HIS:ND1  | 1:G:267:SER:HB2  | 2.21                     | 0.55              |
| 1:G:122:LYS:HE2  | 1:G:159:GLU:OE1  | 2.06                     | 0.55              |
| 1:G:229:ARG:NH2  | 1:G:259:PRO:HG3  | 2.21                     | 0.55              |
| 1:G:405:LEU:HG   | 1:G:409:LEU:CD1  | 2.36                     | 0.55              |
| 1:G:510:MET:HE1  | 1:G:547:TYR:CE1  | 2.41                     | 0.55              |
| 1:A:510:MET:HE2  | 1:A:513:LEU:HD23 | 1.89                     | 0.55              |
| 1:B:205:MET:HG3  | 1:B:231:ALA:CB   | 2.36                     | 0.55              |
| 1:C:322:VAL:HG21 | 1:C:463:ILE:HD11 | 1.89                     | 0.55              |
| 1:D:360:VAL:O    | 1:D:360:VAL:HG23 | 2.07                     | 0.55              |
| 1:E:74:SER:HB3   | 1:E:101:VAL:HG22 | 1.87                     | 0.55              |
| 1:E:165:VAL:HB   | 1:E:175:VAL:HG11 | 1.89                     | 0.55              |
| 1:E:401:GLU:CG   | 1:E:402:THR:H    | 2.19                     | 0.55              |
| 1:F:202:ILE:HD13 | 1:F:223:LEU:HD22 | 1.89                     | 0.55              |
| 1:G:260:TRP:C    | 1:G:262:PRO:HD2  | 2.32                     | 0.55              |
| 1:G:447:THR:HG22 | 1:G:495:LEU:CD2  | 2.26                     | 0.55              |
| 1:A:162:MET:HG2  | 1:A:175:VAL:HB   | 1.89                     | 0.55              |
| 1:A:162:MET:SD   | 1:A:166:MET:HG3  | 2.46                     | 0.55              |
| 1:C:413:ARG:HH21 | 1:C:457:GLY:C    | 2.14                     | 0.55              |
| 1:D:251:MET:CA   | 1:D:251:MET:HE3  | 2.37                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:369:LYS:HG2  | 1:F:279:LEU:CD2  | 2.37                     | 0.55              |
| 1:E:504:ARG:HH21 | 1:E:506:GLN:HG2  | 1.71                     | 0.55              |
| 1:A:126:LYS:NZ   | 1:A:127:ASP:OD1  | 2.40                     | 0.55              |
| 1:A:276:ARG:HG2  | 1:A:276:ARG:HH11 | 1.71                     | 0.55              |
| 1:B:314:SER:O    | 1:B:315:GLY:C    | 2.49                     | 0.55              |
| 1:D:442:ILE:HD12 | 1:D:488:GLY:CA   | 2.36                     | 0.55              |
| 1:E:438:GLU:O    | 1:E:442:ILE:HG22 | 2.07                     | 0.55              |
| 1:F:260:TRP:CB   | 1:F:262:PRO:CD   | 2.44                     | 0.55              |
| 1:F:336:LYS:HB3  | 1:F:418:CYS:HA   | 1.89                     | 0.55              |
| 1:F:471:LYS:HB3  | 1:F:479:ARG:HH11 | 1.72                     | 0.55              |
| 1:A:322:VAL:CG2  | 1:A:463:ILE:HD11 | 2.37                     | 0.54              |
| 1:A:395:ASP:HB3  | 1:C:266:VAL:CG2  | 2.36                     | 0.54              |
| 1:A:425:HIS:HE1  | 1:A:465:HIS:HB2  | 1.71                     | 0.54              |
| 1:C:512:ASN:HD21 | 1:C:537:LYS:HE3  | 1.71                     | 0.54              |
| 1:D:91:CYS:HB3   | 1:D:96:TYR:O     | 2.07                     | 0.54              |
| 1:E:126:LYS:HG2  | 1:E:127:ASP:H    | 1.72                     | 0.54              |
| 1:E:440:LYS:CE   | 1:E:441:MET:HA   | 2.36                     | 0.54              |
| 1:G:166:MET:HE3  | 1:G:171:CYS:CB   | 2.37                     | 0.54              |
| 1:A:79:SER:H     | 1:A:98:ILE:CD1   | 2.20                     | 0.54              |
| 1:A:402:THR:HG23 | 1:A:403:ASP:N    | 2.22                     | 0.54              |
| 1:A:420:VAL:HG22 | 1:A:459:VAL:HB   | 1.88                     | 0.54              |
| 1:B:504:ARG:HH21 | 1:B:506:GLN:CB   | 2.20                     | 0.54              |
| 1:D:126:LYS:HG2  | 1:D:127:ASP:H    | 1.73                     | 0.54              |
| 1:D:359:ARG:HD3  | 1:D:541:TRP:NE1  | 2.20                     | 0.54              |
| 1:E:229:ARG:NE   | 1:E:259:PRO:HB3  | 2.22                     | 0.54              |
| 1:E:303:ARG:CZ   | 1:E:523:PHE:CD1  | 2.90                     | 0.54              |
| 1:E:412:MET:CE   | 1:E:421:ILE:HD13 | 2.36                     | 0.54              |
| 1:E:429:VAL:HG23 | 1:E:430:VAL:H    | 1.72                     | 0.54              |
| 1:F:521:CYS:SG   | 1:F:524:THR:HG23 | 2.47                     | 0.54              |
| 1:A:259:PRO:O    | 1:A:259:PRO:HD2  | 2.08                     | 0.54              |
| 1:B:275:ILE:HD12 | 1:G:382:PHE:HE1  | 1.72                     | 0.54              |
| 1:B:303:ARG:CZ   | 1:B:523:PHE:CD1  | 2.90                     | 0.54              |
| 1:D:288:LEU:HD12 | 1:D:288:LEU:N    | 2.21                     | 0.54              |
| 1:F:91:CYS:HB3   | 1:F:96:TYR:O     | 2.07                     | 0.54              |
| 1:A:311:THR:HA   | 1:A:318:MET:CE   | 2.33                     | 0.54              |
| 1:B:344:GLU:CG   | 1:B:349:THR:HG22 | 2.29                     | 0.54              |
| 1:B:521:CYS:O    | 1:B:525:GLY:N    | 2.35                     | 0.54              |
| 1:D:521:CYS:SG   | 1:D:524:THR:HG23 | 2.48                     | 0.54              |
| 1:F:167:GLU:C    | 1:F:169:GLN:H    | 2.15                     | 0.54              |
| 1:F:286:GLY:O    | 1:F:302:ALA:N    | 2.41                     | 0.54              |
| 1:G:429:VAL:HG23 | 1:G:430:VAL:H    | 1.72                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:232:VAL:O    | 1:A:232:VAL:HG12 | 2.06                     | 0.54              |
| 1:A:318:MET:SD   | 1:A:463:ILE:HD13 | 2.47                     | 0.54              |
| 1:B:141:LEU:CD1  | 1:B:176:VAL:HG21 | 2.34                     | 0.54              |
| 1:C:268:ALA:HA   | 1:C:271:LEU:HD12 | 1.90                     | 0.54              |
| 1:C:486:LEU:HB3  | 1:C:493:ARG:HD2  | 1.90                     | 0.54              |
| 1:E:346:VAL:HB   | 1:E:395:ASP:HB2  | 1.88                     | 0.54              |
| 1:E:496:SER:HB2  | 1:E:499:ILE:HD11 | 1.90                     | 0.54              |
| 1:E:502:LEU:HD12 | 1:E:502:LEU:H    | 1.72                     | 0.54              |
| 1:E:546:SER:O    | 1:E:547:TYR:HB2  | 2.07                     | 0.54              |
| 1:F:74:SER:HB2   | 1:F:99:ALA:HB1   | 1.90                     | 0.54              |
| 1:F:440:LYS:HE2  | 1:F:440:LYS:C    | 2.32                     | 0.54              |
| 1:F:440:LYS:HE2  | 1:F:440:LYS:O    | 2.07                     | 0.54              |
| 1:G:521:CYS:SG   | 1:G:524:THR:HG23 | 2.48                     | 0.54              |
| 1:A:112:ARG:NH2  | 1:A:118:ILE:HD11 | 2.23                     | 0.54              |
| 1:C:536:ASN:HD21 | 1:C:538:GLU:HB2  | 1.71                     | 0.54              |
| 1:D:397:PHE:CD1  | 1:D:397:PHE:C    | 2.86                     | 0.54              |
| 1:E:151:LYS:HG2  | 1:E:200:GLU:OE2  | 2.08                     | 0.54              |
| 1:G:233:LEU:HD22 | 1:G:241:CYS:SG   | 2.48                     | 0.54              |
| 1:G:478:GLY:CA   | 1:G:505:ASN:HB2  | 2.37                     | 0.54              |
| 1:A:443:ASP:HA   | 1:A:491:ALA:CB   | 2.38                     | 0.54              |
| 1:B:265:VAL:HG11 | 1:G:411:TYR:HE1  | 1.73                     | 0.54              |
| 1:B:339:LEU:HB3  | 1:B:341:MET:HE2  | 1.84                     | 0.54              |
| 1:B:421:ILE:HB   | 1:B:460:LEU:HD12 | 1.90                     | 0.54              |
| 1:C:122:LYS:HE3  | 1:C:130:PHE:CE2  | 2.43                     | 0.54              |
| 1:C:317:VAL:HG21 | 1:C:504:ARG:HD2  | 1.90                     | 0.54              |
| 1:D:223:LEU:HD23 | 1:D:224:PRO:HD2  | 1.90                     | 0.54              |
| 1:D:536:ASN:ND2  | 1:D:538:GLU:CB   | 2.71                     | 0.54              |
| 1:E:343:GLU:OE1  | 1:E:343:GLU:HA   | 2.07                     | 0.54              |
| 1:E:521:CYS:O    | 1:E:525:GLY:N    | 2.34                     | 0.54              |
| 1:F:233:LEU:HD22 | 1:F:241:CYS:SG   | 2.48                     | 0.54              |
| 1:F:241:CYS:HB2  | 1:F:250:ILE:HD11 | 1.90                     | 0.54              |
| 1:F:320:THR:HG22 | 1:F:324:GLN:NE2  | 2.23                     | 0.54              |
| 1:G:338:GLY:CA   | 1:G:412:MET:HE1  | 2.38                     | 0.54              |
| 1:B:447:THR:HA   | 1:B:495:LEU:HD23 | 1.90                     | 0.54              |
| 1:C:351:GLU:HB2  | 1:C:363:ARG:HD2  | 1.90                     | 0.54              |
| 1:C:394:TYR:HE1  | 1:C:396:SER:HB2  | 1.73                     | 0.54              |
| 1:C:482:SER:H    | 1:C:485:ASP:CB   | 2.19                     | 0.54              |
| 1:E:241:CYS:HB2  | 1:E:250:ILE:HD11 | 1.89                     | 0.54              |
| 1:E:382:PHE:CE1  | 1:F:272:ARG:HA   | 2.43                     | 0.54              |
| 1:E:392:HIS:ND1  | 1:F:267:SER:HB2  | 2.23                     | 0.54              |
| 1:E:536:ASN:HD22 | 1:E:538:GLU:H    | 1.56                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:186:LYS:CD   | 1:F:218:GLU:HG3  | 2.32                     | 0.54              |
| 1:F:369:LYS:HG2  | 1:G:279:LEU:CD2  | 2.37                     | 0.54              |
| 1:C:153:ILE:HG13 | 1:C:174:PRO:HB2  | 1.89                     | 0.54              |
| 1:C:429:VAL:HG23 | 1:C:430:VAL:H    | 1.72                     | 0.54              |
| 1:D:471:LYS:HB3  | 1:D:479:ARG:HH11 | 1.72                     | 0.54              |
| 1:D:487:ARG:O    | 1:D:493:ARG:HD3  | 2.08                     | 0.54              |
| 1:E:512:ASN:HD21 | 1:E:537:LYS:HE3  | 1.73                     | 0.54              |
| 1:F:111:TYR:CZ   | 1:F:142:PHE:HB2  | 2.43                     | 0.54              |
| 1:F:446:MET:CE   | 1:F:492:LEU:HA   | 2.38                     | 0.54              |
| 1:G:208:MET:HE2  | 1:G:232:VAL:HA   | 1.88                     | 0.54              |
| 1:A:347:GLU:O    | 1:A:351:GLU:HG3  | 2.08                     | 0.54              |
| 1:B:164:THR:O    | 1:B:167:GLU:HB2  | 2.08                     | 0.54              |
| 1:C:145:HIS:CE1  | 1:C:146:LEU:CD2  | 2.91                     | 0.54              |
| 1:C:166:MET:HG2  | 1:C:175:VAL:HG23 | 1.90                     | 0.54              |
| 1:C:411:TYR:CZ   | 1:D:262:PRO:HD3  | 2.42                     | 0.54              |
| 1:C:484:THR:C    | 1:C:486:LEU:N    | 2.64                     | 0.54              |
| 1:D:251:MET:HA   | 1:D:251:MET:HE3  | 1.89                     | 0.54              |
| 1:E:208:MET:HE2  | 1:E:232:VAL:HA   | 1.88                     | 0.54              |
| 1:E:401:GLU:HG2  | 1:E:402:THR:H    | 1.71                     | 0.54              |
| 1:G:166:MET:HG2  | 1:G:175:VAL:HG23 | 1.90                     | 0.54              |
| 1:G:227:LYS:O    | 1:G:229:ARG:HD2  | 2.08                     | 0.54              |
| 1:G:446:MET:HE2  | 1:G:492:LEU:HA   | 1.90                     | 0.54              |
| 1:A:152:LYS:HD3  | 1:A:203:ILE:HD11 | 1.90                     | 0.53              |
| 1:A:321:PHE:CE2  | 1:A:533:MET:HE1  | 2.40                     | 0.53              |
| 1:A:351:GLU:OE1  | 1:C:278:HIS:CD2  | 2.62                     | 0.53              |
| 1:A:437:ASP:OD1  | 1:A:439:ARG:HB2  | 2.07                     | 0.53              |
| 1:A:447:THR:CG2  | 1:A:495:LEU:HD21 | 2.27                     | 0.53              |
| 1:C:195:TYR:O    | 1:C:198:GLN:HB2  | 2.08                     | 0.53              |
| 1:C:316:MET:HE2  | 1:C:320:THR:OG1  | 2.08                     | 0.53              |
| 1:C:382:PHE:C    | 1:C:382:PHE:CD2  | 2.86                     | 0.53              |
| 1:D:111:TYR:CZ   | 1:D:142:PHE:HB2  | 2.43                     | 0.53              |
| 1:D:166:MET:CE   | 1:D:171:CYS:HB3  | 2.37                     | 0.53              |
| 1:D:510:MET:HE1  | 1:D:547:TYR:OH   | 2.08                     | 0.53              |
| 1:E:320:THR:HG22 | 1:E:324:GLN:NE2  | 2.23                     | 0.53              |
| 1:E:515:LEU:HD21 | 1:E:529:ILE:HD12 | 1.91                     | 0.53              |
| 1:F:499:ILE:HG22 | 1:F:519:LEU:CB   | 2.27                     | 0.53              |
| 1:G:241:CYS:HB2  | 1:G:250:ILE:HD11 | 1.89                     | 0.53              |
| 1:G:311:THR:OG1  | 1:G:466:LEU:HD21 | 2.07                     | 0.53              |
| 1:G:450:LYS:CE   | 1:G:454:LYS:CD   | 2.81                     | 0.53              |
| 1:G:471:LYS:HB3  | 1:G:479:ARG:NH1  | 2.23                     | 0.53              |
| 1:G:492:LEU:HD12 | 1:G:492:LEU:N    | 2.12                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:429:VAL:HG23 | 1:B:430:VAL:H    | 1.73                     | 0.53              |
| 1:C:147:TRP:CG   | 1:C:174:PRO:HB3  | 2.42                     | 0.53              |
| 1:C:347:GLU:O    | 1:C:351:GLU:HG3  | 2.09                     | 0.53              |
| 1:C:356:LEU:HD12 | 1:C:541:TRP:NE1  | 2.23                     | 0.53              |
| 1:D:271:LEU:O    | 1:D:272:ARG:C    | 2.51                     | 0.53              |
| 1:D:372:ILE:HG13 | 1:D:378:PHE:HB2  | 1.89                     | 0.53              |
| 1:D:401:GLU:HG2  | 1:D:402:THR:H    | 1.73                     | 0.53              |
| 1:F:372:ILE:HG13 | 1:F:378:PHE:HB2  | 1.90                     | 0.53              |
| 1:G:510:MET:HB3  | 1:G:513:LEU:HB2  | 1.90                     | 0.53              |
| 1:B:413:ARG:O    | 1:B:417:GLY:HA2  | 2.08                     | 0.53              |
| 1:C:446:MET:HE2  | 1:C:492:LEU:CB   | 2.37                     | 0.53              |
| 1:C:486:LEU:HD12 | 1:C:493:ARG:CD   | 2.38                     | 0.53              |
| 1:D:230:VAL:HB   | 1:D:260:TRP:NE1  | 2.22                     | 0.53              |
| 1:D:437:ASP:OD1  | 1:D:439:ARG:HB2  | 2.08                     | 0.53              |
| 1:D:536:ASN:HD21 | 1:D:538:GLU:CB   | 2.20                     | 0.53              |
| 1:E:397:PHE:CD1  | 1:E:397:PHE:C    | 2.87                     | 0.53              |
| 1:E:440:LYS:NZ   | 1:E:441:MET:CA   | 2.55                     | 0.53              |
| 1:E:504:ARG:HD3  | 1:E:506:GLN:CG   | 2.16                     | 0.53              |
| 1:B:86:ILE:HG21  | 1:B:163:LEU:CD1  | 2.38                     | 0.53              |
| 1:B:235:CYS:CB   | 1:B:240:GLU:HG2  | 2.39                     | 0.53              |
| 1:B:441:MET:CE   | 1:B:445:LEU:H    | 2.21                     | 0.53              |
| 1:B:510:MET:HE1  | 1:B:547:TYR:OH   | 2.08                     | 0.53              |
| 1:C:268:ALA:HA   | 1:C:271:LEU:HD13 | 1.90                     | 0.53              |
| 1:C:471:LYS:HB3  | 1:C:479:ARG:HH11 | 1.72                     | 0.53              |
| 1:D:217:GLU:OE2  | 1:D:261:ILE:CA   | 2.54                     | 0.53              |
| 1:D:306:GLU:HA   | 1:D:497:ASP:OD2  | 2.08                     | 0.53              |
| 1:D:318:MET:SD   | 1:D:463:ILE:HG23 | 2.48                     | 0.53              |
| 1:E:370:ARG:CD   | 1:E:370:ARG:C    | 2.81                     | 0.53              |
| 1:G:141:LEU:CD1  | 1:G:176:VAL:HG21 | 2.36                     | 0.53              |
| 1:A:356:LEU:HD12 | 1:A:541:TRP:NE1  | 2.24                     | 0.53              |
| 1:B:167:GLU:C    | 1:B:169:GLN:H    | 2.15                     | 0.53              |
| 1:B:246:HIS:HB3  | 1:B:249:GLU:OE1  | 2.09                     | 0.53              |
| 1:D:345:SER:O    | 1:D:349:THR:CG2  | 2.56                     | 0.53              |
| 1:D:345:SER:O    | 1:D:349:THR:HG23 | 2.08                     | 0.53              |
| 1:D:492:LEU:C    | 1:D:494:GLN:N    | 2.66                     | 0.53              |
| 1:D:512:ASN:HD21 | 1:D:537:LYS:HE3  | 1.73                     | 0.53              |
| 1:E:517:ARG:HB3  | 1:E:519:LEU:CD1  | 2.38                     | 0.53              |
| 1:F:78:TYR:CD2   | 1:F:92:GLN:HG2   | 2.43                     | 0.53              |
| 1:F:305:GLY:O    | 1:F:454:LYS:HD2  | 2.09                     | 0.53              |
| 1:F:496:SER:CB   | 1:F:499:ILE:HD11 | 2.39                     | 0.53              |
| 1:G:166:MET:HE3  | 1:G:171:CYS:CA   | 2.38                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:412:MET:CA   | 1:G:416:LEU:HD12 | 2.28                     | 0.53              |
| 1:G:492:LEU:C    | 1:G:494:GLN:N    | 2.66                     | 0.53              |
| 1:A:397:PHE:CD1  | 1:A:397:PHE:C    | 2.86                     | 0.53              |
| 1:A:510:MET:HE1  | 1:A:547:TYR:CZ   | 2.44                     | 0.53              |
| 1:B:307:VAL:O    | 1:B:307:VAL:HG12 | 2.07                     | 0.53              |
| 1:B:322:VAL:HG21 | 1:B:463:ILE:CG1  | 2.38                     | 0.53              |
| 1:B:345:SER:O    | 1:B:349:THR:CG2  | 2.56                     | 0.53              |
| 1:B:439:ARG:HG2  | 1:B:489:SER:OG   | 2.09                     | 0.53              |
| 1:B:546:SER:O    | 1:B:547:TYR:HB2  | 2.08                     | 0.53              |
| 1:C:531:GLY:C    | 1:C:532:TYR:HD1  | 2.16                     | 0.53              |
| 1:E:447:THR:HA   | 1:E:495:LEU:HD23 | 1.90                     | 0.53              |
| 1:F:447:THR:HA   | 1:F:495:LEU:HD23 | 1.90                     | 0.53              |
| 1:G:256:ASN:O    | 1:G:256:ASN:ND2  | 2.42                     | 0.53              |
| 1:A:166:MET:O    | 1:A:171:CYS:HB3  | 2.08                     | 0.53              |
| 1:A:235:CYS:CB   | 1:A:240:GLU:HG2  | 2.39                     | 0.53              |
| 1:B:154:VAL:HG21 | 1:B:254:VAL:HG22 | 1.90                     | 0.53              |
| 1:B:445:LEU:HD12 | 1:B:445:LEU:O    | 2.09                     | 0.53              |
| 1:C:121:GLN:CB   | 1:C:133:THR:HG23 | 2.39                     | 0.53              |
| 1:C:401:GLU:CG   | 1:C:402:THR:N    | 2.71                     | 0.53              |
| 1:E:152:LYS:O    | 1:E:174:PRO:HD2  | 2.08                     | 0.53              |
| 1:E:164:THR:O    | 1:E:167:GLU:HB2  | 2.09                     | 0.53              |
| 1:E:166:MET:HG2  | 1:E:175:VAL:HG23 | 1.91                     | 0.53              |
| 1:E:294:GLY:O    | 1:E:295:ILE:C    | 2.49                     | 0.53              |
| 1:F:126:LYS:HG2  | 1:F:127:ASP:H    | 1.73                     | 0.53              |
| 1:G:86:ILE:HG21  | 1:G:163:LEU:CD1  | 2.38                     | 0.53              |
| 1:G:343:GLU:OE1  | 1:G:343:GLU:HA   | 2.09                     | 0.53              |
| 1:A:504:ARG:HH21 | 1:A:506:GLN:CG   | 2.21                     | 0.53              |
| 1:A:510:MET:HB2  | 1:A:513:LEU:HB3  | 1.91                     | 0.53              |
| 1:B:91:CYS:HB3   | 1:B:96:TYR:O     | 2.09                     | 0.53              |
| 1:C:382:PHE:CE1  | 1:D:272:ARG:HA   | 2.44                     | 0.53              |
| 1:D:167:GLU:C    | 1:D:169:GLN:H    | 2.13                     | 0.53              |
| 1:D:241:CYS:HB2  | 1:D:250:ILE:HD11 | 1.91                     | 0.53              |
| 1:D:486:LEU:HD12 | 1:D:493:ARG:CD   | 2.38                     | 0.53              |
| 1:D:504:ARG:HH21 | 1:D:506:GLN:CB   | 2.21                     | 0.53              |
| 1:E:312:SER:O    | 1:E:313:GLY:O    | 2.26                     | 0.53              |
| 1:F:286:GLY:O    | 1:F:287:LEU:O    | 2.27                     | 0.53              |
| 1:A:234:PRO:HG2  | 1:A:249:GLU:HG2  | 1.91                     | 0.53              |
| 1:A:324:GLN:OE1  | 1:A:541:TRP:CE3  | 2.61                     | 0.53              |
| 1:A:343:GLU:OE1  | 1:A:343:GLU:HA   | 2.09                     | 0.53              |
| 1:B:536:ASN:ND2  | 1:B:538:GLU:H    | 2.07                     | 0.53              |
| 1:C:406:LEU:HD21 | 1:C:449:LEU:HD23 | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:180:HIS:HB2  | 1:D:184:ALA:HB3  | 1.91                     | 0.53              |
| 1:D:322:VAL:HG21 | 1:D:463:ILE:CG1  | 2.39                     | 0.53              |
| 1:D:394:TYR:CE2  | 1:D:405:LEU:HD12 | 2.44                     | 0.53              |
| 1:E:86:ILE:HG21  | 1:E:163:LEU:CD1  | 2.39                     | 0.53              |
| 1:E:492:LEU:C    | 1:E:494:GLN:N    | 2.65                     | 0.53              |
| 1:F:338:GLY:CA   | 1:F:412:MET:HE1  | 2.39                     | 0.53              |
| 1:A:164:THR:O    | 1:A:167:GLU:HB2  | 2.09                     | 0.53              |
| 1:A:496:SER:O    | 1:A:520:LYS:CE   | 2.56                     | 0.53              |
| 1:D:232:VAL:O    | 1:D:232:VAL:HG12 | 2.07                     | 0.53              |
| 1:E:114:GLN:NE2  | 1:E:195:TYR:HD1  | 2.07                     | 0.53              |
| 1:F:125:ASP:OD1  | 1:F:129:ASN:HB2  | 2.08                     | 0.53              |
| 1:A:259:PRO:O    | 1:A:260:TRP:CB   | 2.46                     | 0.52              |
| 1:A:262:PRO:HB2  | 1:A:265:VAL:HG12 | 1.90                     | 0.52              |
| 1:B:114:GLN:NE2  | 1:B:195:TYR:HD1  | 2.07                     | 0.52              |
| 1:B:152:LYS:O    | 1:B:174:PRO:HD2  | 2.09                     | 0.52              |
| 1:B:216:VAL:CG1  | 1:B:230:VAL:CG2  | 2.85                     | 0.52              |
| 1:C:358:ASN:C    | 1:C:359:ARG:HG2  | 2.32                     | 0.52              |
| 1:C:411:TYR:OH   | 1:D:260:TRP:HA   | 2.09                     | 0.52              |
| 1:D:515:LEU:HD21 | 1:D:529:ILE:HD12 | 1.90                     | 0.52              |
| 1:E:386:PHE:O    | 1:F:269:LEU:CD2  | 2.58                     | 0.52              |
| 1:F:343:GLU:OE1  | 1:F:343:GLU:HA   | 2.09                     | 0.52              |
| 1:G:145:HIS:CE1  | 1:G:146:LEU:CD2  | 2.92                     | 0.52              |
| 1:G:471:LYS:HB3  | 1:G:479:ARG:HH11 | 1.74                     | 0.52              |
| 1:B:126:LYS:HG2  | 1:B:127:ASP:H    | 1.74                     | 0.52              |
| 1:B:359:ARG:HD3  | 1:B:541:TRP:NE1  | 2.23                     | 0.52              |
| 1:C:106:TYR:HB3  | 1:C:123:VAL:HG12 | 1.91                     | 0.52              |
| 1:C:445:LEU:HD12 | 1:C:445:LEU:O    | 2.09                     | 0.52              |
| 1:F:86:ILE:HG21  | 1:F:163:LEU:CD1  | 2.39                     | 0.52              |
| 1:F:268:ALA:HA   | 1:F:271:LEU:HD13 | 1.91                     | 0.52              |
| 1:F:492:LEU:C    | 1:F:494:GLN:N    | 2.67                     | 0.52              |
| 1:G:145:HIS:CE1  | 1:G:146:LEU:HD23 | 2.44                     | 0.52              |
| 1:G:487:ARG:O    | 1:G:493:ARG:HD3  | 2.09                     | 0.52              |
| 1:G:536:ASN:C    | 1:G:536:ASN:HD22 | 2.17                     | 0.52              |
| 1:A:74:SER:HB3   | 1:A:101:VAL:HG22 | 1.90                     | 0.52              |
| 1:A:344:GLU:OE1  | 1:A:349:THR:HB   | 2.10                     | 0.52              |
| 1:A:484:THR:C    | 1:A:486:LEU:N    | 2.66                     | 0.52              |
| 1:A:536:ASN:ND2  | 1:A:538:GLU:H    | 2.08                     | 0.52              |
| 1:B:536:ASN:ND2  | 1:B:538:GLU:CB   | 2.72                     | 0.52              |
| 1:C:145:HIS:CE1  | 1:C:146:LEU:HD23 | 2.45                     | 0.52              |
| 1:D:122:LYS:HE3  | 1:D:130:PHE:CE2  | 2.45                     | 0.52              |
| 1:D:166:MET:HE3  | 1:D:171:CYS:HA   | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:230:VAL:HG11 | 1:D:260:TRP:NE1  | 2.24                     | 0.52              |
| 1:E:167:GLU:C    | 1:E:169:GLN:H    | 2.16                     | 0.52              |
| 1:E:232:VAL:HG12 | 1:E:232:VAL:O    | 2.08                     | 0.52              |
| 1:E:345:SER:O    | 1:E:349:THR:HG23 | 2.08                     | 0.52              |
| 1:F:267:SER:O    | 1:F:270:SER:OG   | 2.26                     | 0.52              |
| 1:G:251:MET:CA   | 1:G:251:MET:HE3  | 2.39                     | 0.52              |
| 1:G:492:LEU:H    | 1:G:492:LEU:CD1  | 2.05                     | 0.52              |
| 1:A:74:SER:HB3   | 1:A:101:VAL:CG2  | 2.40                     | 0.52              |
| 1:A:394:TYR:HE1  | 1:A:396:SER:CB   | 2.21                     | 0.52              |
| 1:A:412:MET:HG2  | 1:C:265:VAL:HG21 | 1.92                     | 0.52              |
| 1:B:478:GLY:O    | 1:B:479:ARG:C    | 2.51                     | 0.52              |
| 1:B:478:GLY:CA   | 1:B:505:ASN:HB2  | 2.39                     | 0.52              |
| 1:C:141:LEU:CD1  | 1:C:176:VAL:HG21 | 2.35                     | 0.52              |
| 1:C:273:GLU:OE2  | 1:C:276:ARG:NH1  | 2.42                     | 0.52              |
| 1:D:344:GLU:OE1  | 1:D:349:THR:HB   | 2.10                     | 0.52              |
| 1:E:410:ALA:HA   | 1:E:452:PHE:CE1  | 2.44                     | 0.52              |
| 1:E:482:SER:H    | 1:E:485:ASP:CB   | 2.17                     | 0.52              |
| 1:F:359:ARG:HD3  | 1:F:541:TRP:NE1  | 2.25                     | 0.52              |
| 1:G:166:MET:HG2  | 1:G:175:VAL:CG2  | 2.39                     | 0.52              |
| 1:G:344:GLU:OE1  | 1:G:349:THR:HB   | 2.09                     | 0.52              |
| 1:A:147:TRP:CG   | 1:A:174:PRO:HB3  | 2.45                     | 0.52              |
| 1:B:229:ARG:CB   | 1:B:258:GLY:O    | 2.58                     | 0.52              |
| 1:D:397:PHE:C    | 1:D:397:PHE:HD1  | 2.17                     | 0.52              |
| 1:F:347:GLU:O    | 1:F:351:GLU:HG3  | 2.09                     | 0.52              |
| 1:F:401:GLU:CG   | 1:F:431:SER:O    | 2.57                     | 0.52              |
| 1:F:445:LEU:CD1  | 1:F:449:LEU:HG   | 2.39                     | 0.52              |
| 1:G:205:MET:HG3  | 1:G:231:ALA:CB   | 2.39                     | 0.52              |
| 1:A:205:MET:HG3  | 1:A:231:ALA:CB   | 2.40                     | 0.52              |
| 1:A:478:GLY:CA   | 1:A:505:ASN:HB2  | 2.40                     | 0.52              |
| 1:B:290:SER:N    | 1:B:325:GLN:HE21 | 2.02                     | 0.52              |
| 1:B:312:SER:H    | 1:B:318:MET:HE2  | 1.75                     | 0.52              |
| 1:B:487:ARG:O    | 1:B:493:ARG:HD3  | 2.10                     | 0.52              |
| 1:C:447:THR:HA   | 1:C:495:LEU:HD23 | 1.91                     | 0.52              |
| 1:C:510:MET:CB   | 1:C:513:LEU:HB2  | 2.39                     | 0.52              |
| 1:C:510:MET:HE1  | 1:C:547:TYR:CE1  | 2.44                     | 0.52              |
| 1:D:318:MET:SD   | 1:D:463:ILE:CD1  | 2.98                     | 0.52              |
| 1:F:194:GLU:CD   | 1:F:194:GLU:N    | 2.66                     | 0.52              |
| 1:F:440:LYS:CE   | 1:F:441:MET:HA   | 2.39                     | 0.52              |
| 1:G:140:ALA:O    | 1:G:141:LEU:HD23 | 2.10                     | 0.52              |
| 1:G:300:LEU:HB3  | 1:G:303:ARG:HH12 | 1.74                     | 0.52              |
| 1:A:428:ILE:HD12 | 1:A:428:ILE:H    | 1.75                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:536:ASN:HD21 | 1:A:538:GLU:CB   | 2.23                     | 0.52              |
| 1:B:140:ALA:O    | 1:B:141:LEU:HD23 | 2.10                     | 0.52              |
| 1:B:162:MET:SD   | 1:B:166:MET:HG3  | 2.49                     | 0.52              |
| 1:B:362:LEU:HD12 | 1:B:362:LEU:O    | 2.10                     | 0.52              |
| 1:B:476:GLU:CD   | 1:B:476:GLU:H    | 2.18                     | 0.52              |
| 1:C:122:LYS:HE2  | 1:C:159:GLU:OE1  | 2.10                     | 0.52              |
| 1:C:140:ALA:O    | 1:C:141:LEU:HD23 | 2.10                     | 0.52              |
| 1:D:341:MET:SD   | 1:D:424:ASP:HB2  | 2.50                     | 0.52              |
| 1:D:359:ARG:HD3  | 1:D:541:TRP:HE1  | 1.75                     | 0.52              |
| 1:E:486:LEU:HD12 | 1:E:493:ARG:CD   | 2.39                     | 0.52              |
| 1:F:208:MET:HE1  | 1:F:232:VAL:HA   | 1.92                     | 0.52              |
| 1:F:446:MET:HE2  | 1:F:492:LEU:CB   | 2.38                     | 0.52              |
| 1:G:114:GLN:NE2  | 1:G:195:TYR:HD1  | 2.07                     | 0.52              |
| 1:A:233:LEU:HD22 | 1:A:241:CYS:SG   | 2.50                     | 0.52              |
| 1:A:368:LEU:HD22 | 1:A:368:LEU:C    | 2.33                     | 0.52              |
| 1:B:352:ASP:OD2  | 1:B:363:ARG:NH1  | 2.43                     | 0.52              |
| 1:B:439:ARG:O    | 1:B:442:ILE:CG2  | 2.57                     | 0.52              |
| 1:C:322:VAL:HG21 | 1:C:463:ILE:CG1  | 2.40                     | 0.52              |
| 1:D:164:THR:O    | 1:D:167:GLU:HB2  | 2.09                     | 0.52              |
| 1:D:318:MET:SD   | 1:D:463:ILE:HD13 | 2.50                     | 0.52              |
| 1:E:91:CYS:HB3   | 1:E:96:TYR:O     | 2.10                     | 0.52              |
| 1:F:287:LEU:HD11 | 1:F:335:LYS:HG3  | 1.92                     | 0.52              |
| 1:F:324:GLN:HE22 | 1:F:542:LEU:H    | 1.58                     | 0.52              |
| 1:F:368:LEU:HD22 | 1:F:368:LEU:C    | 2.35                     | 0.52              |
| 1:F:413:ARG:HH21 | 1:F:457:GLY:C    | 2.18                     | 0.52              |
| 1:G:397:PHE:CD1  | 1:G:397:PHE:C    | 2.86                     | 0.52              |
| 1:G:440:LYS:HE2  | 1:G:440:LYS:O    | 2.10                     | 0.52              |
| 1:G:447:THR:CG2  | 1:G:495:LEU:HD21 | 2.27                     | 0.52              |
| 1:B:304:GLY:HA2  | 1:B:459:VAL:HG22 | 1.92                     | 0.52              |
| 1:B:305:GLY:O    | 1:B:454:LYS:HD2  | 2.10                     | 0.52              |
| 1:B:311:THR:O    | 1:B:312:SER:HB3  | 2.10                     | 0.52              |
| 1:C:345:SER:O    | 1:C:349:THR:HG23 | 2.10                     | 0.52              |
| 1:C:410:ALA:HA   | 1:C:452:PHE:CE1  | 2.45                     | 0.52              |
| 1:C:476:GLU:CD   | 1:C:476:GLU:N    | 2.68                     | 0.52              |
| 1:C:504:ARG:HH21 | 1:C:506:GLN:HG2  | 1.73                     | 0.52              |
| 1:D:208:MET:HE2  | 1:D:232:VAL:HA   | 1.91                     | 0.52              |
| 1:E:140:ALA:O    | 1:E:141:LEU:HD23 | 2.10                     | 0.52              |
| 1:E:234:PRO:CG   | 1:E:249:GLU:HG2  | 2.40                     | 0.52              |
| 1:G:288:LEU:HD12 | 1:G:288:LEU:N    | 2.25                     | 0.52              |
| 1:G:536:ASN:HD22 | 1:G:538:GLU:H    | 1.56                     | 0.52              |
| 1:A:324:GLN:HE22 | 1:A:542:LEU:H    | 1.58                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:345:SER:O    | 1:A:349:THR:CG2  | 2.58                     | 0.52              |
| 1:A:413:ARG:HH21 | 1:A:458:VAL:N    | 2.08                     | 0.52              |
| 1:B:488:GLY:HA3  | 1:B:492:LEU:CD1  | 2.38                     | 0.52              |
| 1:B:499:ILE:CG2  | 1:B:519:LEU:CB   | 2.87                     | 0.52              |
| 1:B:536:ASN:HD21 | 1:B:538:GLU:CB   | 2.22                     | 0.52              |
| 1:C:126:LYS:HG2  | 1:C:127:ASP:H    | 1.73                     | 0.52              |
| 1:C:229:ARG:HB3  | 1:C:259:PRO:HA   | 1.91                     | 0.52              |
| 1:C:276:ARG:HG2  | 1:C:276:ARG:HH11 | 1.75                     | 0.52              |
| 1:C:359:ARG:HD3  | 1:C:541:TRP:NE1  | 2.25                     | 0.52              |
| 1:C:446:MET:CE   | 1:C:492:LEU:HA   | 2.40                     | 0.52              |
| 1:D:322:VAL:CG1  | 1:D:422:ILE:HG21 | 2.40                     | 0.52              |
| 1:D:536:ASN:HD22 | 1:D:536:ASN:C    | 2.16                     | 0.52              |
| 1:F:378:PHE:CD2  | 1:G:276:ARG:HD3  | 2.40                     | 0.52              |
| 1:F:413:ARG:NE   | 1:F:458:VAL:HB   | 2.24                     | 0.52              |
| 1:F:517:ARG:HB3  | 1:F:519:LEU:HD13 | 1.92                     | 0.52              |
| 1:G:372:ILE:HG13 | 1:G:378:PHE:HB2  | 1.91                     | 0.52              |
| 1:G:496:SER:O    | 1:G:520:LYS:HE2  | 2.09                     | 0.52              |
| 1:A:397:PHE:C    | 1:A:397:PHE:HD1  | 2.18                     | 0.51              |
| 1:A:471:LYS:HB3  | 1:A:479:ARG:NH1  | 2.24                     | 0.51              |
| 1:A:484:THR:C    | 1:A:486:LEU:H    | 2.18                     | 0.51              |
| 1:B:324:GLN:HE22 | 1:B:542:LEU:H    | 1.56                     | 0.51              |
| 1:B:492:LEU:C    | 1:B:494:GLN:N    | 2.68                     | 0.51              |
| 1:C:446:MET:O    | 1:C:449:LEU:HB2  | 2.10                     | 0.51              |
| 1:F:378:PHE:CD2  | 1:G:276:ARG:HD2  | 2.44                     | 0.51              |
| 1:F:394:TYR:HE1  | 1:F:396:SER:CB   | 2.21                     | 0.51              |
| 1:G:106:TYR:HB3  | 1:G:123:VAL:HG12 | 1.92                     | 0.51              |
| 1:G:154:VAL:HG21 | 1:G:254:VAL:HG22 | 1.91                     | 0.51              |
| 1:G:531:GLY:C    | 1:G:532:TYR:CD1  | 2.88                     | 0.51              |
| 1:A:406:LEU:HD21 | 1:A:449:LEU:HD23 | 1.93                     | 0.51              |
| 1:A:492:LEU:C    | 1:A:494:GLN:N    | 2.65                     | 0.51              |
| 1:B:486:LEU:HD12 | 1:B:493:ARG:CD   | 2.40                     | 0.51              |
| 1:B:496:SER:O    | 1:B:520:LYS:HE2  | 2.10                     | 0.51              |
| 1:C:125:ASP:OD1  | 1:C:129:ASN:HB2  | 2.10                     | 0.51              |
| 1:C:166:MET:HE3  | 1:C:171:CYS:CB   | 2.40                     | 0.51              |
| 1:C:227:LYS:O    | 1:C:229:ARG:HD2  | 2.10                     | 0.51              |
| 1:C:510:MET:HB2  | 1:C:513:LEU:CB   | 2.39                     | 0.51              |
| 1:E:148:ASN:HD22 | 1:E:198:GLN:HE22 | 1.58                     | 0.51              |
| 1:E:289:PHE:H    | 1:E:296:ASN:ND2  | 1.96                     | 0.51              |
| 1:E:322:VAL:HG21 | 1:E:463:ILE:CG1  | 2.40                     | 0.51              |
| 1:F:232:VAL:O    | 1:F:232:VAL:HG12 | 2.09                     | 0.51              |
| 1:F:322:VAL:HG21 | 1:F:463:ILE:HD11 | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:251:MET:HA   | 1:G:251:MET:HE3  | 1.92                     | 0.51              |
| 1:G:421:ILE:HB   | 1:G:460:LEU:HD12 | 1.92                     | 0.51              |
| 1:A:220:ALA:HB3  | 1:A:261:ILE:CD1  | 2.23                     | 0.51              |
| 1:A:471:LYS:HB3  | 1:A:479:ARG:HH11 | 1.75                     | 0.51              |
| 1:B:440:LYS:CE   | 1:B:441:MET:HA   | 2.41                     | 0.51              |
| 1:C:166:MET:HG2  | 1:C:175:VAL:CG2  | 2.41                     | 0.51              |
| 1:C:504:ARG:HH21 | 1:C:506:GLN:CB   | 2.24                     | 0.51              |
| 1:D:260:TRP:HB2  | 1:D:262:PRO:HD2  | 1.87                     | 0.51              |
| 1:E:111:TYR:CZ   | 1:E:142:PHE:HB2  | 2.44                     | 0.51              |
| 1:E:309:MET:HB3  | 1:E:499:ILE:CD1  | 2.40                     | 0.51              |
| 1:F:162:MET:HG2  | 1:F:175:VAL:HB   | 1.92                     | 0.51              |
| 1:F:362:LEU:HD12 | 1:F:362:LEU:O    | 2.11                     | 0.51              |
| 1:F:401:GLU:HB3  | 1:F:404:ARG:HB3  | 1.92                     | 0.51              |
| 1:F:429:VAL:HG23 | 1:F:430:VAL:H    | 1.75                     | 0.51              |
| 1:F:482:SER:H    | 1:F:485:ASP:CB   | 2.20                     | 0.51              |
| 1:G:180:HIS:HB2  | 1:G:184:ALA:HB3  | 1.92                     | 0.51              |
| 1:G:195:TYR:O    | 1:G:198:GLN:HB2  | 2.09                     | 0.51              |
| 1:G:504:ARG:HH21 | 1:G:506:GLN:HG2  | 1.74                     | 0.51              |
| 1:C:387:GLY:HA2  | 1:D:269:LEU:HD11 | 1.91                     | 0.51              |
| 1:C:428:ILE:H    | 1:C:428:ILE:HD12 | 1.75                     | 0.51              |
| 1:D:369:LYS:CG   | 1:E:279:LEU:CD2  | 2.88                     | 0.51              |
| 1:D:382:PHE:CE1  | 1:E:272:ARG:HA   | 2.45                     | 0.51              |
| 1:D:517:ARG:HB3  | 1:D:519:LEU:HD13 | 1.92                     | 0.51              |
| 1:E:318:MET:CE   | 1:E:465:HIS:CD2  | 2.91                     | 0.51              |
| 1:E:533:MET:HB3  | 1:E:543:GLU:O    | 2.11                     | 0.51              |
| 1:F:447:THR:CG2  | 1:F:495:LEU:HD21 | 2.25                     | 0.51              |
| 1:G:309:MET:HB3  | 1:G:499:ILE:CD1  | 2.39                     | 0.51              |
| 1:A:265:VAL:HG11 | 1:B:411:TYR:HE1  | 1.76                     | 0.51              |
| 1:D:336:LYS:HB3  | 1:D:418:CYS:HA   | 1.92                     | 0.51              |
| 1:E:162:MET:SD   | 1:E:166:MET:HG3  | 2.50                     | 0.51              |
| 1:E:402:THR:HG23 | 1:E:403:ASP:N    | 2.25                     | 0.51              |
| 1:F:208:MET:HE2  | 1:F:232:VAL:HA   | 1.92                     | 0.51              |
| 1:G:397:PHE:C    | 1:G:397:PHE:HD1  | 2.18                     | 0.51              |
| 1:G:437:ASP:OD1  | 1:G:439:ARG:HB2  | 2.09                     | 0.51              |
| 1:A:126:LYS:NZ   | 1:A:127:ASP:CG   | 2.68                     | 0.51              |
| 1:A:339:LEU:HB3  | 1:A:341:MET:HE2  | 1.84                     | 0.51              |
| 1:A:394:TYR:C    | 1:A:394:TYR:HD1  | 2.18                     | 0.51              |
| 1:B:106:TYR:HB3  | 1:B:123:VAL:HG12 | 1.93                     | 0.51              |
| 1:B:401:GLU:HG2  | 1:B:402:THR:N    | 2.26                     | 0.51              |
| 1:D:86:ILE:HG21  | 1:D:163:LEU:CD1  | 2.40                     | 0.51              |
| 1:E:359:ARG:HD3  | 1:E:541:TRP:HE1  | 1.76                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:482:SER:N    | 1:E:485:ASP:HB2  | 2.19                     | 0.51              |
| 1:G:78:TYR:CG    | 1:G:92:GLN:HG2   | 2.45                     | 0.51              |
| 1:A:234:PRO:CG   | 1:A:249:GLU:HG2  | 2.40                     | 0.51              |
| 1:A:346:VAL:HG13 | 1:C:271:LEU:CD2  | 2.40                     | 0.51              |
| 1:A:382:PHE:C    | 1:A:382:PHE:CD2  | 2.88                     | 0.51              |
| 1:A:414:SER:HB3  | 1:C:226:GLY:HA3  | 1.91                     | 0.51              |
| 1:B:401:GLU:HG3  | 1:B:431:SER:O    | 2.10                     | 0.51              |
| 1:C:94:ALA:CB    | 1:C:162:MET:HE1  | 2.41                     | 0.51              |
| 1:C:164:THR:O    | 1:C:167:GLU:HB2  | 2.11                     | 0.51              |
| 1:C:510:MET:HE1  | 1:C:547:TYR:OH   | 2.10                     | 0.51              |
| 1:D:80:ALA:HB2   | 1:D:88:LYS:HB2   | 1.92                     | 0.51              |
| 1:E:411:TYR:CD1  | 1:E:411:TYR:C    | 2.89                     | 0.51              |
| 1:F:402:THR:HG23 | 1:F:403:ASP:N    | 2.26                     | 0.51              |
| 1:F:547:TYR:CD2  | 1:F:548:SER:N    | 2.79                     | 0.51              |
| 1:G:306:GLU:HA   | 1:G:497:ASP:OD2  | 2.10                     | 0.51              |
| 1:A:445:LEU:CD1  | 1:A:449:LEU:HG   | 2.41                     | 0.51              |
| 1:B:492:LEU:H    | 1:B:492:LEU:CD1  | 2.05                     | 0.51              |
| 1:C:74:SER:HB3   | 1:C:101:VAL:HG22 | 1.92                     | 0.51              |
| 1:C:235:CYS:CB   | 1:C:240:GLU:HG2  | 2.40                     | 0.51              |
| 1:C:286:GLY:O    | 1:C:302:ALA:N    | 2.44                     | 0.51              |
| 1:C:411:TYR:OH   | 1:D:260:TRP:CA   | 2.59                     | 0.51              |
| 1:C:486:LEU:HD22 | 1:C:487:ARG:H    | 1.76                     | 0.51              |
| 1:D:520:LYS:HG3  | 1:D:521:CYS:N    | 2.16                     | 0.51              |
| 1:E:421:ILE:HB   | 1:E:460:LEU:HD12 | 1.92                     | 0.51              |
| 1:F:306:GLU:HA   | 1:F:497:ASP:OD2  | 2.11                     | 0.51              |
| 1:F:313:GLY:O    | 1:F:315:GLY:N    | 2.44                     | 0.51              |
| 1:G:91:CYS:HB3   | 1:G:96:TYR:O     | 2.11                     | 0.51              |
| 1:G:271:LEU:O    | 1:G:272:ARG:C    | 2.53                     | 0.51              |
| 1:G:402:THR:HG23 | 1:G:403:ASP:N    | 2.26                     | 0.51              |
| 1:A:346:VAL:HG22 | 1:C:271:LEU:HD21 | 1.91                     | 0.51              |
| 1:B:107:GLN:CB   | 1:B:124:ARG:CG   | 2.84                     | 0.51              |
| 1:C:91:CYS:HB3   | 1:C:96:TYR:O     | 2.11                     | 0.51              |
| 1:C:411:TYR:OH   | 1:D:260:TRP:HB3  | 2.11                     | 0.51              |
| 1:E:107:GLN:CB   | 1:E:124:ARG:CG   | 2.87                     | 0.51              |
| 1:E:492:LEU:C    | 1:E:494:GLN:H    | 2.18                     | 0.51              |
| 1:G:126:LYS:HG2  | 1:G:127:ASP:H    | 1.76                     | 0.51              |
| 1:B:450:LYS:NZ   | 1:B:454:LYS:HD3  | 2.25                     | 0.51              |
| 1:D:112:ARG:HD3  | 1:D:116:GLY:O    | 2.11                     | 0.51              |
| 1:D:122:LYS:HE2  | 1:D:159:GLU:OE1  | 2.11                     | 0.51              |
| 1:D:165:VAL:HB   | 1:D:175:VAL:HG11 | 1.91                     | 0.51              |
| 1:D:268:ALA:HA   | 1:D:271:LEU:HD12 | 1.91                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:394:TYR:HE1  | 1:D:396:SER:CB   | 2.22                     | 0.51              |
| 1:F:424:ASP:O    | 1:F:425:HIS:HB3  | 2.10                     | 0.51              |
| 1:G:165:VAL:HB   | 1:G:175:VAL:HG11 | 1.92                     | 0.51              |
| 1:G:167:GLU:C    | 1:G:169:GLN:H    | 2.15                     | 0.51              |
| 1:G:276:ARG:NH1  | 1:G:276:ARG:CG   | 2.48                     | 0.51              |
| 1:G:351:GLU:HB2  | 1:G:363:ARG:HD2  | 1.92                     | 0.51              |
| 1:G:413:ARG:NE   | 1:G:458:VAL:HB   | 2.24                     | 0.51              |
| 1:A:267:SER:O    | 1:A:270:SER:OG   | 2.27                     | 0.50              |
| 1:B:233:LEU:HD22 | 1:B:241:CYS:SG   | 2.51                     | 0.50              |
| 1:C:368:LEU:HD22 | 1:C:368:LEU:C    | 2.36                     | 0.50              |
| 1:C:536:ASN:ND2  | 1:C:538:GLU:HB2  | 2.26                     | 0.50              |
| 1:D:314:SER:O    | 1:D:315:GLY:C    | 2.53                     | 0.50              |
| 1:D:401:GLU:HB3  | 1:D:404:ARG:HB3  | 1.92                     | 0.50              |
| 1:D:478:GLY:CA   | 1:D:505:ASN:HB2  | 2.40                     | 0.50              |
| 1:E:125:ASP:OD1  | 1:E:129:ASN:HB2  | 2.11                     | 0.50              |
| 1:E:379:ASP:OD1  | 1:F:276:ARG:NH2  | 2.42                     | 0.50              |
| 1:E:413:ARG:HH21 | 1:E:457:GLY:C    | 2.19                     | 0.50              |
| 1:F:180:HIS:HB2  | 1:F:184:ALA:HB3  | 1.93                     | 0.50              |
| 1:F:304:GLY:HA2  | 1:F:459:VAL:HG22 | 1.92                     | 0.50              |
| 1:F:389:ASP:CA   | 1:G:269:LEU:CD2  | 2.87                     | 0.50              |
| 1:A:243:LEU:O    | 1:A:244:ASN:C    | 2.53                     | 0.50              |
| 1:A:286:GLY:O    | 1:A:302:ALA:N    | 2.44                     | 0.50              |
| 1:B:279:LEU:HD23 | 1:G:369:LYS:HG2  | 1.94                     | 0.50              |
| 1:C:166:MET:HE3  | 1:C:171:CYS:CA   | 2.41                     | 0.50              |
| 1:C:330:GLY:HA2  | 1:C:335:LYS:O    | 2.12                     | 0.50              |
| 1:D:283:GLU:CD   | 1:D:286:GLY:HA2  | 2.36                     | 0.50              |
| 1:D:425:HIS:CE1  | 1:D:427:SER:OG   | 2.64                     | 0.50              |
| 1:D:473:LYS:CE   | 1:D:479:ARG:HA   | 2.39                     | 0.50              |
| 1:E:392:HIS:CE1  | 1:F:267:SER:HB2  | 2.45                     | 0.50              |
| 1:F:168:LEU:HD11 | 1:F:250:ILE:HD12 | 1.92                     | 0.50              |
| 1:F:205:MET:HG3  | 1:F:231:ALA:CB   | 2.41                     | 0.50              |
| 1:F:322:VAL:HG21 | 1:F:463:ILE:CG1  | 2.42                     | 0.50              |
| 1:F:484:THR:C    | 1:F:486:LEU:N    | 2.67                     | 0.50              |
| 1:G:425:HIS:CE1  | 1:G:427:SER:CB   | 2.94                     | 0.50              |
| 1:A:326:ALA:HB2  | 1:A:422:ILE:HD12 | 1.92                     | 0.50              |
| 1:B:402:THR:HG23 | 1:B:403:ASP:N    | 2.26                     | 0.50              |
| 1:B:482:SER:N    | 1:B:485:ASP:HB2  | 2.22                     | 0.50              |
| 1:C:168:LEU:HD11 | 1:C:250:ILE:HD12 | 1.92                     | 0.50              |
| 1:C:267:SER:O    | 1:C:270:SER:OG   | 2.28                     | 0.50              |
| 1:C:309:MET:HE2  | 1:C:462:VAL:HG12 | 1.93                     | 0.50              |
| 1:C:401:GLU:N    | 1:C:404:ARG:HD2  | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:168:LEU:HD11 | 1:D:250:ILE:HD12 | 1.93                     | 0.50              |
| 1:D:391:PHE:C    | 1:D:392:HIS:CD2  | 2.89                     | 0.50              |
| 1:D:476:GLU:CD   | 1:D:476:GLU:N    | 2.70                     | 0.50              |
| 1:D:482:SER:H    | 1:D:485:ASP:CB   | 2.23                     | 0.50              |
| 1:E:311:THR:OG1  | 1:E:466:LEU:HD21 | 2.11                     | 0.50              |
| 1:F:521:CYS:O    | 1:F:525:GLY:N    | 2.38                     | 0.50              |
| 1:G:80:ALA:HB2   | 1:G:88:LYS:HB2   | 1.93                     | 0.50              |
| 1:G:220:ALA:HB2  | 1:G:261:ILE:HD13 | 1.94                     | 0.50              |
| 1:G:322:VAL:HG21 | 1:G:463:ILE:CG1  | 2.41                     | 0.50              |
| 1:A:318:MET:SD   | 1:A:463:ILE:HG23 | 2.52                     | 0.50              |
| 1:B:80:ALA:HB2   | 1:B:88:LYS:HB2   | 1.94                     | 0.50              |
| 1:B:112:ARG:HD2  | 1:B:145:HIS:CE1  | 2.46                     | 0.50              |
| 1:B:427:SER:CB   | 1:B:487:ARG:NH1  | 2.74                     | 0.50              |
| 1:B:451:GLY:O    | 1:B:452:PHE:C    | 2.54                     | 0.50              |
| 1:C:194:GLU:CD   | 1:C:194:GLU:N    | 2.67                     | 0.50              |
| 1:C:441:MET:HE1  | 1:C:445:LEU:N    | 2.27                     | 0.50              |
| 1:C:443:ASP:HA   | 1:C:491:ALA:CB   | 2.42                     | 0.50              |
| 1:D:205:MET:HE1  | 1:D:250:ILE:HG23 | 1.92                     | 0.50              |
| 1:E:180:HIS:HB2  | 1:E:184:ALA:HB3  | 1.93                     | 0.50              |
| 1:F:271:LEU:O    | 1:F:272:ARG:C    | 2.53                     | 0.50              |
| 1:F:387:GLY:HA2  | 1:G:269:LEU:HD11 | 1.92                     | 0.50              |
| 1:F:439:ARG:O    | 1:F:442:ILE:CG2  | 2.59                     | 0.50              |
| 1:F:487:ARG:O    | 1:F:493:ARG:HD3  | 2.11                     | 0.50              |
| 1:G:148:ASN:HD22 | 1:G:198:GLN:HE22 | 1.58                     | 0.50              |
| 1:G:316:MET:CE   | 1:G:535:TYR:CZ   | 2.94                     | 0.50              |
| 1:G:502:LEU:N    | 1:G:502:LEU:HD12 | 2.27                     | 0.50              |
| 1:G:504:ARG:HH21 | 1:G:506:GLN:CG   | 2.25                     | 0.50              |
| 1:B:79:SER:H     | 1:B:98:ILE:CD1   | 2.23                     | 0.50              |
| 1:D:351:GLU:HB2  | 1:D:363:ARG:HD2  | 1.93                     | 0.50              |
| 1:D:484:THR:O    | 1:D:486:LEU:N    | 2.45                     | 0.50              |
| 1:E:74:SER:HB3   | 1:E:101:VAL:CG2  | 2.42                     | 0.50              |
| 1:F:309:MET:HE2  | 1:F:462:VAL:HG12 | 1.93                     | 0.50              |
| 1:F:311:THR:O    | 1:F:502:LEU:HD12 | 2.11                     | 0.50              |
| 1:F:473:LYS:CE   | 1:F:479:ARG:HA   | 2.36                     | 0.50              |
| 1:F:478:GLY:O    | 1:F:479:ARG:C    | 2.54                     | 0.50              |
| 1:G:168:LEU:HD11 | 1:G:250:ILE:HD12 | 1.93                     | 0.50              |
| 1:G:202:ILE:HD13 | 1:G:223:LEU:CD2  | 2.41                     | 0.50              |
| 1:G:358:ASN:O    | 1:G:360:VAL:CG1  | 2.47                     | 0.50              |
| 1:G:480:PRO:HA   | 1:G:503:GLU:OE2  | 2.11                     | 0.50              |
| 1:A:186:LYS:CD   | 1:A:218:GLU:HG3  | 2.32                     | 0.50              |
| 1:A:447:THR:HA   | 1:A:495:LEU:HD23 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:502:LEU:HD12 | 1:A:502:LEU:N    | 2.27                     | 0.50              |
| 1:B:165:VAL:HB   | 1:B:175:VAL:HG11 | 1.94                     | 0.50              |
| 1:B:413:ARG:HH21 | 1:B:457:GLY:C    | 2.18                     | 0.50              |
| 1:D:181:GLY:O    | 1:D:182:ALA:C    | 2.55                     | 0.50              |
| 1:D:261:ILE:H    | 1:D:262:PRO:HD3  | 1.75                     | 0.50              |
| 1:D:445:LEU:CD1  | 1:D:449:LEU:HG   | 2.42                     | 0.50              |
| 1:F:322:VAL:CG2  | 1:F:463:ILE:HD11 | 2.42                     | 0.50              |
| 1:F:345:SER:O    | 1:F:349:THR:HG23 | 2.11                     | 0.50              |
| 1:F:397:PHE:CD1  | 1:F:397:PHE:C    | 2.90                     | 0.50              |
| 1:F:410:ALA:HA   | 1:F:452:PHE:CE1  | 2.47                     | 0.50              |
| 1:G:410:ALA:HA   | 1:G:452:PHE:CE1  | 2.45                     | 0.50              |
| 1:A:425:HIS:HE1  | 1:A:427:SER:OG   | 1.90                     | 0.50              |
| 1:B:234:PRO:HG2  | 1:B:249:GLU:HG2  | 1.94                     | 0.50              |
| 1:C:114:GLN:NE2  | 1:C:195:TYR:HD1  | 2.10                     | 0.50              |
| 1:C:397:PHE:C    | 1:C:397:PHE:CD1  | 2.89                     | 0.50              |
| 1:C:463:ILE:CG2  | 1:C:464:CYS:N    | 2.74                     | 0.50              |
| 1:D:166:MET:HE1  | 1:D:171:CYS:HB3  | 1.93                     | 0.50              |
| 1:D:343:GLU:OE1  | 1:D:343:GLU:HA   | 2.11                     | 0.50              |
| 1:E:314:SER:O    | 1:E:315:GLY:C    | 2.54                     | 0.50              |
| 1:F:243:LEU:O    | 1:F:244:ASN:C    | 2.55                     | 0.50              |
| 1:F:473:LYS:HE2  | 1:F:479:ARG:CA   | 2.38                     | 0.50              |
| 1:F:480:PRO:HA   | 1:F:503:GLU:OE2  | 2.11                     | 0.50              |
| 1:G:314:SER:O    | 1:G:315:GLY:C    | 2.55                     | 0.50              |
| 1:A:504:ARG:HH21 | 1:A:506:GLN:CB   | 2.23                     | 0.50              |
| 1:C:162:MET:HG2  | 1:C:175:VAL:HB   | 1.92                     | 0.50              |
| 1:E:81:LEU:HG    | 1:E:91:CYS:SG    | 2.52                     | 0.50              |
| 1:E:112:ARG:HD2  | 1:E:145:HIS:CE1  | 2.47                     | 0.50              |
| 1:F:316:MET:CE   | 1:F:535:TYR:CE2  | 2.94                     | 0.50              |
| 1:F:442:ILE:HD11 | 1:F:492:LEU:CD2  | 2.41                     | 0.50              |
| 1:G:74:SER:HB3   | 1:G:101:VAL:CG2  | 2.42                     | 0.50              |
| 1:G:86:ILE:HD12  | 1:G:163:LEU:HB3  | 1.93                     | 0.50              |
| 1:B:502:LEU:N    | 1:B:502:LEU:HD12 | 2.27                     | 0.50              |
| 1:B:531:GLY:C    | 1:B:532:TYR:CD1  | 2.90                     | 0.50              |
| 1:C:336:LYS:HB3  | 1:C:418:CYS:HA   | 1.92                     | 0.50              |
| 1:D:450:LYS:O    | 1:D:453:ALA:HB3  | 2.12                     | 0.50              |
| 1:F:168:LEU:HD22 | 1:F:247:ASP:OD2  | 2.12                     | 0.50              |
| 1:F:303:ARG:HB2  | 1:F:306:GLU:CD   | 2.37                     | 0.50              |
| 1:F:443:ASP:HA   | 1:F:491:ALA:CB   | 2.41                     | 0.50              |
| 1:B:227:LYS:O    | 1:B:229:ARG:HD2  | 2.11                     | 0.49              |
| 1:C:124:ARG:C    | 1:C:124:ARG:CD   | 2.84                     | 0.49              |
| 1:C:515:LEU:HD21 | 1:C:529:ILE:HD12 | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:114:GLN:NE2  | 1:D:195:TYR:HD1  | 2.10                     | 0.49              |
| 1:D:480:PRO:HA   | 1:D:503:GLU:OE2  | 2.12                     | 0.49              |
| 1:E:246:HIS:HB3  | 1:E:249:GLU:OE1  | 2.12                     | 0.49              |
| 1:F:112:ARG:HB3  | 1:F:117:ASN:C    | 2.34                     | 0.49              |
| 1:F:486:LEU:HD22 | 1:F:487:ARG:H    | 1.77                     | 0.49              |
| 1:G:232:VAL:O    | 1:G:232:VAL:HG12 | 2.12                     | 0.49              |
| 1:G:288:LEU:HD12 | 1:G:288:LEU:H    | 1.77                     | 0.49              |
| 1:G:295:ILE:HD12 | 1:G:516:VAL:HG11 | 1.94                     | 0.49              |
| 1:G:486:LEU:HD12 | 1:G:493:ARG:CD   | 2.42                     | 0.49              |
| 1:A:536:ASN:ND2  | 1:A:538:GLU:CB   | 2.75                     | 0.49              |
| 1:B:122:LYS:HE3  | 1:B:130:PHE:CE2  | 2.47                     | 0.49              |
| 1:C:167:GLU:C    | 1:C:169:GLN:H    | 2.17                     | 0.49              |
| 1:D:286:GLY:O    | 1:D:302:ALA:N    | 2.45                     | 0.49              |
| 1:D:499:ILE:HG22 | 1:D:519:LEU:CB   | 2.31                     | 0.49              |
| 1:E:235:CYS:CB   | 1:E:240:GLU:HG2  | 2.41                     | 0.49              |
| 1:F:401:GLU:HG2  | 1:F:402:THR:N    | 2.26                     | 0.49              |
| 1:G:344:GLU:HB2  | 1:G:348:GLU:OE2  | 2.11                     | 0.49              |
| 1:G:413:ARG:HH21 | 1:G:458:VAL:N    | 2.10                     | 0.49              |
| 1:G:510:MET:CB   | 1:G:513:LEU:HB2  | 2.42                     | 0.49              |
| 1:A:515:LEU:HD21 | 1:A:529:ILE:HD11 | 1.94                     | 0.49              |
| 1:B:234:PRO:CG   | 1:B:249:GLU:HG2  | 2.42                     | 0.49              |
| 1:C:304:GLY:HA2  | 1:C:459:VAL:HG22 | 1.94                     | 0.49              |
| 1:D:78:TYR:CG    | 1:D:92:GLN:HG2   | 2.47                     | 0.49              |
| 1:D:79:SER:H     | 1:D:98:ILE:CD1   | 2.24                     | 0.49              |
| 1:D:482:SER:N    | 1:D:485:ASP:HB2  | 2.22                     | 0.49              |
| 1:E:122:LYS:HE3  | 1:E:130:PHE:CE2  | 2.47                     | 0.49              |
| 1:E:166:MET:HG2  | 1:E:175:VAL:CG2  | 2.41                     | 0.49              |
| 1:E:389:ASP:CA   | 1:F:269:LEU:HD23 | 2.43                     | 0.49              |
| 1:E:392:HIS:ND1  | 1:F:267:SER:HB3  | 2.27                     | 0.49              |
| 1:F:330:GLY:HA2  | 1:F:335:LYS:O    | 2.12                     | 0.49              |
| 1:G:480:PRO:HA   | 1:G:503:GLU:OE1  | 2.12                     | 0.49              |
| 1:A:112:ARG:HD3  | 1:A:116:GLY:O    | 2.12                     | 0.49              |
| 1:B:194:GLU:CD   | 1:B:194:GLU:N    | 2.70                     | 0.49              |
| 1:B:368:LEU:HD22 | 1:B:368:LEU:C    | 2.38                     | 0.49              |
| 1:C:259:PRO:O    | 1:C:260:TRP:CB   | 2.60                     | 0.49              |
| 1:E:86:ILE:HD12  | 1:E:163:LEU:HB3  | 1.94                     | 0.49              |
| 1:E:258:GLY:CA   | 1:E:260:TRP:HZ3  | 2.23                     | 0.49              |
| 1:F:382:PHE:C    | 1:F:382:PHE:CD2  | 2.91                     | 0.49              |
| 1:G:181:GLY:O    | 1:G:182:ALA:C    | 2.54                     | 0.49              |
| 1:G:312:SER:H    | 1:G:318:MET:HE2  | 1.78                     | 0.49              |
| 1:G:492:LEU:C    | 1:G:494:GLN:H    | 2.19                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:272:ARG:HA   | 1:B:382:PHE:CE1  | 2.48                     | 0.49              |
| 1:A:346:VAL:HG23 | 1:A:393:LEU:HB2  | 1.94                     | 0.49              |
| 1:B:316:MET:CE   | 1:B:535:TYR:CZ   | 2.91                     | 0.49              |
| 1:B:445:LEU:CD1  | 1:B:449:LEU:HG   | 2.42                     | 0.49              |
| 1:C:165:VAL:HB   | 1:C:175:VAL:HG11 | 1.93                     | 0.49              |
| 1:C:205:MET:HG3  | 1:C:231:ALA:CB   | 2.42                     | 0.49              |
| 1:C:372:ILE:HG13 | 1:C:378:PHE:HB2  | 1.94                     | 0.49              |
| 1:C:487:ARG:O    | 1:C:493:ARG:HD3  | 2.13                     | 0.49              |
| 1:E:112:ARG:HD3  | 1:E:116:GLY:O    | 2.12                     | 0.49              |
| 1:E:447:THR:O    | 1:E:448:LYS:C    | 2.56                     | 0.49              |
| 1:F:344:GLU:HB2  | 1:F:348:GLU:OE2  | 2.13                     | 0.49              |
| 1:G:345:SER:O    | 1:G:349:THR:HG23 | 2.13                     | 0.49              |
| 1:A:330:GLY:HA2  | 1:A:335:LYS:O    | 2.13                     | 0.49              |
| 1:A:358:ASN:ND2  | 1:A:381:TRP:CE2  | 2.81                     | 0.49              |
| 1:A:512:ASN:HD21 | 1:A:537:LYS:HE3  | 1.77                     | 0.49              |
| 1:B:74:SER:HB3   | 1:B:101:VAL:CG2  | 2.42                     | 0.49              |
| 1:C:413:ARG:NE   | 1:C:458:VAL:HB   | 2.24                     | 0.49              |
| 1:D:205:MET:HG3  | 1:D:231:ALA:HB1  | 1.94                     | 0.49              |
| 1:D:531:GLY:C    | 1:D:532:TYR:CD1  | 2.90                     | 0.49              |
| 1:D:536:ASN:HD21 | 1:D:538:GLU:HB2  | 1.77                     | 0.49              |
| 1:E:121:GLN:HB2  | 1:E:133:THR:HG1  | 1.76                     | 0.49              |
| 1:F:318:MET:SD   | 1:F:463:ILE:HG23 | 2.52                     | 0.49              |
| 1:F:425:HIS:CD2  | 1:F:465:HIS:CE1  | 3.01                     | 0.49              |
| 1:A:369:LYS:CG   | 1:C:279:LEU:HD22 | 2.41                     | 0.49              |
| 1:A:372:ILE:HG13 | 1:A:378:PHE:HB2  | 1.95                     | 0.49              |
| 1:A:536:ASN:C    | 1:A:538:GLU:H    | 2.21                     | 0.49              |
| 1:B:322:VAL:HG21 | 1:B:463:ILE:CD1  | 2.43                     | 0.49              |
| 1:B:504:ARG:HH21 | 1:B:506:GLN:HG2  | 1.77                     | 0.49              |
| 1:C:260:TRP:N    | 1:C:260:TRP:HE3  | 2.10                     | 0.49              |
| 1:D:368:LEU:HD22 | 1:D:368:LEU:C    | 2.36                     | 0.49              |
| 1:D:425:HIS:CE1  | 1:D:427:SER:HB2  | 2.48                     | 0.49              |
| 1:E:260:TRP:C    | 1:E:261:ILE:HG13 | 2.37                     | 0.49              |
| 1:F:492:LEU:C    | 1:F:494:GLN:H    | 2.21                     | 0.49              |
| 1:G:446:MET:HE2  | 1:G:492:LEU:CB   | 2.43                     | 0.49              |
| 1:A:312:SER:O    | 1:A:313:GLY:O    | 2.31                     | 0.49              |
| 1:C:536:ASN:OD1  | 1:C:539:THR:HG23 | 2.12                     | 0.49              |
| 1:D:235:CYS:CB   | 1:D:240:GLU:HG2  | 2.43                     | 0.49              |
| 1:D:401:GLU:CG   | 1:D:431:SER:O    | 2.44                     | 0.49              |
| 1:E:439:ARG:O    | 1:E:442:ILE:CG2  | 2.61                     | 0.49              |
| 1:F:339:LEU:HB3  | 1:F:341:MET:HE3  | 1.88                     | 0.49              |
| 1:A:314:SER:O    | 1:A:315:GLY:C    | 2.54                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:440:LYS:HE2  | 1:A:440:LYS:O    | 2.13                     | 0.49              |
| 1:B:202:ILE:HD13 | 1:B:223:LEU:CD2  | 2.42                     | 0.49              |
| 1:B:322:VAL:CG1  | 1:B:422:ILE:HG21 | 2.43                     | 0.49              |
| 1:B:437:ASP:OD1  | 1:B:439:ARG:HB2  | 2.13                     | 0.49              |
| 1:C:112:ARG:HD3  | 1:C:116:GLY:O    | 2.12                     | 0.49              |
| 1:C:271:LEU:O    | 1:C:272:ARG:C    | 2.54                     | 0.49              |
| 1:D:360:VAL:O    | 1:D:360:VAL:CG2  | 2.59                     | 0.49              |
| 1:E:80:ALA:HB2   | 1:E:88:LYS:HB2   | 1.93                     | 0.49              |
| 1:E:168:LEU:HD11 | 1:E:250:ILE:HD12 | 1.94                     | 0.49              |
| 1:E:389:ASP:HA   | 1:F:269:LEU:CD2  | 2.43                     | 0.49              |
| 1:F:438:GLU:O    | 1:F:442:ILE:HG22 | 2.12                     | 0.49              |
| 1:G:427:SER:HB3  | 1:G:487:ARG:NH1  | 2.25                     | 0.49              |
| 1:G:473:LYS:CE   | 1:G:479:ARG:HA   | 2.42                     | 0.49              |
| 1:A:440:LYS:HE2  | 1:A:440:LYS:C    | 2.38                     | 0.49              |
| 1:B:279:LEU:CD2  | 1:G:369:LYS:HG2  | 2.42                     | 0.49              |
| 1:C:440:LYS:CE   | 1:C:441:MET:HA   | 2.43                     | 0.49              |
| 1:D:229:ARG:HB2  | 1:D:258:GLY:O    | 2.13                     | 0.49              |
| 1:D:408:LYS:NZ   | 1:E:263:ASP:C    | 2.71                     | 0.49              |
| 1:E:452:PHE:O    | 1:E:456:THR:HG23 | 2.12                     | 0.49              |
| 1:F:392:HIS:ND1  | 1:G:267:SER:CB   | 2.75                     | 0.49              |
| 1:G:229:ARG:HH21 | 1:G:259:PRO:HG3  | 1.78                     | 0.49              |
| 1:A:346:VAL:HG22 | 1:C:271:LEU:CD2  | 2.42                     | 0.48              |
| 1:A:536:ASN:HD22 | 1:A:536:ASN:C    | 2.20                     | 0.48              |
| 1:B:401:GLU:CG   | 1:B:402:THR:N    | 2.75                     | 0.48              |
| 1:E:234:PRO:HG2  | 1:E:249:GLU:HG2  | 1.95                     | 0.48              |
| 1:E:352:ASP:CG   | 1:E:363:ARG:HD3  | 2.38                     | 0.48              |
| 1:F:140:ALA:O    | 1:F:141:LEU:HD23 | 2.12                     | 0.48              |
| 1:F:443:ASP:HA   | 1:F:491:ALA:HB3  | 1.95                     | 0.48              |
| 1:A:520:LYS:HG3  | 1:A:521:CYS:N    | 2.24                     | 0.48              |
| 1:B:166:MET:HE3  | 1:B:171:CYS:CB   | 2.42                     | 0.48              |
| 1:B:228:VAL:CB   | 1:B:261:ILE:HD11 | 2.36                     | 0.48              |
| 1:B:401:GLU:HB3  | 1:B:404:ARG:HB3  | 1.94                     | 0.48              |
| 1:B:405:LEU:HG   | 1:B:409:LEU:CD1  | 2.42                     | 0.48              |
| 1:C:482:SER:N    | 1:C:485:ASP:HB2  | 2.22                     | 0.48              |
| 1:D:447:THR:O    | 1:D:448:LYS:C    | 2.56                     | 0.48              |
| 1:D:486:LEU:HD12 | 1:D:493:ARG:CG   | 2.43                     | 0.48              |
| 1:D:496:SER:CB   | 1:D:499:ILE:HD11 | 2.43                     | 0.48              |
| 1:E:204:LEU:HD23 | 1:E:204:LEU:N    | 2.27                     | 0.48              |
| 1:E:326:ALA:HB2  | 1:E:422:ILE:HD12 | 1.95                     | 0.48              |
| 1:F:220:ALA:HB3  | 1:F:261:ILE:HG12 | 1.92                     | 0.48              |
| 1:G:168:LEU:HD22 | 1:G:247:ASP:OD2  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:185:ALA:O    | 1:A:189:CYS:HB2  | 2.12                     | 0.48              |
| 1:A:412:MET:HE2  | 1:A:421:ILE:HD11 | 1.84                     | 0.48              |
| 1:A:469:PRO:O    | 1:A:470:ASP:CB   | 2.54                     | 0.48              |
| 1:C:262:PRO:HB2  | 1:C:265:VAL:HG12 | 1.94                     | 0.48              |
| 1:C:338:GLY:CA   | 1:C:412:MET:HE1  | 2.42                     | 0.48              |
| 1:C:345:SER:O    | 1:C:349:THR:HG22 | 2.13                     | 0.48              |
| 1:D:230:VAL:HB   | 1:D:260:TRP:CE2  | 2.48                     | 0.48              |
| 1:D:438:GLU:O    | 1:D:442:ILE:HG22 | 2.13                     | 0.48              |
| 1:D:439:ARG:O    | 1:D:442:ILE:CG2  | 2.60                     | 0.48              |
| 1:E:439:ARG:HG2  | 1:E:489:SER:OG   | 2.13                     | 0.48              |
| 1:E:454:LYS:HE3  | 1:E:522:ARG:HH22 | 1.78                     | 0.48              |
| 1:F:153:ILE:HG13 | 1:F:174:PRO:CB   | 2.43                     | 0.48              |
| 1:F:531:GLY:C    | 1:F:532:TYR:CD1  | 2.92                     | 0.48              |
| 1:G:267:SER:O    | 1:G:271:LEU:HD12 | 2.14                     | 0.48              |
| 1:G:359:ARG:HD3  | 1:G:541:TRP:NE1  | 2.28                     | 0.48              |
| 1:G:443:ASP:HA   | 1:G:491:ALA:CB   | 2.42                     | 0.48              |
| 1:A:169:GLN:NE2  | 1:A:251:MET:HE2  | 2.27                     | 0.48              |
| 1:A:279:LEU:CD2  | 1:B:369:LYS:HG2  | 2.43                     | 0.48              |
| 1:B:536:ASN:HD21 | 1:B:538:GLU:HB3  | 1.78                     | 0.48              |
| 1:C:229:ARG:NH2  | 1:C:259:PRO:HG3  | 2.27                     | 0.48              |
| 1:E:181:GLY:O    | 1:E:182:ALA:C    | 2.57                     | 0.48              |
| 1:G:510:MET:HE1  | 1:G:547:TYR:OH   | 2.14                     | 0.48              |
| 1:A:121:GLN:HB2  | 1:A:133:THR:HG1  | 1.77                     | 0.48              |
| 1:A:255:TRP:O    | 1:A:256:ASN:OD1  | 2.31                     | 0.48              |
| 1:B:289:PHE:HA   | 1:B:325:GLN:HE21 | 1.77                     | 0.48              |
| 1:D:185:ALA:O    | 1:D:189:CYS:HB2  | 2.13                     | 0.48              |
| 1:D:447:THR:HA   | 1:D:495:LEU:CD2  | 2.42                     | 0.48              |
| 1:E:253:GLN:CA   | 1:E:257:ALA:HB2  | 2.25                     | 0.48              |
| 1:E:451:GLY:O    | 1:E:452:PHE:C    | 2.57                     | 0.48              |
| 1:F:405:LEU:HG   | 1:F:409:LEU:CD1  | 2.41                     | 0.48              |
| 1:G:162:MET:HG2  | 1:G:175:VAL:HB   | 1.96                     | 0.48              |
| 1:G:235:CYS:CB   | 1:G:240:GLU:HG2  | 2.43                     | 0.48              |
| 1:G:402:THR:HG23 | 1:G:403:ASP:H    | 1.79                     | 0.48              |
| 1:A:122:LYS:HE3  | 1:A:130:PHE:CE2  | 2.48                     | 0.48              |
| 1:A:126:LYS:HZ2  | 1:A:127:ASP:CB   | 2.22                     | 0.48              |
| 1:A:216:VAL:CG1  | 1:A:230:VAL:CG2  | 2.90                     | 0.48              |
| 1:B:94:ALA:CB    | 1:B:162:MET:HE1  | 2.43                     | 0.48              |
| 1:C:181:GLY:O    | 1:C:182:ALA:C    | 2.56                     | 0.48              |
| 1:D:106:TYR:HB3  | 1:D:123:VAL:HG12 | 1.95                     | 0.48              |
| 1:D:312:SER:O    | 1:D:313:GLY:O    | 2.30                     | 0.48              |
| 1:D:498:THR:C    | 1:D:499:ILE:HD13 | 2.37                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:289:PHE:HA   | 1:F:325:GLN:HE21 | 1.78                     | 0.48              |
| 1:F:351:GLU:OE1  | 1:G:278:HIS:CD2  | 2.66                     | 0.48              |
| 1:G:330:GLY:HA2  | 1:G:335:LYS:O    | 2.14                     | 0.48              |
| 1:G:394:TYR:CE2  | 1:G:405:LEU:HD12 | 2.49                     | 0.48              |
| 1:G:499:ILE:HG22 | 1:G:519:LEU:CB   | 2.31                     | 0.48              |
| 1:A:268:ALA:HA   | 1:A:271:LEU:HD12 | 1.94                     | 0.48              |
| 1:A:510:MET:CB   | 1:A:513:LEU:HB2  | 2.43                     | 0.48              |
| 1:C:360:VAL:HG23 | 1:C:360:VAL:O    | 2.13                     | 0.48              |
| 1:C:412:MET:HE3  | 1:C:412:MET:HB3  | 1.77                     | 0.48              |
| 1:D:404:ARG:O    | 1:D:408:LYS:HG2  | 2.14                     | 0.48              |
| 1:E:443:ASP:HA   | 1:E:491:ALA:CB   | 2.44                     | 0.48              |
| 1:F:114:GLN:HG3  | 1:F:144:LYS:HE2  | 1.96                     | 0.48              |
| 1:G:246:HIS:HB3  | 1:G:249:GLU:OE1  | 2.14                     | 0.48              |
| 1:G:419:ASP:OD2  | 1:G:419:ASP:N    | 2.47                     | 0.48              |
| 1:A:149:GLY:O    | 1:A:199:PHE:CE2  | 2.67                     | 0.48              |
| 1:A:414:SER:C    | 1:C:226:GLY:HA3  | 2.39                     | 0.48              |
| 1:A:427:SER:CB   | 1:A:487:ARG:HH12 | 2.21                     | 0.48              |
| 1:A:438:GLU:O    | 1:A:442:ILE:HG22 | 2.12                     | 0.48              |
| 1:B:81:LEU:HG    | 1:B:91:CYS:SG    | 2.53                     | 0.48              |
| 1:B:86:ILE:HD12  | 1:B:163:LEU:HB3  | 1.96                     | 0.48              |
| 1:C:368:LEU:CD2  | 1:C:372:ILE:HG23 | 2.43                     | 0.48              |
| 1:D:121:GLN:HB2  | 1:D:133:THR:HG1  | 1.79                     | 0.48              |
| 1:D:202:ILE:HD13 | 1:D:223:LEU:CD2  | 2.44                     | 0.48              |
| 1:D:230:VAL:HG12 | 1:D:260:TRP:CZ2  | 2.49                     | 0.48              |
| 1:F:391:PHE:C    | 1:F:392:HIS:CD2  | 2.91                     | 0.48              |
| 1:G:164:THR:O    | 1:G:167:GLU:HB2  | 2.14                     | 0.48              |
| 1:G:478:GLY:O    | 1:G:479:ARG:C    | 2.57                     | 0.48              |
| 1:G:521:CYS:O    | 1:G:525:GLY:N    | 2.38                     | 0.48              |
| 1:B:145:HIS:CE1  | 1:B:146:LEU:HD23 | 2.49                     | 0.48              |
| 1:C:168:LEU:HD22 | 1:C:247:ASP:OD2  | 2.11                     | 0.48              |
| 1:C:234:PRO:CG   | 1:C:249:GLU:HG2  | 2.44                     | 0.48              |
| 1:C:353:LEU:HD23 | 1:C:353:LEU:HA   | 1.72                     | 0.48              |
| 1:C:359:ARG:HD3  | 1:C:541:TRP:HE1  | 1.79                     | 0.48              |
| 1:C:480:PRO:HA   | 1:C:503:GLU:OE2  | 2.14                     | 0.48              |
| 1:D:420:VAL:HG22 | 1:D:459:VAL:HB   | 1.96                     | 0.48              |
| 1:E:336:LYS:HB3  | 1:E:418:CYS:HA   | 1.95                     | 0.48              |
| 1:F:446:MET:O    | 1:F:449:LEU:HB2  | 2.14                     | 0.48              |
| 1:G:445:LEU:CD1  | 1:G:449:LEU:HG   | 2.43                     | 0.48              |
| 1:A:303:ARG:CZ   | 1:A:523:PHE:CD1  | 2.97                     | 0.48              |
| 1:A:517:ARG:HB3  | 1:A:519:LEU:HD13 | 1.95                     | 0.48              |
| 1:B:162:MET:HG2  | 1:B:175:VAL:HB   | 1.93                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:479:ARG:HA   | 1:C:480:PRO:HD3  | 1.76                     | 0.48              |
| 1:C:510:MET:HB2  | 1:C:513:LEU:HB2  | 1.95                     | 0.48              |
| 1:D:536:ASN:C    | 1:D:538:GLU:H    | 2.22                     | 0.48              |
| 1:E:291:GLY:O    | 1:E:292:CYS:HB2  | 2.13                     | 0.48              |
| 1:E:397:PHE:C    | 1:E:397:PHE:HD1  | 2.21                     | 0.48              |
| 1:G:452:PHE:O    | 1:G:456:THR:HG23 | 2.14                     | 0.48              |
| 1:A:114:GLN:NE2  | 1:A:195:TYR:HD1  | 2.11                     | 0.47              |
| 1:A:322:VAL:CG1  | 1:A:422:ILE:HG21 | 2.43                     | 0.47              |
| 1:A:492:LEU:C    | 1:A:494:GLN:H    | 2.21                     | 0.47              |
| 1:B:306:GLU:HA   | 1:B:497:ASP:OD2  | 2.13                     | 0.47              |
| 1:B:327:LEU:HD11 | 1:B:357:HIS:HA   | 1.96                     | 0.47              |
| 1:B:344:GLU:HB2  | 1:B:348:GLU:OE2  | 2.14                     | 0.47              |
| 1:C:397:PHE:C    | 1:C:397:PHE:HD1  | 2.21                     | 0.47              |
| 1:C:452:PHE:O    | 1:C:456:THR:HG23 | 2.14                     | 0.47              |
| 1:D:492:LEU:H    | 1:D:492:LEU:CD1  | 2.06                     | 0.47              |
| 1:E:300:LEU:HB3  | 1:E:303:ARG:HH12 | 1.79                     | 0.47              |
| 1:E:504:ARG:HH21 | 1:E:506:GLN:CG   | 2.26                     | 0.47              |
| 1:F:166:MET:HG2  | 1:F:175:VAL:HG23 | 1.94                     | 0.47              |
| 1:G:162:MET:SD   | 1:G:166:MET:HG3  | 2.54                     | 0.47              |
| 1:G:345:SER:O    | 1:G:349:THR:CG2  | 2.62                     | 0.47              |
| 1:G:368:LEU:HD22 | 1:G:368:LEU:C    | 2.38                     | 0.47              |
| 1:G:394:TYR:HE1  | 1:G:396:SER:CB   | 2.27                     | 0.47              |
| 1:G:512:ASN:HD21 | 1:G:537:LYS:HE3  | 1.78                     | 0.47              |
| 1:A:467:LYS:H    | 1:A:467:LYS:HG3  | 1.53                     | 0.47              |
| 1:B:125:ASP:OD1  | 1:B:129:ASN:HB2  | 2.14                     | 0.47              |
| 1:B:288:LEU:HD12 | 1:B:288:LEU:H    | 1.79                     | 0.47              |
| 1:C:248:ARG:O    | 1:C:248:ARG:HG2  | 2.14                     | 0.47              |
| 1:C:486:LEU:HD13 | 1:C:487:ARG:O    | 2.14                     | 0.47              |
| 1:D:86:ILE:HD12  | 1:D:163:LEU:HB3  | 1.96                     | 0.47              |
| 1:D:154:VAL:HG21 | 1:D:254:VAL:HG22 | 1.96                     | 0.47              |
| 1:D:411:TYR:HE1  | 1:E:265:VAL:HG11 | 1.78                     | 0.47              |
| 1:E:344:GLU:HB2  | 1:E:348:GLU:OE2  | 2.14                     | 0.47              |
| 1:E:486:LEU:HD12 | 1:E:493:ARG:CG   | 2.44                     | 0.47              |
| 1:F:77:ARG:HE    | 1:F:77:ARG:HB2   | 1.49                     | 0.47              |
| 1:F:106:TYR:HB3  | 1:F:123:VAL:HG12 | 1.96                     | 0.47              |
| 1:F:312:SER:O    | 1:F:313:GLY:O    | 2.32                     | 0.47              |
| 1:F:476:GLU:CD   | 1:F:476:GLU:N    | 2.69                     | 0.47              |
| 1:F:486:LEU:HB3  | 1:F:493:ARG:CD   | 2.44                     | 0.47              |
| 1:G:234:PRO:CG   | 1:G:249:GLU:HG2  | 2.44                     | 0.47              |
| 1:G:413:ARG:HH21 | 1:G:457:GLY:C    | 2.22                     | 0.47              |
| 1:A:111:TYR:CZ   | 1:A:142:PHE:HB2  | 2.48                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:180:HIS:CD2  | 1:A:180:HIS:N    | 2.81                     | 0.47              |
| 1:A:413:ARG:HH21 | 1:A:457:GLY:C    | 2.22                     | 0.47              |
| 1:B:148:ASN:HD22 | 1:B:198:GLN:HE22 | 1.62                     | 0.47              |
| 1:B:402:THR:HG23 | 1:B:403:ASP:H    | 1.79                     | 0.47              |
| 1:B:496:SER:HB2  | 1:B:499:ILE:HD11 | 1.96                     | 0.47              |
| 1:C:148:ASN:HD22 | 1:C:198:GLN:HE22 | 1.61                     | 0.47              |
| 1:D:347:GLU:CD   | 1:E:274:ARG:HG2  | 2.40                     | 0.47              |
| 1:D:419:ASP:OD2  | 1:D:419:ASP:N    | 2.47                     | 0.47              |
| 1:E:106:TYR:HB3  | 1:E:123:VAL:HG12 | 1.95                     | 0.47              |
| 1:E:480:PRO:HA   | 1:E:503:GLU:OE2  | 2.14                     | 0.47              |
| 1:F:265:VAL:HG12 | 1:F:265:VAL:O    | 2.14                     | 0.47              |
| 1:G:439:ARG:O    | 1:G:442:ILE:CG2  | 2.62                     | 0.47              |
| 1:G:513:LEU:HD12 | 1:G:533:MET:O    | 2.15                     | 0.47              |
| 1:G:533:MET:HB3  | 1:G:543:GLU:O    | 2.14                     | 0.47              |
| 1:A:126:LYS:NZ   | 1:A:127:ASP:CB   | 2.76                     | 0.47              |
| 1:A:140:ALA:O    | 1:A:141:LEU:HD23 | 2.15                     | 0.47              |
| 1:A:336:LYS:HB3  | 1:A:418:CYS:HA   | 1.96                     | 0.47              |
| 1:B:181:GLY:O    | 1:B:182:ALA:C    | 2.57                     | 0.47              |
| 1:B:287:LEU:HD23 | 1:B:329:TRP:CE2  | 2.49                     | 0.47              |
| 1:B:347:GLU:O    | 1:B:351:GLU:HG3  | 2.13                     | 0.47              |
| 1:B:440:LYS:O    | 1:B:443:ASP:HB2  | 2.15                     | 0.47              |
| 1:B:520:LYS:HG3  | 1:B:521:CYS:N    | 2.24                     | 0.47              |
| 1:B:536:ASN:HD22 | 1:B:536:ASN:C    | 2.21                     | 0.47              |
| 1:D:151:LYS:HG2  | 1:D:200:GLU:OE2  | 2.13                     | 0.47              |
| 1:D:268:ALA:HA   | 1:D:271:LEU:HD13 | 1.95                     | 0.47              |
| 1:E:78:TYR:CG    | 1:E:92:GLN:HG2   | 2.50                     | 0.47              |
| 1:E:146:LEU:HB2  | 1:E:147:TRP:CE2  | 2.50                     | 0.47              |
| 1:E:510:MET:HB3  | 1:E:513:LEU:HB2  | 1.96                     | 0.47              |
| 1:F:428:ILE:HD12 | 1:F:428:ILE:H    | 1.80                     | 0.47              |
| 1:F:445:LEU:HD12 | 1:F:445:LEU:O    | 2.13                     | 0.47              |
| 1:G:255:TRP:O    | 1:G:256:ASN:C    | 2.57                     | 0.47              |
| 1:G:353:LEU:HA   | 1:G:353:LEU:HD23 | 1.71                     | 0.47              |
| 1:A:442:ILE:HD11 | 1:A:492:LEU:CG   | 2.44                     | 0.47              |
| 1:A:499:ILE:HG22 | 1:A:499:ILE:O    | 2.15                     | 0.47              |
| 1:B:480:PRO:HA   | 1:B:503:GLU:OE2  | 2.15                     | 0.47              |
| 1:D:344:GLU:HB2  | 1:D:348:GLU:OE2  | 2.14                     | 0.47              |
| 1:F:314:SER:O    | 1:F:315:GLY:C    | 2.56                     | 0.47              |
| 1:F:401:GLU:CG   | 1:F:402:THR:N    | 2.77                     | 0.47              |
| 1:F:492:LEU:HD12 | 1:F:492:LEU:N    | 2.21                     | 0.47              |
| 1:G:112:ARG:HD3  | 1:G:116:GLY:O    | 2.14                     | 0.47              |
| 1:G:220:ALA:HB1  | 1:G:261:ILE:CG2  | 2.37                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:440:LYS:HE2  | 1:G:440:LYS:C    | 2.39                     | 0.47              |
| 1:G:484:THR:O    | 1:G:486:LEU:N    | 2.47                     | 0.47              |
| 1:G:486:LEU:HD22 | 1:G:487:ARG:H    | 1.79                     | 0.47              |
| 1:A:223:LEU:HD23 | 1:A:224:PRO:HD2  | 1.96                     | 0.47              |
| 1:A:482:SER:O    | 1:A:485:ASP:CB   | 2.62                     | 0.47              |
| 1:B:205:MET:HG3  | 1:B:231:ALA:HB1  | 1.95                     | 0.47              |
| 1:B:283:GLU:CG   | 1:B:283:GLU:O    | 2.62                     | 0.47              |
| 1:B:517:ARG:HB3  | 1:B:519:LEU:CD1  | 2.45                     | 0.47              |
| 1:C:81:LEU:HG    | 1:C:91:CYS:SG    | 2.54                     | 0.47              |
| 1:D:168:LEU:HD22 | 1:D:247:ASP:OD2  | 2.15                     | 0.47              |
| 1:D:413:ARG:HH21 | 1:D:457:GLY:C    | 2.22                     | 0.47              |
| 1:E:228:VAL:CG2  | 1:E:261:ILE:HD11 | 2.45                     | 0.47              |
| 1:A:152:LYS:NZ   | 1:A:256:ASN:H    | 2.13                     | 0.47              |
| 1:A:235:CYS:HB2  | 1:A:240:GLU:HG2  | 1.96                     | 0.47              |
| 1:A:248:ARG:O    | 1:A:248:ARG:HG2  | 2.14                     | 0.47              |
| 1:A:313:GLY:C    | 1:A:315:GLY:N    | 2.71                     | 0.47              |
| 1:A:445:LEU:O    | 1:A:446:MET:C    | 2.58                     | 0.47              |
| 1:A:487:ARG:O    | 1:A:493:ARG:HD3  | 2.14                     | 0.47              |
| 1:B:166:MET:HE2  | 1:B:166:MET:HB3  | 1.67                     | 0.47              |
| 1:C:153:ILE:O    | 1:C:153:ILE:HG23 | 2.14                     | 0.47              |
| 1:C:202:ILE:HD13 | 1:C:223:LEU:CD2  | 2.44                     | 0.47              |
| 1:C:419:ASP:OD2  | 1:C:419:ASP:N    | 2.47                     | 0.47              |
| 1:C:499:ILE:CG2  | 1:C:519:LEU:CB   | 2.93                     | 0.47              |
| 1:D:74:SER:HB3   | 1:D:101:VAL:CG2  | 2.45                     | 0.47              |
| 1:D:233:LEU:HD22 | 1:D:241:CYS:SG   | 2.54                     | 0.47              |
| 1:D:382:PHE:CZ   | 1:E:272:ARG:HB2  | 2.50                     | 0.47              |
| 1:D:463:ILE:CG2  | 1:D:464:CYS:N    | 2.74                     | 0.47              |
| 1:E:260:TRP:O    | 1:E:261:ILE:CG1  | 2.63                     | 0.47              |
| 1:E:315:GLY:HA2  | 1:E:317:VAL:CG2  | 2.39                     | 0.47              |
| 1:E:324:GLN:HE22 | 1:E:542:LEU:H    | 1.63                     | 0.47              |
| 1:F:163:LEU:N    | 1:F:163:LEU:HD23 | 2.30                     | 0.47              |
| 1:F:217:GLU:CD   | 1:F:261:ILE:HG22 | 2.39                     | 0.47              |
| 1:F:273:GLU:OE2  | 1:F:276:ARG:NH1  | 2.48                     | 0.47              |
| 1:G:125:ASP:OD1  | 1:G:129:ASN:HB2  | 2.15                     | 0.47              |
| 1:G:326:ALA:HB2  | 1:G:422:ILE:CD1  | 2.44                     | 0.47              |
| 1:A:169:GLN:HE22 | 1:A:254:VAL:CG1  | 2.27                     | 0.47              |
| 1:B:78:TYR:CG    | 1:B:92:GLN:HG2   | 2.49                     | 0.47              |
| 1:B:263:ASP:C    | 1:G:408:LYS:NZ   | 2.73                     | 0.47              |
| 1:B:413:ARG:NE   | 1:B:458:VAL:HB   | 2.28                     | 0.47              |
| 1:D:492:LEU:C    | 1:D:494:GLN:H    | 2.22                     | 0.47              |
| 1:D:536:ASN:ND2  | 1:D:538:GLU:HB2  | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:223:LEU:CD2  | 1:E:224:PRO:HD2  | 2.42                     | 0.47              |
| 1:F:164:THR:O    | 1:F:167:GLU:HB2  | 2.15                     | 0.47              |
| 1:F:486:LEU:HD12 | 1:F:493:ARG:HG2  | 1.97                     | 0.47              |
| 1:A:273:GLU:OE2  | 1:A:276:ARG:NH1  | 2.47                     | 0.47              |
| 1:A:446:MET:HE2  | 1:A:492:LEU:CA   | 2.43                     | 0.47              |
| 1:A:542:LEU:HD12 | 1:A:542:LEU:HA   | 1.60                     | 0.47              |
| 1:B:353:LEU:HD23 | 1:B:353:LEU:HA   | 1.69                     | 0.47              |
| 1:C:205:MET:HG3  | 1:C:231:ALA:HB1  | 1.97                     | 0.47              |
| 1:C:309:MET:HB2  | 1:C:309:MET:HE3  | 1.67                     | 0.47              |
| 1:C:486:LEU:HD12 | 1:C:493:ARG:CG   | 2.45                     | 0.47              |
| 1:D:166:MET:HE3  | 1:D:171:CYS:CB   | 2.45                     | 0.47              |
| 1:D:230:VAL:CB   | 1:D:260:TRP:NE1  | 2.78                     | 0.47              |
| 1:F:166:MET:HG2  | 1:F:175:VAL:HG21 | 1.97                     | 0.47              |
| 1:F:216:VAL:CG1  | 1:F:230:VAL:CG2  | 2.93                     | 0.47              |
| 1:F:311:THR:OG1  | 1:F:466:LEU:HD21 | 2.15                     | 0.47              |
| 1:F:322:VAL:HG11 | 1:F:422:ILE:HG21 | 1.97                     | 0.47              |
| 1:G:382:PHE:C    | 1:G:382:PHE:CD2  | 2.92                     | 0.47              |
| 1:G:451:GLY:O    | 1:G:452:PHE:C    | 2.58                     | 0.47              |
| 1:G:493:ARG:H    | 1:G:493:ARG:HG2  | 1.47                     | 0.47              |
| 1:A:322:VAL:HG21 | 1:A:463:ILE:CG1  | 2.44                     | 0.47              |
| 1:A:440:LYS:CE   | 1:A:441:MET:HA   | 2.42                     | 0.47              |
| 1:A:486:LEU:HD12 | 1:A:493:ARG:CD   | 2.45                     | 0.47              |
| 1:B:145:HIS:CE1  | 1:B:146:LEU:CD2  | 2.97                     | 0.47              |
| 1:B:168:LEU:HD11 | 1:B:250:ILE:HD12 | 1.96                     | 0.47              |
| 1:B:220:ALA:HB1  | 1:B:261:ILE:CD1  | 2.41                     | 0.47              |
| 1:C:288:LEU:HD12 | 1:C:288:LEU:H    | 1.77                     | 0.47              |
| 1:D:283:GLU:OE2  | 1:D:286:GLY:CA   | 2.60                     | 0.47              |
| 1:E:162:MET:HG2  | 1:E:175:VAL:HB   | 1.96                     | 0.47              |
| 1:E:268:ALA:HA   | 1:E:271:LEU:HD13 | 1.96                     | 0.47              |
| 1:E:372:ILE:HG13 | 1:E:378:PHE:HB2  | 1.95                     | 0.47              |
| 1:E:536:ASN:HD22 | 1:E:536:ASN:C    | 2.23                     | 0.47              |
| 1:F:151:LYS:HG2  | 1:F:200:GLU:OE2  | 2.14                     | 0.47              |
| 1:F:292:CYS:HB3  | 1:F:295:ILE:CG1  | 2.45                     | 0.47              |
| 1:F:362:LEU:HD12 | 1:F:362:LEU:C    | 2.40                     | 0.47              |
| 1:F:518:ILE:HD13 | 1:F:518:ILE:HA   | 1.79                     | 0.47              |
| 1:G:81:LEU:HG    | 1:G:91:CYS:SG    | 2.54                     | 0.47              |
| 1:A:246:HIS:HB3  | 1:A:249:GLU:OE1  | 2.14                     | 0.46              |
| 1:A:288:LEU:HD12 | 1:A:288:LEU:H    | 1.80                     | 0.46              |
| 1:B:166:MET:HE3  | 1:B:171:CYS:CA   | 2.45                     | 0.46              |
| 1:C:78:TYR:CG    | 1:C:92:GLN:HG2   | 2.49                     | 0.46              |
| 1:C:79:SER:H     | 1:C:98:ILE:CD1   | 2.28                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:326:ALA:HB2  | 1:E:422:ILE:CD1  | 2.45                     | 0.46              |
| 1:E:327:LEU:HA   | 1:E:327:LEU:HD23 | 1.44                     | 0.46              |
| 1:E:369:LYS:HG2  | 1:F:279:LEU:HD22 | 1.97                     | 0.46              |
| 1:E:478:GLY:O    | 1:E:479:ARG:C    | 2.58                     | 0.46              |
| 1:F:124:ARG:HD3  | 1:F:125:ASP:CA   | 2.45                     | 0.46              |
| 1:F:345:SER:O    | 1:F:349:THR:CG2  | 2.63                     | 0.46              |
| 1:F:375:ASN:CG   | 1:F:377:LYS:HG3  | 2.40                     | 0.46              |
| 1:A:412:MET:HE3  | 1:A:412:MET:HB3  | 1.79                     | 0.46              |
| 1:A:414:SER:CB   | 1:C:226:GLY:N    | 2.76                     | 0.46              |
| 1:C:246:HIS:HB3  | 1:C:249:GLU:OE1  | 2.14                     | 0.46              |
| 1:C:307:VAL:O    | 1:C:307:VAL:HG12 | 2.14                     | 0.46              |
| 1:D:450:LYS:HA   | 1:D:450:LYS:HD2  | 1.69                     | 0.46              |
| 1:E:344:GLU:CG   | 1:E:349:THR:HG22 | 2.40                     | 0.46              |
| 1:F:312:SER:CB   | 1:F:502:LEU:O    | 2.54                     | 0.46              |
| 1:F:353:LEU:HD23 | 1:F:353:LEU:HA   | 1.65                     | 0.46              |
| 1:F:510:MET:HB3  | 1:F:513:LEU:HB2  | 1.97                     | 0.46              |
| 1:G:205:MET:HE1  | 1:G:250:ILE:HG23 | 1.97                     | 0.46              |
| 1:G:253:GLN:O    | 1:G:257:ALA:HB2  | 2.16                     | 0.46              |
| 1:G:322:VAL:HG21 | 1:G:463:ILE:CD1  | 2.43                     | 0.46              |
| 1:G:496:SER:CB   | 1:G:499:ILE:HD11 | 2.45                     | 0.46              |
| 1:A:486:LEU:HD13 | 1:A:487:ARG:O    | 2.15                     | 0.46              |
| 1:B:114:GLN:HG3  | 1:B:144:LYS:HE2  | 1.97                     | 0.46              |
| 1:B:267:SER:O    | 1:B:270:SER:OG   | 2.31                     | 0.46              |
| 1:B:443:ASP:HA   | 1:B:491:ALA:HB3  | 1.97                     | 0.46              |
| 1:C:86:ILE:HG21  | 1:C:163:LEU:CD1  | 2.45                     | 0.46              |
| 1:E:168:LEU:HD22 | 1:E:247:ASP:OD2  | 2.12                     | 0.46              |
| 1:E:413:ARG:HH21 | 1:E:458:VAL:N    | 2.13                     | 0.46              |
| 1:F:205:MET:HG3  | 1:F:231:ALA:HB1  | 1.97                     | 0.46              |
| 1:F:229:ARG:HB3  | 1:F:258:GLY:O    | 2.14                     | 0.46              |
| 1:F:326:ALA:HB2  | 1:F:422:ILE:HD12 | 1.97                     | 0.46              |
| 1:F:344:GLU:OE1  | 1:F:349:THR:HB   | 2.15                     | 0.46              |
| 1:F:397:PHE:C    | 1:F:397:PHE:HD1  | 2.22                     | 0.46              |
| 1:G:220:ALA:HB1  | 1:G:261:ILE:HD13 | 1.96                     | 0.46              |
| 1:G:300:LEU:HB3  | 1:G:303:ARG:NH1  | 2.29                     | 0.46              |
| 1:G:429:VAL:HG13 | 1:G:438:GLU:OE1  | 2.15                     | 0.46              |
| 1:G:482:SER:H    | 1:G:485:ASP:CB   | 2.19                     | 0.46              |
| 1:A:536:ASN:OD1  | 1:A:539:THR:HG23 | 2.15                     | 0.46              |
| 1:B:142:PHE:CD2  | 1:B:162:MET:HE3  | 2.50                     | 0.46              |
| 1:B:412:MET:HE2  | 1:B:421:ILE:HD13 | 1.94                     | 0.46              |
| 1:C:513:LEU:HD12 | 1:C:533:MET:O    | 2.16                     | 0.46              |
| 1:E:313:GLY:O    | 1:E:315:GLY:N    | 2.48                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:316:MET:O    | 1:E:319:SER:N    | 2.48                     | 0.46              |
| 1:F:427:SER:HB3  | 1:F:487:ARG:NH1  | 2.29                     | 0.46              |
| 1:F:536:ASN:HD22 | 1:F:536:ASN:C    | 2.22                     | 0.46              |
| 1:G:136:HIS:CD2  | 1:G:180:HIS:CE1  | 3.03                     | 0.46              |
| 1:G:304:GLY:HA2  | 1:G:459:VAL:HG22 | 1.96                     | 0.46              |
| 1:A:160:ILE:O    | 1:A:163:LEU:HB2  | 2.16                     | 0.46              |
| 1:B:394:TYR:HE1  | 1:B:396:SER:CB   | 2.26                     | 0.46              |
| 1:E:295:ILE:HD12 | 1:E:516:VAL:HG11 | 1.98                     | 0.46              |
| 1:E:353:LEU:HD23 | 1:E:353:LEU:HA   | 1.65                     | 0.46              |
| 1:E:406:LEU:HD21 | 1:E:449:LEU:HD23 | 1.98                     | 0.46              |
| 1:F:311:THR:O    | 1:F:312:SER:CB   | 2.59                     | 0.46              |
| 1:F:486:LEU:HD13 | 1:F:487:ARG:O    | 2.15                     | 0.46              |
| 1:F:512:ASN:HD21 | 1:F:537:LYS:HE3  | 1.79                     | 0.46              |
| 1:G:404:ARG:O    | 1:G:408:LYS:HG2  | 2.16                     | 0.46              |
| 1:A:241:CYS:HB2  | 1:A:250:ILE:HD11 | 1.97                     | 0.46              |
| 1:A:322:VAL:HG21 | 1:A:463:ILE:CD1  | 2.46                     | 0.46              |
| 1:B:300:LEU:O    | 1:B:300:LEU:CD1  | 2.64                     | 0.46              |
| 1:B:309:MET:CE   | 1:B:462:VAL:HG12 | 2.44                     | 0.46              |
| 1:B:498:THR:C    | 1:B:499:ILE:HD13 | 2.40                     | 0.46              |
| 1:C:339:LEU:CB   | 1:C:341:MET:HE1  | 2.44                     | 0.46              |
| 1:C:473:LYS:CD   | 1:C:479:ARG:HB2  | 2.46                     | 0.46              |
| 1:D:162:MET:HG2  | 1:D:175:VAL:HB   | 1.98                     | 0.46              |
| 1:D:205:MET:SD   | 1:D:238:ALA:HB2  | 2.56                     | 0.46              |
| 1:D:401:GLU:N    | 1:D:404:ARG:HD2  | 2.31                     | 0.46              |
| 1:F:79:SER:H     | 1:F:98:ILE:CD1   | 2.27                     | 0.46              |
| 1:G:114:GLN:HG3  | 1:G:144:LYS:HE2  | 1.98                     | 0.46              |
| 1:G:234:PRO:HG2  | 1:G:249:GLU:HG2  | 1.98                     | 0.46              |
| 1:G:486:LEU:HD13 | 1:G:487:ARG:O    | 2.15                     | 0.46              |
| 1:A:124:ARG:CD   | 1:A:125:ASP:C    | 2.86                     | 0.46              |
| 1:A:168:LEU:CD1  | 1:A:251:MET:HE1  | 2.42                     | 0.46              |
| 1:A:443:ASP:HA   | 1:A:491:ALA:HB3  | 1.97                     | 0.46              |
| 1:B:492:LEU:C    | 1:B:494:GLN:H    | 2.24                     | 0.46              |
| 1:D:125:ASP:OD1  | 1:D:129:ASN:HB2  | 2.15                     | 0.46              |
| 1:D:166:MET:HE2  | 1:D:166:MET:HB3  | 1.61                     | 0.46              |
| 1:D:276:ARG:HH11 | 1:D:276:ARG:CG   | 2.29                     | 0.46              |
| 1:D:442:ILE:HD11 | 1:D:492:LEU:CG   | 2.46                     | 0.46              |
| 1:E:205:MET:HG3  | 1:E:231:ALA:HB1  | 1.97                     | 0.46              |
| 1:E:322:VAL:CG1  | 1:E:422:ILE:HG21 | 2.45                     | 0.46              |
| 1:E:402:THR:HG23 | 1:E:403:ASP:H    | 1.80                     | 0.46              |
| 1:E:487:ARG:O    | 1:E:493:ARG:HD3  | 2.15                     | 0.46              |
| 1:F:170:ASP:O    | 1:F:172:LYS:HG3  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:311:THR:O    | 1:G:502:LEU:HD12 | 2.16                     | 0.46              |
| 1:G:327:LEU:HD23 | 1:G:327:LEU:HA   | 1.55                     | 0.46              |
| 1:A:152:LYS:O    | 1:A:174:PRO:HD2  | 2.16                     | 0.46              |
| 1:A:154:VAL:HB   | 1:A:175:VAL:CG1  | 2.43                     | 0.46              |
| 1:B:289:PHE:H    | 1:B:296:ASN:ND2  | 2.04                     | 0.46              |
| 1:B:504:ARG:HH21 | 1:B:506:GLN:CG   | 2.29                     | 0.46              |
| 1:C:327:LEU:HD11 | 1:C:357:HIS:HA   | 1.98                     | 0.46              |
| 1:C:425:HIS:HE1  | 1:C:427:SER:CB   | 2.27                     | 0.46              |
| 1:D:140:ALA:O    | 1:D:141:LEU:HD23 | 2.15                     | 0.46              |
| 1:D:412:MET:HE3  | 1:D:412:MET:HB3  | 1.79                     | 0.46              |
| 1:E:260:TRP:C    | 1:E:261:ILE:CG1  | 2.88                     | 0.46              |
| 1:E:351:GLU:HB2  | 1:E:363:ARG:HD2  | 1.98                     | 0.46              |
| 1:F:213:ARG:NE   | 1:F:213:ARG:HA   | 2.30                     | 0.46              |
| 1:F:451:GLY:O    | 1:F:455:SER:HB3  | 2.16                     | 0.46              |
| 1:F:467:LYS:H    | 1:F:467:LYS:HG3  | 1.50                     | 0.46              |
| 1:G:205:MET:HG3  | 1:G:231:ALA:HB1  | 1.98                     | 0.46              |
| 1:G:276:ARG:O    | 1:G:277:GLU:C    | 2.58                     | 0.46              |
| 1:G:294:GLY:C    | 1:G:296:ASN:N    | 2.74                     | 0.46              |
| 1:A:411:TYR:CD1  | 1:A:411:TYR:C    | 2.92                     | 0.46              |
| 1:A:488:GLY:HA3  | 1:A:492:LEU:CD1  | 2.42                     | 0.46              |
| 1:B:442:ILE:HD11 | 1:B:492:LEU:CD2  | 2.45                     | 0.46              |
| 1:C:312:SER:O    | 1:C:313:GLY:O    | 2.34                     | 0.46              |
| 1:D:324:GLN:HE22 | 1:D:542:LEU:H    | 1.63                     | 0.46              |
| 1:E:450:LYS:HD2  | 1:E:450:LYS:HA   | 1.68                     | 0.46              |
| 1:F:80:ALA:HB2   | 1:F:88:LYS:HB2   | 1.97                     | 0.46              |
| 1:F:223:LEU:CD2  | 1:F:224:PRO:HD2  | 2.46                     | 0.46              |
| 1:F:351:GLU:HB2  | 1:F:363:ARG:HD2  | 1.98                     | 0.46              |
| 1:G:228:VAL:HB   | 1:G:261:ILE:HD13 | 1.97                     | 0.46              |
| 1:A:146:LEU:HB2  | 1:A:147:TRP:CE2  | 2.51                     | 0.46              |
| 1:B:510:MET:HB2  | 1:B:513:LEU:CB   | 2.46                     | 0.46              |
| 1:C:241:CYS:HB2  | 1:C:250:ILE:HD11 | 1.98                     | 0.46              |
| 1:D:217:GLU:OE2  | 1:D:261:ILE:C    | 2.59                     | 0.46              |
| 1:D:446:MET:CE   | 1:D:492:LEU:HA   | 2.45                     | 0.46              |
| 1:D:478:GLY:O    | 1:D:479:ARG:C    | 2.59                     | 0.46              |
| 1:E:166:MET:HE3  | 1:E:171:CYS:CB   | 2.45                     | 0.46              |
| 1:F:248:ARG:O    | 1:F:248:ARG:HG2  | 2.15                     | 0.46              |
| 1:F:503:GLU:CD   | 1:F:517:ARG:HE   | 2.24                     | 0.46              |
| 1:F:510:MET:CB   | 1:F:513:LEU:HB2  | 2.45                     | 0.46              |
| 1:G:81:LEU:HD11  | 1:G:96:TYR:CD2   | 2.51                     | 0.46              |
| 1:G:440:LYS:CE   | 1:G:441:MET:HA   | 2.43                     | 0.46              |
| 1:G:446:MET:CE   | 1:G:492:LEU:HA   | 2.46                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:360:VAL:O    | 1:A:360:VAL:HG23 | 2.16                     | 0.45              |
| 1:A:531:GLY:C    | 1:A:532:TYR:CD1  | 2.94                     | 0.45              |
| 1:B:401:GLU:CG   | 1:B:402:THR:H    | 2.29                     | 0.45              |
| 1:B:406:LEU:HD21 | 1:B:449:LEU:HD23 | 1.97                     | 0.45              |
| 1:C:80:ALA:HB2   | 1:C:88:LYS:HB2   | 1.98                     | 0.45              |
| 1:C:180:HIS:HB2  | 1:C:184:ALA:HB3  | 1.98                     | 0.45              |
| 1:C:223:LEU:CD2  | 1:C:224:PRO:HD2  | 2.46                     | 0.45              |
| 1:C:251:MET:HE3  | 1:C:251:MET:N    | 2.31                     | 0.45              |
| 1:C:476:GLU:HB3  | 1:C:506:GLN:OE1  | 2.16                     | 0.45              |
| 1:D:216:VAL:CG1  | 1:D:230:VAL:HG22 | 2.45                     | 0.45              |
| 1:D:312:SER:H    | 1:D:318:MET:HE2  | 1.77                     | 0.45              |
| 1:D:471:LYS:HA   | 1:D:471:LYS:HD2  | 1.60                     | 0.45              |
| 1:F:402:THR:HG23 | 1:F:403:ASP:H    | 1.81                     | 0.45              |
| 1:B:517:ARG:CZ   | 1:B:529:ILE:HD11 | 2.46                     | 0.45              |
| 1:C:234:PRO:HG2  | 1:C:249:GLU:HG2  | 1.98                     | 0.45              |
| 1:C:454:LYS:HE3  | 1:C:522:ARG:HH22 | 1.82                     | 0.45              |
| 1:D:148:ASN:HD22 | 1:D:198:GLN:HE22 | 1.63                     | 0.45              |
| 1:E:205:MET:HE1  | 1:E:250:ILE:HG23 | 1.97                     | 0.45              |
| 1:E:303:ARG:HB2  | 1:E:306:GLU:CD   | 2.42                     | 0.45              |
| 1:E:309:MET:HE3  | 1:E:309:MET:HB2  | 1.63                     | 0.45              |
| 1:F:327:LEU:HD23 | 1:F:327:LEU:HA   | 1.55                     | 0.45              |
| 1:G:269:LEU:HA   | 1:G:269:LEU:HD13 | 1.48                     | 0.45              |
| 1:A:94:ALA:CB    | 1:A:162:MET:HE1  | 2.45                     | 0.45              |
| 1:A:153:ILE:HG23 | 1:A:153:ILE:O    | 2.16                     | 0.45              |
| 1:A:193:TYR:CE1  | 1:A:224:PRO:HA   | 2.51                     | 0.45              |
| 1:B:112:ARG:NH2  | 1:B:118:ILE:HD11 | 2.31                     | 0.45              |
| 1:B:401:GLU:CG   | 1:B:431:SER:O    | 2.64                     | 0.45              |
| 1:C:251:MET:CE   | 1:C:251:MET:CA   | 2.92                     | 0.45              |
| 1:C:327:LEU:HA   | 1:C:327:LEU:HD23 | 1.59                     | 0.45              |
| 1:C:402:THR:HG23 | 1:C:403:ASP:N    | 2.31                     | 0.45              |
| 1:D:193:TYR:CE1  | 1:D:224:PRO:HA   | 2.52                     | 0.45              |
| 1:D:346:VAL:HG13 | 1:E:271:LEU:CD2  | 2.47                     | 0.45              |
| 1:D:427:SER:CB   | 1:D:487:ARG:HH12 | 2.22                     | 0.45              |
| 1:D:443:ASP:HA   | 1:D:491:ALA:CB   | 2.47                     | 0.45              |
| 1:F:124:ARG:HD3  | 1:F:125:ASP:N    | 2.31                     | 0.45              |
| 1:G:447:THR:O    | 1:G:448:LYS:C    | 2.60                     | 0.45              |
| 1:G:506:GLN:H    | 1:G:506:GLN:HG3  | 1.56                     | 0.45              |
| 1:G:517:ARG:HB3  | 1:G:519:LEU:HD13 | 1.96                     | 0.45              |
| 1:A:439:ARG:O    | 1:A:442:ILE:CG2  | 2.62                     | 0.45              |
| 1:A:450:LYS:HA   | 1:A:450:LYS:HD2  | 1.61                     | 0.45              |
| 1:A:491:ALA:O    | 1:A:495:LEU:N    | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:232:VAL:O    | 1:B:232:VAL:HG12 | 2.14                     | 0.45              |
| 1:B:486:LEU:HD12 | 1:B:493:ARG:CG   | 2.47                     | 0.45              |
| 1:C:446:MET:HE2  | 1:C:492:LEU:HA   | 1.97                     | 0.45              |
| 1:C:532:TYR:N    | 1:C:532:TYR:HD1  | 2.14                     | 0.45              |
| 1:C:536:ASN:C    | 1:C:538:GLU:N    | 2.73                     | 0.45              |
| 1:D:267:SER:O    | 1:D:271:LEU:HD12 | 2.17                     | 0.45              |
| 1:D:307:VAL:O    | 1:D:307:VAL:CG1  | 2.64                     | 0.45              |
| 1:D:510:MET:HE2  | 1:D:547:TYR:CE1  | 2.47                     | 0.45              |
| 1:E:193:TYR:CE1  | 1:E:224:PRO:HA   | 2.52                     | 0.45              |
| 1:F:440:LYS:NZ   | 1:F:441:MET:CA   | 2.60                     | 0.45              |
| 1:G:112:ARG:HD2  | 1:G:145:HIS:CE1  | 2.51                     | 0.45              |
| 1:G:142:PHE:CD2  | 1:G:162:MET:HE3  | 2.52                     | 0.45              |
| 1:G:321:PHE:CE2  | 1:G:533:MET:HE1  | 2.46                     | 0.45              |
| 1:A:359:ARG:HD3  | 1:A:541:TRP:HE1  | 1.80                     | 0.45              |
| 1:B:265:VAL:HG11 | 1:G:411:TYR:CE1  | 2.52                     | 0.45              |
| 1:B:311:THR:OG1  | 1:B:466:LEU:HD21 | 2.16                     | 0.45              |
| 1:B:492:LEU:HD12 | 1:B:492:LEU:N    | 2.16                     | 0.45              |
| 1:C:124:ARG:HD3  | 1:C:125:ASP:N    | 2.32                     | 0.45              |
| 1:C:492:LEU:C    | 1:C:494:GLN:N    | 2.73                     | 0.45              |
| 1:C:496:SER:O    | 1:C:520:LYS:CE   | 2.63                     | 0.45              |
| 1:D:502:LEU:N    | 1:D:502:LEU:HD12 | 2.31                     | 0.45              |
| 1:D:536:ASN:OD1  | 1:D:539:THR:HG23 | 2.17                     | 0.45              |
| 1:E:220:ALA:HB1  | 1:E:261:ILE:HG21 | 1.87                     | 0.45              |
| 1:E:248:ARG:HG2  | 1:E:248:ARG:O    | 2.16                     | 0.45              |
| 1:E:345:SER:O    | 1:E:349:THR:HG22 | 2.16                     | 0.45              |
| 1:E:356:LEU:HD12 | 1:E:541:TRP:NE1  | 2.32                     | 0.45              |
| 1:E:482:SER:CB   | 1:E:484:THR:HG23 | 2.46                     | 0.45              |
| 1:F:267:SER:O    | 1:F:271:LEU:HD12 | 2.16                     | 0.45              |
| 1:F:389:ASP:H    | 1:G:269:LEU:CD2  | 2.29                     | 0.45              |
| 1:F:504:ARG:HH21 | 1:F:506:GLN:HG2  | 1.82                     | 0.45              |
| 1:G:122:LYS:HE3  | 1:G:130:PHE:CE2  | 2.52                     | 0.45              |
| 1:A:289:PHE:HA   | 1:A:325:GLN:HE21 | 1.82                     | 0.45              |
| 1:A:478:GLY:O    | 1:A:479:ARG:C    | 2.60                     | 0.45              |
| 1:C:366:ASP:HB2  | 1:D:284:SER:HG   | 1.80                     | 0.45              |
| 1:C:450:LYS:O    | 1:C:453:ALA:HB3  | 2.16                     | 0.45              |
| 1:C:467:LYS:H    | 1:C:467:LYS:HG3  | 1.36                     | 0.45              |
| 1:D:292:CYS:O    | 1:D:293:THR:C    | 2.60                     | 0.45              |
| 1:E:142:PHE:CD2  | 1:E:162:MET:HE3  | 2.51                     | 0.45              |
| 1:E:194:GLU:CD   | 1:E:194:GLU:N    | 2.72                     | 0.45              |
| 1:E:288:LEU:HD12 | 1:E:288:LEU:N    | 2.31                     | 0.45              |
| 1:E:371:GLU:OE1  | 1:E:375:ASN:ND2  | 2.49                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:401:GLU:CB   | 1:E:431:SER:O    | 2.65                     | 0.45              |
| 1:F:515:LEU:HD21 | 1:F:529:ILE:HD12 | 1.95                     | 0.45              |
| 1:G:261:ILE:N    | 1:G:262:PRO:HD2  | 2.30                     | 0.45              |
| 1:A:126:LYS:CE   | 1:A:127:ASP:CG   | 2.90                     | 0.45              |
| 1:A:265:VAL:C    | 1:A:266:VAL:HG23 | 2.41                     | 0.45              |
| 1:A:267:SER:CB   | 1:B:392:HIS:ND1  | 2.80                     | 0.45              |
| 1:A:483:ILE:O    | 1:A:486:LEU:CB   | 2.41                     | 0.45              |
| 1:B:359:ARG:HD3  | 1:B:541:TRP:HE1  | 1.81                     | 0.45              |
| 1:C:294:GLY:O    | 1:C:296:ASN:N    | 2.49                     | 0.45              |
| 1:C:473:LYS:HE2  | 1:C:479:ARG:CB   | 2.46                     | 0.45              |
| 1:C:518:ILE:HD13 | 1:C:518:ILE:HA   | 1.76                     | 0.45              |
| 1:D:246:HIS:HB3  | 1:D:249:GLU:OE1  | 2.17                     | 0.45              |
| 1:D:410:ALA:HA   | 1:D:452:PHE:CE1  | 2.51                     | 0.45              |
| 1:D:536:ASN:C    | 1:D:538:GLU:N    | 2.75                     | 0.45              |
| 1:E:300:LEU:HB3  | 1:E:303:ARG:NH1  | 2.32                     | 0.45              |
| 1:E:320:THR:HG22 | 1:E:324:GLN:HE21 | 1.82                     | 0.45              |
| 1:E:344:GLU:OE1  | 1:E:349:THR:HB   | 2.16                     | 0.45              |
| 1:G:248:ARG:O    | 1:G:248:ARG:HG2  | 2.15                     | 0.45              |
| 1:G:324:GLN:NE2  | 1:G:542:LEU:H    | 2.14                     | 0.45              |
| 1:G:339:LEU:HB3  | 1:G:341:MET:HE1  | 1.94                     | 0.45              |
| 1:G:486:LEU:HD12 | 1:G:493:ARG:CG   | 2.47                     | 0.45              |
| 1:A:166:MET:C    | 1:A:171:CYS:HB3  | 2.42                     | 0.45              |
| 1:A:294:GLY:C    | 1:A:296:ASN:N    | 2.72                     | 0.45              |
| 1:A:338:GLY:CA   | 1:A:412:MET:HE1  | 2.46                     | 0.45              |
| 1:A:446:MET:HB3  | 1:A:491:ALA:HB1  | 1.99                     | 0.45              |
| 1:B:318:MET:HE1  | 1:B:465:HIS:CD2  | 2.50                     | 0.45              |
| 1:B:450:LYS:HE3  | 1:B:454:LYS:CD   | 2.45                     | 0.45              |
| 1:D:234:PRO:CG   | 1:D:249:GLU:HG2  | 2.47                     | 0.45              |
| 1:D:510:MET:HB2  | 1:D:513:LEU:HB3  | 1.98                     | 0.45              |
| 1:E:229:ARG:HB3  | 1:E:259:PRO:CB   | 2.46                     | 0.45              |
| 1:E:548:SER:HB3  | 1:E:549:GLY:H    | 1.61                     | 0.45              |
| 1:F:276:ARG:HH11 | 1:F:276:ARG:CG   | 2.28                     | 0.45              |
| 1:F:504:ARG:HH21 | 1:F:506:GLN:CG   | 2.30                     | 0.45              |
| 1:A:413:ARG:O    | 1:A:413:ARG:HD2  | 2.17                     | 0.45              |
| 1:A:492:LEU:HD12 | 1:A:492:LEU:N    | 2.21                     | 0.45              |
| 1:C:243:LEU:O    | 1:C:244:ASN:O    | 2.35                     | 0.45              |
| 1:C:258:GLY:HA2  | 1:C:259:PRO:HD3  | 1.78                     | 0.45              |
| 1:C:401:GLU:OE2  | 1:C:432:ALA:HB2  | 2.17                     | 0.45              |
| 1:C:510:MET:HE2  | 1:C:547:TYR:CE1  | 2.50                     | 0.45              |
| 1:D:230:VAL:CG1  | 1:D:260:TRP:NE1  | 2.80                     | 0.45              |
| 1:E:145:HIS:CE1  | 1:E:146:LEU:HD23 | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:243:LEU:O    | 1:F:244:ASN:O    | 2.34                     | 0.45              |
| 1:F:288:LEU:N    | 1:F:288:LEU:HD12 | 2.32                     | 0.45              |
| 1:G:286:GLY:O    | 1:G:302:ALA:N    | 2.49                     | 0.45              |
| 1:G:473:LYS:HE2  | 1:G:479:ARG:CA   | 2.46                     | 0.45              |
| 1:A:194:GLU:CD   | 1:A:194:GLU:N    | 2.71                     | 0.45              |
| 1:A:292:CYS:HB3  | 1:A:295:ILE:CG1  | 2.47                     | 0.45              |
| 1:A:450:LYS:HE2  | 1:A:454:LYS:CD   | 2.30                     | 0.45              |
| 1:A:479:ARG:HA   | 1:A:480:PRO:HD3  | 1.85                     | 0.45              |
| 1:C:114:GLN:HG3  | 1:C:144:LYS:HE2  | 1.99                     | 0.45              |
| 1:C:364:GLN:HG3  | 1:D:523:PHE:CZ   | 2.52                     | 0.45              |
| 1:C:478:GLY:O    | 1:C:479:ARG:C    | 2.60                     | 0.45              |
| 1:D:166:MET:HG2  | 1:D:175:VAL:HG23 | 1.99                     | 0.45              |
| 1:D:493:ARG:H    | 1:D:493:ARG:HG2  | 1.40                     | 0.45              |
| 1:E:447:THR:CG2  | 1:E:495:LEU:HD21 | 2.31                     | 0.45              |
| 1:E:493:ARG:H    | 1:E:493:ARG:HG2  | 1.41                     | 0.45              |
| 1:E:510:MET:HB2  | 1:E:513:LEU:HB3  | 1.98                     | 0.45              |
| 1:E:542:LEU:HA   | 1:E:542:LEU:HD12 | 1.56                     | 0.45              |
| 1:F:124:ARG:C    | 1:F:124:ARG:CD   | 2.90                     | 0.45              |
| 1:G:427:SER:CB   | 1:G:487:ARG:HH12 | 2.26                     | 0.45              |
| 1:A:106:TYR:HB3  | 1:A:123:VAL:HG12 | 1.99                     | 0.44              |
| 1:A:130:PHE:O    | 1:A:131:LYS:CG   | 2.64                     | 0.44              |
| 1:A:486:LEU:HD22 | 1:A:487:ARG:H    | 1.83                     | 0.44              |
| 1:A:515:LEU:HD21 | 1:A:529:ILE:HD12 | 1.99                     | 0.44              |
| 1:B:510:MET:CB   | 1:B:513:LEU:HB2  | 2.46                     | 0.44              |
| 1:C:346:VAL:HG23 | 1:C:393:LEU:HB2  | 1.99                     | 0.44              |
| 1:C:504:ARG:HH21 | 1:C:506:GLN:CG   | 2.29                     | 0.44              |
| 1:D:499:ILE:HG22 | 1:D:499:ILE:O    | 2.17                     | 0.44              |
| 1:D:506:GLN:H    | 1:D:506:GLN:HG3  | 1.49                     | 0.44              |
| 1:F:425:HIS:HE1  | 1:F:427:SER:HB2  | 1.60                     | 0.44              |
| 1:F:533:MET:HB3  | 1:F:543:GLU:O    | 2.17                     | 0.44              |
| 1:F:536:ASN:ND2  | 1:F:538:GLU:CB   | 2.80                     | 0.44              |
| 1:G:223:LEU:CD2  | 1:G:224:PRO:HD2  | 2.47                     | 0.44              |
| 1:A:138:SER:HB3  | 1:A:187:LYS:HD3  | 1.99                     | 0.44              |
| 1:A:255:TRP:O    | 1:A:256:ASN:CG   | 2.60                     | 0.44              |
| 1:B:496:SER:CB   | 1:B:499:ILE:HD11 | 2.47                     | 0.44              |
| 1:C:427:SER:CB   | 1:C:487:ARG:HH12 | 2.30                     | 0.44              |
| 1:D:303:ARG:CZ   | 1:D:523:PHE:CD1  | 3.00                     | 0.44              |
| 1:D:496:SER:O    | 1:D:520:LYS:CE   | 2.65                     | 0.44              |
| 1:E:185:ALA:O    | 1:E:189:CYS:HB2  | 2.17                     | 0.44              |
| 1:E:276:ARG:CG   | 1:E:276:ARG:NH1  | 2.76                     | 0.44              |
| 1:E:484:THR:O    | 1:E:486:LEU:N    | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:235:CYS:CB   | 1:F:240:GLU:HG2  | 2.46                     | 0.44              |
| 1:F:491:ALA:O    | 1:F:495:LEU:N    | 2.48                     | 0.44              |
| 1:F:496:SER:O    | 1:F:520:LYS:CE   | 2.65                     | 0.44              |
| 1:G:439:ARG:HG2  | 1:G:489:SER:OG   | 2.16                     | 0.44              |
| 1:G:503:GLU:CD   | 1:G:517:ARG:HE   | 2.25                     | 0.44              |
| 1:A:77:ARG:HE    | 1:A:77:ARG:HB2   | 1.60                     | 0.44              |
| 1:A:320:THR:HG22 | 1:A:324:GLN:NE2  | 2.32                     | 0.44              |
| 1:A:392:HIS:ND1  | 1:C:267:SER:HB2  | 2.32                     | 0.44              |
| 1:C:412:MET:CE   | 1:C:421:ILE:HD13 | 2.42                     | 0.44              |
| 1:C:482:SER:CB   | 1:C:484:THR:HG23 | 2.47                     | 0.44              |
| 1:D:401:GLU:HB2  | 1:D:404:ARG:NH2  | 2.32                     | 0.44              |
| 1:F:74:SER:HB3   | 1:F:101:VAL:CG2  | 2.47                     | 0.44              |
| 1:F:510:MET:HB2  | 1:F:513:LEU:HB3  | 1.98                     | 0.44              |
| 1:F:516:VAL:HG23 | 1:F:531:GLY:O    | 2.17                     | 0.44              |
| 1:G:443:ASP:HA   | 1:G:491:ALA:HB3  | 1.99                     | 0.44              |
| 1:A:121:GLN:CB   | 1:A:133:THR:HG23 | 2.48                     | 0.44              |
| 1:A:220:ALA:HB1  | 1:A:261:ILE:CG2  | 2.47                     | 0.44              |
| 1:A:313:GLY:C    | 1:A:315:GLY:H    | 2.25                     | 0.44              |
| 1:A:510:MET:HB2  | 1:A:513:LEU:CB   | 2.47                     | 0.44              |
| 1:C:316:MET:CE   | 1:C:535:TYR:CZ   | 2.98                     | 0.44              |
| 1:C:362:LEU:O    | 1:C:362:LEU:HD12 | 2.17                     | 0.44              |
| 1:D:321:PHE:CD2  | 1:D:533:MET:CE   | 2.81                     | 0.44              |
| 1:D:510:MET:CB   | 1:D:513:LEU:HB2  | 2.47                     | 0.44              |
| 1:D:513:LEU:HD11 | 1:D:532:TYR:HB3  | 1.99                     | 0.44              |
| 1:E:271:LEU:O    | 1:E:272:ARG:C    | 2.60                     | 0.44              |
| 1:E:503:GLU:CD   | 1:E:517:ARG:HE   | 2.26                     | 0.44              |
| 1:F:106:TYR:N    | 1:F:106:TYR:CD1  | 2.85                     | 0.44              |
| 1:F:107:GLN:H    | 1:F:124:ARG:HG3  | 1.82                     | 0.44              |
| 1:F:209:ASP:O    | 1:F:210:GLU:C    | 2.61                     | 0.44              |
| 1:F:234:PRO:CG   | 1:F:249:GLU:HG2  | 2.48                     | 0.44              |
| 1:F:404:ARG:O    | 1:F:408:LYS:HG2  | 2.16                     | 0.44              |
| 1:F:532:TYR:CD1  | 1:F:532:TYR:N    | 2.85                     | 0.44              |
| 1:B:136:HIS:CD2  | 1:B:180:HIS:CE1  | 3.06                     | 0.44              |
| 1:B:493:ARG:H    | 1:B:493:ARG:HG2  | 1.43                     | 0.44              |
| 1:B:510:MET:HB2  | 1:B:513:LEU:HB3  | 2.00                     | 0.44              |
| 1:C:220:ALA:HB3  | 1:C:261:ILE:HG21 | 2.00                     | 0.44              |
| 1:C:339:LEU:HB3  | 1:C:341:MET:HE2  | 1.88                     | 0.44              |
| 1:C:394:TYR:C    | 1:C:394:TYR:HD1  | 2.25                     | 0.44              |
| 1:C:441:MET:O    | 1:C:442:ILE:C    | 2.61                     | 0.44              |
| 1:D:78:TYR:O     | 1:D:88:LYS:HG3   | 2.17                     | 0.44              |
| 1:E:408:LYS:O    | 1:E:412:MET:HG3  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:446:MET:HE2  | 1:E:492:LEU:HA   | 1.98                     | 0.44              |
| 1:F:437:ASP:CG   | 1:F:439:ARG:HB2  | 2.43                     | 0.44              |
| 1:F:510:MET:HB2  | 1:F:513:LEU:CB   | 2.47                     | 0.44              |
| 1:G:185:ALA:O    | 1:G:189:CYS:HB2  | 2.18                     | 0.44              |
| 1:G:401:GLU:HB3  | 1:G:404:ARG:HB3  | 2.00                     | 0.44              |
| 1:A:100:LYS:HD3  | 1:A:105:MET:HB2  | 1.99                     | 0.44              |
| 1:A:202:ILE:HD13 | 1:A:223:LEU:HD22 | 2.00                     | 0.44              |
| 1:A:440:LYS:O    | 1:A:443:ASP:HB2  | 2.17                     | 0.44              |
| 1:A:546:SER:O    | 1:A:547:TYR:HB2  | 2.17                     | 0.44              |
| 1:B:180:HIS:CD2  | 1:B:180:HIS:N    | 2.85                     | 0.44              |
| 1:B:536:ASN:ND2  | 1:B:538:GLU:HB3  | 2.32                     | 0.44              |
| 1:C:441:MET:HE2  | 1:C:441:MET:C    | 2.38                     | 0.44              |
| 1:C:517:ARG:HB3  | 1:C:519:LEU:HD13 | 1.99                     | 0.44              |
| 1:D:204:LEU:HD13 | 1:D:206:PHE:CZ   | 2.53                     | 0.44              |
| 1:D:532:TYR:CD1  | 1:D:532:TYR:N    | 2.85                     | 0.44              |
| 1:E:79:SER:H     | 1:E:98:ILE:CD1   | 2.29                     | 0.44              |
| 1:E:386:PHE:C    | 1:E:388:ASN:H    | 2.25                     | 0.44              |
| 1:E:394:TYR:C    | 1:E:394:TYR:HD1  | 2.24                     | 0.44              |
| 1:E:463:ILE:CG2  | 1:E:464:CYS:N    | 2.79                     | 0.44              |
| 1:E:488:GLY:HA3  | 1:E:492:LEU:CD1  | 2.44                     | 0.44              |
| 1:F:166:MET:HE3  | 1:F:171:CYS:CB   | 2.47                     | 0.44              |
| 1:G:152:LYS:O    | 1:G:174:PRO:HD2  | 2.17                     | 0.44              |
| 1:G:315:GLY:HA2  | 1:G:317:VAL:CG2  | 2.42                     | 0.44              |
| 1:A:336:LYS:HB3  | 1:A:418:CYS:HB3  | 1.98                     | 0.44              |
| 1:C:273:GLU:CD   | 1:C:276:ARG:HH12 | 2.26                     | 0.44              |
| 1:D:227:LYS:O    | 1:D:229:ARG:HD2  | 2.18                     | 0.44              |
| 1:D:295:ILE:HD12 | 1:D:516:VAL:HG11 | 1.97                     | 0.44              |
| 1:D:304:GLY:HA2  | 1:D:459:VAL:HG22 | 1.98                     | 0.44              |
| 1:D:395:ASP:HB3  | 1:E:266:VAL:HG21 | 2.00                     | 0.44              |
| 1:D:486:LEU:HB3  | 1:D:493:ARG:CD   | 2.45                     | 0.44              |
| 1:E:166:MET:HE3  | 1:E:171:CYS:CA   | 2.47                     | 0.44              |
| 1:E:304:GLY:HA2  | 1:E:459:VAL:HG22 | 1.98                     | 0.44              |
| 1:E:440:LYS:O    | 1:E:443:ASP:HB2  | 2.18                     | 0.44              |
| 1:G:193:TYR:CE1  | 1:G:224:PRO:HA   | 2.53                     | 0.44              |
| 1:G:362:LEU:HD12 | 1:G:362:LEU:O    | 2.17                     | 0.44              |
| 1:B:441:MET:O    | 1:B:442:ILE:C    | 2.60                     | 0.44              |
| 1:C:166:MET:HE1  | 1:C:171:CYS:CB   | 2.44                     | 0.44              |
| 1:C:327:LEU:HB3  | 1:C:328:GLN:H    | 1.70                     | 0.44              |
| 1:C:406:LEU:HD13 | 1:C:406:LEU:HA   | 1.80                     | 0.44              |
| 1:C:409:LEU:HD23 | 1:C:421:ILE:CG2  | 2.33                     | 0.44              |
| 1:D:96:TYR:CE2   | 1:D:107:GLN:HG2  | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:286:GLY:O    | 1:E:302:ALA:N    | 2.51                     | 0.44              |
| 1:E:395:ASP:OD2  | 1:E:395:ASP:C    | 2.61                     | 0.44              |
| 1:E:476:GLU:CD   | 1:E:476:GLU:N    | 2.74                     | 0.44              |
| 1:E:492:LEU:O    | 1:E:494:GLN:N    | 2.51                     | 0.44              |
| 1:E:531:GLY:C    | 1:E:532:TYR:CD1  | 2.96                     | 0.44              |
| 1:F:463:ILE:CG2  | 1:F:464:CYS:N    | 2.78                     | 0.44              |
| 1:G:300:LEU:HA   | 1:G:300:LEU:HD22 | 1.54                     | 0.44              |
| 1:G:339:LEU:HD13 | 1:G:341:MET:CE   | 2.48                     | 0.44              |
| 1:G:488:GLY:HA3  | 1:G:492:LEU:CD1  | 2.46                     | 0.44              |
| 1:A:136:HIS:CD2  | 1:A:180:HIS:CE1  | 3.05                     | 0.44              |
| 1:A:401:GLU:CG   | 1:A:402:THR:N    | 2.76                     | 0.44              |
| 1:A:425:HIS:CE1  | 1:A:465:HIS:HB2  | 2.50                     | 0.44              |
| 1:A:473:LYS:CE   | 1:A:479:ARG:HA   | 2.44                     | 0.44              |
| 1:B:283:GLU:OE2  | 1:B:286:GLY:CA   | 2.61                     | 0.44              |
| 1:B:320:THR:HG22 | 1:B:324:GLN:NE2  | 2.33                     | 0.44              |
| 1:C:71:PHE:CD1   | 1:C:71:PHE:C     | 2.96                     | 0.44              |
| 1:C:124:ARG:HD3  | 1:C:125:ASP:CA   | 2.47                     | 0.44              |
| 1:C:524:THR:C    | 1:C:526:ASP:H    | 2.25                     | 0.44              |
| 1:D:155:VAL:HG12 | 1:D:206:PHE:HE2  | 1.83                     | 0.44              |
| 1:D:322:VAL:HG21 | 1:D:463:ILE:CD1  | 2.47                     | 0.44              |
| 1:D:347:GLU:OE2  | 1:E:274:ARG:CD   | 2.66                     | 0.44              |
| 1:D:405:LEU:HG   | 1:D:409:LEU:CD1  | 2.42                     | 0.44              |
| 1:E:166:MET:HE2  | 1:E:166:MET:HB3  | 1.59                     | 0.44              |
| 1:E:370:ARG:HH12 | 1:E:371:GLU:HG2  | 1.71                     | 0.44              |
| 1:F:401:GLU:CG   | 1:F:402:THR:H    | 2.30                     | 0.44              |
| 1:G:228:VAL:HB   | 1:G:261:ILE:HD12 | 1.99                     | 0.44              |
| 1:G:450:LYS:HD2  | 1:G:450:LYS:HA   | 1.67                     | 0.44              |
| 1:G:510:MET:HB2  | 1:G:513:LEU:HB3  | 2.00                     | 0.44              |
| 1:A:122:LYS:HE3  | 1:A:130:PHE:HE2  | 1.81                     | 0.43              |
| 1:A:125:ASP:OD1  | 1:A:129:ASN:HB2  | 2.18                     | 0.43              |
| 1:A:169:GLN:O    | 1:A:170:ASP:CB   | 2.63                     | 0.43              |
| 1:A:451:GLY:O    | 1:A:452:PHE:C    | 2.61                     | 0.43              |
| 1:A:493:ARG:H    | 1:A:493:ARG:HG2  | 1.40                     | 0.43              |
| 1:A:519:LEU:O    | 1:A:520:LYS:CB   | 2.66                     | 0.43              |
| 1:B:251:MET:CE   | 1:B:251:MET:CA   | 2.96                     | 0.43              |
| 1:B:382:PHE:CD2  | 1:B:382:PHE:C    | 2.96                     | 0.43              |
| 1:B:401:GLU:CA   | 1:B:430:VAL:O    | 2.66                     | 0.43              |
| 1:B:450:LYS:HA   | 1:B:450:LYS:HD2  | 1.67                     | 0.43              |
| 1:C:233:LEU:HD22 | 1:C:241:CYS:SG   | 2.58                     | 0.43              |
| 1:C:513:LEU:HD11 | 1:C:532:TYR:HB3  | 2.00                     | 0.43              |
| 1:D:145:HIS:CE1  | 1:D:146:LEU:HD21 | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:382:PHE:CD2  | 1:D:382:PHE:C    | 2.97                     | 0.43              |
| 1:E:338:GLY:O    | 1:E:421:ILE:HA   | 2.18                     | 0.43              |
| 1:E:363:ARG:H    | 1:E:363:ARG:HG2  | 1.66                     | 0.43              |
| 1:E:441:MET:O    | 1:E:442:ILE:C    | 2.61                     | 0.43              |
| 1:F:313:GLY:C    | 1:F:315:GLY:H    | 2.26                     | 0.43              |
| 1:F:411:TYR:CD1  | 1:F:411:TYR:C    | 2.96                     | 0.43              |
| 1:B:428:ILE:H    | 1:B:428:ILE:HD12 | 1.83                     | 0.43              |
| 1:C:235:CYS:HB2  | 1:C:240:GLU:HG2  | 2.00                     | 0.43              |
| 1:D:319:SER:O    | 1:D:323:ARG:HB2  | 2.18                     | 0.43              |
| 1:D:342:LEU:N    | 1:D:342:LEU:HD23 | 2.32                     | 0.43              |
| 1:D:346:VAL:HG23 | 1:D:393:LEU:HB2  | 2.00                     | 0.43              |
| 1:D:356:LEU:HD12 | 1:D:541:TRP:NE1  | 2.33                     | 0.43              |
| 1:E:112:ARG:NH2  | 1:E:118:ILE:HD11 | 2.33                     | 0.43              |
| 1:E:273:GLU:OE2  | 1:E:276:ARG:NH1  | 2.50                     | 0.43              |
| 1:E:382:PHE:C    | 1:E:382:PHE:CD2  | 2.95                     | 0.43              |
| 1:E:443:ASP:HA   | 1:E:491:ALA:HB3  | 2.00                     | 0.43              |
| 1:F:287:LEU:HD23 | 1:F:329:TRP:CE2  | 2.53                     | 0.43              |
| 1:F:473:LYS:CD   | 1:F:479:ARG:HB2  | 2.48                     | 0.43              |
| 1:F:492:LEU:O    | 1:F:494:GLN:N    | 2.52                     | 0.43              |
| 1:G:406:LEU:HD13 | 1:G:406:LEU:HA   | 1.81                     | 0.43              |
| 1:G:471:LYS:HD2  | 1:G:472:GLY:N    | 2.33                     | 0.43              |
| 1:G:546:SER:O    | 1:G:547:TYR:HB2  | 2.18                     | 0.43              |
| 1:A:141:LEU:HG   | 1:A:192:ASN:ND2  | 2.34                     | 0.43              |
| 1:A:450:LYS:NZ   | 1:A:454:LYS:HD3  | 2.31                     | 0.43              |
| 1:B:121:GLN:HB2  | 1:B:133:THR:HG1  | 1.78                     | 0.43              |
| 1:B:486:LEU:HD23 | 1:B:486:LEU:HA   | 1.71                     | 0.43              |
| 1:C:336:LYS:HB3  | 1:C:418:CYS:HB3  | 2.00                     | 0.43              |
| 1:C:373:ILE:HD11 | 1:D:279:LEU:HB2  | 2.00                     | 0.43              |
| 1:D:71:PHE:C     | 1:D:71:PHE:CD1   | 2.96                     | 0.43              |
| 1:D:352:ASP:OD2  | 1:D:363:ARG:HD3  | 2.17                     | 0.43              |
| 1:D:425:HIS:CE1  | 1:D:427:SER:CB   | 3.01                     | 0.43              |
| 1:E:404:ARG:O    | 1:E:408:LYS:HG2  | 2.18                     | 0.43              |
| 1:E:536:ASN:ND2  | 1:E:538:GLU:H    | 2.17                     | 0.43              |
| 1:F:71:PHE:CD1   | 1:F:71:PHE:C     | 2.96                     | 0.43              |
| 1:F:112:ARG:HD3  | 1:F:116:GLY:O    | 2.18                     | 0.43              |
| 1:F:142:PHE:CD2  | 1:F:162:MET:HE3  | 2.53                     | 0.43              |
| 1:F:368:LEU:HD23 | 1:F:368:LEU:HA   | 1.69                     | 0.43              |
| 1:G:80:ALA:HB2   | 1:G:88:LYS:N     | 2.33                     | 0.43              |
| 1:A:415:GLY:N    | 1:C:226:GLY:HA3  | 2.34                     | 0.43              |
| 1:B:180:HIS:HB2  | 1:B:184:ALA:HB3  | 1.99                     | 0.43              |
| 1:B:193:TYR:CE1  | 1:B:224:PRO:HA   | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:319:SER:O    | 1:B:323:ARG:HB2  | 2.18                     | 0.43              |
| 1:B:440:LYS:HZ3  | 1:B:444:ASN:HB3  | 1.82                     | 0.43              |
| 1:B:510:MET:HE1  | 1:B:547:TYR:CZ   | 2.53                     | 0.43              |
| 1:C:358:ASN:ND2  | 1:C:381:TRP:CE2  | 2.87                     | 0.43              |
| 1:C:483:ILE:O    | 1:C:486:LEU:CB   | 2.48                     | 0.43              |
| 1:D:283:GLU:O    | 1:D:283:GLU:HG2  | 2.16                     | 0.43              |
| 1:D:338:GLY:C    | 1:D:412:MET:HE1  | 2.43                     | 0.43              |
| 1:D:402:THR:HG23 | 1:D:403:ASP:N    | 2.33                     | 0.43              |
| 1:D:473:LYS:HE2  | 1:D:479:ARG:CA   | 2.42                     | 0.43              |
| 1:E:312:SER:C    | 1:E:313:GLY:O    | 2.62                     | 0.43              |
| 1:E:445:LEU:HD12 | 1:E:445:LEU:O    | 2.17                     | 0.43              |
| 1:F:107:GLN:HB3  | 1:F:124:ARG:CG   | 2.49                     | 0.43              |
| 1:F:378:PHE:HD2  | 1:G:276:ARG:HD2  | 1.83                     | 0.43              |
| 1:F:535:TYR:CE1  | 1:F:537:LYS:HA   | 2.53                     | 0.43              |
| 1:G:496:SER:O    | 1:G:520:LYS:CE   | 2.66                     | 0.43              |
| 1:A:101:VAL:C    | 1:A:103:GLY:H    | 2.26                     | 0.43              |
| 1:B:503:GLU:HG3  | 1:B:515:LEU:CD2  | 2.48                     | 0.43              |
| 1:C:450:LYS:HE3  | 1:C:454:LYS:CD   | 2.48                     | 0.43              |
| 1:C:506:GLN:H    | 1:C:506:GLN:HG3  | 1.56                     | 0.43              |
| 1:D:330:GLY:HA2  | 1:D:335:LYS:O    | 2.18                     | 0.43              |
| 1:D:440:LYS:O    | 1:D:443:ASP:HB2  | 2.19                     | 0.43              |
| 1:D:510:MET:HB2  | 1:D:513:LEU:CB   | 2.48                     | 0.43              |
| 1:E:229:ARG:CA   | 1:E:259:PRO:HA   | 2.46                     | 0.43              |
| 1:E:447:THR:HA   | 1:E:495:LEU:CD2  | 2.48                     | 0.43              |
| 1:E:510:MET:CB   | 1:E:513:LEU:HB2  | 2.48                     | 0.43              |
| 1:F:92:GLN:C     | 1:F:92:GLN:HE21  | 2.26                     | 0.43              |
| 1:F:322:VAL:HG11 | 1:F:422:ILE:CG2  | 2.47                     | 0.43              |
| 1:G:289:PHE:HA   | 1:G:325:GLN:HE21 | 1.84                     | 0.43              |
| 1:B:285:VAL:HG22 | 1:B:300:LEU:CD1  | 2.47                     | 0.43              |
| 1:B:303:ARG:HB2  | 1:B:306:GLU:CD   | 2.44                     | 0.43              |
| 1:C:185:ALA:O    | 1:C:189:CYS:HB2  | 2.18                     | 0.43              |
| 1:C:362:LEU:HD12 | 1:C:362:LEU:C    | 2.44                     | 0.43              |
| 1:C:429:VAL:HG13 | 1:C:438:GLU:OE1  | 2.19                     | 0.43              |
| 1:C:439:ARG:O    | 1:C:442:ILE:CG2  | 2.67                     | 0.43              |
| 1:D:320:THR:HG22 | 1:D:324:GLN:NE2  | 2.34                     | 0.43              |
| 1:D:324:GLN:OE1  | 1:D:541:TRP:CE3  | 2.71                     | 0.43              |
| 1:E:430:VAL:O    | 1:E:430:VAL:HG12 | 2.18                     | 0.43              |
| 1:E:446:MET:CE   | 1:E:492:LEU:HA   | 2.48                     | 0.43              |
| 1:E:486:LEU:HB3  | 1:E:493:ARG:CD   | 2.48                     | 0.43              |
| 1:F:394:TYR:C    | 1:F:394:TYR:HD1  | 2.24                     | 0.43              |
| 1:G:316:MET:CE   | 1:G:535:TYR:CE2  | 2.96                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:442:ILE:HD11 | 1:G:492:LEU:CD2  | 2.47                     | 0.43              |
| 1:B:204:LEU:HD13 | 1:B:206:PHE:CZ   | 2.54                     | 0.43              |
| 1:B:286:GLY:O    | 1:B:302:ALA:O    | 2.35                     | 0.43              |
| 1:B:312:SER:HB3  | 1:B:502:LEU:H    | 1.83                     | 0.43              |
| 1:B:492:LEU:O    | 1:B:494:GLN:N    | 2.52                     | 0.43              |
| 1:C:122:LYS:HE3  | 1:C:130:PHE:HE2  | 1.81                     | 0.43              |
| 1:C:440:LYS:O    | 1:C:443:ASP:HB2  | 2.19                     | 0.43              |
| 1:D:81:LEU:HG    | 1:D:91:CYS:SG    | 2.59                     | 0.43              |
| 1:D:141:LEU:CD1  | 1:D:176:VAL:HG21 | 2.43                     | 0.43              |
| 1:D:147:TRP:CD2  | 1:D:174:PRO:HB3  | 2.54                     | 0.43              |
| 1:D:220:ALA:HB1  | 1:D:261:ILE:HG12 | 2.01                     | 0.43              |
| 1:D:510:MET:HE1  | 1:D:547:TYR:CZ   | 2.53                     | 0.43              |
| 1:E:136:HIS:CD2  | 1:E:180:HIS:CE1  | 3.06                     | 0.43              |
| 1:F:193:TYR:CE1  | 1:F:224:PRO:HA   | 2.54                     | 0.43              |
| 1:F:536:ASN:HD21 | 1:F:538:GLU:CB   | 2.32                     | 0.43              |
| 1:G:124:ARG:HD3  | 1:G:125:ASP:O    | 2.19                     | 0.43              |
| 1:G:412:MET:HE3  | 1:G:412:MET:HB3  | 1.76                     | 0.43              |
| 1:A:105:MET:O    | 1:A:105:MET:HG2  | 2.18                     | 0.43              |
| 1:A:114:GLN:HG3  | 1:A:144:LYS:HE2  | 2.01                     | 0.43              |
| 1:A:401:GLU:N    | 1:A:404:ARG:HD2  | 2.34                     | 0.43              |
| 1:B:124:ARG:CD   | 1:B:124:ARG:C    | 2.91                     | 0.43              |
| 1:B:248:ARG:NH1  | 1:B:248:ARG:CG   | 2.70                     | 0.43              |
| 1:B:251:MET:HE3  | 1:B:251:MET:N    | 2.34                     | 0.43              |
| 1:B:454:LYS:HZ3  | 1:G:344:GLU:HA   | 1.73                     | 0.43              |
| 1:C:260:TRP:O    | 1:C:261:ILE:HD13 | 2.19                     | 0.43              |
| 1:C:427:SER:HB3  | 1:C:487:ARG:NH1  | 2.33                     | 0.43              |
| 1:C:442:ILE:HD11 | 1:C:492:LEU:CD1  | 2.47                     | 0.43              |
| 1:D:451:GLY:O    | 1:D:452:PHE:C    | 2.60                     | 0.43              |
| 1:E:338:GLY:C    | 1:E:412:MET:HE1  | 2.43                     | 0.43              |
| 1:F:122:LYS:HE3  | 1:F:130:PHE:CE2  | 2.53                     | 0.43              |
| 1:F:149:GLY:O    | 1:F:199:PHE:CE2  | 2.71                     | 0.43              |
| 1:F:285:VAL:HG13 | 1:F:300:LEU:CD1  | 2.49                     | 0.43              |
| 1:F:309:MET:HB2  | 1:F:309:MET:HE3  | 1.72                     | 0.43              |
| 1:F:320:THR:HG22 | 1:F:324:GLN:HE21 | 1.84                     | 0.43              |
| 1:F:366:ASP:CB   | 1:G:284:SER:CB   | 2.92                     | 0.43              |
| 1:F:440:LYS:O    | 1:F:443:ASP:HB2  | 2.18                     | 0.43              |
| 1:G:510:MET:HE3  | 1:G:547:TYR:CE1  | 2.32                     | 0.43              |
| 1:C:124:ARG:HD3  | 1:C:124:ARG:C    | 2.44                     | 0.43              |
| 1:C:149:GLY:O    | 1:C:199:PHE:CE2  | 2.72                     | 0.43              |
| 1:C:360:VAL:O    | 1:C:360:VAL:CG2  | 2.67                     | 0.43              |
| 1:C:364:GLN:HA   | 1:D:523:PHE:HZ   | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:322:VAL:HG11 | 1:D:422:ILE:HG21 | 2.01                     | 0.43              |
| 1:D:394:TYR:C    | 1:D:394:TYR:HD1  | 2.22                     | 0.43              |
| 1:E:124:ARG:CD   | 1:E:124:ARG:C    | 2.91                     | 0.43              |
| 1:E:145:HIS:CE1  | 1:E:146:LEU:CD2  | 3.02                     | 0.43              |
| 1:E:153:ILE:HG23 | 1:E:153:ILE:O    | 2.18                     | 0.43              |
| 1:F:425:HIS:C    | 1:F:425:HIS:ND1  | 2.76                     | 0.43              |
| 1:F:450:LYS:HA   | 1:F:450:LYS:HD2  | 1.72                     | 0.43              |
| 1:G:268:ALA:HA   | 1:G:271:LEU:HD12 | 1.98                     | 0.43              |
| 1:G:425:HIS:NE2  | 1:G:465:HIS:ND1  | 2.66                     | 0.43              |
| 1:G:428:ILE:H    | 1:G:428:ILE:HD12 | 1.83                     | 0.43              |
| 1:G:536:ASN:ND2  | 1:G:538:GLU:H    | 2.16                     | 0.43              |
| 1:A:216:VAL:HG11 | 1:A:230:VAL:HG22 | 1.99                     | 0.43              |
| 1:A:327:LEU:HA   | 1:A:327:LEU:HD23 | 1.43                     | 0.43              |
| 1:A:427:SER:CB   | 1:A:487:ARG:NH1  | 2.81                     | 0.43              |
| 1:A:510:MET:CB   | 1:A:513:LEU:CB   | 2.97                     | 0.43              |
| 1:B:344:GLU:OE1  | 1:B:349:THR:HB   | 2.19                     | 0.43              |
| 1:C:441:MET:CE   | 1:C:445:LEU:H    | 2.32                     | 0.43              |
| 1:D:166:MET:HE3  | 1:D:171:CYS:CA   | 2.49                     | 0.43              |
| 1:E:368:LEU:CD2  | 1:E:372:ILE:HG23 | 2.43                     | 0.43              |
| 1:E:401:GLU:HG3  | 1:E:431:SER:O    | 2.19                     | 0.43              |
| 1:E:442:ILE:HD11 | 1:E:492:LEU:HD11 | 1.95                     | 0.43              |
| 1:E:446:MET:HE2  | 1:E:492:LEU:CB   | 2.45                     | 0.43              |
| 1:E:517:ARG:CG   | 1:E:517:ARG:HH11 | 2.30                     | 0.43              |
| 1:F:259:PRO:O    | 1:F:259:PRO:CG   | 2.64                     | 0.43              |
| 1:F:313:GLY:C    | 1:F:315:GLY:N    | 2.76                     | 0.43              |
| 1:F:318:MET:SD   | 1:F:463:ILE:HD13 | 2.59                     | 0.43              |
| 1:F:445:LEU:HD12 | 1:F:445:LEU:C    | 2.44                     | 0.43              |
| 1:G:536:ASN:OD1  | 1:G:539:THR:HG23 | 2.19                     | 0.43              |
| 1:A:265:VAL:HG21 | 1:B:412:MET:HG2  | 2.01                     | 0.42              |
| 1:A:450:LYS:HE3  | 1:A:454:LYS:CD   | 2.47                     | 0.42              |
| 1:B:248:ARG:O    | 1:B:248:ARG:HG2  | 2.19                     | 0.42              |
| 1:B:445:LEU:HD12 | 1:B:445:LEU:C    | 2.43                     | 0.42              |
| 1:C:145:HIS:CE1  | 1:C:146:LEU:HD21 | 2.53                     | 0.42              |
| 1:C:290:SER:N    | 1:C:325:GLN:HE22 | 2.03                     | 0.42              |
| 1:C:442:ILE:HD11 | 1:C:492:LEU:CG   | 2.48                     | 0.42              |
| 1:C:491:ALA:O    | 1:C:495:LEU:N    | 2.47                     | 0.42              |
| 1:E:122:LYS:HE3  | 1:E:130:PHE:HE2  | 1.84                     | 0.42              |
| 1:E:379:ASP:CG   | 1:F:276:ARG:HH21 | 2.26                     | 0.42              |
| 1:E:449:LEU:O    | 1:E:452:PHE:HB3  | 2.18                     | 0.42              |
| 1:F:382:PHE:CZ   | 1:G:272:ARG:HA   | 2.54                     | 0.42              |
| 1:G:327:LEU:HD11 | 1:G:357:HIS:HA   | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:424:ASP:O    | 1:G:425:HIS:HB3  | 2.19                     | 0.42              |
| 1:A:145:HIS:CE1  | 1:A:146:LEU:HD21 | 2.54                     | 0.42              |
| 1:A:309:MET:HE2  | 1:A:462:VAL:HG12 | 2.00                     | 0.42              |
| 1:A:346:VAL:CG1  | 1:C:271:LEU:HD21 | 2.50                     | 0.42              |
| 1:A:401:GLU:CB   | 1:A:431:SER:O    | 2.67                     | 0.42              |
| 1:B:473:LYS:HE2  | 1:B:479:ARG:CA   | 2.44                     | 0.42              |
| 1:C:86:ILE:HD12  | 1:C:163:LEU:HB3  | 2.02                     | 0.42              |
| 1:C:427:SER:HB2  | 1:D:494:GLN:HE22 | 1.84                     | 0.42              |
| 1:D:317:VAL:HG21 | 1:D:504:ARG:HD2  | 2.01                     | 0.42              |
| 1:D:327:LEU:HA   | 1:D:327:LEU:HD23 | 1.47                     | 0.42              |
| 1:D:440:LYS:NZ   | 1:D:441:MET:HG2  | 2.34                     | 0.42              |
| 1:E:81:LEU:HD11  | 1:E:96:TYR:CD2   | 2.54                     | 0.42              |
| 1:E:178:LEU:HD23 | 1:E:178:LEU:HA   | 1.83                     | 0.42              |
| 1:E:411:TYR:CZ   | 1:F:262:PRO:HB3  | 2.52                     | 0.42              |
| 1:E:445:LEU:CD1  | 1:E:449:LEU:HG   | 2.49                     | 0.42              |
| 1:E:479:ARG:HA   | 1:E:480:PRO:HD3  | 1.83                     | 0.42              |
| 1:E:520:LYS:HG3  | 1:E:521:CYS:N    | 2.25                     | 0.42              |
| 1:F:180:HIS:CD2  | 1:F:180:HIS:N    | 2.87                     | 0.42              |
| 1:F:285:VAL:HA   | 1:F:300:LEU:HD12 | 2.00                     | 0.42              |
| 1:G:121:GLN:HB2  | 1:G:133:THR:HG1  | 1.83                     | 0.42              |
| 1:A:126:LYS:HD3  | 1:A:127:ASP:CG   | 2.44                     | 0.42              |
| 1:A:318:MET:HE1  | 1:A:464:CYS:O    | 2.19                     | 0.42              |
| 1:B:170:ASP:O    | 1:B:172:LYS:HG3  | 2.20                     | 0.42              |
| 1:B:320:THR:O    | 1:B:321:PHE:C    | 2.59                     | 0.42              |
| 1:B:336:LYS:HB3  | 1:B:418:CYS:HA   | 2.00                     | 0.42              |
| 1:B:441:MET:HE1  | 1:B:445:LEU:H    | 1.84                     | 0.42              |
| 1:B:476:GLU:HB3  | 1:B:506:GLN:OE1  | 2.19                     | 0.42              |
| 1:C:146:LEU:HB2  | 1:C:147:TRP:CE2  | 2.54                     | 0.42              |
| 1:C:204:LEU:HD13 | 1:C:206:PHE:CZ   | 2.54                     | 0.42              |
| 1:C:437:ASP:CG   | 1:C:439:ARG:HB2  | 2.45                     | 0.42              |
| 1:D:208:MET:HE1  | 1:D:232:VAL:HG22 | 2.01                     | 0.42              |
| 1:D:290:SER:N    | 1:D:325:GLN:HE22 | 2.08                     | 0.42              |
| 1:D:311:THR:O    | 1:D:502:LEU:HD12 | 2.18                     | 0.42              |
| 1:D:542:LEU:HD12 | 1:D:542:LEU:HA   | 1.56                     | 0.42              |
| 1:E:518:ILE:HA   | 1:E:518:ILE:HD13 | 1.75                     | 0.42              |
| 1:F:303:ARG:CZ   | 1:F:523:PHE:CD1  | 3.02                     | 0.42              |
| 1:F:401:GLU:HG2  | 1:F:402:THR:H    | 1.85                     | 0.42              |
| 1:F:442:ILE:HD11 | 1:F:492:LEU:CG   | 2.49                     | 0.42              |
| 1:A:168:LEU:O    | 1:A:169:GLN:CB   | 2.55                     | 0.42              |
| 1:A:406:LEU:HA   | 1:A:406:LEU:HD13 | 1.74                     | 0.42              |
| 1:A:499:ILE:HG22 | 1:A:519:LEU:CB   | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:263:ASP:C    | 1:G:408:LYS:HZ1  | 2.27                     | 0.42              |
| 1:C:411:TYR:CD1  | 1:C:411:TYR:C    | 2.98                     | 0.42              |
| 1:D:220:ALA:CB   | 1:D:261:ILE:HG23 | 2.47                     | 0.42              |
| 1:D:482:SER:O    | 1:D:485:ASP:CB   | 2.68                     | 0.42              |
| 1:E:267:SER:O    | 1:E:271:LEU:HD12 | 2.19                     | 0.42              |
| 1:E:442:ILE:HD11 | 1:E:492:LEU:CG   | 2.48                     | 0.42              |
| 1:F:322:VAL:CG1  | 1:F:422:ILE:HD13 | 2.49                     | 0.42              |
| 1:A:141:LEU:CD1  | 1:A:176:VAL:HG21 | 2.43                     | 0.42              |
| 1:A:339:LEU:HB3  | 1:A:341:MET:HE3  | 1.88                     | 0.42              |
| 1:B:114:GLN:NE2  | 1:B:195:TYR:CD1  | 2.88                     | 0.42              |
| 1:B:235:CYS:HB2  | 1:B:240:GLU:HG2  | 2.01                     | 0.42              |
| 1:B:271:LEU:O    | 1:B:272:ARG:C    | 2.62                     | 0.42              |
| 1:C:443:ASP:HA   | 1:C:491:ALA:HB3  | 2.00                     | 0.42              |
| 1:D:251:MET:HE3  | 1:D:251:MET:N    | 2.35                     | 0.42              |
| 1:D:309:MET:HB2  | 1:D:309:MET:HE3  | 1.67                     | 0.42              |
| 1:F:121:GLN:HB3  | 1:F:133:THR:CG2  | 2.45                     | 0.42              |
| 1:F:178:LEU:HB3  | 1:F:181:GLY:CA   | 2.40                     | 0.42              |
| 1:F:513:LEU:HD12 | 1:F:533:MET:O    | 2.18                     | 0.42              |
| 1:G:124:ARG:CZ   | 1:G:126:LYS:HA   | 2.49                     | 0.42              |
| 1:G:520:LYS:HG3  | 1:G:521:CYS:N    | 2.30                     | 0.42              |
| 1:A:300:LEU:HD22 | 1:A:300:LEU:HA   | 1.78                     | 0.42              |
| 1:A:401:GLU:CA   | 1:A:430:VAL:O    | 2.67                     | 0.42              |
| 1:A:536:ASN:HD21 | 1:A:538:GLU:HB2  | 1.83                     | 0.42              |
| 1:B:406:LEU:HA   | 1:B:406:LEU:HD13 | 1.59                     | 0.42              |
| 1:C:121:GLN:HB3  | 1:C:133:THR:CG2  | 2.47                     | 0.42              |
| 1:C:124:ARG:CZ   | 1:C:126:LYS:HA   | 2.50                     | 0.42              |
| 1:C:141:LEU:HG   | 1:C:192:ASN:ND2  | 2.34                     | 0.42              |
| 1:C:278:HIS:CD2  | 1:C:278:HIS:C    | 2.97                     | 0.42              |
| 1:C:445:LEU:HD12 | 1:C:445:LEU:C    | 2.44                     | 0.42              |
| 1:D:107:GLN:CB   | 1:D:124:ARG:CG   | 2.93                     | 0.42              |
| 1:D:124:ARG:C    | 1:D:124:ARG:CD   | 2.92                     | 0.42              |
| 1:D:289:PHE:HA   | 1:D:325:GLN:HE21 | 1.84                     | 0.42              |
| 1:D:444:ASN:OD1  | 1:D:448:LYS:HE3  | 2.19                     | 0.42              |
| 1:E:114:GLN:NE2  | 1:E:195:TYR:CD1  | 2.87                     | 0.42              |
| 1:E:251:MET:HE3  | 1:E:251:MET:N    | 2.35                     | 0.42              |
| 1:F:217:GLU:OE2  | 1:F:261:ILE:HG23 | 2.18                     | 0.42              |
| 1:F:498:THR:C    | 1:F:499:ILE:HD13 | 2.44                     | 0.42              |
| 1:G:153:ILE:HG23 | 1:G:153:ILE:O    | 2.20                     | 0.42              |
| 1:A:124:ARG:CD   | 1:A:124:ARG:C    | 2.92                     | 0.42              |
| 1:A:229:ARG:NH2  | 1:A:259:PRO:HB3  | 2.34                     | 0.42              |
| 1:A:352:ASP:OD2  | 1:A:363:ARG:HD3  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:74:SER:HB3   | 1:C:101:VAL:CG2  | 2.50                     | 0.42              |
| 1:C:344:GLU:OE1  | 1:C:349:THR:CB   | 2.66                     | 0.42              |
| 1:C:510:MET:HB2  | 1:C:513:LEU:HB3  | 2.00                     | 0.42              |
| 1:D:115:ASN:HB3  | 1:D:117:ASN:HD21 | 1.84                     | 0.42              |
| 1:D:167:GLU:O    | 1:D:168:LEU:C    | 2.59                     | 0.42              |
| 1:D:347:GLU:O    | 1:D:351:GLU:HG3  | 2.20                     | 0.42              |
| 1:D:486:LEU:HD22 | 1:D:487:ARG:H    | 1.85                     | 0.42              |
| 1:D:546:SER:O    | 1:D:547:TYR:HB2  | 2.20                     | 0.42              |
| 1:E:94:ALA:CB    | 1:E:162:MET:HE1  | 2.47                     | 0.42              |
| 1:E:341:MET:SD   | 1:E:424:ASP:HB2  | 2.59                     | 0.42              |
| 1:E:429:VAL:HG13 | 1:E:438:GLU:OE1  | 2.19                     | 0.42              |
| 1:E:486:LEU:HD22 | 1:E:487:ARG:H    | 1.85                     | 0.42              |
| 1:E:517:ARG:CZ   | 1:E:529:ILE:HD11 | 2.50                     | 0.42              |
| 1:F:260:TRP:CD1  | 1:F:262:PRO:HD2  | 2.55                     | 0.42              |
| 1:G:318:MET:HE1  | 1:G:465:HIS:CD2  | 2.54                     | 0.42              |
| 1:G:363:ARG:H    | 1:G:363:ARG:HG2  | 1.55                     | 0.42              |
| 1:G:445:LEU:HD12 | 1:G:445:LEU:O    | 2.19                     | 0.42              |
| 1:C:70:ASN:HD22  | 1:C:70:ASN:HA    | 1.69                     | 0.42              |
| 1:C:441:MET:HE1  | 1:C:445:LEU:H    | 1.84                     | 0.42              |
| 1:D:243:LEU:O    | 1:D:244:ASN:C    | 2.62                     | 0.42              |
| 1:E:278:HIS:CD2  | 1:E:278:HIS:C    | 2.98                     | 0.42              |
| 1:E:427:SER:HB3  | 1:E:487:ARG:NH1  | 2.28                     | 0.42              |
| 1:F:356:LEU:HD12 | 1:F:541:TRP:CD1  | 2.54                     | 0.42              |
| 1:F:415:GLY:HA2  | 1:G:226:GLY:H    | 1.82                     | 0.42              |
| 1:A:269:LEU:HD21 | 1:B:389:ASP:H    | 1.84                     | 0.42              |
| 1:B:248:ARG:HD2  | 1:B:249:GLU:OE2  | 2.20                     | 0.42              |
| 1:B:404:ARG:O    | 1:B:408:LYS:HG2  | 2.19                     | 0.42              |
| 1:B:429:VAL:HG13 | 1:B:438:GLU:OE1  | 2.19                     | 0.42              |
| 1:B:446:MET:HE2  | 1:B:492:LEU:HB3  | 2.01                     | 0.42              |
| 1:C:233:LEU:CD2  | 1:C:250:ILE:HG12 | 2.50                     | 0.42              |
| 1:C:401:GLU:HG3  | 1:C:431:SER:O    | 2.20                     | 0.42              |
| 1:D:142:PHE:CE2  | 1:D:162:MET:CE   | 2.99                     | 0.42              |
| 1:D:388:ASN:O    | 1:D:389:ASP:C    | 2.63                     | 0.42              |
| 1:D:451:GLY:O    | 1:D:455:SER:HB3  | 2.19                     | 0.42              |
| 1:E:71:PHE:C     | 1:E:71:PHE:CD1   | 2.98                     | 0.42              |
| 1:E:229:ARG:HB3  | 1:E:259:PRO:CA   | 2.50                     | 0.42              |
| 1:E:294:GLY:C    | 1:E:296:ASN:N    | 2.77                     | 0.42              |
| 1:E:368:LEU:HD22 | 1:E:372:ILE:CG2  | 2.46                     | 0.42              |
| 1:F:165:VAL:HB   | 1:F:175:VAL:HG11 | 2.02                     | 0.42              |
| 1:F:307:VAL:HG12 | 1:F:496:SER:HA   | 2.01                     | 0.42              |
| 1:F:488:GLY:HA3  | 1:F:492:LEU:CD1  | 2.45                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:368:LEU:C    | 1:G:368:LEU:CD2  | 2.93                     | 0.42              |
| 1:G:440:LYS:NZ   | 1:G:441:MET:HG2  | 2.35                     | 0.42              |
| 1:A:242:HIS:O    | 1:A:244:ASN:N    | 2.53                     | 0.42              |
| 1:A:440:LYS:NZ   | 1:A:441:MET:HG2  | 2.34                     | 0.42              |
| 1:B:71:PHE:CD1   | 1:B:71:PHE:C     | 2.98                     | 0.42              |
| 1:B:401:GLU:CB   | 1:B:431:SER:O    | 2.68                     | 0.42              |
| 1:B:479:ARG:HA   | 1:B:480:PRO:HD3  | 1.85                     | 0.42              |
| 1:B:482:SER:H    | 1:B:485:ASP:CB   | 2.23                     | 0.42              |
| 1:C:204:LEU:N    | 1:C:204:LEU:HD23 | 2.35                     | 0.42              |
| 1:C:442:ILE:HD11 | 1:C:492:LEU:CD2  | 2.49                     | 0.42              |
| 1:C:536:ASN:CG   | 1:C:539:THR:HG23 | 2.45                     | 0.42              |
| 1:D:259:PRO:O    | 1:D:260:TRP:CE3  | 2.72                     | 0.42              |
| 1:D:492:LEU:O    | 1:D:494:GLN:N    | 2.53                     | 0.42              |
| 1:E:124:ARG:HD3  | 1:E:125:ASP:O    | 2.19                     | 0.42              |
| 1:E:370:ARG:HD2  | 1:E:371:GLU:CA   | 2.49                     | 0.42              |
| 1:F:378:PHE:CE2  | 1:G:276:ARG:CG   | 3.03                     | 0.42              |
| 1:F:442:ILE:HD11 | 1:F:492:LEU:HD11 | 1.98                     | 0.42              |
| 1:G:77:ARG:HE    | 1:G:77:ARG:HB2   | 1.61                     | 0.42              |
| 1:G:170:ASP:O    | 1:G:172:LYS:HG3  | 2.20                     | 0.42              |
| 1:G:307:VAL:HG22 | 1:G:460:LEU:HB3  | 2.02                     | 0.42              |
| 1:G:476:GLU:CD   | 1:G:476:GLU:N    | 2.76                     | 0.42              |
| 1:A:476:GLU:CD   | 1:A:476:GLU:N    | 2.75                     | 0.41              |
| 1:B:122:LYS:HE3  | 1:B:130:PHE:HE2  | 1.85                     | 0.41              |
| 1:B:542:LEU:HD12 | 1:B:542:LEU:HA   | 1.64                     | 0.41              |
| 1:C:322:VAL:HG21 | 1:C:463:ILE:CD1  | 2.49                     | 0.41              |
| 1:C:366:ASP:CB   | 1:D:284:SER:OG   | 2.67                     | 0.41              |
| 1:C:504:ARG:HD3  | 1:C:506:GLN:CG   | 2.26                     | 0.41              |
| 1:D:251:MET:CE   | 1:D:251:MET:CA   | 2.97                     | 0.41              |
| 1:E:447:THR:HG22 | 1:E:495:LEU:CD2  | 2.31                     | 0.41              |
| 1:E:496:SER:O    | 1:E:520:LYS:CE   | 2.67                     | 0.41              |
| 1:F:285:VAL:HA   | 1:F:300:LEU:CD1  | 2.49                     | 0.41              |
| 1:F:295:ILE:HD12 | 1:F:516:VAL:HG11 | 2.02                     | 0.41              |
| 1:F:482:SER:CB   | 1:F:484:THR:HG23 | 2.49                     | 0.41              |
| 1:G:124:ARG:C    | 1:G:124:ARG:CD   | 2.93                     | 0.41              |
| 1:G:425:HIS:CE1  | 1:G:427:SER:HB2  | 2.55                     | 0.41              |
| 1:G:517:ARG:CZ   | 1:G:529:ILE:HD11 | 2.50                     | 0.41              |
| 1:G:532:TYR:CD1  | 1:G:532:TYR:N    | 2.88                     | 0.41              |
| 1:A:129:ASN:C    | 1:A:130:PHE:CD1  | 2.98                     | 0.41              |
| 1:A:173:TYR:CD1  | 1:A:173:TYR:N    | 2.88                     | 0.41              |
| 1:A:276:ARG:HH11 | 1:A:276:ARG:CG   | 2.30                     | 0.41              |
| 1:A:492:LEU:H    | 1:A:492:LEU:CD1  | 2.13                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:106:TYR:HB3  | 1:B:123:VAL:CG1  | 2.50                     | 0.41              |
| 1:B:185:ALA:O    | 1:B:189:CYS:HB2  | 2.19                     | 0.41              |
| 1:B:316:MET:HE2  | 1:B:320:THR:OG1  | 2.21                     | 0.41              |
| 1:B:324:GLN:OE1  | 1:B:541:TRP:CE3  | 2.73                     | 0.41              |
| 1:B:486:LEU:HB3  | 1:B:493:ARG:CD   | 2.50                     | 0.41              |
| 1:C:229:ARG:NH2  | 1:C:259:PRO:CG   | 2.83                     | 0.41              |
| 1:C:369:LYS:NZ   | 1:D:284:SER:H    | 2.19                     | 0.41              |
| 1:C:440:LYS:NZ   | 1:C:441:MET:CA   | 2.58                     | 0.41              |
| 1:D:152:LYS:O    | 1:D:174:PRO:HD2  | 2.19                     | 0.41              |
| 1:D:445:LEU:O    | 1:D:445:LEU:HD12 | 2.20                     | 0.41              |
| 1:E:170:ASP:O    | 1:E:172:LYS:HG3  | 2.20                     | 0.41              |
| 1:F:147:TRP:CE2  | 1:F:174:PRO:HA   | 2.55                     | 0.41              |
| 1:F:366:ASP:HA   | 1:G:284:SER:OG   | 2.20                     | 0.41              |
| 1:F:414:SER:O    | 1:G:225:ALA:HB1  | 2.19                     | 0.41              |
| 1:G:71:PHE:CD1   | 1:G:71:PHE:C     | 2.99                     | 0.41              |
| 1:G:272:ARG:CG   | 1:G:273:GLU:N    | 2.81                     | 0.41              |
| 1:G:284:SER:O    | 1:G:300:LEU:HD12 | 2.19                     | 0.41              |
| 1:G:292:CYS:O    | 1:G:293:THR:C    | 2.60                     | 0.41              |
| 1:A:166:MET:HG2  | 1:A:175:VAL:HG21 | 2.02                     | 0.41              |
| 1:A:173:TYR:HA   | 1:A:174:PRO:HD3  | 1.94                     | 0.41              |
| 1:A:267:SER:O    | 1:A:271:LEU:HD12 | 2.20                     | 0.41              |
| 1:A:368:LEU:O    | 1:A:369:LYS:C    | 2.63                     | 0.41              |
| 1:A:424:ASP:HA   | 1:A:463:ILE:HB   | 2.01                     | 0.41              |
| 1:A:437:ASP:CG   | 1:A:439:ARG:HB2  | 2.45                     | 0.41              |
| 1:A:548:SER:HB3  | 1:A:549:GLY:H    | 1.60                     | 0.41              |
| 1:B:81:LEU:HD12  | 1:B:86:ILE:HB    | 2.02                     | 0.41              |
| 1:B:204:LEU:N    | 1:B:204:LEU:HD23 | 2.36                     | 0.41              |
| 1:B:262:PRO:CB   | 1:B:265:VAL:HG12 | 2.49                     | 0.41              |
| 1:B:283:GLU:HG3  | 1:B:283:GLU:O    | 2.20                     | 0.41              |
| 1:B:330:GLY:HA2  | 1:B:335:LYS:O    | 2.20                     | 0.41              |
| 1:C:402:THR:HG23 | 1:C:403:ASP:H    | 1.85                     | 0.41              |
| 1:C:441:MET:HE3  | 1:C:444:ASN:HB3  | 1.98                     | 0.41              |
| 1:C:447:THR:HG22 | 1:C:495:LEU:CD2  | 2.32                     | 0.41              |
| 1:D:129:ASN:OD1  | 1:E:89:GLU:OE1   | 2.38                     | 0.41              |
| 1:D:533:MET:HB3  | 1:D:543:GLU:O    | 2.20                     | 0.41              |
| 1:E:346:VAL:HG23 | 1:E:393:LEU:HB2  | 2.02                     | 0.41              |
| 1:E:437:ASP:CG   | 1:E:439:ARG:HB2  | 2.45                     | 0.41              |
| 1:F:360:VAL:O    | 1:F:360:VAL:HG23 | 2.20                     | 0.41              |
| 1:F:412:MET:HA   | 1:F:416:LEU:HD11 | 1.96                     | 0.41              |
| 1:F:446:MET:HE2  | 1:F:492:LEU:CA   | 2.49                     | 0.41              |
| 1:F:486:LEU:HD22 | 1:F:487:ARG:N    | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:81:LEU:HD22  | 1:G:107:GLN:NE2  | 2.35                     | 0.41              |
| 1:A:227:LYS:O    | 1:A:229:ARG:HD2  | 2.21                     | 0.41              |
| 1:A:347:GLU:OE2  | 1:C:274:ARG:HD2  | 2.21                     | 0.41              |
| 1:A:368:LEU:HD23 | 1:A:368:LEU:HA   | 1.67                     | 0.41              |
| 1:A:498:THR:C    | 1:A:499:ILE:HD13 | 2.45                     | 0.41              |
| 1:B:283:GLU:O    | 1:B:286:GLY:N    | 2.53                     | 0.41              |
| 1:B:286:GLY:O    | 1:B:287:LEU:CB   | 2.68                     | 0.41              |
| 1:C:170:ASP:O    | 1:C:172:LYS:HG3  | 2.20                     | 0.41              |
| 1:C:180:HIS:CD2  | 1:C:180:HIS:N    | 2.88                     | 0.41              |
| 1:C:216:VAL:CG1  | 1:C:230:VAL:HG22 | 2.47                     | 0.41              |
| 1:C:366:ASP:HA   | 1:D:284:SER:OG   | 2.21                     | 0.41              |
| 1:C:442:ILE:HG23 | 1:C:443:ASP:N    | 2.35                     | 0.41              |
| 1:C:477:GLU:HG3  | 1:C:507:GLN:HE22 | 1.86                     | 0.41              |
| 1:D:313:GLY:O    | 1:D:315:GLY:N    | 2.53                     | 0.41              |
| 1:E:411:TYR:O    | 1:E:411:TYR:CG   | 2.73                     | 0.41              |
| 1:E:450:LYS:HE3  | 1:E:454:LYS:CD   | 2.48                     | 0.41              |
| 1:E:513:LEU:HD12 | 1:E:533:MET:O    | 2.20                     | 0.41              |
| 1:E:517:ARG:CG   | 1:E:517:ARG:NH1  | 2.82                     | 0.41              |
| 1:F:368:LEU:C    | 1:F:368:LEU:CD2  | 2.92                     | 0.41              |
| 1:G:145:HIS:CE1  | 1:G:146:LEU:HD21 | 2.55                     | 0.41              |
| 1:G:318:MET:SD   | 1:G:463:ILE:HG23 | 2.60                     | 0.41              |
| 1:A:165:VAL:HB   | 1:A:175:VAL:HG11 | 2.03                     | 0.41              |
| 1:A:439:ARG:HG2  | 1:A:489:SER:OG   | 2.20                     | 0.41              |
| 1:A:447:THR:HA   | 1:A:495:LEU:CD2  | 2.50                     | 0.41              |
| 1:A:529:ILE:HD13 | 1:A:529:ILE:HA   | 1.88                     | 0.41              |
| 1:A:533:MET:HB3  | 1:A:543:GLU:O    | 2.20                     | 0.41              |
| 1:B:253:GLN:O    | 1:B:257:ALA:HB2  | 2.21                     | 0.41              |
| 1:B:311:THR:O    | 1:B:312:SER:CB   | 2.68                     | 0.41              |
| 1:B:363:ARG:H    | 1:B:363:ARG:HG2  | 1.52                     | 0.41              |
| 1:C:97:TRP:HZ3   | 1:C:99:ALA:HB2   | 1.76                     | 0.41              |
| 1:C:178:LEU:HA   | 1:C:178:LEU:HD23 | 1.81                     | 0.41              |
| 1:C:294:GLY:C    | 1:C:296:ASN:N    | 2.75                     | 0.41              |
| 1:C:503:GLU:CD   | 1:C:517:ARG:HE   | 2.27                     | 0.41              |
| 1:C:505:ASN:O    | 1:C:505:ASN:CG   | 2.64                     | 0.41              |
| 1:D:147:TRP:CE2  | 1:D:174:PRO:HA   | 2.55                     | 0.41              |
| 1:D:486:LEU:HD13 | 1:D:487:ARG:O    | 2.20                     | 0.41              |
| 1:D:536:ASN:HD21 | 1:D:538:GLU:HB3  | 1.86                     | 0.41              |
| 1:F:234:PRO:HG2  | 1:F:249:GLU:HG2  | 2.02                     | 0.41              |
| 1:F:300:LEU:HD22 | 1:F:300:LEU:HA   | 1.79                     | 0.41              |
| 1:G:233:LEU:CD2  | 1:G:250:ILE:HG12 | 2.50                     | 0.41              |
| 1:G:442:ILE:HD11 | 1:G:492:LEU:CG   | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:142:PHE:CD2  | 1:A:162:MET:HE3  | 2.55                     | 0.41              |
| 1:A:229:ARG:HA   | 1:A:259:PRO:HA   | 2.02                     | 0.41              |
| 1:B:205:MET:HE1  | 1:B:250:ILE:HG23 | 2.03                     | 0.41              |
| 1:C:243:LEU:O    | 1:C:244:ASN:C    | 2.63                     | 0.41              |
| 1:C:296:ASN:O    | 1:C:300:LEU:N    | 2.35                     | 0.41              |
| 1:D:353:LEU:HA   | 1:D:353:LEU:HD23 | 1.56                     | 0.41              |
| 1:D:401:GLU:HB2  | 1:D:404:ARG:HH21 | 1.85                     | 0.41              |
| 1:F:101:VAL:HG12 | 1:F:102:ASP:OD2  | 2.20                     | 0.41              |
| 1:F:404:ARG:HH21 | 1:F:404:ARG:CB   | 2.33                     | 0.41              |
| 1:G:317:VAL:HG21 | 1:G:504:ARG:HD2  | 2.02                     | 0.41              |
| 1:G:517:ARG:HG3  | 1:G:529:ILE:HD13 | 2.03                     | 0.41              |
| 1:A:353:LEU:HA   | 1:A:353:LEU:HD23 | 1.59                     | 0.41              |
| 1:A:430:VAL:O    | 1:A:430:VAL:HG12 | 2.20                     | 0.41              |
| 1:A:473:LYS:HE2  | 1:A:479:ARG:CA   | 2.47                     | 0.41              |
| 1:B:115:ASN:HB3  | 1:B:117:ASN:HD21 | 1.85                     | 0.41              |
| 1:B:147:TRP:CD2  | 1:B:174:PRO:HB3  | 2.54                     | 0.41              |
| 1:B:155:VAL:HG22 | 1:B:176:VAL:CG2  | 2.51                     | 0.41              |
| 1:C:81:LEU:HD11  | 1:C:96:TYR:CD2   | 2.55                     | 0.41              |
| 1:C:493:ARG:H    | 1:C:493:ARG:HG2  | 1.43                     | 0.41              |
| 1:C:529:ILE:HD13 | 1:C:529:ILE:HA   | 1.80                     | 0.41              |
| 1:D:136:HIS:CD2  | 1:D:180:HIS:CE1  | 3.07                     | 0.41              |
| 1:D:223:LEU:CD2  | 1:D:224:PRO:HD2  | 2.51                     | 0.41              |
| 1:D:499:ILE:HG21 | 1:D:519:LEU:CB   | 2.50                     | 0.41              |
| 1:D:510:MET:HB3  | 1:D:513:LEU:HB2  | 2.02                     | 0.41              |
| 1:E:233:LEU:CD2  | 1:E:250:ILE:HG12 | 2.50                     | 0.41              |
| 1:E:260:TRP:O    | 1:E:261:ILE:HG12 | 2.20                     | 0.41              |
| 1:E:300:LEU:C    | 1:E:303:ARG:HH12 | 2.28                     | 0.41              |
| 1:E:370:ARG:CD   | 1:E:371:GLU:CA   | 2.99                     | 0.41              |
| 1:E:391:PHE:C    | 1:E:392:HIS:CD2  | 2.98                     | 0.41              |
| 1:E:427:SER:CB   | 1:E:487:ARG:HH12 | 2.27                     | 0.41              |
| 1:E:450:LYS:NZ   | 1:E:454:LYS:HD3  | 2.35                     | 0.41              |
| 1:F:386:PHE:C    | 1:F:388:ASN:H    | 2.28                     | 0.41              |
| 1:F:471:LYS:HA   | 1:F:471:LYS:HD2  | 1.61                     | 0.41              |
| 1:F:486:LEU:HD23 | 1:F:486:LEU:HA   | 1.77                     | 0.41              |
| 1:G:324:GLN:HE22 | 1:G:542:LEU:HB2  | 1.84                     | 0.41              |
| 1:A:263:ASP:C    | 1:B:408:LYS:NZ   | 2.79                     | 0.41              |
| 1:A:347:GLU:OE2  | 1:C:274:ARG:HG2  | 2.21                     | 0.41              |
| 1:A:386:PHE:O    | 1:A:388:ASN:N    | 2.50                     | 0.41              |
| 1:A:401:GLU:CD   | 1:A:403:ASP:HB2  | 2.46                     | 0.41              |
| 1:A:486:LEU:HB3  | 1:A:493:ARG:CD   | 2.51                     | 0.41              |
| 1:B:225:ALA:HB1  | 1:G:414:SER:CB   | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:233:LEU:CD2  | 1:B:250:ILE:HG12 | 2.50                     | 0.41              |
| 1:B:261:ILE:H    | 1:B:262:PRO:CD   | 2.34                     | 0.41              |
| 1:B:268:ALA:HA   | 1:B:271:LEU:HD12 | 2.01                     | 0.41              |
| 1:B:362:LEU:HD12 | 1:B:362:LEU:C    | 2.43                     | 0.41              |
| 1:B:413:ARG:HA   | 1:B:413:ARG:HD3  | 1.92                     | 0.41              |
| 1:C:106:TYR:HB3  | 1:C:123:VAL:CG1  | 2.50                     | 0.41              |
| 1:C:379:ASP:CG   | 1:D:276:ARG:HH21 | 2.29                     | 0.41              |
| 1:D:300:LEU:C    | 1:D:303:ARG:HH12 | 2.28                     | 0.41              |
| 1:D:325:GLN:O    | 1:D:326:ALA:C    | 2.64                     | 0.41              |
| 1:D:443:ASP:HA   | 1:D:491:ALA:HB3  | 2.03                     | 0.41              |
| 1:E:124:ARG:CZ   | 1:E:126:LYS:HA   | 2.51                     | 0.41              |
| 1:F:409:LEU:HD23 | 1:F:421:ILE:CG2  | 2.32                     | 0.41              |
| 1:G:216:VAL:CG1  | 1:G:230:VAL:HG22 | 2.49                     | 0.41              |
| 1:G:375:ASN:CG   | 1:G:377:LYS:HG3  | 2.45                     | 0.41              |
| 1:G:510:MET:HB2  | 1:G:513:LEU:CB   | 2.50                     | 0.41              |
| 1:A:81:LEU:HD11  | 1:A:96:TYR:CD2   | 2.56                     | 0.41              |
| 1:A:209:ASP:O    | 1:A:210:GLU:C    | 2.63                     | 0.41              |
| 1:A:262:PRO:HB3  | 1:B:411:TYR:CE1  | 2.56                     | 0.41              |
| 1:A:271:LEU:O    | 1:A:272:ARG:C    | 2.64                     | 0.41              |
| 1:A:499:ILE:HD12 | 1:A:499:ILE:HA   | 1.83                     | 0.41              |
| 1:A:503:GLU:HG3  | 1:A:515:LEU:CD2  | 2.51                     | 0.41              |
| 1:A:536:ASN:C    | 1:A:538:GLU:N    | 2.75                     | 0.41              |
| 1:B:121:GLN:CB   | 1:B:133:THR:CG2  | 2.98                     | 0.41              |
| 1:B:223:LEU:CD2  | 1:B:224:PRO:HD2  | 2.50                     | 0.41              |
| 1:B:440:LYS:NZ   | 1:B:441:MET:CA   | 2.64                     | 0.41              |
| 1:B:503:GLU:HG3  | 1:B:515:LEU:HD23 | 2.02                     | 0.41              |
| 1:B:515:LEU:HD21 | 1:B:529:ILE:HD12 | 2.03                     | 0.41              |
| 1:C:229:ARG:HH21 | 1:C:259:PRO:CB   | 2.32                     | 0.41              |
| 1:C:394:TYR:HE1  | 1:C:396:SER:CB   | 2.32                     | 0.41              |
| 1:C:445:LEU:CD1  | 1:C:449:LEU:HG   | 2.51                     | 0.41              |
| 1:C:446:MET:HB3  | 1:C:491:ALA:HB1  | 2.03                     | 0.41              |
| 1:C:469:PRO:HD3  | 1:C:475:HIS:HE1  | 1.86                     | 0.41              |
| 1:C:492:LEU:C    | 1:C:494:GLN:H    | 2.29                     | 0.41              |
| 1:C:536:ASN:C    | 1:C:536:ASN:ND2  | 2.74                     | 0.41              |
| 1:D:112:ARG:HD2  | 1:D:145:HIS:CE1  | 2.55                     | 0.41              |
| 1:D:200:GLU:O    | 1:D:227:LYS:HE3  | 2.21                     | 0.41              |
| 1:D:243:LEU:O    | 1:D:244:ASN:O    | 2.37                     | 0.41              |
| 1:D:273:GLU:OE2  | 1:D:276:ARG:NH1  | 2.53                     | 0.41              |
| 1:D:327:LEU:HD11 | 1:D:357:HIS:HA   | 2.03                     | 0.41              |
| 1:D:454:LYS:HE3  | 1:D:522:ARG:HH22 | 1.85                     | 0.41              |
| 1:D:504:ARG:HH21 | 1:D:506:GLN:HG2  | 1.86                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:124:ARG:HD3  | 1:E:125:ASP:N    | 2.35                     | 0.41              |
| 1:E:235:CYS:HB2  | 1:E:240:GLU:HG2  | 2.03                     | 0.41              |
| 1:E:313:GLY:C    | 1:E:315:GLY:N    | 2.79                     | 0.41              |
| 1:E:401:GLU:N    | 1:E:430:VAL:O    | 2.54                     | 0.41              |
| 1:E:473:LYS:HE2  | 1:E:479:ARG:CA   | 2.43                     | 0.41              |
| 1:E:510:MET:HE1  | 1:E:547:TYR:CE1  | 2.51                     | 0.41              |
| 1:F:167:GLU:O    | 1:F:168:LEU:C    | 2.60                     | 0.41              |
| 1:F:204:LEU:HD23 | 1:F:204:LEU:N    | 2.36                     | 0.41              |
| 1:F:291:GLY:O    | 1:F:292:CYS:HB2  | 2.21                     | 0.41              |
| 1:F:427:SER:CB   | 1:F:487:ARG:HH12 | 2.30                     | 0.41              |
| 1:F:447:THR:O    | 1:F:448:LYS:C    | 2.64                     | 0.41              |
| 1:A:152:LYS:HD3  | 1:A:203:ILE:CD1  | 2.51                     | 0.41              |
| 1:A:265:VAL:CG2  | 1:B:412:MET:HG2  | 2.51                     | 0.41              |
| 1:A:386:PHE:C    | 1:A:388:ASN:H    | 2.29                     | 0.41              |
| 1:B:412:MET:HE2  | 1:B:421:ILE:HD12 | 2.02                     | 0.41              |
| 1:B:413:ARG:HH21 | 1:B:458:VAL:N    | 2.19                     | 0.41              |
| 1:C:166:MET:HE2  | 1:C:166:MET:HB3  | 1.62                     | 0.41              |
| 1:C:322:VAL:HG11 | 1:C:422:ILE:CG2  | 2.51                     | 0.41              |
| 1:C:484:THR:O    | 1:C:486:LEU:N    | 2.54                     | 0.41              |
| 1:C:521:CYS:O    | 1:C:522:ARG:C    | 2.64                     | 0.41              |
| 1:D:368:LEU:O    | 1:D:369:LYS:C    | 2.62                     | 0.41              |
| 1:D:411:TYR:CD1  | 1:D:411:TYR:C    | 2.99                     | 0.41              |
| 1:E:216:VAL:CG1  | 1:E:230:VAL:HG22 | 2.49                     | 0.41              |
| 1:E:228:VAL:HG23 | 1:E:261:ILE:HD11 | 2.01                     | 0.41              |
| 1:E:309:MET:HE2  | 1:E:462:VAL:HG12 | 2.02                     | 0.41              |
| 1:E:499:ILE:HG21 | 1:E:519:LEU:CB   | 2.51                     | 0.41              |
| 1:F:78:TYR:CG    | 1:F:92:GLN:HG2   | 2.55                     | 0.41              |
| 1:F:316:MET:CE   | 1:F:535:TYR:CZ   | 2.99                     | 0.41              |
| 1:F:327:LEU:HD11 | 1:F:357:HIS:HA   | 2.03                     | 0.41              |
| 1:G:204:LEU:N    | 1:G:204:LEU:HD23 | 2.35                     | 0.41              |
| 1:G:316:MET:HE2  | 1:G:320:THR:OG1  | 2.21                     | 0.41              |
| 1:G:336:LYS:HB3  | 1:G:418:CYS:HB3  | 2.03                     | 0.41              |
| 1:A:446:MET:O    | 1:A:449:LEU:HB2  | 2.20                     | 0.40              |
| 1:B:312:SER:C    | 1:B:313:GLY:O    | 2.63                     | 0.40              |
| 1:B:467:LYS:H    | 1:B:467:LYS:HG3  | 1.50                     | 0.40              |
| 1:D:260:TRP:CB   | 1:D:262:PRO:HG3  | 2.35                     | 0.40              |
| 1:G:463:ILE:CG2  | 1:G:464:CYS:N    | 2.78                     | 0.40              |
| 1:A:316:MET:CE   | 1:A:535:TYR:CZ   | 3.00                     | 0.40              |
| 1:A:482:SER:O    | 1:A:485:ASP:HB2  | 2.21                     | 0.40              |
| 1:A:492:LEU:O    | 1:A:494:GLN:N    | 2.54                     | 0.40              |
| 1:B:295:ILE:HD12 | 1:B:516:VAL:HG11 | 2.04                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:267:SER:O    | 1:D:270:SER:OG   | 2.32                     | 0.40              |
| 1:F:323:ARG:O    | 1:F:326:ALA:HB3  | 2.22                     | 0.40              |
| 1:F:338:GLY:HA2  | 1:F:392:HIS:O    | 2.21                     | 0.40              |
| 1:F:401:GLU:N    | 1:F:404:ARG:HD2  | 2.36                     | 0.40              |
| 1:G:114:GLN:NE2  | 1:G:195:TYR:CD1  | 2.88                     | 0.40              |
| 1:G:155:VAL:HG22 | 1:G:176:VAL:CG2  | 2.51                     | 0.40              |
| 1:G:194:GLU:CD   | 1:G:194:GLU:N    | 2.74                     | 0.40              |
| 1:G:285:VAL:HA   | 1:G:300:LEU:CD1  | 2.51                     | 0.40              |
| 1:G:447:THR:HA   | 1:G:495:LEU:CD2  | 2.50                     | 0.40              |
| 1:G:492:LEU:O    | 1:G:494:GLN:N    | 2.53                     | 0.40              |
| 1:A:536:ASN:HD21 | 1:A:538:GLU:HB3  | 1.86                     | 0.40              |
| 1:B:80:ALA:HB2   | 1:B:88:LYS:N     | 2.36                     | 0.40              |
| 1:B:168:LEU:HD22 | 1:B:247:ASP:OD2  | 2.15                     | 0.40              |
| 1:B:391:PHE:C    | 1:B:392:HIS:CD2  | 2.99                     | 0.40              |
| 1:B:440:LYS:HZ2  | 1:B:441:MET:HA   | 1.76                     | 0.40              |
| 1:C:142:PHE:CD2  | 1:C:162:MET:HE3  | 2.56                     | 0.40              |
| 1:C:229:ARG:HH21 | 1:C:259:PRO:HB3  | 1.82                     | 0.40              |
| 1:D:309:MET:HE2  | 1:D:462:VAL:HG12 | 2.03                     | 0.40              |
| 1:D:442:ILE:HG23 | 1:D:443:ASP:N    | 2.36                     | 0.40              |
| 1:D:446:MET:HE2  | 1:D:492:LEU:HA   | 2.03                     | 0.40              |
| 1:F:502:LEU:HD12 | 1:F:502:LEU:N    | 2.35                     | 0.40              |
| 1:F:542:LEU:HA   | 1:F:542:LEU:HD12 | 1.63                     | 0.40              |
| 1:G:322:VAL:CG1  | 1:G:422:ILE:HG21 | 2.51                     | 0.40              |
| 1:G:482:SER:CB   | 1:G:484:THR:HG23 | 2.51                     | 0.40              |
| 1:G:495:LEU:N    | 1:G:495:LEU:CD1  | 2.84                     | 0.40              |
| 1:G:504:ARG:CG   | 1:G:506:GLN:HG2  | 2.51                     | 0.40              |
| 1:A:471:LYS:HA   | 1:A:471:LYS:HD2  | 1.64                     | 0.40              |
| 1:A:536:ASN:ND2  | 1:A:538:GLU:HB2  | 2.36                     | 0.40              |
| 1:B:81:LEU:HD22  | 1:B:107:GLN:NE2  | 2.36                     | 0.40              |
| 1:B:149:GLY:O    | 1:B:199:PHE:CE2  | 2.75                     | 0.40              |
| 1:B:273:GLU:O    | 1:B:274:ARG:C    | 2.65                     | 0.40              |
| 1:B:300:LEU:O    | 1:B:300:LEU:HD13 | 2.21                     | 0.40              |
| 1:C:152:LYS:O    | 1:C:174:PRO:HD2  | 2.21                     | 0.40              |
| 1:C:232:VAL:O    | 1:C:232:VAL:HG12 | 2.20                     | 0.40              |
| 1:C:401:GLU:HG2  | 1:C:402:THR:H    | 1.86                     | 0.40              |
| 1:C:408:LYS:O    | 1:C:412:MET:HG3  | 2.21                     | 0.40              |
| 1:C:471:LYS:HD2  | 1:C:472:GLY:N    | 2.36                     | 0.40              |
| 1:C:502:LEU:N    | 1:C:502:LEU:HD12 | 2.37                     | 0.40              |
| 1:C:536:ASN:HD21 | 1:C:538:GLU:HB3  | 1.83                     | 0.40              |
| 1:D:74:SER:O     | 1:D:76:GLY:N     | 2.54                     | 0.40              |
| 1:D:170:ASP:O    | 1:D:172:LYS:HG3  | 2.20                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:248:ARG:O    | 1:D:248:ARG:HG2  | 2.22                     | 0.40              |
| 1:D:318:MET:SD   | 1:D:463:ILE:HD12 | 2.61                     | 0.40              |
| 1:D:346:VAL:CB   | 1:D:395:ASP:HB2  | 2.50                     | 0.40              |
| 1:E:386:PHE:HB3  | 1:F:269:LEU:HD13 | 2.03                     | 0.40              |
| 1:F:121:GLN:CB   | 1:F:133:THR:CG2  | 2.99                     | 0.40              |
| 1:F:125:ASP:O    | 1:F:126:LYS:C    | 2.64                     | 0.40              |
| 1:F:322:VAL:HG21 | 1:F:463:ILE:CD1  | 2.52                     | 0.40              |
| 1:F:429:VAL:HG13 | 1:F:438:GLU:OE1  | 2.22                     | 0.40              |
| 1:F:447:THR:HA   | 1:F:495:LEU:CD2  | 2.52                     | 0.40              |
| 1:G:79:SER:H     | 1:G:98:ILE:CD1   | 2.29                     | 0.40              |
| 1:G:413:ARG:HA   | 1:G:413:ARG:HD3  | 1.86                     | 0.40              |
| 1:A:265:VAL:C    | 1:A:266:VAL:CG2  | 2.94                     | 0.40              |
| 1:A:324:GLN:OE1  | 1:A:541:TRP:HE3  | 2.05                     | 0.40              |
| 1:B:481:VAL:HG13 | 1:B:503:GLU:OE2  | 2.20                     | 0.40              |
| 1:C:90:THR:O     | 1:C:91:CYS:C     | 2.62                     | 0.40              |
| 1:C:276:ARG:HH11 | 1:C:276:ARG:CG   | 2.34                     | 0.40              |
| 1:C:443:ASP:O    | 1:C:447:THR:HG23 | 2.22                     | 0.40              |
| 1:C:498:THR:C    | 1:C:499:ILE:HD13 | 2.46                     | 0.40              |
| 1:D:122:LYS:HE3  | 1:D:130:PHE:HE2  | 1.86                     | 0.40              |
| 1:D:427:SER:CB   | 1:D:487:ARG:NH1  | 2.84                     | 0.40              |
| 1:D:439:ARG:HG2  | 1:D:489:SER:OG   | 2.21                     | 0.40              |
| 1:E:80:ALA:HB2   | 1:E:88:LYS:N     | 2.36                     | 0.40              |
| 1:E:180:HIS:CD2  | 1:E:180:HIS:N    | 2.89                     | 0.40              |
| 1:E:345:SER:OG   | 1:E:347:GLU:HG2  | 2.21                     | 0.40              |
| 1:E:405:LEU:HD21 | 1:E:409:LEU:HD11 | 2.04                     | 0.40              |
| 1:G:112:ARG:NH2  | 1:G:118:ILE:HD11 | 2.36                     | 0.40              |
| 1:G:445:LEU:HD11 | 1:G:449:LEU:HG   | 2.03                     | 0.40              |
| 1:G:454:LYS:HE3  | 1:G:522:ARG:HH22 | 1.87                     | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 479/503 (95%)   | 377 (79%)  | 68 (14%)  | 34 (7%)  | 1           | 10 |
| 1   | B     | 479/503 (95%)   | 384 (80%)  | 65 (14%)  | 30 (6%)  | 1           | 12 |
| 1   | C     | 479/503 (95%)   | 385 (80%)  | 57 (12%)  | 37 (8%)  | 1           | 8  |
| 1   | D     | 479/503 (95%)   | 377 (79%)  | 66 (14%)  | 36 (8%)  | 1           | 9  |
| 1   | E     | 479/503 (95%)   | 381 (80%)  | 65 (14%)  | 33 (7%)  | 1           | 10 |
| 1   | F     | 479/503 (95%)   | 380 (79%)  | 63 (13%)  | 36 (8%)  | 1           | 9  |
| 1   | G     | 479/503 (95%)   | 386 (81%)  | 67 (14%)  | 26 (5%)  | 1           | 14 |
| All | All   | 3353/3521 (95%) | 2670 (80%) | 451 (14%) | 232 (7%) | 1           | 10 |

All (232) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 128 | LYS  |
| 1   | A     | 182 | ALA  |
| 1   | A     | 244 | ASN  |
| 1   | A     | 258 | GLY  |
| 1   | A     | 261 | ILE  |
| 1   | A     | 432 | ALA  |
| 1   | B     | 128 | LYS  |
| 1   | B     | 182 | ALA  |
| 1   | B     | 244 | ASN  |
| 1   | B     | 261 | ILE  |
| 1   | B     | 313 | GLY  |
| 1   | B     | 429 | VAL  |
| 1   | B     | 432 | ALA  |
| 1   | C     | 128 | LYS  |
| 1   | C     | 182 | ALA  |
| 1   | C     | 244 | ASN  |
| 1   | C     | 261 | ILE  |
| 1   | C     | 284 | SER  |
| 1   | C     | 315 | GLY  |
| 1   | C     | 327 | LEU  |
| 1   | C     | 429 | VAL  |
| 1   | C     | 432 | ALA  |
| 1   | D     | 128 | LYS  |
| 1   | D     | 182 | ALA  |
| 1   | D     | 244 | ASN  |
| 1   | D     | 284 | SER  |
| 1   | D     | 432 | ALA  |
| 1   | E     | 128 | LYS  |
| 1   | E     | 182 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 244 | ASN  |
| 1   | E     | 261 | ILE  |
| 1   | E     | 425 | HIS  |
| 1   | E     | 432 | ALA  |
| 1   | F     | 128 | LYS  |
| 1   | F     | 182 | ALA  |
| 1   | F     | 244 | ASN  |
| 1   | F     | 259 | PRO  |
| 1   | F     | 261 | ILE  |
| 1   | F     | 284 | SER  |
| 1   | F     | 425 | HIS  |
| 1   | F     | 429 | VAL  |
| 1   | F     | 432 | ALA  |
| 1   | G     | 128 | LYS  |
| 1   | G     | 182 | ALA  |
| 1   | G     | 244 | ASN  |
| 1   | G     | 261 | ILE  |
| 1   | G     | 313 | GLY  |
| 1   | G     | 429 | VAL  |
| 1   | G     | 432 | ALA  |
| 1   | A     | 126 | LYS  |
| 1   | A     | 169 | GLN  |
| 1   | A     | 171 | CYS  |
| 1   | A     | 210 | GLU  |
| 1   | A     | 257 | ALA  |
| 1   | A     | 287 | LEU  |
| 1   | A     | 292 | CYS  |
| 1   | A     | 313 | GLY  |
| 1   | A     | 314 | SER  |
| 1   | A     | 315 | GLY  |
| 1   | A     | 425 | HIS  |
| 1   | A     | 429 | VAL  |
| 1   | A     | 472 | GLY  |
| 1   | B     | 168 | LEU  |
| 1   | B     | 210 | GLU  |
| 1   | B     | 243 | LEU  |
| 1   | B     | 315 | GLY  |
| 1   | B     | 425 | HIS  |
| 1   | B     | 472 | GLY  |
| 1   | B     | 485 | ASP  |
| 1   | C     | 168 | LEU  |
| 1   | C     | 210 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 243 | LEU  |
| 1   | C     | 313 | GLY  |
| 1   | C     | 425 | HIS  |
| 1   | C     | 472 | GLY  |
| 1   | D     | 168 | LEU  |
| 1   | D     | 210 | GLU  |
| 1   | D     | 243 | LEU  |
| 1   | D     | 260 | TRP  |
| 1   | D     | 287 | LEU  |
| 1   | D     | 313 | GLY  |
| 1   | D     | 315 | GLY  |
| 1   | D     | 425 | HIS  |
| 1   | D     | 429 | VAL  |
| 1   | D     | 472 | GLY  |
| 1   | E     | 168 | LEU  |
| 1   | E     | 210 | GLU  |
| 1   | E     | 243 | LEU  |
| 1   | E     | 292 | CYS  |
| 1   | E     | 313 | GLY  |
| 1   | E     | 314 | SER  |
| 1   | E     | 315 | GLY  |
| 1   | E     | 429 | VAL  |
| 1   | E     | 472 | GLY  |
| 1   | F     | 168 | LEU  |
| 1   | F     | 181 | GLY  |
| 1   | F     | 210 | GLU  |
| 1   | F     | 287 | LEU  |
| 1   | F     | 313 | GLY  |
| 1   | F     | 315 | GLY  |
| 1   | F     | 472 | GLY  |
| 1   | F     | 548 | SER  |
| 1   | G     | 168 | LEU  |
| 1   | G     | 210 | GLU  |
| 1   | G     | 243 | LEU  |
| 1   | G     | 315 | GLY  |
| 1   | G     | 425 | HIS  |
| 1   | G     | 472 | GLY  |
| 1   | A     | 243 | LEU  |
| 1   | A     | 256 | ASN  |
| 1   | A     | 259 | PRO  |
| 1   | A     | 284 | SER  |
| 1   | A     | 523 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 292 | CYS  |
| 1   | B     | 317 | VAL  |
| 1   | C     | 181 | GLY  |
| 1   | C     | 287 | LEU  |
| 1   | C     | 292 | CYS  |
| 1   | D     | 292 | CYS  |
| 1   | D     | 314 | SER  |
| 1   | D     | 485 | ASP  |
| 1   | E     | 259 | PRO  |
| 1   | E     | 287 | LEU  |
| 1   | E     | 485 | ASP  |
| 1   | E     | 523 | PHE  |
| 1   | F     | 243 | LEU  |
| 1   | F     | 292 | CYS  |
| 1   | F     | 314 | SER  |
| 1   | F     | 453 | ALA  |
| 1   | F     | 485 | ASP  |
| 1   | F     | 493 | ARG  |
| 1   | G     | 287 | LEU  |
| 1   | G     | 317 | VAL  |
| 1   | G     | 485 | ASP  |
| 1   | B     | 181 | GLY  |
| 1   | B     | 469 | PRO  |
| 1   | B     | 487 | ARG  |
| 1   | B     | 520 | LYS  |
| 1   | C     | 260 | TRP  |
| 1   | C     | 431 | SER  |
| 1   | C     | 469 | PRO  |
| 1   | C     | 479 | ARG  |
| 1   | C     | 485 | ASP  |
| 1   | C     | 547 | TYR  |
| 1   | D     | 75  | ASN  |
| 1   | D     | 453 | ALA  |
| 1   | D     | 469 | PRO  |
| 1   | E     | 181 | GLY  |
| 1   | E     | 317 | VAL  |
| 1   | E     | 469 | PRO  |
| 1   | E     | 493 | ARG  |
| 1   | F     | 469 | PRO  |
| 1   | F     | 520 | LYS  |
| 1   | F     | 547 | TYR  |
| 1   | G     | 181 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 292 | CYS  |
| 1   | G     | 523 | PHE  |
| 1   | A     | 430 | VAL  |
| 1   | A     | 431 | SER  |
| 1   | A     | 469 | PRO  |
| 1   | A     | 474 | ALA  |
| 1   | A     | 485 | ASP  |
| 1   | A     | 520 | LYS  |
| 1   | A     | 548 | SER  |
| 1   | B     | 430 | VAL  |
| 1   | B     | 431 | SER  |
| 1   | B     | 479 | ARG  |
| 1   | B     | 493 | ARG  |
| 1   | B     | 495 | LEU  |
| 1   | C     | 75  | ASN  |
| 1   | C     | 259 | PRO  |
| 1   | C     | 262 | PRO  |
| 1   | C     | 295 | ILE  |
| 1   | C     | 430 | VAL  |
| 1   | C     | 453 | ALA  |
| 1   | C     | 548 | SER  |
| 1   | D     | 430 | VAL  |
| 1   | D     | 431 | SER  |
| 1   | D     | 520 | LYS  |
| 1   | E     | 364 | GLN  |
| 1   | E     | 430 | VAL  |
| 1   | E     | 431 | SER  |
| 1   | E     | 520 | LYS  |
| 1   | F     | 312 | SER  |
| 1   | F     | 389 | ASP  |
| 1   | F     | 430 | VAL  |
| 1   | F     | 431 | SER  |
| 1   | F     | 479 | ARG  |
| 1   | F     | 523 | PHE  |
| 1   | G     | 75  | ASN  |
| 1   | G     | 430 | VAL  |
| 1   | G     | 431 | SER  |
| 1   | G     | 469 | PRO  |
| 1   | G     | 479 | ARG  |
| 1   | A     | 434 | GLY  |
| 1   | A     | 479 | ARG  |
| 1   | C     | 436 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 181 | GLY  |
| 1   | D     | 327 | LEU  |
| 1   | D     | 474 | ALA  |
| 1   | D     | 479 | ARG  |
| 1   | D     | 493 | ARG  |
| 1   | D     | 548 | SER  |
| 1   | E     | 75  | ASN  |
| 1   | E     | 453 | ALA  |
| 1   | F     | 317 | VAL  |
| 1   | F     | 364 | GLN  |
| 1   | G     | 295 | ILE  |
| 1   | B     | 286 | GLY  |
| 1   | C     | 317 | VAL  |
| 1   | C     | 354 | ILE  |
| 1   | D     | 317 | VAL  |
| 1   | F     | 434 | GLY  |
| 1   | B     | 354 | ILE  |
| 1   | B     | 434 | GLY  |
| 1   | C     | 434 | GLY  |
| 1   | D     | 434 | GLY  |
| 1   | E     | 434 | GLY  |
| 1   | G     | 434 | GLY  |
| 1   | B     | 295 | ILE  |
| 1   | D     | 285 | VAL  |
| 1   | E     | 285 | VAL  |
| 1   | E     | 479 | ARG  |
| 1   | A     | 285 | VAL  |
| 1   | C     | 266 | VAL  |
| 1   | C     | 285 | VAL  |
| 1   | D     | 259 | PRO  |
| 1   | D     | 264 | GLY  |
| 1   | D     | 295 | ILE  |
| 1   | E     | 262 | PRO  |
| 1   | F     | 285 | VAL  |
| 1   | B     | 285 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |   |
|-----|-------|-----------------|------------|------------|-------------|---|
| 1   | A     | 401/421 (95%)   | 240 (60%)  | 161 (40%)  | 0           | 1 |
| 1   | B     | 401/421 (95%)   | 247 (62%)  | 154 (38%)  | 0           | 1 |
| 1   | C     | 401/421 (95%)   | 245 (61%)  | 156 (39%)  | 0           | 1 |
| 1   | D     | 401/421 (95%)   | 250 (62%)  | 151 (38%)  | 0           | 1 |
| 1   | E     | 401/421 (95%)   | 244 (61%)  | 157 (39%)  | 0           | 1 |
| 1   | F     | 401/421 (95%)   | 241 (60%)  | 160 (40%)  | 0           | 1 |
| 1   | G     | 401/421 (95%)   | 248 (62%)  | 153 (38%)  | 0           | 1 |
| All | All   | 2807/2947 (95%) | 1715 (61%) | 1092 (39%) | 0           | 1 |

All (1092) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 65  | THR  |
| 1   | A     | 68  | VAL  |
| 1   | A     | 74  | SER  |
| 1   | A     | 77  | ARG  |
| 1   | A     | 89  | GLU  |
| 1   | A     | 90  | THR  |
| 1   | A     | 93  | LYS  |
| 1   | A     | 100 | LYS  |
| 1   | A     | 104 | VAL  |
| 1   | A     | 105 | MET  |
| 1   | A     | 107 | GLN  |
| 1   | A     | 108 | VAL  |
| 1   | A     | 112 | ARG  |
| 1   | A     | 115 | ASN  |
| 1   | A     | 117 | ASN  |
| 1   | A     | 118 | ILE  |
| 1   | A     | 119 | VAL  |
| 1   | A     | 121 | GLN  |
| 1   | A     | 122 | LYS  |
| 1   | A     | 123 | VAL  |
| 1   | A     | 124 | ARG  |
| 1   | A     | 126 | LYS  |
| 1   | A     | 127 | ASP  |
| 1   | A     | 128 | LYS  |
| 1   | A     | 131 | LYS  |
| 1   | A     | 132 | THR  |
| 1   | A     | 133 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 141 | LEU  |
| 1   | A     | 144 | LYS  |
| 1   | A     | 147 | TRP  |
| 1   | A     | 148 | ASN  |
| 1   | A     | 153 | ILE  |
| 1   | A     | 160 | ILE  |
| 1   | A     | 163 | LEU  |
| 1   | A     | 166 | MET  |
| 1   | A     | 167 | GLU  |
| 1   | A     | 168 | LEU  |
| 1   | A     | 169 | GLN  |
| 1   | A     | 172 | LYS  |
| 1   | A     | 175 | VAL  |
| 1   | A     | 177 | SER  |
| 1   | A     | 183 | SER  |
| 1   | A     | 186 | LYS  |
| 1   | A     | 187 | LYS  |
| 1   | A     | 188 | THR  |
| 1   | A     | 189 | CYS  |
| 1   | A     | 194 | GLU  |
| 1   | A     | 200 | GLU  |
| 1   | A     | 203 | ILE  |
| 1   | A     | 204 | LEU  |
| 1   | A     | 210 | GLU  |
| 1   | A     | 213 | ARG  |
| 1   | A     | 214 | LYS  |
| 1   | A     | 218 | GLU  |
| 1   | A     | 221 | GLN  |
| 1   | A     | 223 | LEU  |
| 1   | A     | 228 | VAL  |
| 1   | A     | 229 | ARG  |
| 1   | A     | 230 | VAL  |
| 1   | A     | 235 | CYS  |
| 1   | A     | 243 | LEU  |
| 1   | A     | 246 | HIS  |
| 1   | A     | 248 | ARG  |
| 1   | A     | 249 | GLU  |
| 1   | A     | 251 | MET  |
| 1   | A     | 255 | TRP  |
| 1   | A     | 261 | ILE  |
| 1   | A     | 265 | VAL  |
| 1   | A     | 269 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 272 | ARG  |
| 1   | A     | 274 | ARG  |
| 1   | A     | 276 | ARG  |
| 1   | A     | 277 | GLU  |
| 1   | A     | 281 | SER  |
| 1   | A     | 282 | GLU  |
| 1   | A     | 283 | GLU  |
| 1   | A     | 284 | SER  |
| 1   | A     | 285 | VAL  |
| 1   | A     | 287 | LEU  |
| 1   | A     | 290 | SER  |
| 1   | A     | 295 | ILE  |
| 1   | A     | 300 | LEU  |
| 1   | A     | 307 | VAL  |
| 1   | A     | 309 | MET  |
| 1   | A     | 316 | MET  |
| 1   | A     | 317 | VAL  |
| 1   | A     | 319 | SER  |
| 1   | A     | 323 | ARG  |
| 1   | A     | 324 | GLN  |
| 1   | A     | 325 | GLN  |
| 1   | A     | 327 | LEU  |
| 1   | A     | 328 | GLN  |
| 1   | A     | 336 | LYS  |
| 1   | A     | 347 | GLU  |
| 1   | A     | 349 | THR  |
| 1   | A     | 363 | ARG  |
| 1   | A     | 368 | LEU  |
| 1   | A     | 369 | LYS  |
| 1   | A     | 370 | ARG  |
| 1   | A     | 371 | GLU  |
| 1   | A     | 377 | LYS  |
| 1   | A     | 388 | ASN  |
| 1   | A     | 390 | THR  |
| 1   | A     | 393 | LEU  |
| 1   | A     | 394 | TYR  |
| 1   | A     | 395 | ASP  |
| 1   | A     | 406 | LEU  |
| 1   | A     | 409 | LEU  |
| 1   | A     | 412 | MET  |
| 1   | A     | 416 | LEU  |
| 1   | A     | 418 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 419 | ASP  |
| 1   | A     | 426 | ILE  |
| 1   | A     | 430 | VAL  |
| 1   | A     | 431 | SER  |
| 1   | A     | 433 | SER  |
| 1   | A     | 435 | GLU  |
| 1   | A     | 437 | ASP  |
| 1   | A     | 438 | GLU  |
| 1   | A     | 440 | LYS  |
| 1   | A     | 441 | MET  |
| 1   | A     | 442 | ILE  |
| 1   | A     | 446 | MET  |
| 1   | A     | 454 | LYS  |
| 1   | A     | 455 | SER  |
| 1   | A     | 461 | VAL  |
| 1   | A     | 463 | ILE  |
| 1   | A     | 464 | CYS  |
| 1   | A     | 467 | LYS  |
| 1   | A     | 468 | ASN  |
| 1   | A     | 470 | ASP  |
| 1   | A     | 471 | LYS  |
| 1   | A     | 476 | GLU  |
| 1   | A     | 479 | ARG  |
| 1   | A     | 481 | VAL  |
| 1   | A     | 483 | ILE  |
| 1   | A     | 484 | THR  |
| 1   | A     | 485 | ASP  |
| 1   | A     | 486 | LEU  |
| 1   | A     | 487 | ARG  |
| 1   | A     | 492 | LEU  |
| 1   | A     | 493 | ARG  |
| 1   | A     | 499 | ILE  |
| 1   | A     | 502 | LEU  |
| 1   | A     | 503 | GLU  |
| 1   | A     | 504 | ARG  |
| 1   | A     | 506 | GLN  |
| 1   | A     | 507 | GLN  |
| 1   | A     | 511 | PRO  |
| 1   | A     | 514 | VAL  |
| 1   | A     | 516 | VAL  |
| 1   | A     | 517 | ARG  |
| 1   | A     | 520 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 522 | ARG  |
| 1   | A     | 524 | THR  |
| 1   | A     | 533 | MET  |
| 1   | A     | 534 | GLU  |
| 1   | A     | 538 | GLU  |
| 1   | A     | 542 | LEU  |
| 1   | A     | 543 | GLU  |
| 1   | A     | 548 | SER  |
| 1   | B     | 65  | THR  |
| 1   | B     | 68  | VAL  |
| 1   | B     | 89  | GLU  |
| 1   | B     | 90  | THR  |
| 1   | B     | 92  | GLN  |
| 1   | B     | 100 | LYS  |
| 1   | B     | 104 | VAL  |
| 1   | B     | 105 | MET  |
| 1   | B     | 107 | GLN  |
| 1   | B     | 108 | VAL  |
| 1   | B     | 112 | ARG  |
| 1   | B     | 115 | ASN  |
| 1   | B     | 117 | ASN  |
| 1   | B     | 119 | VAL  |
| 1   | B     | 121 | GLN  |
| 1   | B     | 122 | LYS  |
| 1   | B     | 124 | ARG  |
| 1   | B     | 126 | LYS  |
| 1   | B     | 127 | ASP  |
| 1   | B     | 131 | LYS  |
| 1   | B     | 132 | THR  |
| 1   | B     | 133 | THR  |
| 1   | B     | 141 | LEU  |
| 1   | B     | 147 | TRP  |
| 1   | B     | 148 | ASN  |
| 1   | B     | 151 | LYS  |
| 1   | B     | 153 | ILE  |
| 1   | B     | 160 | ILE  |
| 1   | B     | 163 | LEU  |
| 1   | B     | 166 | MET  |
| 1   | B     | 167 | GLU  |
| 1   | B     | 175 | VAL  |
| 1   | B     | 177 | SER  |
| 1   | B     | 183 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 186 | LYS  |
| 1   | B     | 187 | LYS  |
| 1   | B     | 188 | THR  |
| 1   | B     | 189 | CYS  |
| 1   | B     | 194 | GLU  |
| 1   | B     | 200 | GLU  |
| 1   | B     | 203 | ILE  |
| 1   | B     | 204 | LEU  |
| 1   | B     | 210 | GLU  |
| 1   | B     | 213 | ARG  |
| 1   | B     | 214 | LYS  |
| 1   | B     | 218 | GLU  |
| 1   | B     | 221 | GLN  |
| 1   | B     | 223 | LEU  |
| 1   | B     | 228 | VAL  |
| 1   | B     | 229 | ARG  |
| 1   | B     | 230 | VAL  |
| 1   | B     | 235 | CYS  |
| 1   | B     | 243 | LEU  |
| 1   | B     | 244 | ASN  |
| 1   | B     | 246 | HIS  |
| 1   | B     | 248 | ARG  |
| 1   | B     | 249 | GLU  |
| 1   | B     | 251 | MET  |
| 1   | B     | 255 | TRP  |
| 1   | B     | 261 | ILE  |
| 1   | B     | 265 | VAL  |
| 1   | B     | 269 | LEU  |
| 1   | B     | 272 | ARG  |
| 1   | B     | 276 | ARG  |
| 1   | B     | 277 | GLU  |
| 1   | B     | 280 | SER  |
| 1   | B     | 281 | SER  |
| 1   | B     | 282 | GLU  |
| 1   | B     | 287 | LEU  |
| 1   | B     | 290 | SER  |
| 1   | B     | 295 | ILE  |
| 1   | B     | 300 | LEU  |
| 1   | B     | 307 | VAL  |
| 1   | B     | 309 | MET  |
| 1   | B     | 316 | MET  |
| 1   | B     | 317 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 319 | SER  |
| 1   | B     | 323 | ARG  |
| 1   | B     | 324 | GLN  |
| 1   | B     | 325 | GLN  |
| 1   | B     | 327 | LEU  |
| 1   | B     | 328 | GLN  |
| 1   | B     | 333 | MET  |
| 1   | B     | 336 | LYS  |
| 1   | B     | 343 | GLU  |
| 1   | B     | 347 | GLU  |
| 1   | B     | 349 | THR  |
| 1   | B     | 356 | LEU  |
| 1   | B     | 363 | ARG  |
| 1   | B     | 368 | LEU  |
| 1   | B     | 369 | LYS  |
| 1   | B     | 370 | ARG  |
| 1   | B     | 371 | GLU  |
| 1   | B     | 377 | LYS  |
| 1   | B     | 388 | ASN  |
| 1   | B     | 390 | THR  |
| 1   | B     | 393 | LEU  |
| 1   | B     | 395 | ASP  |
| 1   | B     | 404 | ARG  |
| 1   | B     | 406 | LEU  |
| 1   | B     | 409 | LEU  |
| 1   | B     | 412 | MET  |
| 1   | B     | 416 | LEU  |
| 1   | B     | 418 | CYS  |
| 1   | B     | 419 | ASP  |
| 1   | B     | 426 | ILE  |
| 1   | B     | 430 | VAL  |
| 1   | B     | 431 | SER  |
| 1   | B     | 433 | SER  |
| 1   | B     | 435 | GLU  |
| 1   | B     | 437 | ASP  |
| 1   | B     | 440 | LYS  |
| 1   | B     | 441 | MET  |
| 1   | B     | 442 | ILE  |
| 1   | B     | 446 | MET  |
| 1   | B     | 454 | LYS  |
| 1   | B     | 455 | SER  |
| 1   | B     | 461 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 463 | ILE  |
| 1   | B     | 464 | CYS  |
| 1   | B     | 467 | LYS  |
| 1   | B     | 468 | ASN  |
| 1   | B     | 470 | ASP  |
| 1   | B     | 471 | LYS  |
| 1   | B     | 476 | GLU  |
| 1   | B     | 479 | ARG  |
| 1   | B     | 481 | VAL  |
| 1   | B     | 483 | ILE  |
| 1   | B     | 484 | THR  |
| 1   | B     | 485 | ASP  |
| 1   | B     | 486 | LEU  |
| 1   | B     | 487 | ARG  |
| 1   | B     | 492 | LEU  |
| 1   | B     | 493 | ARG  |
| 1   | B     | 495 | LEU  |
| 1   | B     | 499 | ILE  |
| 1   | B     | 502 | LEU  |
| 1   | B     | 503 | GLU  |
| 1   | B     | 504 | ARG  |
| 1   | B     | 505 | ASN  |
| 1   | B     | 506 | GLN  |
| 1   | B     | 507 | GLN  |
| 1   | B     | 514 | VAL  |
| 1   | B     | 516 | VAL  |
| 1   | B     | 517 | ARG  |
| 1   | B     | 520 | LYS  |
| 1   | B     | 522 | ARG  |
| 1   | B     | 524 | THR  |
| 1   | B     | 533 | MET  |
| 1   | B     | 534 | GLU  |
| 1   | B     | 538 | GLU  |
| 1   | B     | 542 | LEU  |
| 1   | B     | 543 | GLU  |
| 1   | B     | 548 | SER  |
| 1   | C     | 65  | THR  |
| 1   | C     | 68  | VAL  |
| 1   | C     | 77  | ARG  |
| 1   | C     | 89  | GLU  |
| 1   | C     | 90  | THR  |
| 1   | C     | 92  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 100 | LYS  |
| 1   | C     | 104 | VAL  |
| 1   | C     | 105 | MET  |
| 1   | C     | 107 | GLN  |
| 1   | C     | 108 | VAL  |
| 1   | C     | 112 | ARG  |
| 1   | C     | 115 | ASN  |
| 1   | C     | 117 | ASN  |
| 1   | C     | 119 | VAL  |
| 1   | C     | 121 | GLN  |
| 1   | C     | 122 | LYS  |
| 1   | C     | 124 | ARG  |
| 1   | C     | 126 | LYS  |
| 1   | C     | 127 | ASP  |
| 1   | C     | 131 | LYS  |
| 1   | C     | 132 | THR  |
| 1   | C     | 133 | THR  |
| 1   | C     | 141 | LEU  |
| 1   | C     | 147 | TRP  |
| 1   | C     | 148 | ASN  |
| 1   | C     | 151 | LYS  |
| 1   | C     | 153 | ILE  |
| 1   | C     | 163 | LEU  |
| 1   | C     | 166 | MET  |
| 1   | C     | 167 | GLU  |
| 1   | C     | 175 | VAL  |
| 1   | C     | 177 | SER  |
| 1   | C     | 183 | SER  |
| 1   | C     | 186 | LYS  |
| 1   | C     | 187 | LYS  |
| 1   | C     | 188 | THR  |
| 1   | C     | 189 | CYS  |
| 1   | C     | 194 | GLU  |
| 1   | C     | 200 | GLU  |
| 1   | C     | 203 | ILE  |
| 1   | C     | 204 | LEU  |
| 1   | C     | 208 | MET  |
| 1   | C     | 210 | GLU  |
| 1   | C     | 213 | ARG  |
| 1   | C     | 214 | LYS  |
| 1   | C     | 218 | GLU  |
| 1   | C     | 221 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 223 | LEU  |
| 1   | C     | 228 | VAL  |
| 1   | C     | 229 | ARG  |
| 1   | C     | 230 | VAL  |
| 1   | C     | 235 | CYS  |
| 1   | C     | 243 | LEU  |
| 1   | C     | 246 | HIS  |
| 1   | C     | 248 | ARG  |
| 1   | C     | 249 | GLU  |
| 1   | C     | 251 | MET  |
| 1   | C     | 255 | TRP  |
| 1   | C     | 260 | TRP  |
| 1   | C     | 261 | ILE  |
| 1   | C     | 265 | VAL  |
| 1   | C     | 269 | LEU  |
| 1   | C     | 272 | ARG  |
| 1   | C     | 274 | ARG  |
| 1   | C     | 276 | ARG  |
| 1   | C     | 277 | GLU  |
| 1   | C     | 281 | SER  |
| 1   | C     | 282 | GLU  |
| 1   | C     | 283 | GLU  |
| 1   | C     | 284 | SER  |
| 1   | C     | 285 | VAL  |
| 1   | C     | 287 | LEU  |
| 1   | C     | 290 | SER  |
| 1   | C     | 295 | ILE  |
| 1   | C     | 300 | LEU  |
| 1   | C     | 307 | VAL  |
| 1   | C     | 309 | MET  |
| 1   | C     | 316 | MET  |
| 1   | C     | 317 | VAL  |
| 1   | C     | 319 | SER  |
| 1   | C     | 323 | ARG  |
| 1   | C     | 324 | GLN  |
| 1   | C     | 325 | GLN  |
| 1   | C     | 327 | LEU  |
| 1   | C     | 336 | LYS  |
| 1   | C     | 343 | GLU  |
| 1   | C     | 347 | GLU  |
| 1   | C     | 349 | THR  |
| 1   | C     | 363 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 368 | LEU  |
| 1   | C     | 369 | LYS  |
| 1   | C     | 370 | ARG  |
| 1   | C     | 371 | GLU  |
| 1   | C     | 377 | LYS  |
| 1   | C     | 388 | ASN  |
| 1   | C     | 393 | LEU  |
| 1   | C     | 394 | TYR  |
| 1   | C     | 395 | ASP  |
| 1   | C     | 406 | LEU  |
| 1   | C     | 409 | LEU  |
| 1   | C     | 412 | MET  |
| 1   | C     | 416 | LEU  |
| 1   | C     | 418 | CYS  |
| 1   | C     | 419 | ASP  |
| 1   | C     | 426 | ILE  |
| 1   | C     | 430 | VAL  |
| 1   | C     | 431 | SER  |
| 1   | C     | 435 | GLU  |
| 1   | C     | 437 | ASP  |
| 1   | C     | 438 | GLU  |
| 1   | C     | 440 | LYS  |
| 1   | C     | 441 | MET  |
| 1   | C     | 442 | ILE  |
| 1   | C     | 446 | MET  |
| 1   | C     | 454 | LYS  |
| 1   | C     | 455 | SER  |
| 1   | C     | 461 | VAL  |
| 1   | C     | 463 | ILE  |
| 1   | C     | 464 | CYS  |
| 1   | C     | 467 | LYS  |
| 1   | C     | 468 | ASN  |
| 1   | C     | 470 | ASP  |
| 1   | C     | 471 | LYS  |
| 1   | C     | 476 | GLU  |
| 1   | C     | 479 | ARG  |
| 1   | C     | 481 | VAL  |
| 1   | C     | 483 | ILE  |
| 1   | C     | 484 | THR  |
| 1   | C     | 485 | ASP  |
| 1   | C     | 486 | LEU  |
| 1   | C     | 487 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 492 | LEU  |
| 1   | C     | 493 | ARG  |
| 1   | C     | 495 | LEU  |
| 1   | C     | 496 | SER  |
| 1   | C     | 499 | ILE  |
| 1   | C     | 502 | LEU  |
| 1   | C     | 503 | GLU  |
| 1   | C     | 505 | ASN  |
| 1   | C     | 506 | GLN  |
| 1   | C     | 507 | GLN  |
| 1   | C     | 514 | VAL  |
| 1   | C     | 516 | VAL  |
| 1   | C     | 517 | ARG  |
| 1   | C     | 520 | LYS  |
| 1   | C     | 522 | ARG  |
| 1   | C     | 524 | THR  |
| 1   | C     | 529 | ILE  |
| 1   | C     | 532 | TYR  |
| 1   | C     | 533 | MET  |
| 1   | C     | 534 | GLU  |
| 1   | C     | 538 | GLU  |
| 1   | C     | 542 | LEU  |
| 1   | C     | 543 | GLU  |
| 1   | C     | 548 | SER  |
| 1   | D     | 65  | THR  |
| 1   | D     | 68  | VAL  |
| 1   | D     | 89  | GLU  |
| 1   | D     | 90  | THR  |
| 1   | D     | 92  | GLN  |
| 1   | D     | 100 | LYS  |
| 1   | D     | 104 | VAL  |
| 1   | D     | 105 | MET  |
| 1   | D     | 107 | GLN  |
| 1   | D     | 108 | VAL  |
| 1   | D     | 112 | ARG  |
| 1   | D     | 115 | ASN  |
| 1   | D     | 117 | ASN  |
| 1   | D     | 119 | VAL  |
| 1   | D     | 121 | GLN  |
| 1   | D     | 122 | LYS  |
| 1   | D     | 124 | ARG  |
| 1   | D     | 126 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 127 | ASP  |
| 1   | D     | 131 | LYS  |
| 1   | D     | 132 | THR  |
| 1   | D     | 133 | THR  |
| 1   | D     | 141 | LEU  |
| 1   | D     | 147 | TRP  |
| 1   | D     | 148 | ASN  |
| 1   | D     | 151 | LYS  |
| 1   | D     | 153 | ILE  |
| 1   | D     | 163 | LEU  |
| 1   | D     | 166 | MET  |
| 1   | D     | 167 | GLU  |
| 1   | D     | 175 | VAL  |
| 1   | D     | 177 | SER  |
| 1   | D     | 183 | SER  |
| 1   | D     | 186 | LYS  |
| 1   | D     | 187 | LYS  |
| 1   | D     | 188 | THR  |
| 1   | D     | 189 | CYS  |
| 1   | D     | 194 | GLU  |
| 1   | D     | 200 | GLU  |
| 1   | D     | 203 | ILE  |
| 1   | D     | 204 | LEU  |
| 1   | D     | 210 | GLU  |
| 1   | D     | 213 | ARG  |
| 1   | D     | 214 | LYS  |
| 1   | D     | 218 | GLU  |
| 1   | D     | 221 | GLN  |
| 1   | D     | 223 | LEU  |
| 1   | D     | 228 | VAL  |
| 1   | D     | 229 | ARG  |
| 1   | D     | 230 | VAL  |
| 1   | D     | 232 | VAL  |
| 1   | D     | 235 | CYS  |
| 1   | D     | 243 | LEU  |
| 1   | D     | 246 | HIS  |
| 1   | D     | 248 | ARG  |
| 1   | D     | 249 | GLU  |
| 1   | D     | 251 | MET  |
| 1   | D     | 255 | TRP  |
| 1   | D     | 261 | ILE  |
| 1   | D     | 265 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 269 | LEU  |
| 1   | D     | 272 | ARG  |
| 1   | D     | 276 | ARG  |
| 1   | D     | 277 | GLU  |
| 1   | D     | 281 | SER  |
| 1   | D     | 282 | GLU  |
| 1   | D     | 283 | GLU  |
| 1   | D     | 284 | SER  |
| 1   | D     | 285 | VAL  |
| 1   | D     | 287 | LEU  |
| 1   | D     | 290 | SER  |
| 1   | D     | 295 | ILE  |
| 1   | D     | 300 | LEU  |
| 1   | D     | 307 | VAL  |
| 1   | D     | 309 | MET  |
| 1   | D     | 316 | MET  |
| 1   | D     | 317 | VAL  |
| 1   | D     | 319 | SER  |
| 1   | D     | 324 | GLN  |
| 1   | D     | 325 | GLN  |
| 1   | D     | 327 | LEU  |
| 1   | D     | 328 | GLN  |
| 1   | D     | 336 | LYS  |
| 1   | D     | 341 | MET  |
| 1   | D     | 347 | GLU  |
| 1   | D     | 349 | THR  |
| 1   | D     | 363 | ARG  |
| 1   | D     | 368 | LEU  |
| 1   | D     | 369 | LYS  |
| 1   | D     | 370 | ARG  |
| 1   | D     | 371 | GLU  |
| 1   | D     | 377 | LYS  |
| 1   | D     | 388 | ASN  |
| 1   | D     | 390 | THR  |
| 1   | D     | 393 | LEU  |
| 1   | D     | 394 | TYR  |
| 1   | D     | 395 | ASP  |
| 1   | D     | 404 | ARG  |
| 1   | D     | 406 | LEU  |
| 1   | D     | 409 | LEU  |
| 1   | D     | 412 | MET  |
| 1   | D     | 416 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 418 | CYS  |
| 1   | D     | 419 | ASP  |
| 1   | D     | 426 | ILE  |
| 1   | D     | 430 | VAL  |
| 1   | D     | 431 | SER  |
| 1   | D     | 433 | SER  |
| 1   | D     | 435 | GLU  |
| 1   | D     | 437 | ASP  |
| 1   | D     | 440 | LYS  |
| 1   | D     | 441 | MET  |
| 1   | D     | 442 | ILE  |
| 1   | D     | 446 | MET  |
| 1   | D     | 454 | LYS  |
| 1   | D     | 455 | SER  |
| 1   | D     | 461 | VAL  |
| 1   | D     | 463 | ILE  |
| 1   | D     | 464 | CYS  |
| 1   | D     | 467 | LYS  |
| 1   | D     | 468 | ASN  |
| 1   | D     | 470 | ASP  |
| 1   | D     | 471 | LYS  |
| 1   | D     | 476 | GLU  |
| 1   | D     | 479 | ARG  |
| 1   | D     | 481 | VAL  |
| 1   | D     | 483 | ILE  |
| 1   | D     | 484 | THR  |
| 1   | D     | 485 | ASP  |
| 1   | D     | 486 | LEU  |
| 1   | D     | 487 | ARG  |
| 1   | D     | 489 | SER  |
| 1   | D     | 492 | LEU  |
| 1   | D     | 493 | ARG  |
| 1   | D     | 499 | ILE  |
| 1   | D     | 502 | LEU  |
| 1   | D     | 503 | GLU  |
| 1   | D     | 504 | ARG  |
| 1   | D     | 506 | GLN  |
| 1   | D     | 507 | GLN  |
| 1   | D     | 514 | VAL  |
| 1   | D     | 516 | VAL  |
| 1   | D     | 517 | ARG  |
| 1   | D     | 520 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 522 | ARG  |
| 1   | D     | 524 | THR  |
| 1   | D     | 533 | MET  |
| 1   | D     | 538 | GLU  |
| 1   | D     | 542 | LEU  |
| 1   | D     | 543 | GLU  |
| 1   | D     | 548 | SER  |
| 1   | E     | 65  | THR  |
| 1   | E     | 68  | VAL  |
| 1   | E     | 77  | ARG  |
| 1   | E     | 89  | GLU  |
| 1   | E     | 90  | THR  |
| 1   | E     | 92  | GLN  |
| 1   | E     | 100 | LYS  |
| 1   | E     | 104 | VAL  |
| 1   | E     | 105 | MET  |
| 1   | E     | 107 | GLN  |
| 1   | E     | 108 | VAL  |
| 1   | E     | 112 | ARG  |
| 1   | E     | 115 | ASN  |
| 1   | E     | 117 | ASN  |
| 1   | E     | 119 | VAL  |
| 1   | E     | 121 | GLN  |
| 1   | E     | 122 | LYS  |
| 1   | E     | 124 | ARG  |
| 1   | E     | 126 | LYS  |
| 1   | E     | 127 | ASP  |
| 1   | E     | 131 | LYS  |
| 1   | E     | 132 | THR  |
| 1   | E     | 133 | THR  |
| 1   | E     | 141 | LEU  |
| 1   | E     | 147 | TRP  |
| 1   | E     | 148 | ASN  |
| 1   | E     | 151 | LYS  |
| 1   | E     | 153 | ILE  |
| 1   | E     | 160 | ILE  |
| 1   | E     | 163 | LEU  |
| 1   | E     | 166 | MET  |
| 1   | E     | 167 | GLU  |
| 1   | E     | 175 | VAL  |
| 1   | E     | 177 | SER  |
| 1   | E     | 183 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 186 | LYS  |
| 1   | E     | 187 | LYS  |
| 1   | E     | 188 | THR  |
| 1   | E     | 189 | CYS  |
| 1   | E     | 194 | GLU  |
| 1   | E     | 200 | GLU  |
| 1   | E     | 203 | ILE  |
| 1   | E     | 204 | LEU  |
| 1   | E     | 210 | GLU  |
| 1   | E     | 213 | ARG  |
| 1   | E     | 214 | LYS  |
| 1   | E     | 218 | GLU  |
| 1   | E     | 221 | GLN  |
| 1   | E     | 223 | LEU  |
| 1   | E     | 228 | VAL  |
| 1   | E     | 229 | ARG  |
| 1   | E     | 230 | VAL  |
| 1   | E     | 235 | CYS  |
| 1   | E     | 243 | LEU  |
| 1   | E     | 246 | HIS  |
| 1   | E     | 248 | ARG  |
| 1   | E     | 249 | GLU  |
| 1   | E     | 251 | MET  |
| 1   | E     | 255 | TRP  |
| 1   | E     | 261 | ILE  |
| 1   | E     | 265 | VAL  |
| 1   | E     | 269 | LEU  |
| 1   | E     | 272 | ARG  |
| 1   | E     | 274 | ARG  |
| 1   | E     | 276 | ARG  |
| 1   | E     | 277 | GLU  |
| 1   | E     | 280 | SER  |
| 1   | E     | 281 | SER  |
| 1   | E     | 282 | GLU  |
| 1   | E     | 283 | GLU  |
| 1   | E     | 285 | VAL  |
| 1   | E     | 287 | LEU  |
| 1   | E     | 290 | SER  |
| 1   | E     | 295 | ILE  |
| 1   | E     | 300 | LEU  |
| 1   | E     | 307 | VAL  |
| 1   | E     | 309 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 316 | MET  |
| 1   | E     | 317 | VAL  |
| 1   | E     | 319 | SER  |
| 1   | E     | 323 | ARG  |
| 1   | E     | 324 | GLN  |
| 1   | E     | 325 | GLN  |
| 1   | E     | 327 | LEU  |
| 1   | E     | 328 | GLN  |
| 1   | E     | 333 | MET  |
| 1   | E     | 336 | LYS  |
| 1   | E     | 343 | GLU  |
| 1   | E     | 347 | GLU  |
| 1   | E     | 349 | THR  |
| 1   | E     | 356 | LEU  |
| 1   | E     | 363 | ARG  |
| 1   | E     | 368 | LEU  |
| 1   | E     | 369 | LYS  |
| 1   | E     | 370 | ARG  |
| 1   | E     | 371 | GLU  |
| 1   | E     | 377 | LYS  |
| 1   | E     | 388 | ASN  |
| 1   | E     | 390 | THR  |
| 1   | E     | 393 | LEU  |
| 1   | E     | 394 | TYR  |
| 1   | E     | 395 | ASP  |
| 1   | E     | 404 | ARG  |
| 1   | E     | 406 | LEU  |
| 1   | E     | 409 | LEU  |
| 1   | E     | 412 | MET  |
| 1   | E     | 416 | LEU  |
| 1   | E     | 418 | CYS  |
| 1   | E     | 419 | ASP  |
| 1   | E     | 426 | ILE  |
| 1   | E     | 430 | VAL  |
| 1   | E     | 431 | SER  |
| 1   | E     | 433 | SER  |
| 1   | E     | 435 | GLU  |
| 1   | E     | 437 | ASP  |
| 1   | E     | 438 | GLU  |
| 1   | E     | 440 | LYS  |
| 1   | E     | 441 | MET  |
| 1   | E     | 442 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 446 | MET  |
| 1   | E     | 454 | LYS  |
| 1   | E     | 455 | SER  |
| 1   | E     | 461 | VAL  |
| 1   | E     | 463 | ILE  |
| 1   | E     | 464 | CYS  |
| 1   | E     | 467 | LYS  |
| 1   | E     | 468 | ASN  |
| 1   | E     | 470 | ASP  |
| 1   | E     | 471 | LYS  |
| 1   | E     | 476 | GLU  |
| 1   | E     | 479 | ARG  |
| 1   | E     | 481 | VAL  |
| 1   | E     | 483 | ILE  |
| 1   | E     | 484 | THR  |
| 1   | E     | 485 | ASP  |
| 1   | E     | 486 | LEU  |
| 1   | E     | 492 | LEU  |
| 1   | E     | 493 | ARG  |
| 1   | E     | 499 | ILE  |
| 1   | E     | 502 | LEU  |
| 1   | E     | 503 | GLU  |
| 1   | E     | 504 | ARG  |
| 1   | E     | 506 | GLN  |
| 1   | E     | 507 | GLN  |
| 1   | E     | 514 | VAL  |
| 1   | E     | 516 | VAL  |
| 1   | E     | 517 | ARG  |
| 1   | E     | 520 | LYS  |
| 1   | E     | 522 | ARG  |
| 1   | E     | 524 | THR  |
| 1   | E     | 529 | ILE  |
| 1   | E     | 533 | MET  |
| 1   | E     | 534 | GLU  |
| 1   | E     | 538 | GLU  |
| 1   | E     | 542 | LEU  |
| 1   | E     | 543 | GLU  |
| 1   | E     | 548 | SER  |
| 1   | F     | 65  | THR  |
| 1   | F     | 68  | VAL  |
| 1   | F     | 73  | GLU  |
| 1   | F     | 89  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 90  | THR  |
| 1   | F     | 92  | GLN  |
| 1   | F     | 100 | LYS  |
| 1   | F     | 104 | VAL  |
| 1   | F     | 105 | MET  |
| 1   | F     | 106 | TYR  |
| 1   | F     | 107 | GLN  |
| 1   | F     | 108 | VAL  |
| 1   | F     | 112 | ARG  |
| 1   | F     | 115 | ASN  |
| 1   | F     | 119 | VAL  |
| 1   | F     | 121 | GLN  |
| 1   | F     | 122 | LYS  |
| 1   | F     | 124 | ARG  |
| 1   | F     | 126 | LYS  |
| 1   | F     | 127 | ASP  |
| 1   | F     | 131 | LYS  |
| 1   | F     | 132 | THR  |
| 1   | F     | 133 | THR  |
| 1   | F     | 141 | LEU  |
| 1   | F     | 144 | LYS  |
| 1   | F     | 147 | TRP  |
| 1   | F     | 148 | ASN  |
| 1   | F     | 151 | LYS  |
| 1   | F     | 153 | ILE  |
| 1   | F     | 163 | LEU  |
| 1   | F     | 166 | MET  |
| 1   | F     | 167 | GLU  |
| 1   | F     | 175 | VAL  |
| 1   | F     | 177 | SER  |
| 1   | F     | 183 | SER  |
| 1   | F     | 186 | LYS  |
| 1   | F     | 187 | LYS  |
| 1   | F     | 188 | THR  |
| 1   | F     | 189 | CYS  |
| 1   | F     | 194 | GLU  |
| 1   | F     | 200 | GLU  |
| 1   | F     | 203 | ILE  |
| 1   | F     | 204 | LEU  |
| 1   | F     | 210 | GLU  |
| 1   | F     | 213 | ARG  |
| 1   | F     | 214 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 218 | GLU  |
| 1   | F     | 221 | GLN  |
| 1   | F     | 223 | LEU  |
| 1   | F     | 228 | VAL  |
| 1   | F     | 229 | ARG  |
| 1   | F     | 230 | VAL  |
| 1   | F     | 232 | VAL  |
| 1   | F     | 235 | CYS  |
| 1   | F     | 243 | LEU  |
| 1   | F     | 246 | HIS  |
| 1   | F     | 248 | ARG  |
| 1   | F     | 249 | GLU  |
| 1   | F     | 251 | MET  |
| 1   | F     | 255 | TRP  |
| 1   | F     | 260 | TRP  |
| 1   | F     | 261 | ILE  |
| 1   | F     | 265 | VAL  |
| 1   | F     | 269 | LEU  |
| 1   | F     | 272 | ARG  |
| 1   | F     | 274 | ARG  |
| 1   | F     | 276 | ARG  |
| 1   | F     | 277 | GLU  |
| 1   | F     | 280 | SER  |
| 1   | F     | 281 | SER  |
| 1   | F     | 282 | GLU  |
| 1   | F     | 283 | GLU  |
| 1   | F     | 284 | SER  |
| 1   | F     | 285 | VAL  |
| 1   | F     | 287 | LEU  |
| 1   | F     | 290 | SER  |
| 1   | F     | 295 | ILE  |
| 1   | F     | 300 | LEU  |
| 1   | F     | 307 | VAL  |
| 1   | F     | 309 | MET  |
| 1   | F     | 312 | SER  |
| 1   | F     | 314 | SER  |
| 1   | F     | 316 | MET  |
| 1   | F     | 317 | VAL  |
| 1   | F     | 319 | SER  |
| 1   | F     | 323 | ARG  |
| 1   | F     | 324 | GLN  |
| 1   | F     | 325 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 327 | LEU  |
| 1   | F     | 328 | GLN  |
| 1   | F     | 336 | LYS  |
| 1   | F     | 343 | GLU  |
| 1   | F     | 347 | GLU  |
| 1   | F     | 349 | THR  |
| 1   | F     | 363 | ARG  |
| 1   | F     | 368 | LEU  |
| 1   | F     | 369 | LYS  |
| 1   | F     | 370 | ARG  |
| 1   | F     | 371 | GLU  |
| 1   | F     | 377 | LYS  |
| 1   | F     | 388 | ASN  |
| 1   | F     | 390 | THR  |
| 1   | F     | 393 | LEU  |
| 1   | F     | 394 | TYR  |
| 1   | F     | 395 | ASP  |
| 1   | F     | 404 | ARG  |
| 1   | F     | 406 | LEU  |
| 1   | F     | 409 | LEU  |
| 1   | F     | 412 | MET  |
| 1   | F     | 416 | LEU  |
| 1   | F     | 418 | CYS  |
| 1   | F     | 419 | ASP  |
| 1   | F     | 426 | ILE  |
| 1   | F     | 430 | VAL  |
| 1   | F     | 431 | SER  |
| 1   | F     | 433 | SER  |
| 1   | F     | 435 | GLU  |
| 1   | F     | 437 | ASP  |
| 1   | F     | 440 | LYS  |
| 1   | F     | 441 | MET  |
| 1   | F     | 442 | ILE  |
| 1   | F     | 446 | MET  |
| 1   | F     | 454 | LYS  |
| 1   | F     | 455 | SER  |
| 1   | F     | 461 | VAL  |
| 1   | F     | 463 | ILE  |
| 1   | F     | 464 | CYS  |
| 1   | F     | 467 | LYS  |
| 1   | F     | 468 | ASN  |
| 1   | F     | 470 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 471 | LYS  |
| 1   | F     | 476 | GLU  |
| 1   | F     | 479 | ARG  |
| 1   | F     | 481 | VAL  |
| 1   | F     | 483 | ILE  |
| 1   | F     | 484 | THR  |
| 1   | F     | 485 | ASP  |
| 1   | F     | 486 | LEU  |
| 1   | F     | 487 | ARG  |
| 1   | F     | 492 | LEU  |
| 1   | F     | 493 | ARG  |
| 1   | F     | 499 | ILE  |
| 1   | F     | 502 | LEU  |
| 1   | F     | 503 | GLU  |
| 1   | F     | 504 | ARG  |
| 1   | F     | 506 | GLN  |
| 1   | F     | 507 | GLN  |
| 1   | F     | 514 | VAL  |
| 1   | F     | 516 | VAL  |
| 1   | F     | 517 | ARG  |
| 1   | F     | 520 | LYS  |
| 1   | F     | 522 | ARG  |
| 1   | F     | 524 | THR  |
| 1   | F     | 529 | ILE  |
| 1   | F     | 533 | MET  |
| 1   | F     | 534 | GLU  |
| 1   | F     | 538 | GLU  |
| 1   | F     | 542 | LEU  |
| 1   | F     | 543 | GLU  |
| 1   | F     | 548 | SER  |
| 1   | G     | 65  | THR  |
| 1   | G     | 68  | VAL  |
| 1   | G     | 77  | ARG  |
| 1   | G     | 89  | GLU  |
| 1   | G     | 90  | THR  |
| 1   | G     | 92  | GLN  |
| 1   | G     | 100 | LYS  |
| 1   | G     | 104 | VAL  |
| 1   | G     | 105 | MET  |
| 1   | G     | 107 | GLN  |
| 1   | G     | 108 | VAL  |
| 1   | G     | 112 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 115 | ASN  |
| 1   | G     | 117 | ASN  |
| 1   | G     | 119 | VAL  |
| 1   | G     | 121 | GLN  |
| 1   | G     | 122 | LYS  |
| 1   | G     | 124 | ARG  |
| 1   | G     | 126 | LYS  |
| 1   | G     | 127 | ASP  |
| 1   | G     | 131 | LYS  |
| 1   | G     | 132 | THR  |
| 1   | G     | 133 | THR  |
| 1   | G     | 141 | LEU  |
| 1   | G     | 147 | TRP  |
| 1   | G     | 148 | ASN  |
| 1   | G     | 151 | LYS  |
| 1   | G     | 153 | ILE  |
| 1   | G     | 163 | LEU  |
| 1   | G     | 166 | MET  |
| 1   | G     | 167 | GLU  |
| 1   | G     | 175 | VAL  |
| 1   | G     | 177 | SER  |
| 1   | G     | 183 | SER  |
| 1   | G     | 186 | LYS  |
| 1   | G     | 187 | LYS  |
| 1   | G     | 188 | THR  |
| 1   | G     | 189 | CYS  |
| 1   | G     | 194 | GLU  |
| 1   | G     | 200 | GLU  |
| 1   | G     | 203 | ILE  |
| 1   | G     | 204 | LEU  |
| 1   | G     | 210 | GLU  |
| 1   | G     | 213 | ARG  |
| 1   | G     | 214 | LYS  |
| 1   | G     | 218 | GLU  |
| 1   | G     | 221 | GLN  |
| 1   | G     | 223 | LEU  |
| 1   | G     | 228 | VAL  |
| 1   | G     | 229 | ARG  |
| 1   | G     | 230 | VAL  |
| 1   | G     | 235 | CYS  |
| 1   | G     | 243 | LEU  |
| 1   | G     | 246 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 248 | ARG  |
| 1   | G     | 249 | GLU  |
| 1   | G     | 251 | MET  |
| 1   | G     | 255 | TRP  |
| 1   | G     | 260 | TRP  |
| 1   | G     | 261 | ILE  |
| 1   | G     | 265 | VAL  |
| 1   | G     | 269 | LEU  |
| 1   | G     | 272 | ARG  |
| 1   | G     | 274 | ARG  |
| 1   | G     | 276 | ARG  |
| 1   | G     | 277 | GLU  |
| 1   | G     | 280 | SER  |
| 1   | G     | 281 | SER  |
| 1   | G     | 282 | GLU  |
| 1   | G     | 283 | GLU  |
| 1   | G     | 284 | SER  |
| 1   | G     | 285 | VAL  |
| 1   | G     | 287 | LEU  |
| 1   | G     | 290 | SER  |
| 1   | G     | 295 | ILE  |
| 1   | G     | 300 | LEU  |
| 1   | G     | 307 | VAL  |
| 1   | G     | 309 | MET  |
| 1   | G     | 316 | MET  |
| 1   | G     | 317 | VAL  |
| 1   | G     | 319 | SER  |
| 1   | G     | 323 | ARG  |
| 1   | G     | 324 | GLN  |
| 1   | G     | 325 | GLN  |
| 1   | G     | 327 | LEU  |
| 1   | G     | 328 | GLN  |
| 1   | G     | 336 | LYS  |
| 1   | G     | 341 | MET  |
| 1   | G     | 347 | GLU  |
| 1   | G     | 349 | THR  |
| 1   | G     | 356 | LEU  |
| 1   | G     | 363 | ARG  |
| 1   | G     | 368 | LEU  |
| 1   | G     | 369 | LYS  |
| 1   | G     | 370 | ARG  |
| 1   | G     | 371 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 377 | LYS  |
| 1   | G     | 388 | ASN  |
| 1   | G     | 390 | THR  |
| 1   | G     | 393 | LEU  |
| 1   | G     | 394 | TYR  |
| 1   | G     | 395 | ASP  |
| 1   | G     | 406 | LEU  |
| 1   | G     | 409 | LEU  |
| 1   | G     | 412 | MET  |
| 1   | G     | 416 | LEU  |
| 1   | G     | 418 | CYS  |
| 1   | G     | 419 | ASP  |
| 1   | G     | 426 | ILE  |
| 1   | G     | 430 | VAL  |
| 1   | G     | 431 | SER  |
| 1   | G     | 433 | SER  |
| 1   | G     | 435 | GLU  |
| 1   | G     | 437 | ASP  |
| 1   | G     | 438 | GLU  |
| 1   | G     | 440 | LYS  |
| 1   | G     | 441 | MET  |
| 1   | G     | 442 | ILE  |
| 1   | G     | 446 | MET  |
| 1   | G     | 454 | LYS  |
| 1   | G     | 455 | SER  |
| 1   | G     | 461 | VAL  |
| 1   | G     | 463 | ILE  |
| 1   | G     | 467 | LYS  |
| 1   | G     | 468 | ASN  |
| 1   | G     | 470 | ASP  |
| 1   | G     | 471 | LYS  |
| 1   | G     | 476 | GLU  |
| 1   | G     | 479 | ARG  |
| 1   | G     | 481 | VAL  |
| 1   | G     | 483 | ILE  |
| 1   | G     | 484 | THR  |
| 1   | G     | 485 | ASP  |
| 1   | G     | 486 | LEU  |
| 1   | G     | 492 | LEU  |
| 1   | G     | 493 | ARG  |
| 1   | G     | 499 | ILE  |
| 1   | G     | 502 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 503 | GLU  |
| 1   | G     | 504 | ARG  |
| 1   | G     | 506 | GLN  |
| 1   | G     | 507 | GLN  |
| 1   | G     | 514 | VAL  |
| 1   | G     | 516 | VAL  |
| 1   | G     | 517 | ARG  |
| 1   | G     | 520 | LYS  |
| 1   | G     | 522 | ARG  |
| 1   | G     | 524 | THR  |
| 1   | G     | 533 | MET  |
| 1   | G     | 538 | GLU  |
| 1   | G     | 542 | LEU  |
| 1   | G     | 543 | GLU  |
| 1   | G     | 548 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 70  | ASN  |
| 1   | A     | 75  | ASN  |
| 1   | A     | 107 | GLN  |
| 1   | A     | 114 | GLN  |
| 1   | A     | 145 | HIS  |
| 1   | A     | 169 | GLN  |
| 1   | A     | 180 | HIS  |
| 1   | A     | 198 | GLN  |
| 1   | A     | 201 | GLN  |
| 1   | A     | 244 | ASN  |
| 1   | A     | 278 | HIS  |
| 1   | A     | 296 | ASN  |
| 1   | A     | 324 | GLN  |
| 1   | A     | 325 | GLN  |
| 1   | A     | 358 | ASN  |
| 1   | A     | 364 | GLN  |
| 1   | A     | 425 | HIS  |
| 1   | A     | 475 | HIS  |
| 1   | A     | 512 | ASN  |
| 1   | A     | 536 | ASN  |
| 1   | B     | 70  | ASN  |
| 1   | B     | 75  | ASN  |
| 1   | B     | 92  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 107 | GLN  |
| 1   | B     | 117 | ASN  |
| 1   | B     | 145 | HIS  |
| 1   | B     | 169 | GLN  |
| 1   | B     | 180 | HIS  |
| 1   | B     | 198 | GLN  |
| 1   | B     | 201 | GLN  |
| 1   | B     | 244 | ASN  |
| 1   | B     | 278 | HIS  |
| 1   | B     | 296 | ASN  |
| 1   | B     | 324 | GLN  |
| 1   | B     | 325 | GLN  |
| 1   | B     | 358 | ASN  |
| 1   | B     | 380 | GLN  |
| 1   | B     | 425 | HIS  |
| 1   | B     | 475 | HIS  |
| 1   | B     | 536 | ASN  |
| 1   | C     | 70  | ASN  |
| 1   | C     | 75  | ASN  |
| 1   | C     | 92  | GLN  |
| 1   | C     | 107 | GLN  |
| 1   | C     | 114 | GLN  |
| 1   | C     | 145 | HIS  |
| 1   | C     | 169 | GLN  |
| 1   | C     | 180 | HIS  |
| 1   | C     | 198 | GLN  |
| 1   | C     | 201 | GLN  |
| 1   | C     | 244 | ASN  |
| 1   | C     | 256 | ASN  |
| 1   | C     | 278 | HIS  |
| 1   | C     | 296 | ASN  |
| 1   | C     | 324 | GLN  |
| 1   | C     | 325 | GLN  |
| 1   | C     | 358 | ASN  |
| 1   | C     | 380 | GLN  |
| 1   | C     | 425 | HIS  |
| 1   | C     | 475 | HIS  |
| 1   | C     | 512 | ASN  |
| 1   | C     | 536 | ASN  |
| 1   | D     | 70  | ASN  |
| 1   | D     | 92  | GLN  |
| 1   | D     | 107 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 145 | HIS  |
| 1   | D     | 169 | GLN  |
| 1   | D     | 180 | HIS  |
| 1   | D     | 198 | GLN  |
| 1   | D     | 201 | GLN  |
| 1   | D     | 244 | ASN  |
| 1   | D     | 278 | HIS  |
| 1   | D     | 296 | ASN  |
| 1   | D     | 324 | GLN  |
| 1   | D     | 325 | GLN  |
| 1   | D     | 358 | ASN  |
| 1   | D     | 425 | HIS  |
| 1   | D     | 475 | HIS  |
| 1   | D     | 512 | ASN  |
| 1   | D     | 536 | ASN  |
| 1   | E     | 70  | ASN  |
| 1   | E     | 92  | GLN  |
| 1   | E     | 107 | GLN  |
| 1   | E     | 114 | GLN  |
| 1   | E     | 145 | HIS  |
| 1   | E     | 148 | ASN  |
| 1   | E     | 169 | GLN  |
| 1   | E     | 180 | HIS  |
| 1   | E     | 198 | GLN  |
| 1   | E     | 201 | GLN  |
| 1   | E     | 244 | ASN  |
| 1   | E     | 256 | ASN  |
| 1   | E     | 278 | HIS  |
| 1   | E     | 296 | ASN  |
| 1   | E     | 324 | GLN  |
| 1   | E     | 325 | GLN  |
| 1   | E     | 358 | ASN  |
| 1   | E     | 425 | HIS  |
| 1   | E     | 475 | HIS  |
| 1   | E     | 536 | ASN  |
| 1   | F     | 70  | ASN  |
| 1   | F     | 75  | ASN  |
| 1   | F     | 92  | GLN  |
| 1   | F     | 107 | GLN  |
| 1   | F     | 114 | GLN  |
| 1   | F     | 145 | HIS  |
| 1   | F     | 169 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 180 | HIS  |
| 1   | F     | 198 | GLN  |
| 1   | F     | 201 | GLN  |
| 1   | F     | 244 | ASN  |
| 1   | F     | 278 | HIS  |
| 1   | F     | 296 | ASN  |
| 1   | F     | 324 | GLN  |
| 1   | F     | 325 | GLN  |
| 1   | F     | 358 | ASN  |
| 1   | F     | 380 | GLN  |
| 1   | F     | 425 | HIS  |
| 1   | F     | 475 | HIS  |
| 1   | F     | 494 | GLN  |
| 1   | F     | 536 | ASN  |
| 1   | G     | 70  | ASN  |
| 1   | G     | 75  | ASN  |
| 1   | G     | 92  | GLN  |
| 1   | G     | 107 | GLN  |
| 1   | G     | 114 | GLN  |
| 1   | G     | 145 | HIS  |
| 1   | G     | 169 | GLN  |
| 1   | G     | 180 | HIS  |
| 1   | G     | 198 | GLN  |
| 1   | G     | 201 | GLN  |
| 1   | G     | 244 | ASN  |
| 1   | G     | 278 | HIS  |
| 1   | G     | 296 | ASN  |
| 1   | G     | 324 | GLN  |
| 1   | G     | 325 | GLN  |
| 1   | G     | 358 | ASN  |
| 1   | G     | 380 | GLN  |
| 1   | G     | 425 | HIS  |
| 1   | G     | 475 | HIS  |
| 1   | G     | 512 | ASN  |
| 1   | G     | 536 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 483/503 (96%)   | 0.03   | 5 (1%) 79 56  | 59, 136, 136, 136     | 0     |
| 1   | B     | 483/503 (96%)   | -0.10  | 6 (1%) 76 53  | 94, 94, 178, 178      | 0     |
| 1   | C     | 483/503 (96%)   | 0.08   | 8 (1%) 69 44  | 120, 120, 178, 178    | 0     |
| 1   | D     | 483/503 (96%)   | 0.13   | 9 (1%) 66 42  | 132, 132, 178, 178    | 0     |
| 1   | E     | 483/503 (96%)   | 0.07   | 8 (1%) 69 44  | 115, 115, 178, 178    | 0     |
| 1   | F     | 483/503 (96%)   | 0.40   | 20 (4%) 41 24 | 103, 164, 164, 164    | 0     |
| 1   | G     | 483/503 (96%)   | -0.03  | 11 (2%) 61 38 | 129, 129, 178, 178    | 0     |
| All | All   | 3381/3521 (96%) | 0.08   | 67 (1%) 65 41 | 59, 132, 178, 178     | 0     |

All (67) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 317 | VAL  | 9.0  |
| 1   | C     | 238 | ALA  | 4.6  |
| 1   | D     | 254 | VAL  | 4.5  |
| 1   | G     | 109 | ALA  | 4.0  |
| 1   | G     | 158 | GLY  | 4.0  |
| 1   | D     | 153 | ILE  | 3.9  |
| 1   | B     | 433 | SER  | 3.9  |
| 1   | A     | 262 | PRO  | 3.6  |
| 1   | F     | 391 | PHE  | 3.5  |
| 1   | A     | 127 | ASP  | 3.5  |
| 1   | G     | 268 | ALA  | 3.4  |
| 1   | G     | 261 | ILE  | 3.4  |
| 1   | E     | 156 | THR  | 3.3  |
| 1   | D     | 196 | PHE  | 3.1  |
| 1   | B     | 261 | ILE  | 3.1  |
| 1   | C     | 250 | ILE  | 3.1  |
| 1   | F     | 373 | ILE  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 205 | MET  | 3.0  |
| 1   | F     | 243 | LEU  | 2.9  |
| 1   | C     | 262 | PRO  | 2.9  |
| 1   | E     | 433 | SER  | 2.9  |
| 1   | F     | 284 | SER  | 2.8  |
| 1   | B     | 79  | SER  | 2.8  |
| 1   | A     | 170 | ASP  | 2.7  |
| 1   | F     | 492 | LEU  | 2.7  |
| 1   | C     | 165 | VAL  | 2.7  |
| 1   | G     | 265 | VAL  | 2.7  |
| 1   | B     | 226 | GLY  | 2.6  |
| 1   | D     | 223 | LEU  | 2.6  |
| 1   | E     | 216 | VAL  | 2.6  |
| 1   | F     | 530 | ALA  | 2.6  |
| 1   | C     | 205 | MET  | 2.6  |
| 1   | B     | 317 | VAL  | 2.5  |
| 1   | E     | 69  | TRP  | 2.5  |
| 1   | C     | 254 | VAL  | 2.5  |
| 1   | D     | 202 | ILE  | 2.4  |
| 1   | B     | 315 | GLY  | 2.4  |
| 1   | G     | 250 | ILE  | 2.4  |
| 1   | D     | 484 | THR  | 2.4  |
| 1   | E     | 181 | GLY  | 2.3  |
| 1   | A     | 171 | CYS  | 2.3  |
| 1   | D     | 386 | PHE  | 2.3  |
| 1   | F     | 115 | ASN  | 2.3  |
| 1   | G     | 438 | GLU  | 2.3  |
| 1   | G     | 115 | ASN  | 2.3  |
| 1   | F     | 262 | PRO  | 2.3  |
| 1   | F     | 542 | LEU  | 2.3  |
| 1   | E     | 432 | ALA  | 2.2  |
| 1   | F     | 116 | GLY  | 2.2  |
| 1   | F     | 453 | ALA  | 2.2  |
| 1   | F     | 275 | ILE  | 2.2  |
| 1   | C     | 233 | LEU  | 2.2  |
| 1   | F     | 300 | LEU  | 2.2  |
| 1   | G     | 239 | ASN  | 2.2  |
| 1   | D     | 238 | ALA  | 2.2  |
| 1   | F     | 483 | ILE  | 2.2  |
| 1   | F     | 117 | ASN  | 2.2  |
| 1   | G     | 238 | ALA  | 2.1  |
| 1   | F     | 265 | VAL  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 169 | GLN  | 2.1  |
| 1   | F     | 321 | PHE  | 2.1  |
| 1   | F     | 436 | SER  | 2.1  |
| 1   | D     | 393 | LEU  | 2.1  |
| 1   | E     | 233 | LEU  | 2.1  |
| 1   | F     | 372 | ILE  | 2.0  |
| 1   | C     | 132 | THR  | 2.0  |
| 1   | E     | 196 | PHE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.