



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:49 am GMT

PDB ID : 4LNN  
Title : B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: structure of apo form of GS  
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.  
Deposited on : 2013-07-11  
Resolution : 3.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Mogul                          | : | 1.7.2 (RC1), CSD as538be (2017)                                    |
| Xtriage (Phenix)               | : | 1.9-1692   |
| EDS                            | : | trunk28620   |
| Percentile statistics          | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac                         | : | 5.8.0135   |
| CCP4                           | : | 6.5.0  |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | recalc28949  |

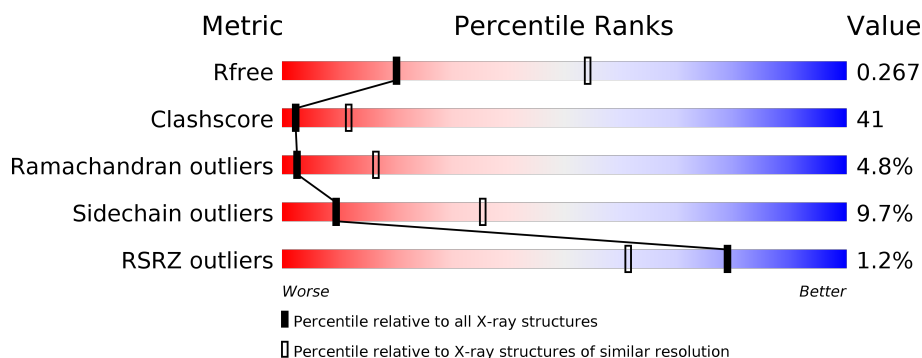
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1001 (3.12-3.08)                                      |
| Clashscore            | 112137                      | 1099 (3.12-3.08)                                      |
| Ramachandran outliers | 110173                      | 1057 (3.12-3.08)                                      |
| Sidechain outliers    | 110143                      | 1057 (3.12-3.08)                                      |
| RSRZ outliers         | 101464                      | 1006 (3.12-3.08)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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     | 443    | <div> <div>36%</div> <div>55%</div> <div>7%</div> <div>..</div> </div>              |
| 1   | B     | 443    | <div> <div>41%</div> <div>51%</div> <div>7%</div> <div>.</div> </div>               |
| 1   | C     | 443    | <div> <div>39%</div> <div>50%</div> <div>10%</div> <div>.</div> </div>              |
| 1   | D     | 443    | <div> <div>36%</div> <div>55%</div> <div>8%</div> <div>.</div> </div>               |
| 1   | E     | 443    | <div> <div>37%</div> <div>51%</div> <div>10%</div> <div>..</div> </div>             |
| 1   | F     | 443    | <div> <div>2%</div> <div>33%</div> <div>58%</div> <div>8%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | G     | 443    |  |
| 1   | H     | 443    |  |
| 1   | I     | 443    |  |
| 1   | J     | 443    |  |
| 1   | K     | 443    |  |
| 1   | L     | 443    |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | MG   | C     | 501 | -         | -        | -       | X                |
| 3   | SO4  | D     | 501 | -         | -        | -       | X                |
| 3   | SO4  | F     | 503 | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 42284 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 Glutamine synthetase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 439      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3505  | 2240 | 586 | 663 | 16 |         |         |       |
| 1   | B     | 439      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3505  | 2240 | 586 | 663 | 16 |         |         |       |
| 1   | C     | 438      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3498  | 2235 | 585 | 662 | 16 |         |         |       |
| 1   | D     | 439      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3505  | 2240 | 586 | 663 | 16 |         |         |       |
| 1   | E     | 438      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3498  | 2235 | 585 | 662 | 16 |         |         |       |
| 1   | F     | 437      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3491  | 2230 | 584 | 661 | 16 |         |         |       |
| 1   | G     | 438      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3498  | 2235 | 585 | 662 | 16 |         |         |       |
| 1   | H     | 437      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3491  | 2230 | 584 | 661 | 16 |         |         |       |
| 1   | I     | 436      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3485  | 2227 | 583 | 660 | 15 |         |         |       |
| 1   | J     | 438      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3498  | 2235 | 585 | 662 | 16 |         |         |       |
| 1   | K     | 438      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3498  | 2235 | 585 | 662 | 16 |         |         |       |
| 1   | L     | 440      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3509  | 2242 | 587 | 664 | 16 |         |         |       |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

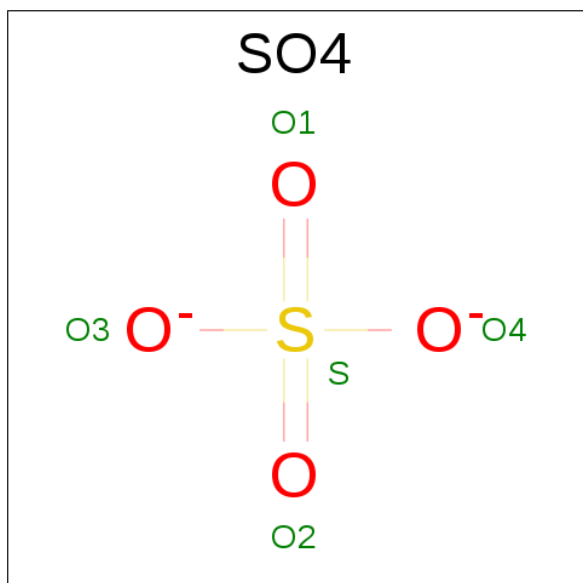
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | G     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | J     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | D     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 2   | K     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 2   | E     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 2   | H     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 2   | B     | 3        | Total<br>3 | Mg<br>3 | 0       | 0       |
| 2   | I     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 2   | C     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 2   | A     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 2   | L     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 2   | F     | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 3   | D     | 1        | Total<br>5 | O<br>4 | S<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

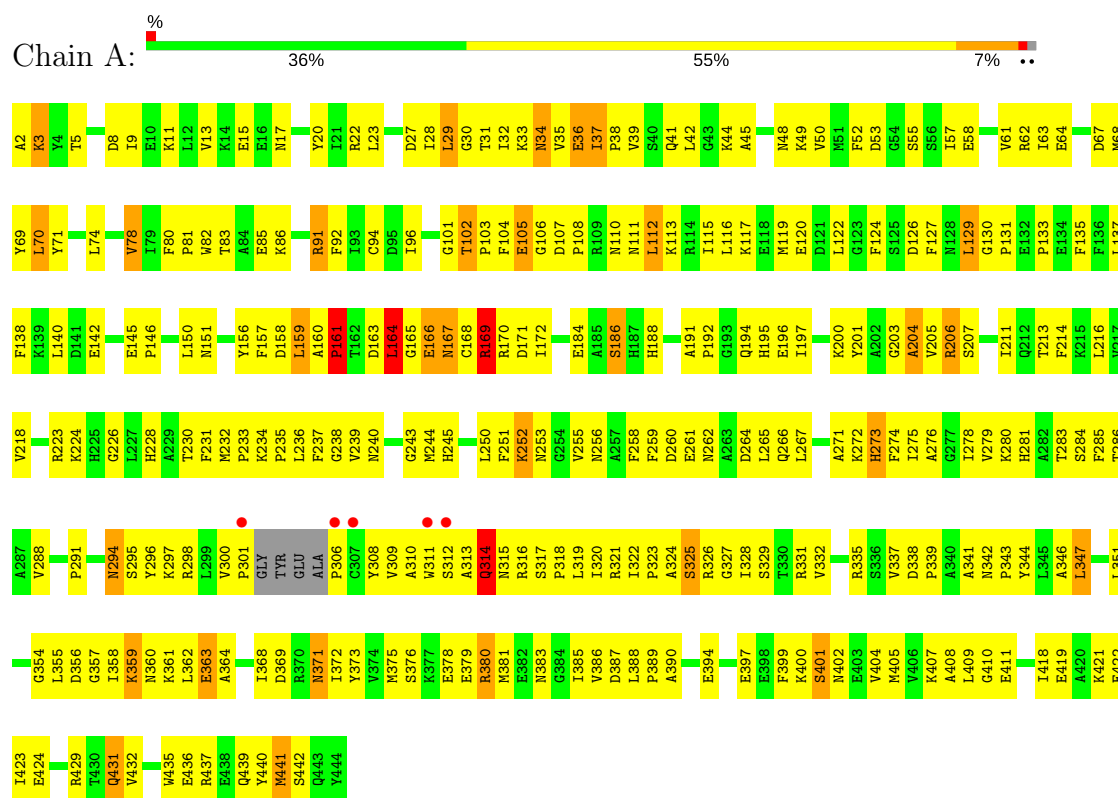
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 4   | B     | 27       | Total | O  | 0       | 0       |
|     |       |          | 27    | 27 |         |         |
| 4   | C     | 28       | Total | O  | 0       | 0       |
|     |       |          | 28    | 28 |         |         |
| 4   | D     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 4   | E     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 4   | F     | 24       | Total | O  | 0       | 0       |
|     |       |          | 24    | 24 |         |         |
| 4   | G     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 4   | H     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 4   | I     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |
| 4   | J     | 12       | Total | O  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |
| 4   | K     | 22       | Total | O  | 0       | 0       |
|     |       |          | 22    | 22 |         |         |
| 4   | L     | 22       | Total | O  | 0       | 0       |
|     |       |          | 22    | 22 |         |         |

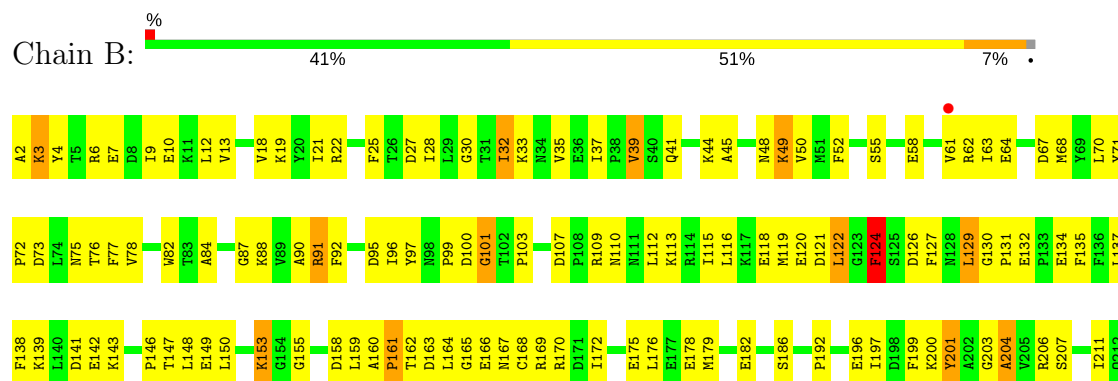
### 3 Residue-property plots

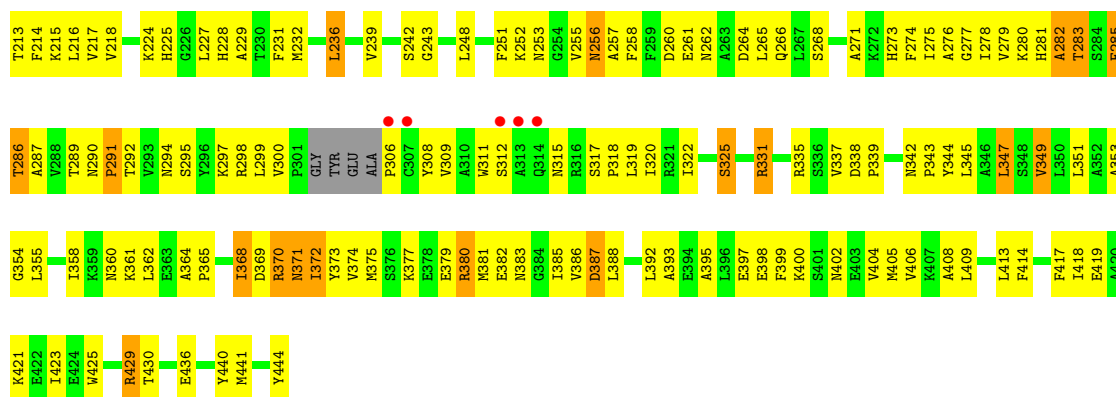
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: Glutamine synthetase

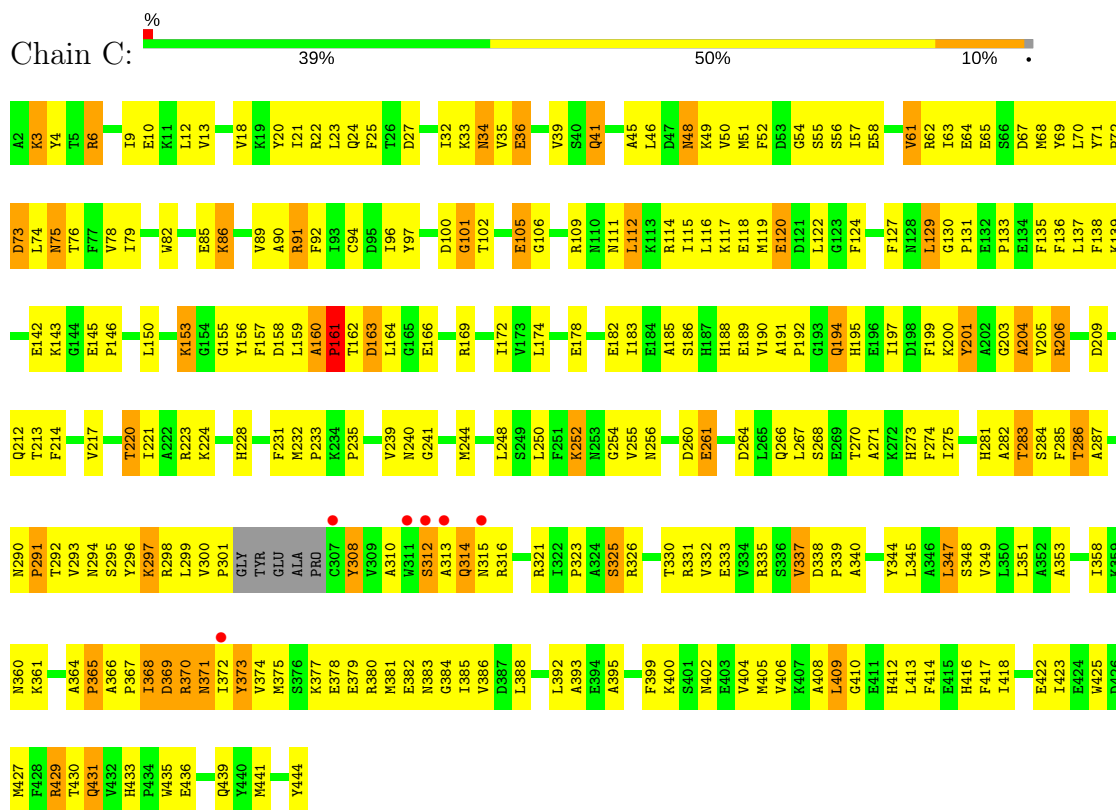


#### • Molecule 1: Glutamine synthetase

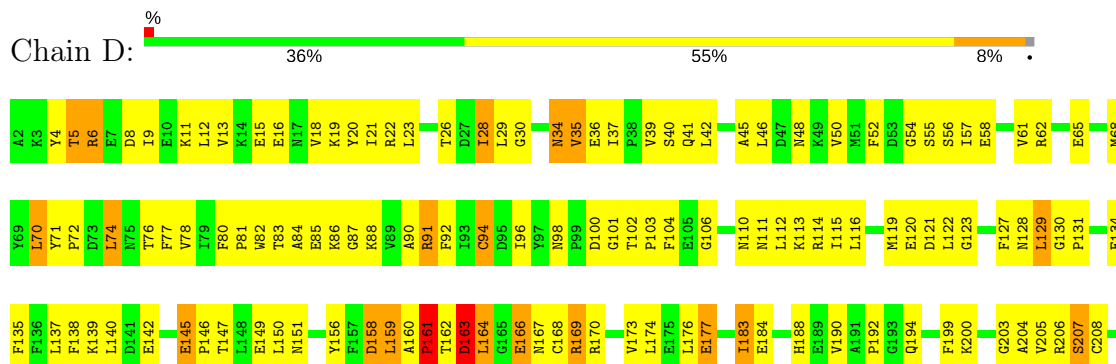




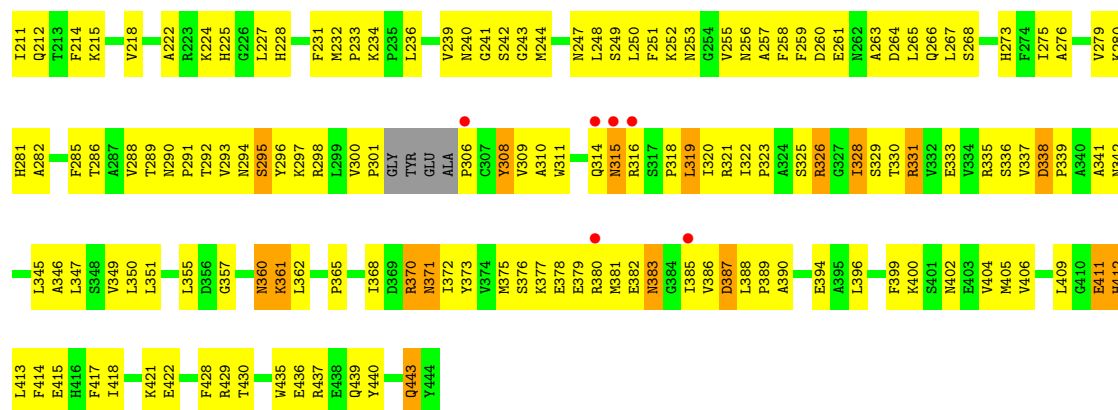
• Molecule 1: Glutamine synthetase



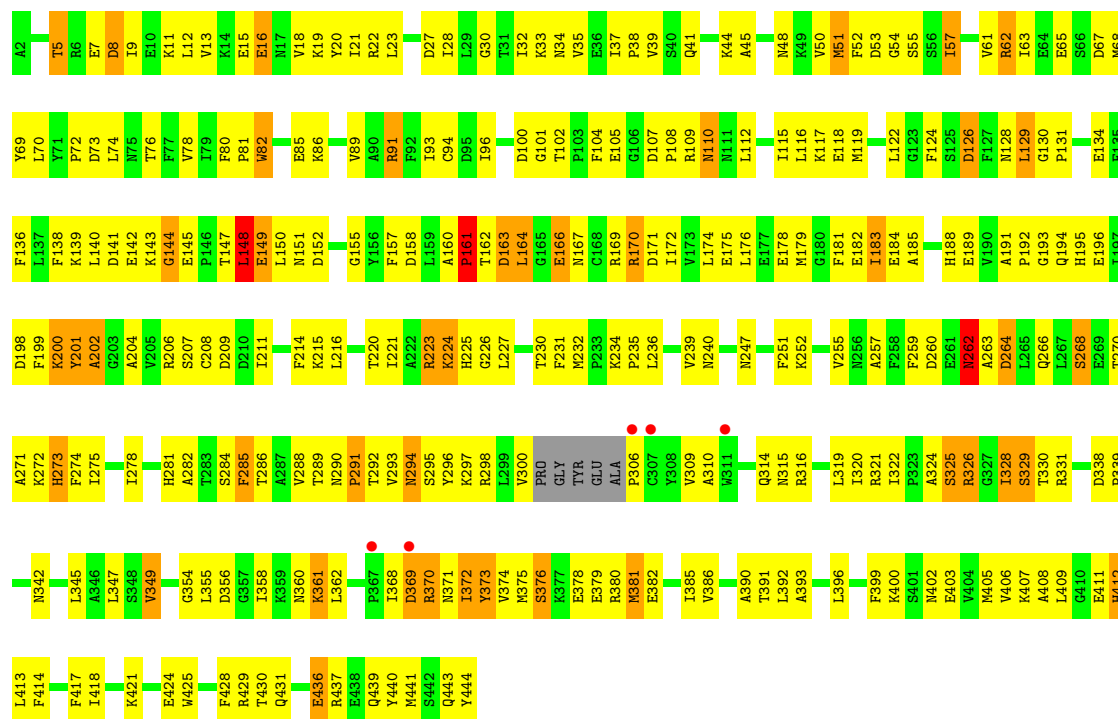
• Molecule 1: Glutamine synthetase



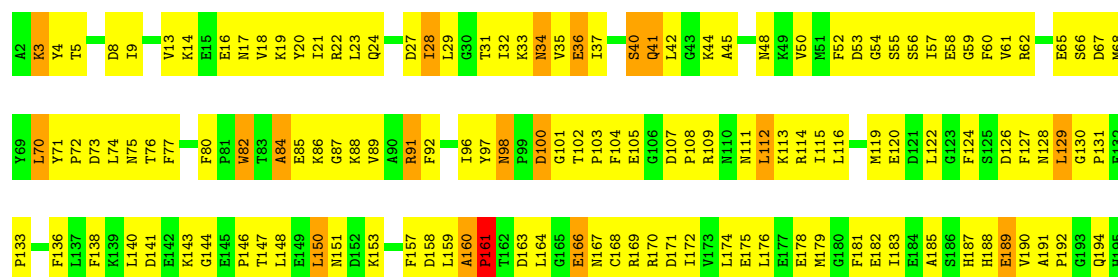




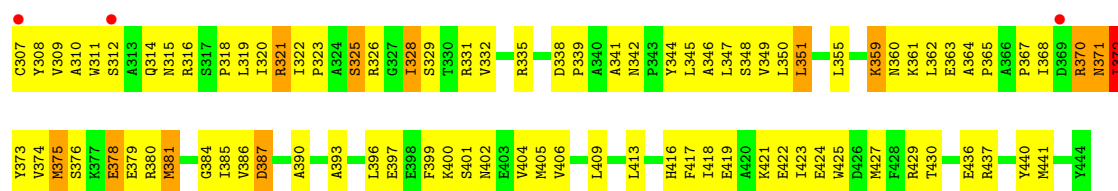
### • Molecule 1: Glutamine synthetase



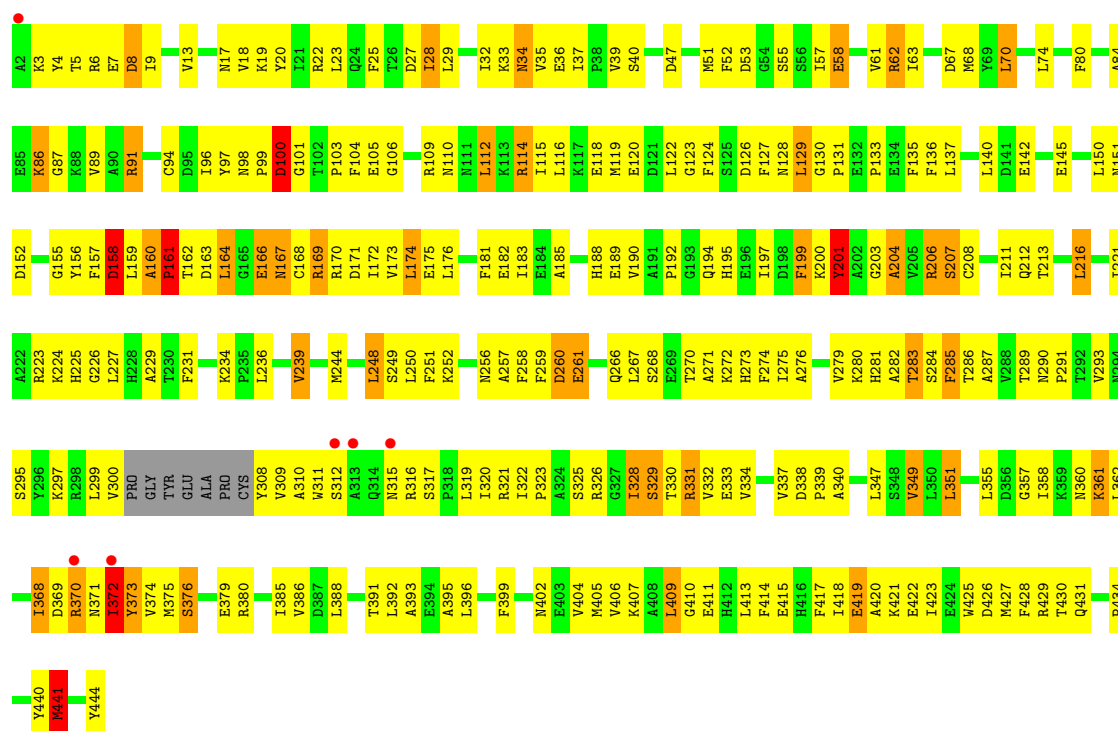
### • Molecule 1: Glutamine synthetase



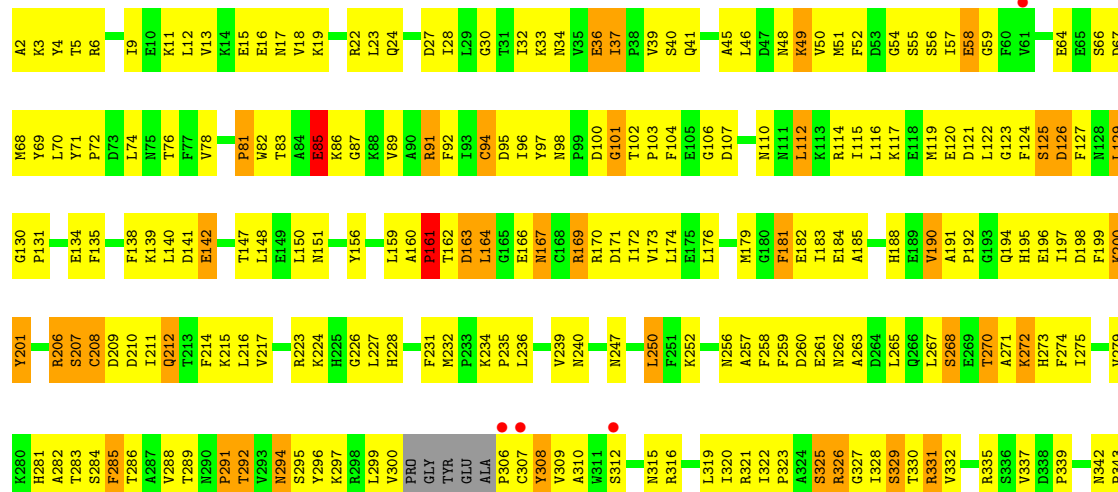


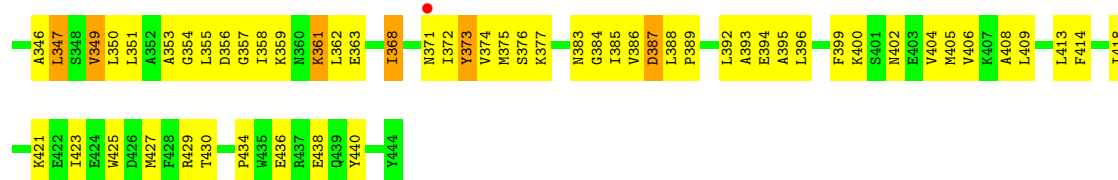


● Molecule 1: Glutamine synthetase

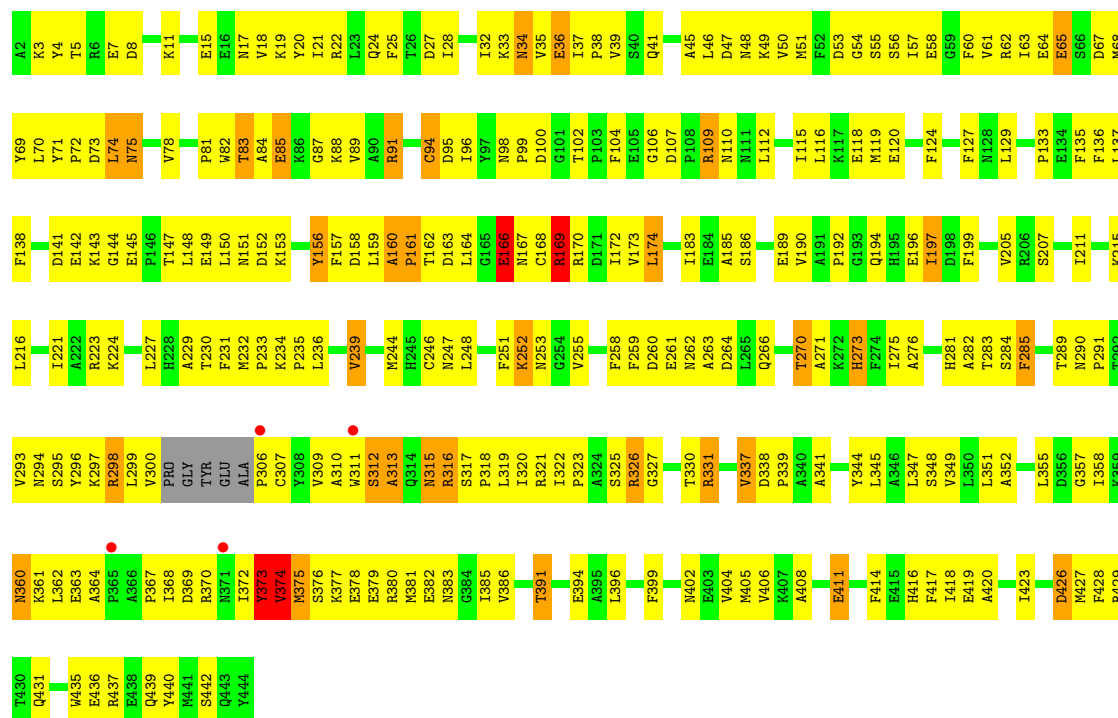


● Molecule 1: Glutamine synthetase

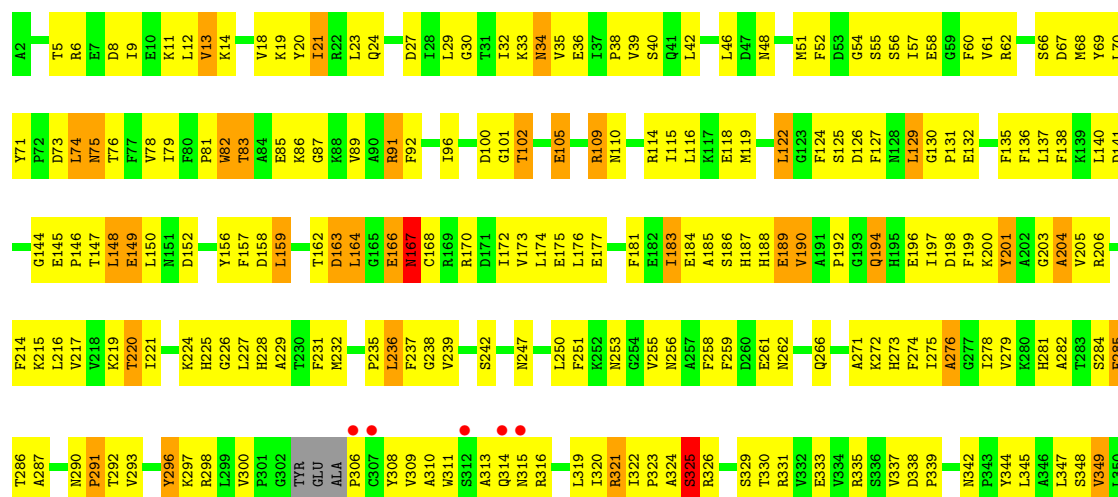


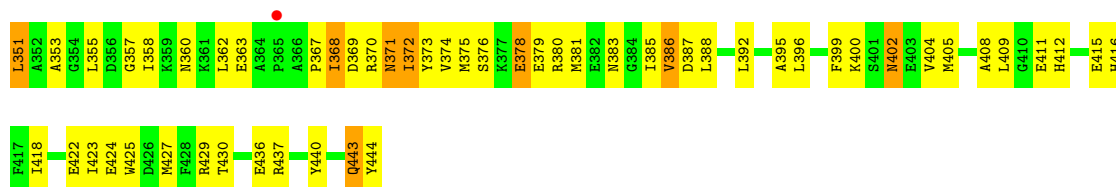


• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 109.99Å 138.38Å 138.74Å<br>119.80° 90.19° 93.85°            | Depositor        |
| Resolution (Å)  | 84.25 – 3.10<br>84.25 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 85.7 (84.25-3.10)<br>71.7 (84.25-3.10)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.49 (at 3.13Å)   | Xtriage          |
| Refinement program  | CNS 1.2   | Depositor        |
| R, $R_{free}$   | 0.217 , 0.267<br>0.217 , 0.267                              | Depositor<br>DCC |
| $R_{free}$ test set   | 8288 reflections (7.53%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 70.3  | Xtriage          |
| Anisotropy  | 0.300   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 40.6   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction   | 0.327 for -h,-k-l,l   | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 42284   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 66.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.39         | 0/3586  | 0.61        | 0/4849         |
| 1   | B     | 0.40         | 0/3586  | 0.62        | 0/4849         |
| 1   | C     | 0.42         | 0/3578  | 0.62        | 0/4838         |
| 1   | D     | 0.41         | 0/3586  | 0.61        | 0/4849         |
| 1   | E     | 0.41         | 0/3578  | 0.60        | 0/4837         |
| 1   | F     | 0.43         | 0/3570  | 0.62        | 0/4826         |
| 1   | G     | 0.41         | 0/3578  | 0.61        | 0/4837         |
| 1   | H     | 0.41         | 0/3570  | 0.62        | 0/4826         |
| 1   | I     | 0.42         | 0/3564  | 0.63        | 0/4818         |
| 1   | J     | 0.43         | 0/3578  | 0.63        | 1/4837 (0.0%)  |
| 1   | K     | 0.39         | 0/3578  | 0.61        | 0/4837         |
| 1   | L     | 0.42         | 0/3590  | 0.63        | 0/4854         |
| All | All   | 0.41         | 0/42942 | 0.62        | 1/58057 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | L     | 0                   | 1                   |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | J     | 2   | ALA  | CA-C-N | -6.09 | 103.80      | 117.20   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | L     | 296 | TYR  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3505  | 0        | 3443     | 310     | 0            |
| 1   | B     | 3505  | 0        | 3443     | 285     | 0            |
| 1   | C     | 3498  | 0        | 3435     | 295     | 0            |
| 1   | D     | 3505  | 0        | 3443     | 308     | 0            |
| 1   | E     | 3498  | 0        | 3436     | 329     | 0            |
| 1   | F     | 3491  | 0        | 3428     | 342     | 0            |
| 1   | G     | 3498  | 0        | 3436     | 303     | 0            |
| 1   | H     | 3491  | 0        | 3428     | 294     | 0            |
| 1   | I     | 3485  | 0        | 3423     | 298     | 0            |
| 1   | J     | 3498  | 0        | 3436     | 318     | 0            |
| 1   | K     | 3498  | 0        | 3436     | 314     | 0            |
| 1   | L     | 3509  | 0        | 3446     | 301     | 0            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |
| 2   | B     | 3     | 0        | 0        | 0       | 0            |
| 2   | C     | 2     | 0        | 0        | 0       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 2   | E     | 2     | 0        | 0        | 0       | 0            |
| 2   | F     | 2     | 0        | 0        | 0       | 0            |
| 2   | G     | 2     | 0        | 0        | 0       | 0            |
| 2   | H     | 2     | 0        | 0        | 0       | 0            |
| 2   | I     | 2     | 0        | 0        | 0       | 0            |
| 2   | J     | 2     | 0        | 0        | 0       | 0            |
| 2   | K     | 2     | 0        | 0        | 0       | 0            |
| 2   | L     | 2     | 0        | 0        | 0       | 0            |
| 3   | D     | 10    | 0        | 0        | 0       | 0            |
| 3   | E     | 5     | 0        | 0        | 0       | 0            |
| 3   | F     | 5     | 0        | 0        | 0       | 0            |
| 3   | H     | 5     | 0        | 0        | 0       | 0            |
| 4   | A     | 17    | 0        | 0        | 4       | 0            |
| 4   | B     | 27    | 0        | 0        | 1       | 0            |
| 4   | C     | 28    | 0        | 0        | 1       | 0            |
| 4   | D     | 20    | 0        | 0        | 3       | 0            |
| 4   | E     | 17    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | F     | 24    | 0        | 0        | 1       | 0            |
| 4   | G     | 21    | 0        | 0        | 4       | 0            |
| 4   | H     | 20    | 0        | 0        | 2       | 0            |
| 4   | I     | 23    | 0        | 0        | 2       | 0            |
| 4   | J     | 12    | 0        | 0        | 1       | 0            |
| 4   | K     | 22    | 0        | 0        | 1       | 0            |
| 4   | L     | 22    | 0        | 0        | 2       | 0            |
| All | All   | 42284 | 0        | 41233    | 3435    | 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 41.

All (3435) 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:K:83:THR:HG21  | 1:K:89:VAL:H     | 1.13                     | 1.09              |
| 1:F:286:THR:HG23 | 1:F:290:ASN:HD22 | 1.19                     | 1.07              |
| 1:I:173:VAL:HG13 | 1:I:183:ILE:HD12 | 1.31                     | 1.07              |
| 1:I:372:ILE:HG22 | 1:I:385:ILE:HD13 | 1.37                     | 1.05              |
| 1:G:371:ASN:HD22 | 1:G:375:MET:HB3  | 1.18                     | 1.04              |
| 1:E:9:ILE:HG13   | 1:E:74:LEU:HD12  | 1.39                     | 1.04              |
| 1:C:372:ILE:HG22 | 1:C:385:ILE:HD13 | 1.40                     | 1.02              |
| 1:E:319:LEU:HG   | 1:E:320:ILE:HD12 | 1.40                     | 1.02              |
| 1:G:27:ASP:HA    | 1:G:57:ILE:HG23  | 1.41                     | 1.02              |
| 1:I:261:GLU:HA   | 1:I:266:GLN:HG2  | 1.37                     | 1.02              |
| 1:B:126:ASP:HB2  | 1:B:251:PHE:HB2  | 1.37                     | 1.02              |
| 1:J:98:ASN:HD22  | 1:J:102:THR:HG23 | 1.24                     | 1.02              |
| 1:G:258:PHE:HB2  | 1:G:271:ALA:HB2  | 1.40                     | 1.01              |
| 1:J:272:LYS:HA   | 1:J:275:ILE:HD12 | 1.42                     | 1.01              |
| 1:F:13:VAL:HG13  | 1:F:18:VAL:HB    | 1.43                     | 1.00              |
| 1:B:153:LYS:H    | 1:B:153:LYS:HE2  | 1.23                     | 0.99              |
| 1:J:182:GLU:HB3  | 1:J:200:LYS:HE2  | 1.44                     | 0.99              |
| 1:H:182:GLU:HB3  | 1:H:200:LYS:HD2  | 1.42                     | 0.98              |
| 1:A:380:ARG:HH11 | 1:A:380:ARG:HB2  | 1.28                     | 0.97              |
| 1:A:160:ALA:HB1  | 1:A:161:PRO:HD2  | 1.45                     | 0.97              |
| 1:H:321:ARG:HG2  | 1:H:335:ARG:HD2  | 1.45                     | 0.97              |
| 1:K:315:ASN:HD21 | 1:K:370:ARG:H    | 1.10                     | 0.95              |
| 1:H:140:LEU:HD21 | 1:H:223:ARG:NH2  | 1.81                     | 0.95              |
| 1:H:129:LEU:HD13 | 1:H:131:PRO:HD3  | 1.46                     | 0.94              |
| 1:I:328:ILE:H    | 1:I:328:ILE:HD13 | 1.32                     | 0.94              |
| 1:L:52:PHE:HE2   | 1:L:56:SER:HG    | 1.13                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:129:LEU:HD22 | 1:I:131:PRO:HG3  | 1.49                     | 0.94              |
| 1:K:160:ALA:HB1  | 1:K:161:PRO:HD2  | 1.50                     | 0.93              |
| 1:K:370:ARG:HH21 | 1:K:374:VAL:HG22 | 1.32                     | 0.93              |
| 1:D:129:LEU:HD13 | 1:D:131:PRO:HD3  | 1.51                     | 0.92              |
| 1:H:5:THR:H      | 1:H:8:ASP:HB2    | 1.34                     | 0.92              |
| 1:F:371:ASN:HD21 | 1:F:373:TYR:HB2  | 1.32                     | 0.92              |
| 1:J:386:VAL:HG12 | 1:J:387:ASP:H    | 1.31                     | 0.92              |
| 1:B:325:SER:HB2  | 1:B:331:ARG:NH2  | 1.85                     | 0.92              |
| 1:F:146:PRO:HG3  | 1:F:228:HIS:CD2  | 2.04                     | 0.92              |
| 1:J:281:HIS:CD2  | 1:J:402:ASN:HD21 | 1.88                     | 0.92              |
| 1:G:182:GLU:HB3  | 1:G:200:LYS:HD2  | 1.52                     | 0.91              |
| 1:K:33:LYS:HA    | 1:L:158:ASP:HA   | 1.53                     | 0.91              |
| 1:L:315:ASN:HD21 | 1:L:370:ARG:HA   | 1.36                     | 0.91              |
| 1:F:429:ARG:HH21 | 1:L:300:VAL:HG22 | 1.33                     | 0.91              |
| 1:H:74:LEU:H     | 1:H:74:LEU:HD22  | 1.35                     | 0.91              |
| 1:I:57:ILE:HD11  | 1:I:96:ILE:HG12  | 1.53                     | 0.91              |
| 1:E:325:SER:HB2  | 1:E:331:ARG:HH22 | 1.34                     | 0.90              |
| 1:K:316:ARG:HH11 | 1:K:316:ARG:H    | 1.16                     | 0.90              |
| 1:J:281:HIS:HD2  | 1:J:402:ASN:HD21 | 1.20                     | 0.90              |
| 1:J:371:ASN:HD22 | 1:J:374:VAL:HG22 | 1.34                     | 0.90              |
| 1:H:13:VAL:HG13  | 1:H:18:VAL:HB    | 1.51                     | 0.90              |
| 1:B:370:ARG:HH22 | 1:B:375:MET:HG3  | 1.36                     | 0.90              |
| 1:I:63:ILE:HG22  | 1:J:316:ARG:HD3  | 1.55                     | 0.89              |
| 1:G:370:ARG:H    | 1:G:370:ARG:HD3  | 1.35                     | 0.89              |
| 1:F:300:VAL:HG22 | 1:L:429:ARG:NH2  | 1.88                     | 0.89              |
| 1:J:377:LYS:H    | 1:J:377:LYS:HD2  | 1.37                     | 0.88              |
| 1:I:86:LYS:HB3   | 1:J:174:LEU:HD13 | 1.55                     | 0.88              |
| 1:J:160:ALA:HB3  | 1:J:169:ARG:HH12 | 1.38                     | 0.88              |
| 1:I:248:LEU:HD11 | 1:I:334:VAL:HG23 | 1.54                     | 0.88              |
| 1:J:13:VAL:HG13  | 1:J:18:VAL:HB    | 1.52                     | 0.88              |
| 1:L:55:SER:HB2   | 1:L:62:ARG:HG3   | 1.56                     | 0.88              |
| 1:G:281:HIS:NE2  | 1:G:404:VAL:HG11 | 1.88                     | 0.87              |
| 1:B:201:TYR:HB2  | 4:B:602:HOH:O    | 1.73                     | 0.87              |
| 1:A:306:PRO:HB3  | 1:A:319:LEU:HA   | 1.53                     | 0.87              |
| 1:F:300:VAL:HG22 | 1:L:429:ARG:HH22 | 1.39                     | 0.87              |
| 1:B:429:ARG:HH21 | 1:H:390:ALA:HB1  | 1.37                     | 0.87              |
| 1:D:150:LEU:HD13 | 1:D:192:PRO:HB2  | 1.56                     | 0.87              |
| 1:E:57:ILE:HD11  | 1:E:96:ILE:HG12  | 1.55                     | 0.86              |
| 1:F:286:THR:HG23 | 1:F:290:ASN:ND2  | 1.89                     | 0.86              |
| 1:G:310:ALA:HB1  | 1:G:368:ILE:HG12 | 1.55                     | 0.86              |
| 1:E:13:VAL:HG13  | 1:E:18:VAL:HB    | 1.56                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:281:HIS:HD2  | 1:E:402:ASN:HD21 | 1.20                     | 0.86              |
| 1:K:313:ALA:HA   | 1:K:321:ARG:HG3  | 1.56                     | 0.86              |
| 1:E:319:LEU:HG   | 1:E:320:ILE:CD1  | 2.05                     | 0.85              |
| 1:G:32:ILE:HD13  | 1:G:216:LEU:HD12 | 1.56                     | 0.85              |
| 1:D:319:LEU:HD23 | 1:D:320:ILE:HG12 | 1.59                     | 0.85              |
| 1:B:3:LYS:HB3    | 1:B:75:ASN:OD1   | 1.77                     | 0.84              |
| 1:E:129:LEU:HD23 | 1:E:347:LEU:HD21 | 1.59                     | 0.84              |
| 1:G:160:ALA:HB1  | 1:G:161:PRO:HD2  | 1.57                     | 0.84              |
| 1:B:182:GLU:HB3  | 1:B:200:LYS:HD2  | 1.59                     | 0.84              |
| 1:G:115:ILE:HG22 | 1:G:351:LEU:HD13 | 1.59                     | 0.84              |
| 1:B:153:LYS:N    | 1:B:153:LYS:HE2  | 1.92                     | 0.84              |
| 1:E:316:ARG:HB3  | 1:E:372:ILE:HD11 | 1.60                     | 0.84              |
| 1:J:236:LEU:HB2  | 1:J:239:VAL:HG21 | 1.60                     | 0.84              |
| 1:F:368:ILE:HG23 | 1:F:372:ILE:HD11 | 1.57                     | 0.84              |
| 1:J:54:GLY:O     | 1:J:57:ILE:HG12  | 1.77                     | 0.83              |
| 1:F:3:LYS:HB3    | 1:F:75:ASN:OD1   | 1.77                     | 0.83              |
| 1:J:9:ILE:HG13   | 1:J:74:LEU:HD12  | 1.58                     | 0.83              |
| 1:J:236:LEU:HB2  | 1:J:239:VAL:CG2  | 2.06                     | 0.83              |
| 1:L:57:ILE:HD11  | 1:L:96:ILE:HG12  | 1.60                     | 0.83              |
| 1:F:45:ALA:HA    | 1:F:50:VAL:HG23  | 1.59                     | 0.83              |
| 1:G:371:ASN:HB3  | 1:G:375:MET:HG2  | 1.60                     | 0.83              |
| 1:I:280:LYS:HE3  | 1:I:281:HIS:HE2  | 1.43                     | 0.83              |
| 1:J:231:PHE:HB3  | 1:J:339:PRO:HB2  | 1.61                     | 0.83              |
| 1:B:236:LEU:HD12 | 1:B:239:VAL:HG21 | 1.61                     | 0.83              |
| 1:B:27:ASP:OD1   | 1:B:33:LYS:HE3   | 1.79                     | 0.83              |
| 1:H:129:LEU:CD1  | 1:H:131:PRO:HD3  | 2.09                     | 0.83              |
| 1:L:27:ASP:HA    | 1:L:57:ILE:HG23  | 1.60                     | 0.82              |
| 1:F:182:GLU:HB3  | 1:F:200:LYS:HD2  | 1.60                     | 0.82              |
| 1:G:236:LEU:HB2  | 1:G:239:VAL:CG2  | 2.09                     | 0.82              |
| 1:D:160:ALA:HB1  | 1:D:161:PRO:HD2  | 1.59                     | 0.82              |
| 1:L:386:VAL:HG12 | 1:L:387:ASP:H    | 1.43                     | 0.82              |
| 1:J:275:ILE:O    | 1:J:279:VAL:HG23 | 1.80                     | 0.82              |
| 1:F:300:VAL:HG21 | 1:L:430:THR:HG22 | 1.60                     | 0.82              |
| 1:A:338:ASP:HB2  | 1:A:339:PRO:HD2  | 1.61                     | 0.82              |
| 1:L:375:MET:HG3  | 1:L:379:GLU:HG3  | 1.60                     | 0.82              |
| 1:F:136:PHE:CD1  | 1:F:235:PRO:HG2  | 2.14                     | 0.81              |
| 1:K:83:THR:HG21  | 1:K:89:VAL:N     | 1.94                     | 0.81              |
| 1:B:150:LEU:HD13 | 1:B:192:PRO:O    | 1.80                     | 0.81              |
| 1:J:306:PRO:HG2  | 1:J:335:ARG:HB2  | 1.61                     | 0.81              |
| 1:L:127:PHE:CE2  | 1:L:351:LEU:HG   | 2.15                     | 0.81              |
| 1:L:52:PHE:CZ    | 1:L:54:GLY:HA2   | 2.14                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:325:SER:HB2  | 1:G:331:ARG:NH2  | 1.94                     | 0.81              |
| 1:F:297:LYS:HD3  | 1:L:429:ARG:O    | 1.79                     | 0.81              |
| 1:A:252:LYS:NZ   | 1:A:252:LYS:HB2  | 1.96                     | 0.81              |
| 1:E:310:ALA:HB1  | 1:E:368:ILE:HG12 | 1.63                     | 0.81              |
| 1:G:236:LEU:HB2  | 1:G:239:VAL:HG21 | 1.62                     | 0.81              |
| 1:B:132:GLU:HB3  | 1:B:196:GLU:OE1  | 1.80                     | 0.81              |
| 1:G:129:LEU:HD13 | 1:G:131:PRO:HD3  | 1.63                     | 0.81              |
| 1:B:370:ARG:HH22 | 1:B:375:MET:CG   | 1.95                     | 0.80              |
| 1:C:402:ASN:O    | 1:C:406:VAL:HG23 | 1.82                     | 0.80              |
| 1:L:51:MET:HE1   | 1:L:67:ASP:HB3   | 1.61                     | 0.80              |
| 1:B:325:SER:HB2  | 1:B:331:ARG:HH22 | 1.46                     | 0.80              |
| 1:B:281:HIS:NE2  | 1:B:404:VAL:HG21 | 1.97                     | 0.80              |
| 1:C:51:MET:HE3   | 1:C:67:ASP:HB3   | 1.64                     | 0.80              |
| 1:H:41:GLN:HE22  | 1:I:200:LYS:NZ   | 1.78                     | 0.80              |
| 1:E:286:THR:HG23 | 1:E:290:ASN:HD22 | 1.47                     | 0.80              |
| 1:L:166:GLU:O    | 1:L:168:CYS:N    | 2.14                     | 0.80              |
| 1:J:212:GLN:HA   | 1:J:212:GLN:OE1  | 1.81                     | 0.80              |
| 1:E:314:GLN:HE22 | 1:E:321:ARG:HH21 | 1.30                     | 0.80              |
| 1:H:160:ALA:HB1  | 1:H:161:PRO:HD2  | 1.63                     | 0.80              |
| 1:C:310:ALA:HB2  | 1:C:385:ILE:HG23 | 1.64                     | 0.79              |
| 1:F:16:GLU:O     | 1:F:88:LYS:HE2   | 1.82                     | 0.79              |
| 1:I:5:THR:HG23   | 1:I:8:ASP:H      | 1.47                     | 0.79              |
| 1:K:152:ASP:HB3  | 1:K:161:PRO:HG3  | 1.64                     | 0.79              |
| 1:D:273:HIS:O    | 1:D:276:ALA:HB3  | 1.82                     | 0.79              |
| 1:E:406:VAL:HG22 | 1:E:414:PHE:CE1  | 2.18                     | 0.79              |
| 1:E:314:GLN:NE2  | 1:E:321:ARG:HH21 | 1.81                     | 0.79              |
| 1:G:371:ASN:ND2  | 1:G:375:MET:HB3  | 1.97                     | 0.79              |
| 1:J:389:PRO:HB2  | 1:J:394:GLU:HB3  | 1.64                     | 0.79              |
| 1:E:140:LEU:HD12 | 1:E:226:GLY:C    | 2.03                     | 0.79              |
| 1:I:27:ASP:HA    | 1:I:57:ILE:HG23  | 1.63                     | 0.79              |
| 1:L:83:THR:HG21  | 1:L:89:VAL:HB    | 1.65                     | 0.79              |
| 1:A:310:ALA:HB3  | 1:A:372:ILE:HD13 | 1.62                     | 0.78              |
| 1:A:355:LEU:O    | 1:A:359:LYS:HG2  | 1.83                     | 0.78              |
| 1:B:345:LEU:HD22 | 1:B:409:LEU:HD21 | 1.64                     | 0.78              |
| 1:C:281:HIS:CE1  | 1:C:404:VAL:HG11 | 2.18                     | 0.78              |
| 1:F:57:ILE:HD11  | 1:F:96:ILE:HG12  | 1.64                     | 0.78              |
| 1:J:190:VAL:HG13 | 1:J:191:ALA:H    | 1.47                     | 0.78              |
| 1:K:270:THR:HG22 | 1:K:358:ILE:HD12 | 1.63                     | 0.78              |
| 1:E:285:PHE:HB2  | 1:E:349:VAL:CG1  | 2.14                     | 0.78              |
| 1:J:98:ASN:ND2   | 1:J:102:THR:HG23 | 1.98                     | 0.78              |
| 1:F:286:THR:CG2  | 1:F:290:ASN:HD22 | 1.95                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:368:ILE:CG2  | 1:F:372:ILE:HD11 | 2.12                     | 0.78              |
| 1:H:272:LYS:HE3  | 1:H:363:GLU:HA   | 1.64                     | 0.78              |
| 1:H:98:ASN:HD21  | 1:H:104:PHE:HA   | 1.46                     | 0.78              |
| 1:J:156:TYR:HB2  | 1:J:190:VAL:HA   | 1.65                     | 0.78              |
| 1:K:357:GLY:HA2  | 1:K:362:LEU:HD13 | 1.64                     | 0.78              |
| 1:L:291:PRO:O    | 1:L:392:LEU:HD13 | 1.84                     | 0.78              |
| 1:L:67:ASP:O     | 1:L:68:MET:HG3   | 1.83                     | 0.78              |
| 1:E:372:ILE:HD12 | 1:E:373:TYR:N    | 1.99                     | 0.78              |
| 1:G:250:LEU:HB2  | 1:G:258:PHE:CZ   | 2.19                     | 0.78              |
| 1:I:150:LEU:HD13 | 1:I:192:PRO:O    | 1.83                     | 0.78              |
| 1:G:132:GLU:HA   | 1:G:198:ASP:HB3  | 1.64                     | 0.77              |
| 1:H:380:ARG:NH1  | 1:H:380:ARG:HB2  | 1.98                     | 0.77              |
| 1:G:160:ALA:HB2  | 1:G:188:HIS:HD2  | 1.50                     | 0.77              |
| 1:C:436:GLU:OE2  | 1:I:297:LYS:HE3  | 1.85                     | 0.77              |
| 1:F:232:MET:CE   | 1:L:440:TYR:HB2  | 2.13                     | 0.77              |
| 1:A:135:PHE:HB3  | 1:A:231:PHE:CE1  | 2.19                     | 0.77              |
| 1:D:111:ASN:HD21 | 1:D:409:LEU:HA   | 1.50                     | 0.77              |
| 1:E:257:ALA:O    | 1:E:270:THR:HB   | 1.84                     | 0.77              |
| 1:G:13:VAL:HG13  | 1:G:18:VAL:HB    | 1.65                     | 0.77              |
| 1:A:41:GLN:HE22  | 1:F:200:LYS:HE2  | 1.48                     | 0.77              |
| 1:E:136:PHE:CD1  | 1:E:235:PRO:HG2  | 2.20                     | 0.77              |
| 1:F:309:VAL:HB   | 1:F:386:VAL:HG23 | 1.65                     | 0.77              |
| 1:K:115:ILE:HG22 | 1:K:351:LEU:HD12 | 1.64                     | 0.77              |
| 1:A:200:LYS:HZ1  | 1:B:41:GLN:HE22  | 1.32                     | 0.77              |
| 1:D:241:GLY:HA3  | 1:D:298:ARG:HG3  | 1.66                     | 0.77              |
| 1:E:91:ARG:HD2   | 1:E:91:ARG:C     | 2.05                     | 0.77              |
| 1:L:78:VAL:HG13  | 1:L:91:ARG:HG3   | 1.66                     | 0.77              |
| 1:E:160:ALA:HB1  | 1:E:161:PRO:HD2  | 1.67                     | 0.77              |
| 1:G:86:LYS:HG3   | 1:H:174:LEU:HB3  | 1.66                     | 0.77              |
| 1:K:316:ARG:HH12 | 1:K:372:ILE:HG13 | 1.49                     | 0.77              |
| 1:B:271:ALA:O    | 1:B:275:ILE:HD12 | 1.85                     | 0.77              |
| 1:C:164:LEU:HD11 | 1:D:224:LYS:HD3  | 1.65                     | 0.77              |
| 1:D:91:ARG:HD2   | 1:D:91:ARG:C     | 2.05                     | 0.77              |
| 1:I:406:VAL:HG22 | 1:I:414:PHE:CE1  | 2.20                     | 0.77              |
| 1:K:127:PHE:CZ   | 1:K:248:LEU:HD22 | 2.19                     | 0.77              |
| 1:E:273:HIS:CD2  | 1:E:361:LYS:HA   | 2.20                     | 0.76              |
| 1:F:160:ALA:HB1  | 1:F:161:PRO:HD2  | 1.65                     | 0.76              |
| 1:J:328:ILE:HD12 | 1:J:329:SER:N    | 2.00                     | 0.76              |
| 1:H:273:HIS:CD2  | 1:H:361:LYS:HA   | 2.20                     | 0.76              |
| 1:A:372:ILE:HG23 | 1:A:385:ILE:HD13 | 1.67                     | 0.76              |
| 1:C:429:ARG:HH22 | 1:I:300:VAL:HA   | 1.49                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:9:ILE:O      | 1:I:13:VAL:HG23  | 1.85                     | 0.76              |
| 1:B:159:LEU:CD1  | 1:C:22:ARG:HH11  | 1.99                     | 0.76              |
| 1:G:399:PHE:HZ   | 1:G:409:LEU:HD22 | 1.49                     | 0.76              |
| 1:G:21:ILE:HD13  | 1:G:42:LEU:HD13  | 1.66                     | 0.76              |
| 1:J:30:GLY:HA2   | 1:J:342:ASN:ND2  | 2.01                     | 0.76              |
| 1:H:309:VAL:HG23 | 1:H:386:VAL:O    | 1.86                     | 0.75              |
| 1:L:109:ARG:HD2  | 1:L:344:TYR:CE2  | 2.21                     | 0.75              |
| 1:A:273:HIS:CD2  | 1:A:361:LYS:HA   | 2.21                     | 0.75              |
| 1:B:429:ARG:HH12 | 1:H:300:VAL:HG23 | 1.51                     | 0.75              |
| 1:C:136:PHE:HB3  | 1:C:138:PHE:HE1  | 1.52                     | 0.75              |
| 1:E:96:ILE:H     | 1:E:96:ILE:HD12  | 1.50                     | 0.75              |
| 1:H:98:ASN:ND2   | 1:H:104:PHE:HA   | 2.00                     | 0.75              |
| 1:A:129:LEU:HG   | 1:A:347:LEU:HD21 | 1.69                     | 0.75              |
| 1:J:176:LEU:HB2  | 1:J:183:ILE:HD11 | 1.68                     | 0.75              |
| 1:J:83:THR:HG21  | 1:J:89:VAL:HB    | 1.66                     | 0.75              |
| 1:H:372:ILE:HD13 | 1:H:372:ILE:H    | 1.50                     | 0.75              |
| 1:C:105:GLU:OE1  | 1:C:412:HIS:HB2  | 1.86                     | 0.75              |
| 1:E:281:HIS:CD2  | 1:E:402:ASN:HD21 | 2.04                     | 0.75              |
| 1:F:434:PRO:HA   | 1:F:437:ARG:HH12 | 1.51                     | 0.75              |
| 1:J:160:ALA:HB3  | 1:J:169:ARG:NH1  | 2.02                     | 0.75              |
| 1:G:4:TYR:HB3    | 1:G:9:ILE:HD11   | 1.69                     | 0.75              |
| 1:H:242:SER:O    | 1:H:339:PRO:HD2  | 1.87                     | 0.75              |
| 1:K:11:LYS:HG3   | 1:K:15:GLU:OE2   | 1.87                     | 0.75              |
| 1:E:21:ILE:HD13  | 1:E:39:VAL:HA    | 1.68                     | 0.74              |
| 1:F:98:ASN:N     | 1:F:98:ASN:HD22  | 1.83                     | 0.74              |
| 1:F:232:MET:HE3  | 1:L:440:TYR:HB2  | 1.68                     | 0.74              |
| 1:B:338:ASP:HB2  | 1:B:339:PRO:HD2  | 1.69                     | 0.74              |
| 1:K:273:HIS:CD2  | 1:K:361:LYS:HA   | 2.21                     | 0.74              |
| 1:D:129:LEU:HD22 | 1:D:130:GLY:N    | 2.03                     | 0.74              |
| 1:F:312:SER:HB2  | 1:F:368:ILE:HB   | 1.69                     | 0.74              |
| 1:I:225:HIS:O    | 1:I:227:LEU:HG   | 1.88                     | 0.74              |
| 1:A:380:ARG:NH1  | 1:A:380:ARG:HB2  | 2.03                     | 0.73              |
| 1:B:129:LEU:HG   | 1:B:347:LEU:HD21 | 1.70                     | 0.73              |
| 1:H:106:GLY:O    | 1:H:413:LEU:HD21 | 1.86                     | 0.73              |
| 1:E:100:ASP:O    | 1:E:102:THR:HG23 | 1.88                     | 0.73              |
| 1:E:136:PHE:HD1  | 1:E:235:PRO:HG2  | 1.52                     | 0.73              |
| 1:A:206:ARG:HG2  | 1:A:206:ARG:HH11 | 1.52                     | 0.73              |
| 1:D:309:VAL:HG13 | 1:D:319:LEU:HD22 | 1.70                     | 0.73              |
| 1:H:41:GLN:HE22  | 1:I:200:LYS:HZ2  | 1.34                     | 0.73              |
| 1:I:260:ASP:O    | 1:I:266:GLN:HA   | 1.88                     | 0.73              |
| 1:J:70:LEU:O     | 1:J:72:PRO:HD3   | 1.88                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:76:THR:O     | 1:E:78:VAL:HG23  | 1.89                     | 0.73              |
| 1:F:380:ARG:HA   | 1:F:385:ILE:HB   | 1.71                     | 0.73              |
| 1:L:150:LEU:HD13 | 1:L:192:PRO:O    | 1.86                     | 0.73              |
| 1:I:68:MET:HE3   | 1:I:98:ASN:HA    | 1.70                     | 0.73              |
| 1:K:3:LYS:H      | 1:K:75:ASN:HB3   | 1.53                     | 0.73              |
| 1:C:129:LEU:HD22 | 1:C:131:PRO:HD3  | 1.69                     | 0.73              |
| 1:D:252:LYS:O    | 1:D:255:VAL:HG22 | 1.88                     | 0.73              |
| 1:J:121:ASP:O    | 1:J:122:LEU:HD22 | 1.89                     | 0.73              |
| 1:J:125:SER:H    | 1:J:252:LYS:HA   | 1.53                     | 0.73              |
| 1:K:129:LEU:HD22 | 1:K:347:LEU:HD21 | 1.70                     | 0.73              |
| 1:D:328:ILE:HD12 | 1:D:329:SER:H    | 1.52                     | 0.73              |
| 1:F:98:ASN:HD21  | 1:F:104:PHE:HA   | 1.54                     | 0.73              |
| 1:B:148:LEU:HD21 | 1:H:437:ARG:HD3  | 1.71                     | 0.72              |
| 1:E:158:ASP:OD1  | 1:F:33:LYS:HE2   | 1.89                     | 0.72              |
| 1:J:282:ALA:HA   | 1:J:285:PHE:CZ   | 2.23                     | 0.72              |
| 1:D:243:GLY:HA3  | 1:D:298:ARG:HH12 | 1.55                     | 0.72              |
| 1:K:247:ASN:HB3  | 1:K:331:ARG:HG3  | 1.70                     | 0.72              |
| 1:D:310:ALA:HB1  | 1:D:368:ILE:HG21 | 1.71                     | 0.72              |
| 1:E:371:ASN:HB3  | 1:E:375:MET:SD   | 2.28                     | 0.72              |
| 1:B:377:LYS:O    | 1:B:381:MET:HG2  | 1.88                     | 0.72              |
| 1:D:259:PHE:CE2  | 1:D:326:ARG:HB3  | 2.24                     | 0.72              |
| 1:F:308:TYR:HA   | 1:F:387:ASP:HA   | 1.70                     | 0.72              |
| 1:H:172:ILE:HD12 | 1:H:218:VAL:HA   | 1.72                     | 0.72              |
| 1:J:310:ALA:HB1  | 1:J:368:ILE:HG21 | 1.71                     | 0.72              |
| 1:D:390:ALA:HB1  | 1:J:429:ARG:HE   | 1.55                     | 0.72              |
| 1:L:116:LEU:O    | 1:L:119:MET:HG2  | 1.89                     | 0.72              |
| 1:L:287:ALA:HB2  | 1:L:395:ALA:HB1  | 1.70                     | 0.72              |
| 1:B:349:VAL:HG22 | 1:B:405:MET:SD   | 2.30                     | 0.72              |
| 1:E:191:ALA:HB2  | 1:E:240:ASN:HB3  | 1.70                     | 0.72              |
| 1:F:22:ARG:HD2   | 1:F:80:PHE:HE1   | 1.53                     | 0.72              |
| 1:G:128:ASN:HA   | 1:G:202:ALA:O    | 1.89                     | 0.72              |
| 1:H:57:ILE:HD11  | 1:H:96:ILE:HG12  | 1.70                     | 0.72              |
| 1:I:355:LEU:HD23 | 1:I:358:ILE:HD12 | 1.71                     | 0.72              |
| 1:A:3:LYS:HB3    | 1:A:3:LYS:NZ     | 2.05                     | 0.72              |
| 1:C:182:GLU:HG3  | 1:C:200:LYS:HD2  | 1.69                     | 0.72              |
| 1:I:267:LEU:HD11 | 1:I:322:ILE:HD13 | 1.70                     | 0.72              |
| 1:A:429:ARG:NH2  | 1:G:300:VAL:HG22 | 2.05                     | 0.72              |
| 1:I:96:ILE:H     | 1:I:96:ILE:HD12  | 1.54                     | 0.72              |
| 1:K:291:PRO:HG3  | 1:K:341:ALA:HA   | 1.71                     | 0.72              |
| 1:K:67:ASP:O     | 1:K:68:MET:HG3   | 1.90                     | 0.72              |
| 1:C:55:SER:HB2   | 1:C:62:ARG:HG2   | 1.72                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:112:LEU:O    | 1:H:116:LEU:HG   | 1.90                     | 0.71              |
| 1:L:375:MET:HG2  | 1:L:380:ARG:HG2  | 1.71                     | 0.71              |
| 1:L:51:MET:CE    | 1:L:67:ASP:HB3   | 2.20                     | 0.71              |
| 1:C:366:ALA:HB1  | 1:C:367:PRO:HD2  | 1.70                     | 0.71              |
| 1:D:140:LEU:HD21 | 1:D:228:HIS:HB2  | 1.72                     | 0.71              |
| 1:A:429:ARG:HH22 | 1:G:300:VAL:HG22 | 1.56                     | 0.71              |
| 1:K:310:ALA:HB2  | 1:K:372:ILE:HG21 | 1.71                     | 0.71              |
| 1:G:183:ILE:HD12 | 1:G:183:ILE:H    | 1.55                     | 0.71              |
| 1:D:236:LEU:HB2  | 1:D:239:VAL:CG2  | 2.20                     | 0.71              |
| 1:G:338:ASP:HB2  | 1:G:339:PRO:HD2  | 1.73                     | 0.71              |
| 1:L:82:TRP:HH2   | 1:L:217:VAL:HG22 | 1.55                     | 0.71              |
| 1:G:23:LEU:HB2   | 1:G:35:VAL:HG13  | 1.73                     | 0.71              |
| 1:G:91:ARG:C     | 1:G:91:ARG:HD2   | 2.11                     | 0.71              |
| 1:J:72:PRO:HA    | 1:J:94:CYS:HB3   | 1.71                     | 0.71              |
| 1:A:294:ASN:HB2  | 1:G:436:GLU:OE2  | 1.91                     | 0.71              |
| 1:A:300:VAL:HG22 | 1:G:429:ARG:HH22 | 1.56                     | 0.71              |
| 1:B:211:ILE:HG22 | 1:B:215:LYS:HE3  | 1.73                     | 0.71              |
| 1:B:160:ALA:HB1  | 1:B:161:PRO:HD2  | 1.72                     | 0.71              |
| 1:G:375:MET:HB2  | 1:G:379:GLU:HB2  | 1.73                     | 0.71              |
| 1:I:248:LEU:O    | 1:I:331:ARG:HB2  | 1.91                     | 0.71              |
| 1:J:52:PHE:CE2   | 1:J:54:GLY:HA2   | 2.26                     | 0.71              |
| 1:K:316:ARG:NH1  | 1:K:316:ARG:H    | 1.88                     | 0.71              |
| 1:L:189:GLU:HB2  | 1:L:194:GLN:HB3  | 1.72                     | 0.71              |
| 1:C:150:LEU:CD1  | 1:C:192:PRO:HG2  | 2.21                     | 0.70              |
| 1:D:345:LEU:HD22 | 1:D:409:LEU:HD22 | 1.73                     | 0.70              |
| 1:F:437:ARG:HH11 | 1:F:437:ARG:HB2  | 1.56                     | 0.70              |
| 1:A:45:ALA:HA    | 1:A:50:VAL:HG23  | 1.72                     | 0.70              |
| 1:E:236:LEU:O    | 1:E:239:VAL:HG22 | 1.91                     | 0.70              |
| 1:G:34:ASN:HD22  | 1:G:34:ASN:C     | 1.93                     | 0.70              |
| 1:G:402:ASN:O    | 1:G:406:VAL:HG23 | 1.91                     | 0.70              |
| 1:L:91:ARG:C     | 1:L:91:ARG:HD2   | 2.11                     | 0.70              |
| 1:A:252:LYS:HE3  | 1:A:253:ASN:HD22 | 1.56                     | 0.70              |
| 1:C:267:LEU:HD21 | 1:C:326:ARG:NH1  | 2.07                     | 0.70              |
| 1:J:231:PHE:HB3  | 1:J:339:PRO:CB   | 2.20                     | 0.70              |
| 1:J:371:ASN:ND2  | 1:J:374:VAL:HG22 | 2.05                     | 0.70              |
| 1:A:34:ASN:HD22  | 1:A:34:ASN:C     | 1.94                     | 0.70              |
| 1:L:402:ASN:ND2  | 1:L:404:VAL:HG12 | 2.07                     | 0.70              |
| 1:C:380:ARG:HB2  | 1:C:380:ARG:HH11 | 1.55                     | 0.70              |
| 1:F:129:LEU:HD22 | 1:F:131:PRO:HD3  | 1.73                     | 0.70              |
| 1:A:224:LYS:HB2  | 1:F:164:LEU:HD11 | 1.73                     | 0.70              |
| 1:G:375:MET:SD   | 1:G:380:ARG:HG2  | 2.31                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:201:TYR:H    | 1:B:201:TYR:HD1  | 1.39                     | 0.70              |
| 1:C:182:GLU:CG   | 1:C:200:LYS:HD2  | 2.22                     | 0.70              |
| 1:A:112:LEU:O    | 1:A:116:LEU:HG   | 1.92                     | 0.70              |
| 1:A:372:ILE:HG22 | 1:A:380:ARG:HH21 | 1.56                     | 0.70              |
| 1:E:320:ILE:HG22 | 1:E:321:ARG:N    | 2.07                     | 0.70              |
| 1:I:338:ASP:HB2  | 1:I:339:PRO:HD2  | 1.74                     | 0.70              |
| 1:L:323:PRO:HD2  | 1:L:331:ARG:O    | 1.92                     | 0.70              |
| 1:J:414:PHE:O    | 1:J:418:ILE:HG12 | 1.91                     | 0.70              |
| 1:B:368:ILE:HG21 | 1:B:385:ILE:HD11 | 1.73                     | 0.70              |
| 1:C:58:GLU:O     | 1:C:61:VAL:HG23  | 1.91                     | 0.70              |
| 1:D:142:GLU:CD   | 1:D:142:GLU:H    | 1.95                     | 0.70              |
| 1:D:289:THR:O    | 1:D:341:ALA:HB2  | 1.92                     | 0.70              |
| 1:F:59:GLY:O     | 1:F:62:ARG:HG3   | 1.91                     | 0.70              |
| 1:J:310:ALA:HA   | 1:J:368:ILE:HG13 | 1.74                     | 0.70              |
| 1:A:252:LYS:O    | 1:A:252:LYS:HG3  | 1.90                     | 0.69              |
| 1:C:73:ASP:OD2   | 1:C:76:THR:HG23  | 1.90                     | 0.69              |
| 1:H:279:VAL:HG13 | 1:H:309:VAL:HG12 | 1.72                     | 0.69              |
| 1:I:328:ILE:H    | 1:I:328:ILE:CD1  | 2.05                     | 0.69              |
| 1:K:404:VAL:HG23 | 1:K:405:MET:HE3  | 1.73                     | 0.69              |
| 1:B:281:HIS:CD2  | 1:B:402:ASN:HD21 | 2.09                     | 0.69              |
| 1:J:119:MET:SD   | 1:J:127:PHE:HB2  | 2.32                     | 0.69              |
| 1:L:378:GLU:OE1  | 1:L:381:MET:HG3  | 1.92                     | 0.69              |
| 1:A:127:PHE:CD2  | 1:A:351:LEU:HD13 | 2.28                     | 0.69              |
| 1:K:325:SER:HB2  | 1:K:331:ARG:HH22 | 1.57                     | 0.69              |
| 1:K:325:SER:HB2  | 1:K:331:ARG:NH2  | 2.06                     | 0.69              |
| 1:K:404:VAL:HG23 | 1:K:405:MET:CE   | 2.22                     | 0.69              |
| 1:K:85:GLU:HG2   | 1:L:170:ARG:HH12 | 1.58                     | 0.69              |
| 1:G:368:ILE:HD13 | 1:G:372:ILE:HD11 | 1.72                     | 0.69              |
| 1:H:310:ALA:HB1  | 1:H:368:ILE:HG12 | 1.72                     | 0.69              |
| 1:E:285:PHE:HB2  | 1:E:349:VAL:HG11 | 1.73                     | 0.69              |
| 1:F:136:PHE:HB3  | 1:F:138:PHE:CE1  | 2.26                     | 0.69              |
| 1:I:375:MET:HB3  | 1:I:379:GLU:HB3  | 1.75                     | 0.69              |
| 1:H:272:LYS:HD3  | 1:H:272:LYS:C    | 2.13                     | 0.69              |
| 1:J:281:HIS:HD2  | 1:J:402:ASN:ND2  | 1.91                     | 0.69              |
| 1:A:231:PHE:HB3  | 1:A:339:PRO:HB2  | 1.73                     | 0.69              |
| 1:C:293:VAL:HG23 | 1:I:440:TYR:OH   | 1.92                     | 0.69              |
| 1:D:231:PHE:HB3  | 1:D:339:PRO:HB2  | 1.74                     | 0.69              |
| 1:G:377:LYS:HA   | 1:G:380:ARG:NH1  | 2.08                     | 0.69              |
| 1:J:129:LEU:HD23 | 1:J:130:GLY:N    | 2.07                     | 0.69              |
| 1:K:293:VAL:HG11 | 1:K:428:PHE:CD2  | 2.28                     | 0.69              |
| 1:B:236:LEU:HB2  | 1:B:239:VAL:CG2  | 2.23                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:119:MET:SD   | 1:D:127:PHE:HB2  | 2.33                     | 0.69              |
| 1:D:21:ILE:HD13  | 1:D:42:LEU:HD13  | 1.74                     | 0.69              |
| 1:E:325:SER:HB3  | 1:E:329:SER:HB2  | 1.75                     | 0.69              |
| 1:E:440:TYR:HB2  | 1:K:232:MET:HE2  | 1.73                     | 0.69              |
| 1:G:111:ASN:O    | 1:G:115:ILE:HD13 | 1.93                     | 0.69              |
| 1:B:429:ARG:HH21 | 1:H:390:ALA:CB   | 2.06                     | 0.68              |
| 1:C:287:ALA:HB2  | 1:C:395:ALA:HB1  | 1.75                     | 0.68              |
| 1:E:96:ILE:N     | 1:E:96:ILE:HD12  | 2.08                     | 0.68              |
| 1:G:55:SER:O     | 1:G:62:ARG:HG2   | 1.91                     | 0.68              |
| 1:L:353:ALA:HB2  | 1:L:405:MET:HE1  | 1.75                     | 0.68              |
| 1:C:48:ASN:HB3   | 1:C:71:TYR:CD1   | 2.28                     | 0.68              |
| 1:D:236:LEU:O    | 1:D:239:VAL:HG22 | 1.92                     | 0.68              |
| 1:D:247:ASN:HB3  | 1:D:331:ARG:HG3  | 1.75                     | 0.68              |
| 1:H:437:ARG:NH1  | 4:H:602:HOH:O    | 2.26                     | 0.68              |
| 1:E:440:TYR:HB2  | 1:K:232:MET:CE   | 2.22                     | 0.68              |
| 1:D:13:VAL:HG13  | 1:D:18:VAL:HB    | 1.75                     | 0.68              |
| 1:F:423:ILE:HD12 | 1:F:423:ILE:C    | 2.13                     | 0.68              |
| 1:I:80:PHE:HE1   | 1:I:91:ARG:HG2   | 1.57                     | 0.68              |
| 1:L:368:ILE:HD12 | 1:L:368:ILE:H    | 1.59                     | 0.68              |
| 1:L:129:LEU:HG   | 1:L:347:LEU:HD21 | 1.76                     | 0.68              |
| 1:L:125:SER:HB3  | 1:L:251:PHE:O    | 1.93                     | 0.68              |
| 1:G:370:ARG:N    | 1:G:370:ARG:HD3  | 2.08                     | 0.68              |
| 1:L:386:VAL:HG12 | 1:L:387:ASP:N    | 2.08                     | 0.68              |
| 1:B:178:GLU:OE1  | 1:C:86:LYS:HD3   | 1.93                     | 0.68              |
| 1:I:281:HIS:CE1  | 1:I:404:VAL:HG11 | 2.28                     | 0.68              |
| 1:C:372:ILE:CG2  | 1:C:385:ILE:HD13 | 2.22                     | 0.68              |
| 1:E:129:LEU:HD13 | 1:E:130:GLY:N    | 2.08                     | 0.68              |
| 1:K:315:ASN:ND2  | 1:K:370:ARG:H    | 1.86                     | 0.68              |
| 1:I:167:ASN:OD1  | 1:I:170:ARG:HB3  | 1.93                     | 0.68              |
| 1:J:182:GLU:O    | 1:J:200:LYS:HB2  | 1.92                     | 0.68              |
| 1:A:363:GLU:CD   | 1:A:363:GLU:H    | 1.96                     | 0.68              |
| 1:G:323:PRO:HG3  | 1:G:331:ARG:HG2  | 1.75                     | 0.68              |
| 1:B:441:MET:O    | 1:H:228:HIS:HE1  | 1.77                     | 0.68              |
| 1:J:67:ASP:O     | 1:J:68:MET:HG3   | 1.93                     | 0.68              |
| 1:K:316:ARG:HH11 | 1:K:316:ARG:N    | 1.90                     | 0.68              |
| 1:C:402:ASN:OD1  | 1:C:404:VAL:HG12 | 1.94                     | 0.68              |
| 1:E:314:GLN:HE22 | 1:E:321:ARG:NH2  | 1.91                     | 0.68              |
| 1:K:233:PRO:C    | 1:K:235:PRO:HD3  | 2.14                     | 0.68              |
| 1:C:129:LEU:O    | 1:C:201:TYR:HA   | 1.94                     | 0.67              |
| 1:C:169:ARG:HH22 | 1:C:188:HIS:HB2  | 1.59                     | 0.67              |
| 1:D:300:VAL:HG13 | 1:D:301:PRO:HD2  | 1.73                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:83:THR:HG22  | 1:D:88:LYS:HD3   | 1.76                     | 0.67              |
| 1:G:260:ASP:O    | 1:G:266:GLN:HA   | 1.94                     | 0.67              |
| 1:G:34:ASN:ND2   | 1:G:34:ASN:C     | 2.47                     | 0.67              |
| 1:E:52:PHE:CE2   | 1:E:54:GLY:HA2   | 2.30                     | 0.67              |
| 1:G:160:ALA:HB1  | 1:G:161:PRO:CD   | 2.24                     | 0.67              |
| 1:I:114:ARG:HH11 | 1:I:114:ARG:HB3  | 1.58                     | 0.67              |
| 1:K:316:ARG:NH1  | 1:K:316:ARG:HB2  | 2.08                     | 0.67              |
| 1:E:178:GLU:OE2  | 1:F:86:LYS:HD2   | 1.95                     | 0.67              |
| 1:E:309:VAL:HG21 | 1:E:386:VAL:HG23 | 1.75                     | 0.67              |
| 1:H:312:SER:HB2  | 1:H:368:ILE:HG22 | 1.74                     | 0.67              |
| 1:J:295:SER:O    | 1:J:299:LEU:HD13 | 1.94                     | 0.67              |
| 1:A:419:GLU:O    | 1:A:423:ILE:HD13 | 1.93                     | 0.67              |
| 1:K:316:ARG:HH11 | 1:K:316:ARG:HB2  | 1.59                     | 0.67              |
| 1:K:109:ARG:HD2  | 1:K:344:TYR:CE2  | 2.30                     | 0.67              |
| 1:C:13:VAL:HG13  | 1:C:18:VAL:HB    | 1.76                     | 0.67              |
| 1:D:116:LEU:O    | 1:D:120:GLU:HG3  | 1.95                     | 0.67              |
| 1:E:320:ILE:CG2  | 1:E:321:ARG:N    | 2.58                     | 0.67              |
| 1:I:280:LYS:HE3  | 1:I:281:HIS:NE2  | 2.09                     | 0.67              |
| 1:K:259:PHE:HD1  | 1:K:326:ARG:HD2  | 1.58                     | 0.67              |
| 1:K:58:GLU:O     | 1:K:61:VAL:HG22  | 1.95                     | 0.67              |
| 1:C:423:ILE:O    | 1:C:427:MET:HG3  | 1.93                     | 0.67              |
| 1:F:40:SER:O     | 1:F:41:GLN:HG2   | 1.93                     | 0.67              |
| 1:F:423:ILE:HD12 | 1:F:424:GLU:N    | 2.09                     | 0.67              |
| 1:G:160:ALA:HB2  | 1:G:188:HIS:CD2  | 2.29                     | 0.67              |
| 1:I:23:LEU:HB2   | 1:I:35:VAL:HG13  | 1.77                     | 0.67              |
| 1:K:282:ALA:HA   | 1:K:285:PHE:CZ   | 2.30                     | 0.67              |
| 1:A:30:GLY:HA2   | 1:A:342:ASN:ND2  | 2.10                     | 0.67              |
| 1:B:319:LEU:HG   | 1:B:320:ILE:HG13 | 1.77                     | 0.67              |
| 1:C:232:MET:HE3  | 1:C:235:PRO:HB3  | 1.76                     | 0.67              |
| 1:H:30:GLY:HA2   | 1:H:342:ASN:ND2  | 2.09                     | 0.67              |
| 1:I:127:PHE:CD2  | 1:I:351:LEU:HG   | 2.29                     | 0.67              |
| 1:L:21:ILE:HG12  | 1:L:42:LEU:HD13  | 1.76                     | 0.67              |
| 1:I:310:ALA:HB2  | 1:I:368:ILE:HD12 | 1.75                     | 0.67              |
| 1:K:112:LEU:O    | 1:K:116:LEU:HG   | 1.95                     | 0.67              |
| 1:E:155:GLY:HA3  | 4:E:616:HOH:O    | 1.94                     | 0.66              |
| 1:G:267:LEU:HD21 | 1:G:326:ARG:HH12 | 1.61                     | 0.66              |
| 1:I:97:TYR:CZ    | 1:I:103:PRO:HG3  | 2.30                     | 0.66              |
| 1:J:142:GLU:H    | 1:J:142:GLU:CD   | 1.97                     | 0.66              |
| 1:K:309:VAL:HG13 | 1:K:319:LEU:HD23 | 1.76                     | 0.66              |
| 1:A:431:GLN:HE21 | 1:A:432:VAL:N    | 1.93                     | 0.66              |
| 1:D:402:ASN:O    | 1:D:406:VAL:HG23 | 1.96                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:260:ASP:HB3  | 1:H:267:LEU:O    | 1.96                     | 0.66              |
| 1:L:129:LEU:HD12 | 1:L:347:LEU:HD11 | 1.76                     | 0.66              |
| 1:A:200:LYS:NZ   | 1:B:41:GLN:HE22  | 1.93                     | 0.66              |
| 1:C:32:ILE:N     | 1:C:32:ILE:HD12  | 2.10                     | 0.66              |
| 1:E:444:TYR:OXT  | 1:K:231:PHE:HB2  | 1.95                     | 0.66              |
| 1:C:160:ALA:HB1  | 1:C:161:PRO:HD2  | 1.77                     | 0.66              |
| 1:F:319:LEU:HD12 | 1:F:336:SER:HB3  | 1.78                     | 0.66              |
| 1:C:232:MET:HE2  | 1:I:441:MET:HA   | 1.77                     | 0.66              |
| 1:K:323:PRO:HD2  | 1:K:331:ARG:O    | 1.96                     | 0.66              |
| 1:K:402:ASN:OD1  | 1:K:404:VAL:HG22 | 1.96                     | 0.66              |
| 1:A:32:ILE:HD13  | 1:A:216:LEU:HD13 | 1.77                     | 0.66              |
| 1:D:265:LEU:O    | 1:D:267:LEU:HD13 | 1.94                     | 0.66              |
| 1:E:57:ILE:CD1   | 1:E:96:ILE:HG12  | 2.24                     | 0.66              |
| 1:G:224:LYS:HD2  | 1:H:164:LEU:HD11 | 1.78                     | 0.66              |
| 1:L:349:VAL:HG22 | 1:L:405:MET:SD   | 2.34                     | 0.66              |
| 1:B:414:PHE:O    | 1:B:418:ILE:HD13 | 1.95                     | 0.66              |
| 1:D:183:ILE:HD11 | 1:E:38:PRO:HG3   | 1.77                     | 0.66              |
| 1:F:189:GLU:HA   | 1:F:189:GLU:OE1  | 1.96                     | 0.66              |
| 1:H:244:MET:H    | 1:H:338:ASP:HA   | 1.61                     | 0.66              |
| 1:H:322:ILE:HD13 | 1:H:332:VAL:HA   | 1.77                     | 0.66              |
| 1:I:105:GLU:HB3  | 4:I:608:HOH:O    | 1.96                     | 0.66              |
| 1:K:295:SER:O    | 1:K:299:LEU:HD13 | 1.95                     | 0.66              |
| 1:A:131:PRO:CB   | 1:A:211:ILE:HD11 | 2.25                     | 0.66              |
| 1:B:372:ILE:HG21 | 1:B:385:ILE:HG21 | 1.77                     | 0.66              |
| 1:B:345:LEU:HD22 | 1:B:409:LEU:CD2  | 2.25                     | 0.66              |
| 1:D:411:GLU:O    | 1:D:415:GLU:HG2  | 1.96                     | 0.66              |
| 1:E:331:ARG:HG2  | 1:E:331:ARG:HH21 | 1.60                     | 0.66              |
| 1:H:5:THR:OG1    | 1:H:7:GLU:HG3    | 1.96                     | 0.66              |
| 1:L:189:GLU:HA   | 1:L:189:GLU:OE1  | 1.93                     | 0.66              |
| 1:E:234:LYS:HE3  | 1:E:239:VAL:O    | 1.96                     | 0.66              |
| 1:E:378:GLU:HA   | 1:E:381:MET:HB3  | 1.77                     | 0.66              |
| 1:I:182:GLU:HB3  | 1:I:200:LYS:HE2  | 1.76                     | 0.66              |
| 1:J:160:ALA:CB   | 1:J:169:ARG:HH12 | 2.08                     | 0.66              |
| 1:B:129:LEU:HD22 | 1:B:130:GLY:N    | 2.10                     | 0.65              |
| 1:G:314:GLN:HE22 | 1:L:66:SER:HA    | 1.59                     | 0.65              |
| 1:L:82:TRP:HE1   | 1:L:221:ILE:CD1  | 2.09                     | 0.65              |
| 1:A:310:ALA:HB2  | 1:A:385:ILE:HG23 | 1.77                     | 0.65              |
| 1:B:84:ALA:HB3   | 1:B:87:GLY:O     | 1.95                     | 0.65              |
| 1:E:300:VAL:HG22 | 1:K:429:ARG:NH2  | 2.11                     | 0.65              |
| 1:I:368:ILE:HG21 | 1:I:372:ILE:HG23 | 1.78                     | 0.65              |
| 1:J:236:LEU:O    | 1:J:239:VAL:HG22 | 1.95                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:68:MET:HG2   | 1:B:99:PRO:HD3   | 1.79                     | 0.65              |
| 1:D:236:LEU:HB2  | 1:D:239:VAL:HG22 | 1.77                     | 0.65              |
| 1:D:18:VAL:HA    | 1:D:88:LYS:HB2   | 1.78                     | 0.65              |
| 1:K:78:VAL:HB    | 1:K:91:ARG:HG3   | 1.77                     | 0.65              |
| 1:L:313:ALA:HA   | 1:L:322:ILE:H    | 1.60                     | 0.65              |
| 1:C:119:MET:SD   | 1:C:127:PHE:HB2  | 2.37                     | 0.65              |
| 1:E:264:ASP:N    | 1:E:264:ASP:OD2  | 2.29                     | 0.65              |
| 1:F:4:TYR:HB3    | 1:F:9:ILE:HD11   | 1.78                     | 0.65              |
| 1:L:135:PHE:HB3  | 1:L:231:PHE:CE1  | 2.31                     | 0.65              |
| 1:B:129:LEU:HD12 | 1:B:207:SER:HB3  | 1.79                     | 0.65              |
| 1:B:200:LYS:HE2  | 1:C:41:GLN:OE1   | 1.96                     | 0.65              |
| 1:C:331:ARG:HG2  | 1:C:331:ARG:HH21 | 1.61                     | 0.65              |
| 1:F:168:CYS:O    | 1:F:172:ILE:HG12 | 1.97                     | 0.65              |
| 1:A:191:ALA:HB2  | 1:A:240:ASN:HB3  | 1.79                     | 0.65              |
| 1:C:52:PHE:CE1   | 1:C:70:LEU:HD13  | 2.31                     | 0.65              |
| 1:E:129:LEU:CD2  | 1:E:347:LEU:HD21 | 2.26                     | 0.65              |
| 1:A:37:ILE:HG22  | 1:F:185:ALA:HA   | 1.77                     | 0.65              |
| 1:I:274:PHE:CE2  | 1:I:332:VAL:HG21 | 2.32                     | 0.65              |
| 1:I:248:LEU:CD1  | 1:I:334:VAL:HG23 | 2.26                     | 0.65              |
| 1:K:315:ASN:HB3  | 1:K:318:PRO:HG3  | 1.78                     | 0.65              |
| 1:A:357:GLY:HA2  | 1:A:362:LEU:HB2  | 1.78                     | 0.65              |
| 1:G:383:ASN:HB2  | 1:G:385:ILE:HG12 | 1.78                     | 0.65              |
| 1:E:429:ARG:HH22 | 1:K:300:VAL:HG12 | 1.61                     | 0.65              |
| 1:A:400:LYS:HE2  | 1:A:418:ILE:HD13 | 1.79                     | 0.65              |
| 1:C:273:HIS:NE2  | 1:C:361:LYS:HE3  | 2.10                     | 0.65              |
| 1:D:205:VAL:HG23 | 1:D:206:ARG:H    | 1.61                     | 0.65              |
| 1:F:205:VAL:HG13 | 1:F:206:ARG:N    | 2.12                     | 0.65              |
| 1:K:261:GLU:HA   | 1:K:266:GLN:NE2  | 2.12                     | 0.65              |
| 1:C:314:GLN:HE22 | 1:D:65:GLU:C     | 2.01                     | 0.65              |
| 1:G:267:LEU:HD21 | 1:G:326:ARG:NH1  | 2.11                     | 0.65              |
| 1:G:421:LYS:HD3  | 1:G:424:GLU:OE2  | 1.96                     | 0.65              |
| 1:H:328:ILE:H    | 1:H:328:ILE:HD13 | 1.61                     | 0.65              |
| 1:K:136:PHE:HB2  | 1:K:230:THR:HG23 | 1.78                     | 0.65              |
| 1:L:271:ALA:O    | 1:L:275:ILE:HG12 | 1.96                     | 0.65              |
| 1:A:22:ARG:HH22  | 1:F:167:ASN:HD21 | 1.44                     | 0.65              |
| 1:F:282:ALA:CB   | 1:F:319:LEU:HD21 | 2.27                     | 0.65              |
| 1:H:315:ASN:HD22 | 1:H:373:TYR:HE1  | 1.45                     | 0.65              |
| 1:H:37:ILE:HG22  | 1:I:185:ALA:HB2  | 1.79                     | 0.65              |
| 1:K:33:LYS:HG2   | 1:L:158:ASP:HB3  | 1.78                     | 0.65              |
| 1:B:159:LEU:HD12 | 1:C:22:ARG:HH11  | 1.62                     | 0.64              |
| 1:I:114:ARG:NH1  | 1:I:114:ARG:HB3  | 2.12                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:244:MET:H    | 1:A:338:ASP:HA   | 1.61                     | 0.64              |
| 1:A:431:GLN:NE2  | 1:A:432:VAL:H    | 1.94                     | 0.64              |
| 1:B:289:THR:HB   | 1:B:337:VAL:HG22 | 1.78                     | 0.64              |
| 1:L:351:LEU:HD22 | 1:L:355:LEU:HG   | 1.78                     | 0.64              |
| 1:A:131:PRO:CG   | 1:A:211:ILE:HD11 | 2.28                     | 0.64              |
| 1:B:261:GLU:C    | 1:B:262:ASN:HD22 | 2.00                     | 0.64              |
| 1:G:91:ARG:HD2   | 1:G:92:PHE:N     | 2.12                     | 0.64              |
| 1:H:250:LEU:HB2  | 1:H:258:PHE:CE2  | 2.32                     | 0.64              |
| 1:I:176:LEU:O    | 1:I:181:PHE:HB2  | 1.95                     | 0.64              |
| 1:B:370:ARG:NH2  | 1:B:375:MET:HG3  | 2.10                     | 0.64              |
| 1:C:160:ALA:HB2  | 1:C:169:ARG:HH22 | 1.61                     | 0.64              |
| 1:C:297:LYS:HG2  | 1:I:431:GLN:O    | 1.96                     | 0.64              |
| 1:L:399:PHE:HD2  | 1:L:418:ILE:HD11 | 1.62                     | 0.64              |
| 1:A:161:PRO:HD3  | 4:A:616:HOH:O    | 1.96                     | 0.64              |
| 1:C:116:LEU:O    | 1:C:119:MET:HB3  | 1.97                     | 0.64              |
| 1:C:160:ALA:HB2  | 1:C:169:ARG:NH2  | 2.12                     | 0.64              |
| 1:F:338:ASP:HB2  | 1:F:339:PRO:HD2  | 1.80                     | 0.64              |
| 1:F:19:LYS:HG3   | 1:F:86:LYS:O     | 1.97                     | 0.64              |
| 1:G:122:LEU:HD11 | 1:G:359:LYS:HG3  | 1.79                     | 0.64              |
| 1:H:272:LYS:HZ1  | 1:H:364:ALA:H    | 1.45                     | 0.64              |
| 1:C:24:GLN:NE2   | 1:C:91:ARG:HH11  | 1.95                     | 0.64              |
| 1:D:127:PHE:CE2  | 1:D:351:LEU:HD23 | 2.33                     | 0.64              |
| 1:E:158:ASP:HA   | 1:F:33:LYS:HG2   | 1.78                     | 0.64              |
| 1:K:293:VAL:HG11 | 1:K:428:PHE:CE2  | 2.32                     | 0.64              |
| 1:A:150:LEU:HD13 | 1:A:192:PRO:O    | 1.98                     | 0.64              |
| 1:A:23:LEU:HB2   | 1:A:35:VAL:HG13  | 1.78                     | 0.64              |
| 1:D:48:ASN:HB3   | 1:D:71:TYR:CE1   | 2.33                     | 0.64              |
| 1:G:129:LEU:CD1  | 1:G:131:PRO:HD3  | 2.27                     | 0.64              |
| 1:J:91:ARG:HD2   | 1:J:91:ARG:C     | 2.18                     | 0.64              |
| 1:K:251:PHE:HA   | 1:K:255:VAL:O    | 1.97                     | 0.64              |
| 1:L:306:PRO:HG2  | 1:L:335:ARG:O    | 1.98                     | 0.64              |
| 1:C:261:GLU:HA   | 1:C:266:GLN:HE21 | 1.62                     | 0.64              |
| 1:C:409:LEU:O    | 1:C:413:LEU:HB2  | 1.98                     | 0.64              |
| 1:H:396:LEU:O    | 1:H:400:LYS:HG2  | 1.97                     | 0.64              |
| 1:J:160:ALA:HB1  | 1:J:161:PRO:HD2  | 1.79                     | 0.64              |
| 1:A:34:ASN:ND2   | 1:A:34:ASN:C     | 2.51                     | 0.64              |
| 1:C:136:PHE:HB3  | 1:C:138:PHE:CE1  | 2.31                     | 0.64              |
| 1:D:281:HIS:HD2  | 1:D:402:ASN:HD21 | 1.45                     | 0.64              |
| 1:D:396:LEU:HD11 | 1:D:421:LYS:HB3  | 1.77                     | 0.64              |
| 1:D:45:ALA:HA    | 1:D:50:VAL:HG23  | 1.80                     | 0.64              |
| 1:E:322:ILE:HD12 | 1:E:322:ILE:N    | 2.13                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:187:HIS:HE1  | 1:F:196:GLU:OE1  | 1.81                     | 0.64              |
| 1:L:9:ILE:HA     | 1:L:12:LEU:HD12  | 1.80                     | 0.64              |
| 1:B:236:LEU:HB2  | 1:B:239:VAL:HG22 | 1.78                     | 0.64              |
| 1:F:73:ASP:OD1   | 1:F:76:THR:HG23  | 1.97                     | 0.64              |
| 1:H:236:LEU:HB2  | 1:H:239:VAL:CG2  | 2.27                     | 0.64              |
| 1:E:300:VAL:HG22 | 1:K:429:ARG:HH22 | 1.63                     | 0.64              |
| 1:K:46:LEU:O     | 1:K:47:ASP:HB2   | 1.98                     | 0.64              |
| 1:A:311:TRP:HB3  | 1:A:320:ILE:HB   | 1.80                     | 0.63              |
| 1:B:147:THR:CG2  | 1:B:149:GLU:HG3  | 2.28                     | 0.63              |
| 1:C:241:GLY:HA3  | 1:C:298:ARG:HG3  | 1.81                     | 0.63              |
| 1:F:377:LYS:HA   | 1:F:380:ARG:HG3  | 1.80                     | 0.63              |
| 1:I:135:PHE:HB3  | 1:I:231:PHE:CE1  | 2.33                     | 0.63              |
| 1:L:315:ASN:ND2  | 1:L:370:ARG:HA   | 2.11                     | 0.63              |
| 1:K:309:VAL:HB   | 1:K:386:VAL:O    | 1.99                     | 0.63              |
| 1:L:48:ASN:HB3   | 1:L:71:TYR:CE1   | 2.33                     | 0.63              |
| 1:A:37:ILE:HG22  | 1:F:185:ALA:CB   | 2.29                     | 0.63              |
| 1:D:291:PRO:HG3  | 1:D:341:ALA:HA   | 1.78                     | 0.63              |
| 1:F:402:ASN:O    | 1:F:406:VAL:HG23 | 1.97                     | 0.63              |
| 1:I:98:ASN:HB3   | 1:I:100:ASP:OD1  | 1.98                     | 0.63              |
| 1:I:279:VAL:HG13 | 1:I:309:VAL:HG12 | 1.81                     | 0.63              |
| 1:I:295:SER:O    | 1:I:299:LEU:HD23 | 1.99                     | 0.63              |
| 1:J:72:PRO:CA    | 1:J:94:CYS:HB3   | 2.27                     | 0.63              |
| 1:K:307:CYS:H    | 1:K:317:SER:HB2  | 1.63                     | 0.63              |
| 1:B:19:LYS:HA    | 1:B:39:VAL:HG11  | 1.80                     | 0.63              |
| 1:C:150:LEU:HD13 | 1:C:192:PRO:HG2  | 1.80                     | 0.63              |
| 1:F:440:TYR:HB2  | 1:L:232:MET:HE3  | 1.79                     | 0.63              |
| 1:G:160:ALA:HB3  | 1:G:169:ARG:NH1  | 2.14                     | 0.63              |
| 1:J:386:VAL:HG12 | 1:J:387:ASP:N    | 2.07                     | 0.63              |
| 1:K:35:VAL:HG11  | 1:K:70:LEU:HD11  | 1.79                     | 0.63              |
| 1:A:78:VAL:HG12  | 1:A:91:ARG:HG3   | 1.80                     | 0.63              |
| 1:B:58:GLU:HB3   | 1:B:61:VAL:HG23  | 1.81                     | 0.63              |
| 1:C:178:GLU:OE1  | 1:D:86:LYS:HD3   | 1.99                     | 0.63              |
| 1:E:9:ILE:O      | 1:E:13:VAL:HG23  | 1.99                     | 0.63              |
| 1:E:368:ILE:HG21 | 1:E:372:ILE:HG23 | 1.81                     | 0.63              |
| 1:F:34:ASN:C     | 1:F:34:ASN:HD22  | 2.00                     | 0.63              |
| 1:B:13:VAL:HG13  | 1:B:18:VAL:HB    | 1.80                     | 0.63              |
| 1:K:316:ARG:HE   | 1:K:370:ARG:CZ   | 2.11                     | 0.63              |
| 1:K:310:ALA:HB3  | 1:K:372:ILE:HD13 | 1.80                     | 0.63              |
| 1:E:264:ASP:C    | 1:E:266:GLN:H    | 2.02                     | 0.63              |
| 1:E:402:ASN:O    | 1:E:406:VAL:HG23 | 1.99                     | 0.63              |
| 1:F:150:LEU:HD13 | 1:F:192:PRO:HB2  | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:21:ILE:HG22  | 1:H:90:ALA:HB3   | 1.80                     | 0.63              |
| 1:I:129:LEU:HD22 | 1:I:131:PRO:CG   | 2.27                     | 0.63              |
| 1:A:22:ARG:NH2   | 1:F:167:ASN:HD21 | 1.97                     | 0.63              |
| 1:A:418:ILE:O    | 1:A:422:GLU:HG3  | 1.99                     | 0.63              |
| 1:F:98:ASN:ND2   | 1:F:98:ASN:N     | 2.47                     | 0.63              |
| 1:G:306:PRO:HG2  | 1:G:335:ARG:HH21 | 1.64                     | 0.63              |
| 1:G:406:VAL:HG22 | 1:G:414:PHE:CE1  | 2.33                     | 0.63              |
| 1:I:55:SER:O     | 1:I:58:GLU:HB2   | 1.97                     | 0.63              |
| 1:J:399:PHE:CE1  | 1:J:405:MET:HB3  | 2.34                     | 0.63              |
| 1:E:430:THR:HG22 | 1:K:300:VAL:HG11 | 1.80                     | 0.63              |
| 1:A:207:SER:O    | 1:A:211:ILE:HG12 | 1.99                     | 0.62              |
| 1:B:19:LYS:HA    | 1:B:39:VAL:CG1   | 2.29                     | 0.62              |
| 1:D:300:VAL:CG1  | 1:D:301:PRO:HD2  | 2.28                     | 0.62              |
| 1:E:290:ASN:HB3  | 1:E:295:SER:HB3  | 1.81                     | 0.62              |
| 1:D:183:ILE:CD1  | 1:E:38:PRO:HG3   | 2.29                     | 0.62              |
| 1:F:129:LEU:HD23 | 1:F:130:GLY:N    | 2.14                     | 0.62              |
| 1:J:234:LYS:HB3  | 1:J:294:ASN:HD21 | 1.63                     | 0.62              |
| 1:K:98:ASN:ND2   | 1:K:104:PHE:HA   | 2.14                     | 0.62              |
| 1:K:298:ARG:O    | 1:K:298:ARG:HG3  | 1.97                     | 0.62              |
| 1:A:159:LEU:HD21 | 1:B:22:ARG:HE    | 1.64                     | 0.62              |
| 1:A:184:GLU:HG2  | 4:A:604:HOH:O    | 1.97                     | 0.62              |
| 1:B:311:TRP:CE3  | 1:B:322:ILE:HD13 | 2.34                     | 0.62              |
| 1:E:129:LEU:HD12 | 1:E:131:PRO:HD3  | 1.81                     | 0.62              |
| 1:G:37:ILE:HG13  | 1:G:37:ILE:O     | 1.99                     | 0.62              |
| 1:G:48:ASN:OD1   | 1:G:71:TYR:HA    | 1.98                     | 0.62              |
| 1:I:189:GLU:HB3  | 1:I:194:GLN:NE2  | 2.14                     | 0.62              |
| 1:C:169:ARG:HD2  | 1:D:36:GLU:OE1   | 1.99                     | 0.62              |
| 1:E:9:ILE:CG1    | 1:E:74:LEU:HD12  | 2.24                     | 0.62              |
| 1:F:434:PRO:HA   | 1:F:437:ARG:NH1  | 2.14                     | 0.62              |
| 1:H:316:ARG:HB3  | 1:H:373:TYR:CD1  | 2.33                     | 0.62              |
| 1:H:20:TYR:HB3   | 1:H:89:VAL:HG22  | 1.80                     | 0.62              |
| 1:I:274:PHE:HE2  | 1:I:332:VAL:HG21 | 1.64                     | 0.62              |
| 1:C:112:LEU:HD12 | 1:C:344:TYR:HD2  | 1.64                     | 0.62              |
| 1:D:162:THR:O    | 1:D:164:LEU:N    | 2.29                     | 0.62              |
| 1:F:282:ALA:HB1  | 1:F:319:LEU:HD21 | 1.81                     | 0.62              |
| 1:L:114:ARG:NH2  | 1:L:115:ILE:HD11 | 2.14                     | 0.62              |
| 1:E:285:PHE:HB2  | 1:E:349:VAL:HG13 | 1.81                     | 0.62              |
| 1:F:33:LYS:NZ    | 1:F:56:SER:O     | 2.33                     | 0.62              |
| 1:F:24:GLN:NE2   | 1:F:91:ARG:HH11  | 1.98                     | 0.62              |
| 1:A:283:THR:HG22 | 1:A:388:LEU:HA   | 1.80                     | 0.62              |
| 1:A:431:GLN:HE21 | 1:A:432:VAL:H    | 1.48                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:370:ARG:HH11 | 1:H:370:ARG:HG3  | 1.65                     | 0.62              |
| 1:B:232:MET:CE   | 1:H:440:TYR:HB2  | 2.30                     | 0.62              |
| 1:B:232:MET:HE3  | 1:H:440:TYR:HB2  | 1.81                     | 0.62              |
| 1:J:104:PHE:CZ   | 1:J:106:GLY:HA3  | 2.35                     | 0.62              |
| 1:J:95:ASP:HB3   | 1:J:110:ASN:HD21 | 1.63                     | 0.62              |
| 1:J:402:ASN:O    | 1:J:406:VAL:HG23 | 1.99                     | 0.62              |
| 1:D:104:PHE:CZ   | 1:D:106:GLY:HA3  | 2.34                     | 0.62              |
| 1:E:169:ARG:HH11 | 1:E:195:HIS:HD2  | 1.46                     | 0.62              |
| 1:J:115:ILE:HD11 | 1:J:408:ALA:O    | 2.00                     | 0.62              |
| 1:J:325:SER:HB3  | 1:J:329:SER:HB3  | 1.80                     | 0.62              |
| 1:K:253:ASN:O    | 1:K:255:VAL:HG23 | 1.99                     | 0.62              |
| 1:E:282:ALA:HA   | 1:E:285:PHE:CZ   | 2.35                     | 0.62              |
| 1:F:21:ILE:HG13  | 1:F:42:LEU:HD13  | 1.81                     | 0.62              |
| 1:F:371:ASN:ND2  | 1:F:373:TYR:HB2  | 2.10                     | 0.62              |
| 1:H:380:ARG:HH11 | 1:H:380:ARG:HB2  | 1.64                     | 0.62              |
| 1:L:372:ILE:CG2  | 1:L:385:ILE:HG21 | 2.30                     | 0.62              |
| 1:A:312:SER:HB3  | 1:A:315:ASN:HD22 | 1.64                     | 0.62              |
| 1:B:197:ILE:HD12 | 1:B:214:PHE:CZ   | 2.35                     | 0.62              |
| 1:D:273:HIS:CE1  | 1:D:361:LYS:HA   | 2.35                     | 0.62              |
| 1:F:183:ILE:HD12 | 1:F:197:ILE:HG22 | 1.80                     | 0.62              |
| 1:H:138:PHE:HB3  | 1:H:147:THR:O    | 2.00                     | 0.62              |
| 1:L:355:LEU:HD23 | 1:L:358:ILE:HD12 | 1.82                     | 0.62              |
| 1:D:243:GLY:HA3  | 1:D:298:ARG:NH1  | 2.14                     | 0.62              |
| 1:L:74:LEU:H     | 1:L:74:LEU:HD22  | 1.64                     | 0.62              |
| 1:C:267:LEU:HD21 | 1:C:326:ARG:HH12 | 1.64                     | 0.61              |
| 1:C:380:ARG:HB2  | 1:C:380:ARG:NH1  | 2.15                     | 0.61              |
| 1:F:321:ARG:C    | 1:F:322:ILE:HD12 | 2.20                     | 0.61              |
| 1:H:86:LYS:HE2   | 1:H:86:LYS:HA    | 1.81                     | 0.61              |
| 1:C:282:ALA:C    | 1:C:284:SER:H    | 2.03                     | 0.61              |
| 1:C:96:ILE:N     | 1:C:96:ILE:HD12  | 2.14                     | 0.61              |
| 1:D:289:THR:C    | 1:D:290:ASN:HD22 | 2.03                     | 0.61              |
| 1:E:161:PRO:O    | 1:E:167:ASN:ND2  | 2.33                     | 0.61              |
| 1:H:308:TYR:HB3  | 1:H:385:ILE:HG23 | 1.81                     | 0.61              |
| 1:H:4:TYR:HB3    | 1:H:9:ILE:HG13   | 1.82                     | 0.61              |
| 1:L:9:ILE:HG21   | 1:L:92:PHE:HZ    | 1.64                     | 0.61              |
| 1:A:252:LYS:HE3  | 1:A:253:ASN:ND2  | 2.15                     | 0.61              |
| 1:B:381:MET:HE2  | 1:B:381:MET:N    | 2.16                     | 0.61              |
| 1:B:77:PHE:HB2   | 1:B:92:PHE:HE2   | 1.65                     | 0.61              |
| 1:D:396:LEU:O    | 1:D:400:LYS:HG3  | 2.00                     | 0.61              |
| 1:G:267:LEU:HD11 | 1:G:322:ILE:HG21 | 1.83                     | 0.61              |
| 1:H:160:ALA:HB1  | 1:H:161:PRO:CD   | 2.31                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:287:ALA:HB2  | 1:I:395:ALA:HB1  | 1.82                     | 0.61              |
| 1:I:57:ILE:CD1   | 1:I:96:ILE:HG12  | 2.27                     | 0.61              |
| 1:L:236:LEU:HD12 | 1:L:239:VAL:HG21 | 1.83                     | 0.61              |
| 1:D:338:ASP:HB2  | 1:D:339:PRO:HD2  | 1.82                     | 0.61              |
| 1:H:202:ALA:HB3  | 1:H:207:SER:HB2  | 1.81                     | 0.61              |
| 1:L:273:HIS:HB3  | 1:L:357:GLY:O    | 2.00                     | 0.61              |
| 1:L:316:ARG:HD3  | 1:L:370:ARG:HH22 | 1.66                     | 0.61              |
| 1:B:164:LEU:HD11 | 1:C:224:LYS:HG3  | 1.83                     | 0.61              |
| 1:D:264:ASP:C    | 1:D:266:GLN:H    | 2.03                     | 0.61              |
| 1:E:20:TYR:O     | 1:E:89:VAL:HG13  | 2.01                     | 0.61              |
| 1:F:244:MET:H    | 1:F:338:ASP:HA   | 1.65                     | 0.61              |
| 1:F:399:PHE:CE1  | 1:F:405:MET:HB3  | 2.35                     | 0.61              |
| 1:I:35:VAL:HG11  | 1:I:70:LEU:CD2   | 2.30                     | 0.61              |
| 1:J:156:TYR:HA   | 1:J:188:HIS:O    | 2.00                     | 0.61              |
| 1:A:211:ILE:HG21 | 1:A:343:PRO:HG3  | 1.82                     | 0.61              |
| 1:B:315:ASN:HB3  | 1:B:318:PRO:HD3  | 1.83                     | 0.61              |
| 1:B:281:HIS:HD2  | 1:B:402:ASN:HD21 | 1.46                     | 0.61              |
| 1:E:136:PHE:CE2  | 1:E:194:GLN:HB2  | 2.35                     | 0.61              |
| 1:F:16:GLU:O     | 1:F:17:ASN:HB3   | 2.01                     | 0.61              |
| 1:G:236:LEU:HB2  | 1:G:239:VAL:HG22 | 1.83                     | 0.61              |
| 1:I:127:PHE:CE2  | 1:I:351:LEU:HG   | 2.35                     | 0.61              |
| 1:I:129:LEU:O    | 1:I:201:TYR:HA   | 2.00                     | 0.61              |
| 1:K:45:ALA:HA    | 1:K:50:VAL:HG21  | 1.82                     | 0.61              |
| 1:F:436:GLU:OE2  | 1:L:297:LYS:HE3  | 2.01                     | 0.61              |
| 1:B:282:ALA:HA   | 1:B:285:PHE:CZ   | 2.36                     | 0.61              |
| 1:E:139:LYS:HA   | 1:E:227:LEU:HD23 | 1.83                     | 0.61              |
| 1:F:119:MET:HA   | 1:F:355:LEU:HD11 | 1.82                     | 0.61              |
| 1:I:320:ILE:N    | 1:I:320:ILE:HD12 | 2.16                     | 0.61              |
| 1:I:289:THR:HB   | 1:I:337:VAL:HG22 | 1.83                     | 0.61              |
| 1:J:176:LEU:O    | 1:J:181:PHE:HB2  | 1.99                     | 0.61              |
| 1:K:236:LEU:HB2  | 1:K:239:VAL:CG2  | 2.30                     | 0.61              |
| 1:K:281:HIS:CD2  | 1:K:402:ASN:HD21 | 2.19                     | 0.61              |
| 1:L:372:ILE:HG21 | 1:L:385:ILE:HG21 | 1.82                     | 0.61              |
| 1:A:45:ALA:HA    | 1:A:50:VAL:CG2   | 2.30                     | 0.61              |
| 1:A:5:THR:H      | 1:A:8:ASP:HB2    | 1.66                     | 0.61              |
| 1:C:337:VAL:HG12 | 1:C:338:ASP:N    | 2.16                     | 0.61              |
| 1:E:148:LEU:HD22 | 1:E:148:LEU:H    | 1.64                     | 0.61              |
| 1:E:306:PRO:HB3  | 1:E:319:LEU:HA   | 1.81                     | 0.61              |
| 1:G:311:TRP:CB   | 1:G:320:ILE:HB   | 2.31                     | 0.61              |
| 1:H:311:TRP:CZ2  | 1:H:367:PRO:HB3  | 2.36                     | 0.61              |
| 1:I:310:ALA:CB   | 1:I:368:ILE:HD12 | 2.31                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:131:PRO:HB3  | 1:A:211:ILE:HD11 | 1.83                     | 0.61              |
| 1:A:400:LYS:HB3  | 1:A:418:ILE:CD1  | 2.30                     | 0.61              |
| 1:B:120:GLU:C    | 1:B:122:LEU:H    | 2.02                     | 0.61              |
| 1:H:183:ILE:N    | 1:H:183:ILE:HD12 | 2.15                     | 0.61              |
| 1:B:436:GLU:OE2  | 1:H:297:LYS:HE3  | 2.01                     | 0.60              |
| 1:B:163:ASP:OD1  | 1:C:89:VAL:HG21  | 2.01                     | 0.60              |
| 1:D:248:LEU:O    | 1:D:331:ARG:HB2  | 2.00                     | 0.60              |
| 1:F:236:LEU:HD12 | 1:F:239:VAL:HG22 | 1.82                     | 0.60              |
| 1:G:312:SER:HB3  | 1:G:315:ASN:HB2  | 1.82                     | 0.60              |
| 1:I:32:ILE:HG21  | 1:I:216:LEU:HD12 | 1.82                     | 0.60              |
| 1:K:160:ALA:HB1  | 1:K:161:PRO:CD   | 2.26                     | 0.60              |
| 1:A:252:LYS:HB2  | 1:A:252:LYS:HZ2  | 1.64                     | 0.60              |
| 1:A:127:PHE:CE2  | 1:A:351:LEU:HD13 | 2.37                     | 0.60              |
| 1:D:249:SER:HB3  | 1:D:331:ARG:HB3  | 1.84                     | 0.60              |
| 1:D:260:ASP:O    | 1:D:266:GLN:HA   | 2.01                     | 0.60              |
| 1:H:57:ILE:CD1   | 1:H:96:ILE:HG12  | 2.31                     | 0.60              |
| 1:C:231:PHE:HB2  | 1:I:444:TYR:OXT  | 2.01                     | 0.60              |
| 1:K:380:ARG:HA   | 1:K:383:ASN:HD22 | 1.65                     | 0.60              |
| 1:A:9:ILE:HG13   | 1:A:74:LEU:HD12  | 1.82                     | 0.60              |
| 1:B:197:ILE:HD12 | 1:B:214:PHE:CE1  | 2.36                     | 0.60              |
| 1:C:159:LEU:HD11 | 1:D:22:ARG:HD3   | 1.83                     | 0.60              |
| 1:D:259:PHE:CD2  | 1:D:326:ARG:HB3  | 2.36                     | 0.60              |
| 1:D:316:ARG:NH1  | 1:E:63:ILE:HA    | 2.16                     | 0.60              |
| 1:G:169:ARG:HG3  | 1:G:195:HIS:ND1  | 2.16                     | 0.60              |
| 1:G:20:TYR:CZ    | 1:G:36:GLU:HB3   | 2.36                     | 0.60              |
| 1:H:166:GLU:OE2  | 1:H:227:LEU:HD11 | 2.01                     | 0.60              |
| 1:I:118:GLU:O    | 1:I:122:LEU:HD13 | 2.02                     | 0.60              |
| 1:I:150:LEU:CD1  | 1:I:192:PRO:HB2  | 2.32                     | 0.60              |
| 1:I:349:VAL:HG22 | 1:I:405:MET:SD   | 2.41                     | 0.60              |
| 1:J:129:LEU:HD23 | 1:J:130:GLY:H    | 1.67                     | 0.60              |
| 1:K:150:LEU:CD1  | 1:K:192:PRO:HG2  | 2.31                     | 0.60              |
| 1:L:323:PRO:HG3  | 1:L:331:ARG:HG3  | 1.82                     | 0.60              |
| 1:D:111:ASN:O    | 1:D:115:ILE:HD13 | 2.00                     | 0.60              |
| 1:D:377:LYS:HG3  | 1:D:380:ARG:NH2  | 2.15                     | 0.60              |
| 1:F:27:ASP:HB2   | 1:F:57:ILE:O     | 2.01                     | 0.60              |
| 1:H:84:ALA:HB3   | 1:H:87:GLY:O     | 2.02                     | 0.60              |
| 1:K:248:LEU:O    | 1:K:331:ARG:HB2  | 2.02                     | 0.60              |
| 1:B:96:ILE:HD12  | 1:B:96:ILE:H     | 1.65                     | 0.60              |
| 1:D:129:LEU:HD12 | 1:D:207:SER:HB3  | 1.82                     | 0.60              |
| 1:E:297:LYS:HE3  | 1:K:436:GLU:OE1  | 2.02                     | 0.60              |
| 1:F:283:THR:O    | 1:F:398:GLU:HG2  | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:2:ALA:N      | 4:H:613:HOH:O    | 2.34                     | 0.60              |
| 1:J:236:LEU:HB2  | 1:J:239:VAL:HG22 | 1.80                     | 0.60              |
| 1:K:37:ILE:HD13  | 1:K:41:GLN:HB2   | 1.82                     | 0.60              |
| 1:A:329:SER:O    | 1:A:331:ARG:HG2  | 2.02                     | 0.60              |
| 1:F:440:TYR:OH   | 1:L:293:VAL:HB   | 2.02                     | 0.60              |
| 1:I:316:ARG:HB3  | 1:I:373:TYR:CE1  | 2.37                     | 0.60              |
| 1:J:57:ILE:HG13  | 1:J:96:ILE:HD13  | 1.84                     | 0.60              |
| 1:K:338:ASP:HB2  | 1:K:339:PRO:HD2  | 1.83                     | 0.60              |
| 1:L:145:GLU:OE2  | 1:L:146:PRO:HD2  | 2.01                     | 0.60              |
| 1:A:206:ARG:HH11 | 1:A:206:ARG:CG   | 2.13                     | 0.60              |
| 1:D:282:ALA:HA   | 1:D:285:PHE:CE2  | 2.35                     | 0.60              |
| 1:D:6:ARG:HH11   | 1:D:6:ARG:HG3    | 1.67                     | 0.60              |
| 1:F:32:ILE:HD13  | 1:F:216:LEU:HD13 | 1.83                     | 0.60              |
| 1:G:224:LYS:CD   | 1:H:164:LEU:HD11 | 2.32                     | 0.60              |
| 1:B:430:THR:HG22 | 1:H:300:VAL:HG21 | 1.83                     | 0.60              |
| 1:I:136:PHE:CE2  | 1:I:194:GLN:HB2  | 2.36                     | 0.60              |
| 1:K:55:SER:O     | 1:K:62:ARG:HG2   | 2.02                     | 0.60              |
| 1:K:83:THR:HB    | 1:K:88:LYS:HA    | 1.84                     | 0.60              |
| 1:L:286:THR:HG23 | 1:L:290:ASN:ND2  | 2.17                     | 0.60              |
| 1:E:326:ARG:HG2  | 1:E:326:ARG:NH1  | 2.17                     | 0.60              |
| 1:E:19:LYS:HD3   | 1:E:39:VAL:HG11  | 1.83                     | 0.60              |
| 1:F:100:ASP:O    | 1:F:102:THR:N    | 2.34                     | 0.60              |
| 1:J:206:ARG:HG3  | 1:J:206:ARG:HH11 | 1.65                     | 0.60              |
| 1:L:48:ASN:HB3   | 1:L:71:TYR:CD1   | 2.36                     | 0.60              |
| 1:A:319:LEU:HD22 | 1:A:320:ILE:CD1  | 2.31                     | 0.60              |
| 1:B:159:LEU:HD11 | 1:C:22:ARG:HH11  | 1.65                     | 0.60              |
| 1:E:271:ALA:O    | 1:E:275:ILE:HG12 | 2.02                     | 0.60              |
| 1:I:285:PHE:HB2  | 1:I:349:VAL:CG1  | 2.32                     | 0.60              |
| 1:K:119:MET:HG2  | 1:K:124:PHE:HB2  | 1.84                     | 0.60              |
| 1:D:325:SER:HB3  | 1:D:331:ARG:HH21 | 1.66                     | 0.60              |
| 1:H:21:ILE:HD13  | 1:H:21:ILE:H     | 1.66                     | 0.60              |
| 1:H:96:ILE:HD12  | 1:H:96:ILE:N     | 2.17                     | 0.60              |
| 1:B:139:LYS:O    | 1:B:147:THR:HB   | 2.02                     | 0.59              |
| 1:C:197:ILE:HD12 | 1:C:214:PHE:CE1  | 2.37                     | 0.59              |
| 1:D:183:ILE:H    | 1:D:183:ILE:HD13 | 1.66                     | 0.59              |
| 1:E:176:LEU:O    | 1:E:181:PHE:HB2  | 2.01                     | 0.59              |
| 1:G:282:ALA:HA   | 1:G:285:PHE:CZ   | 2.37                     | 0.59              |
| 1:C:260:ASP:HB2  | 1:C:268:SER:HB3  | 1.84                     | 0.59              |
| 1:C:402:ASN:HD21 | 1:C:404:VAL:CG1  | 2.15                     | 0.59              |
| 1:D:325:SER:HB3  | 1:D:331:ARG:NH2  | 2.16                     | 0.59              |
| 1:D:91:ARG:HD2   | 1:D:92:PHE:N     | 2.17                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:127:PHE:HE2  | 1:H:347:LEU:HD12 | 1.67                     | 0.59              |
| 1:H:146:PRO:HG3  | 1:H:228:HIS:CD2  | 2.36                     | 0.59              |
| 1:H:328:ILE:N    | 1:H:328:ILE:HD13 | 2.17                     | 0.59              |
| 1:A:300:VAL:HG22 | 1:G:429:ARG:HH12 | 1.66                     | 0.59              |
| 1:D:372:ILE:HG13 | 1:D:373:TYR:HD1  | 1.66                     | 0.59              |
| 1:I:160:ALA:HB1  | 1:I:161:PRO:HD2  | 1.83                     | 0.59              |
| 1:I:372:ILE:HG13 | 1:I:373:TYR:CE1  | 2.38                     | 0.59              |
| 1:K:306:PRO:HB3  | 1:K:319:LEU:HA   | 1.85                     | 0.59              |
| 1:K:383:ASN:HB2  | 1:K:385:ILE:HG13 | 1.83                     | 0.59              |
| 1:E:314:GLN:NE2  | 1:F:65:GLU:HB3   | 2.16                     | 0.59              |
| 1:F:437:ARG:HD3  | 1:L:148:LEU:HD21 | 1.84                     | 0.59              |
| 1:F:96:ILE:N     | 1:F:96:ILE:HD12  | 2.17                     | 0.59              |
| 1:G:258:PHE:HB3  | 1:G:270:THR:HB   | 1.83                     | 0.59              |
| 1:H:127:PHE:CE2  | 1:H:347:LEU:HD12 | 2.38                     | 0.59              |
| 1:I:163:ASP:HA   | 1:I:167:ASN:HD22 | 1.67                     | 0.59              |
| 1:J:11:LYS:HG3   | 1:J:15:GLU:CD    | 2.22                     | 0.59              |
| 1:A:122:LEU:HD21 | 1:A:359:LYS:HB3  | 1.84                     | 0.59              |
| 1:C:200:LYS:HE2  | 1:D:41:GLN:OE1   | 2.01                     | 0.59              |
| 1:D:316:ARG:HH11 | 1:E:63:ILE:HA    | 1.66                     | 0.59              |
| 1:E:161:PRO:HB3  | 1:F:223:ARG:HH12 | 1.67                     | 0.59              |
| 1:G:325:SER:HB2  | 1:G:331:ARG:HH22 | 1.67                     | 0.59              |
| 1:K:315:ASN:HD21 | 1:K:370:ARG:N    | 1.91                     | 0.59              |
| 1:D:83:THR:CG2   | 1:D:88:LYS:HD3   | 2.32                     | 0.59              |
| 1:G:368:ILE:HD13 | 1:G:372:ILE:CD1  | 2.31                     | 0.59              |
| 1:G:57:ILE:C     | 1:G:59:GLY:H     | 2.06                     | 0.59              |
| 1:C:85:GLU:O     | 1:C:86:LYS:HB2   | 2.01                     | 0.59              |
| 1:E:273:HIS:NE2  | 1:E:361:LYS:HA   | 2.18                     | 0.59              |
| 1:F:380:ARG:HH11 | 1:F:385:ILE:CG2  | 2.15                     | 0.59              |
| 1:G:4:TYR:HB3    | 1:G:9:ILE:CD1    | 2.32                     | 0.59              |
| 1:J:368:ILE:HD12 | 1:J:385:ILE:HG23 | 1.83                     | 0.59              |
| 1:K:17:ASN:HD22  | 1:K:87:GLY:HA2   | 1.67                     | 0.59              |
| 1:K:316:ARG:HD3  | 1:K:316:ARG:N    | 2.18                     | 0.59              |
| 1:E:293:VAL:HG23 | 1:K:440:TYR:OH   | 2.02                     | 0.59              |
| 1:L:168:CYS:O    | 1:L:172:ILE:HG13 | 2.02                     | 0.59              |
| 1:L:306:PRO:HG2  | 1:L:335:ARG:C    | 2.23                     | 0.59              |
| 1:A:41:GLN:HE22  | 1:F:200:LYS:CE   | 2.15                     | 0.59              |
| 1:H:63:ILE:N     | 1:H:63:ILE:HD12  | 2.18                     | 0.59              |
| 1:J:357:GLY:HA2  | 1:J:362:LEU:HG   | 1.85                     | 0.59              |
| 1:K:260:ASP:O    | 1:K:266:GLN:HA   | 2.02                     | 0.59              |
| 1:K:5:THR:HG22   | 1:K:8:ASP:CG     | 2.23                     | 0.59              |
| 1:A:244:MET:N    | 1:A:338:ASP:HA   | 2.17                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:131:PRO:HG2  | 1:E:199:PHE:HD1  | 1.68                     | 0.59              |
| 1:F:115:ILE:HG22 | 1:F:351:LEU:HD13 | 1.84                     | 0.59              |
| 1:I:376:SER:O    | 1:I:380:ARG:HG3  | 2.03                     | 0.59              |
| 1:J:371:ASN:ND2  | 1:J:374:VAL:H    | 2.01                     | 0.59              |
| 1:L:136:PHE:HB3  | 1:L:138:PHE:HE1  | 1.68                     | 0.59              |
| 1:A:191:ALA:HB3  | 1:A:194:GLN:HE21 | 1.68                     | 0.59              |
| 1:B:370:ARG:NH2  | 1:B:375:MET:SD   | 2.76                     | 0.59              |
| 1:E:207:SER:O    | 1:E:211:ILE:HG12 | 2.03                     | 0.59              |
| 1:H:280:LYS:HG2  | 1:H:281:HIS:CD2  | 2.38                     | 0.59              |
| 1:H:402:ASN:O    | 1:H:406:VAL:HG23 | 2.03                     | 0.59              |
| 1:I:282:ALA:C    | 1:I:284:SER:H    | 2.05                     | 0.59              |
| 1:L:55:SER:CB    | 1:L:62:ARG:HG3   | 2.30                     | 0.59              |
| 1:A:172:ILE:HD13 | 1:A:218:VAL:HG22 | 1.85                     | 0.58              |
| 1:A:319:LEU:HB3  | 1:A:320:ILE:HD12 | 1.84                     | 0.58              |
| 1:A:306:PRO:HG2  | 1:A:335:ARG:C    | 2.23                     | 0.58              |
| 1:D:68:MET:CE    | 1:D:98:ASN:HA    | 2.33                     | 0.58              |
| 1:D:68:MET:HE3   | 1:D:98:ASN:HA    | 1.84                     | 0.58              |
| 1:E:140:LEU:HD12 | 1:E:226:GLY:CA   | 2.33                     | 0.58              |
| 1:E:273:HIS:NE2  | 1:E:361:LYS:HG2  | 2.16                     | 0.58              |
| 1:L:443:GLN:HG2  | 1:L:444:TYR:CE2  | 2.38                     | 0.58              |
| 1:A:138:PHE:CZ   | 1:A:236:LEU:HD11 | 2.38                     | 0.58              |
| 1:D:139:LYS:HE3  | 1:D:149:GLU:HB3  | 1.84                     | 0.58              |
| 1:F:218:VAL:HG12 | 1:F:219:LYS:N    | 2.16                     | 0.58              |
| 1:J:184:GLU:OE1  | 1:J:200:LYS:HG3  | 2.03                     | 0.58              |
| 1:K:360:ASN:N    | 1:K:360:ASN:HD22 | 2.00                     | 0.58              |
| 1:L:425:TRP:CZ3  | 1:L:429:ARG:HD2  | 2.38                     | 0.58              |
| 1:B:129:LEU:HD13 | 1:B:131:PRO:HD3  | 1.86                     | 0.58              |
| 1:C:6:ARG:O      | 1:C:10:GLU:HG3   | 2.03                     | 0.58              |
| 1:C:189:GLU:HB2  | 1:C:194:GLN:HB3  | 1.83                     | 0.58              |
| 1:C:9:ILE:HA     | 1:C:12:LEU:HD12  | 1.84                     | 0.58              |
| 1:F:96:ILE:HD13  | 1:F:107:ASP:CG   | 2.23                     | 0.58              |
| 1:J:299:LEU:HD12 | 1:J:299:LEU:N    | 2.17                     | 0.58              |
| 1:K:169:ARG:HH21 | 1:K:169:ARG:HG3  | 1.68                     | 0.58              |
| 1:K:380:ARG:HA   | 1:K:383:ASN:ND2  | 2.18                     | 0.58              |
| 1:D:310:ALA:O    | 1:D:318:PRO:HB2  | 2.03                     | 0.58              |
| 1:E:152:ASP:OD1  | 1:E:193:GLY:HA2  | 2.03                     | 0.58              |
| 1:E:247:ASN:HD22 | 1:E:331:ARG:HE   | 1.51                     | 0.58              |
| 1:E:396:LEU:HD11 | 1:E:421:LYS:HB3  | 1.84                     | 0.58              |
| 1:F:141:ASP:O    | 1:F:144:GLY:N    | 2.28                     | 0.58              |
| 1:H:267:LEU:CD2  | 1:H:326:ARG:HH12 | 2.14                     | 0.58              |
| 1:I:9:ILE:HG13   | 1:I:74:LEU:HD12  | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:140:LEU:HD21 | 1:J:228:HIS:HB2  | 1.84                     | 0.58              |
| 1:J:9:ILE:HG21   | 1:J:92:PHE:HZ    | 1.68                     | 0.58              |
| 4:K:620:HOH:O    | 1:L:177:GLU:HG2  | 2.03                     | 0.58              |
| 1:L:127:PHE:CD2  | 1:L:351:LEU:HG   | 2.38                     | 0.58              |
| 1:B:134:GLU:O    | 1:B:242:SER:HB3  | 2.04                     | 0.58              |
| 1:B:429:ARG:NH1  | 1:H:300:VAL:HG23 | 2.16                     | 0.58              |
| 1:D:114:ARG:HH21 | 1:D:115:ILE:HD11 | 1.68                     | 0.58              |
| 1:D:146:PRO:HG3  | 1:D:228:HIS:CD2  | 2.38                     | 0.58              |
| 1:D:52:PHE:HZ    | 1:D:57:ILE:HD11  | 1.68                     | 0.58              |
| 1:F:109:ARG:HH21 | 1:F:109:ARG:HG2  | 1.68                     | 0.58              |
| 1:F:437:ARG:CD   | 1:L:148:LEU:HD21 | 2.34                     | 0.58              |
| 1:G:160:ALA:O    | 1:G:161:PRO:C    | 2.42                     | 0.58              |
| 1:J:100:ASP:OD1  | 1:J:102:THR:HG22 | 2.03                     | 0.58              |
| 1:J:123:GLY:O    | 1:J:252:LYS:HG3  | 2.03                     | 0.58              |
| 1:J:346:ALA:O    | 1:J:350:LEU:HB2  | 2.03                     | 0.58              |
| 1:C:375:MET:HE3  | 1:C:379:GLU:HB3  | 1.86                     | 0.58              |
| 1:G:371:ASN:HB3  | 1:G:375:MET:CG   | 2.33                     | 0.58              |
| 1:G:77:PHE:CZ    | 1:G:79:ILE:HD11  | 2.38                     | 0.58              |
| 1:I:189:GLU:OE1  | 1:I:190:VAL:HG23 | 2.03                     | 0.58              |
| 1:I:27:ASP:OD1   | 1:I:33:LYS:HE3   | 2.04                     | 0.58              |
| 1:L:231:PHE:HB3  | 1:L:339:PRO:HB2  | 1.84                     | 0.58              |
| 1:C:191:ALA:HB2  | 1:C:240:ASN:HB3  | 1.85                     | 0.58              |
| 1:E:282:ALA:HA   | 1:E:285:PHE:CE1  | 2.38                     | 0.58              |
| 1:K:380:ARG:HB3  | 1:K:385:ILE:HD12 | 1.85                     | 0.58              |
| 1:E:232:MET:HE3  | 1:K:437:ARG:HA   | 1.85                     | 0.58              |
| 1:C:3:LYS:HG2    | 1:C:4:TYR:CD1    | 2.39                     | 0.58              |
| 1:E:122:LEU:HD12 | 1:E:355:LEU:HD22 | 1.85                     | 0.58              |
| 1:E:68:MET:HE1   | 1:E:104:PHE:CD1  | 2.39                     | 0.58              |
| 1:G:281:HIS:HD2  | 1:G:402:ASN:HD21 | 1.50                     | 0.58              |
| 1:B:429:ARG:NH2  | 1:H:390:ALA:HB1  | 2.15                     | 0.58              |
| 1:I:261:GLU:HA   | 1:I:266:GLN:CG   | 2.24                     | 0.58              |
| 1:E:429:ARG:HH12 | 1:K:300:VAL:HG12 | 1.69                     | 0.58              |
| 1:L:250:LEU:C    | 1:L:251:PHE:HD1  | 2.07                     | 0.58              |
| 1:D:48:ASN:HB3   | 1:D:71:TYR:CD1   | 2.39                     | 0.58              |
| 1:E:12:LEU:O     | 1:E:16:GLU:HB2   | 2.04                     | 0.58              |
| 1:E:140:LEU:HD22 | 1:E:144:GLY:O    | 2.04                     | 0.58              |
| 1:E:325:SER:HB2  | 1:E:331:ARG:NH2  | 2.14                     | 0.58              |
| 1:G:177:GLU:HB2  | 1:G:183:ILE:HD11 | 1.85                     | 0.58              |
| 1:G:308:TYR:HD2  | 1:G:380:ARG:HD3  | 1.68                     | 0.58              |
| 1:H:122:LEU:HD21 | 1:H:359:LYS:HD3  | 1.86                     | 0.58              |
| 1:L:287:ALA:HB2  | 1:L:395:ALA:CB   | 2.33                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:265:LEU:N    | 1:G:265:LEU:HD12 | 2.19                     | 0.58              |
| 1:H:279:VAL:HG13 | 1:H:309:VAL:CG1  | 2.32                     | 0.58              |
| 1:H:5:THR:C      | 1:H:7:GLU:H      | 2.07                     | 0.58              |
| 1:J:404:VAL:HG13 | 1:J:405:MET:HE2  | 1.86                     | 0.58              |
| 1:L:291:PRO:HG2  | 1:L:292:THR:H    | 1.69                     | 0.58              |
| 1:B:48:ASN:OD1   | 1:B:72:PRO:HD2   | 2.04                     | 0.57              |
| 1:C:118:GLU:O    | 1:C:122:LEU:HD23 | 2.04                     | 0.57              |
| 1:C:150:LEU:HD13 | 1:C:192:PRO:O    | 2.04                     | 0.57              |
| 1:D:22:ARG:O     | 1:D:91:ARG:HB2   | 2.04                     | 0.57              |
| 1:G:380:ARG:HD2  | 1:G:387:ASP:OD2  | 2.04                     | 0.57              |
| 1:J:119:MET:O    | 1:J:124:PHE:HB2  | 2.03                     | 0.57              |
| 1:K:325:SER:CB   | 1:K:331:ARG:HH22 | 2.17                     | 0.57              |
| 1:L:402:ASN:HD21 | 1:L:404:VAL:HG12 | 1.67                     | 0.57              |
| 1:C:124:PHE:CD2  | 1:C:250:LEU:HD13 | 2.39                     | 0.57              |
| 1:D:52:PHE:CZ    | 1:D:54:GLY:HA2   | 2.38                     | 0.57              |
| 1:E:429:ARG:O    | 1:K:297:LYS:HD3  | 2.04                     | 0.57              |
| 1:F:34:ASN:ND2   | 1:F:34:ASN:C     | 2.57                     | 0.57              |
| 1:H:140:LEU:HD21 | 1:H:223:ARG:HH22 | 1.67                     | 0.57              |
| 1:I:399:PHE:CE1  | 1:I:405:MET:HB3  | 2.39                     | 0.57              |
| 1:L:118:GLU:O    | 1:L:122:LEU:HD23 | 2.03                     | 0.57              |
| 1:A:142:GLU:H    | 1:A:142:GLU:CD   | 2.08                     | 0.57              |
| 1:A:52:PHE:CE1   | 1:A:70:LEU:HD13  | 2.38                     | 0.57              |
| 1:A:63:ILE:O     | 1:F:316:ARG:HD2  | 2.03                     | 0.57              |
| 1:C:201:TYR:C    | 1:C:201:TYR:CD1  | 2.77                     | 0.57              |
| 1:E:13:VAL:CG1   | 1:E:18:VAL:HB    | 2.32                     | 0.57              |
| 1:F:298:ARG:NH2  | 1:F:338:ASP:HB3  | 2.20                     | 0.57              |
| 1:G:370:ARG:CD   | 1:G:370:ARG:H    | 2.11                     | 0.57              |
| 1:H:215:LYS:HG2  | 1:H:231:PHE:CE2  | 2.39                     | 0.57              |
| 1:J:81:PRO:HG2   | 1:J:82:TRP:H     | 1.69                     | 0.57              |
| 1:K:150:LEU:HD13 | 1:K:192:PRO:HG2  | 1.87                     | 0.57              |
| 1:K:323:PRO:HG3  | 1:K:331:ARG:NE   | 2.18                     | 0.57              |
| 1:D:129:LEU:CD1  | 1:D:131:PRO:HD3  | 2.31                     | 0.57              |
| 1:E:32:ILE:HD12  | 1:E:216:LEU:HD13 | 1.84                     | 0.57              |
| 1:H:155:GLY:O    | 1:H:158:ASP:HB2  | 2.05                     | 0.57              |
| 1:I:112:LEU:HD21 | 1:I:347:LEU:HD12 | 1.86                     | 0.57              |
| 1:K:319:LEU:O    | 1:K:320:ILE:HD13 | 2.03                     | 0.57              |
| 1:K:45:ALA:HA    | 1:K:50:VAL:CG2   | 2.35                     | 0.57              |
| 1:A:274:PHE:CE1  | 1:A:354:GLY:HA3  | 2.39                     | 0.57              |
| 1:B:116:LEU:O    | 1:B:119:MET:HB3  | 2.04                     | 0.57              |
| 1:C:65:GLU:O     | 1:C:65:GLU:HG3   | 2.04                     | 0.57              |
| 1:F:232:MET:HE2  | 1:L:440:TYR:HB2  | 1.84                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:98:ASN:HD21  | 1:F:104:PHE:CA   | 2.17                     | 0.57              |
| 1:A:436:GLU:CD   | 1:G:297:LYS:HZ2  | 2.08                     | 0.57              |
| 1:H:166:GLU:O    | 1:H:168:CYS:N    | 2.37                     | 0.57              |
| 1:H:351:LEU:HD22 | 1:H:355:LEU:HG   | 1.87                     | 0.57              |
| 1:I:323:PRO:HD2  | 1:I:331:ARG:O    | 2.05                     | 0.57              |
| 1:J:273:HIS:CE1  | 1:J:361:LYS:HA   | 2.39                     | 0.57              |
| 1:K:28:ILE:HD11  | 1:K:417:PHE:CA   | 2.34                     | 0.57              |
| 1:A:233:PRO:HG2  | 1:A:295:SER:OG   | 2.04                     | 0.57              |
| 1:A:55:SER:O     | 1:A:58:GLU:HG2   | 2.05                     | 0.57              |
| 1:C:63:ILE:HG22  | 1:C:64:GLU:HG3   | 1.87                     | 0.57              |
| 1:D:212:GLN:OE1  | 1:D:212:GLN:HA   | 2.05                     | 0.57              |
| 1:D:34:ASN:C     | 1:D:34:ASN:ND2   | 2.56                     | 0.57              |
| 1:H:123:GLY:O    | 1:H:252:LYS:HG3  | 2.05                     | 0.57              |
| 1:I:347:LEU:O    | 1:I:347:LEU:HD13 | 2.04                     | 0.57              |
| 1:L:51:MET:HE1   | 1:L:67:ASP:CB    | 2.32                     | 0.57              |
| 1:A:205:VAL:HG23 | 4:A:602:HOH:O    | 2.04                     | 0.57              |
| 1:B:142:GLU:HG3  | 1:B:143:LYS:N    | 2.20                     | 0.57              |
| 1:B:164:LEU:HB2  | 1:C:82:TRP:CD1   | 2.38                     | 0.57              |
| 1:D:160:ALA:O    | 1:D:161:PRO:O    | 2.23                     | 0.57              |
| 1:D:243:GLY:CA   | 1:D:298:ARG:NH1  | 2.68                     | 0.57              |
| 1:G:342:ASN:C    | 1:G:342:ASN:HD22 | 2.08                     | 0.57              |
| 1:I:22:ARG:NH1   | 1:J:159:LEU:HD21 | 2.20                     | 0.57              |
| 1:K:310:ALA:CB   | 1:K:372:ILE:HG21 | 2.34                     | 0.57              |
| 1:A:223:ARG:HG3  | 1:A:223:ARG:HH11 | 1.69                     | 0.57              |
| 1:D:214:PHE:O    | 1:D:218:VAL:HG23 | 2.04                     | 0.57              |
| 1:F:114:ARG:HH21 | 1:F:115:ILE:HD11 | 1.68                     | 0.57              |
| 1:F:91:ARG:HD2   | 1:F:92:PHE:N     | 2.20                     | 0.57              |
| 1:G:169:ARG:NE   | 1:L:36:GLU:OE1   | 2.38                     | 0.57              |
| 1:E:440:TYR:OH   | 1:K:293:VAL:HG23 | 2.05                     | 0.57              |
| 1:K:316:ARG:HH11 | 1:K:316:ARG:CB   | 2.18                     | 0.57              |
| 1:F:429:ARG:NH2  | 1:L:300:VAL:HG22 | 2.13                     | 0.57              |
| 1:B:147:THR:HG21 | 1:B:149:GLU:HG3  | 1.85                     | 0.57              |
| 1:E:170:ARG:NH1  | 1:E:171:ASP:OD2  | 2.38                     | 0.57              |
| 1:G:375:MET:HB2  | 1:G:379:GLU:CB   | 2.33                     | 0.57              |
| 1:I:309:VAL:HG23 | 1:I:386:VAL:O    | 2.04                     | 0.57              |
| 1:K:370:ARG:NH2  | 1:K:374:VAL:HG22 | 2.13                     | 0.57              |
| 1:A:135:PHE:HB3  | 1:A:231:PHE:CD1  | 2.40                     | 0.57              |
| 1:A:311:TRP:CB   | 1:A:320:ILE:HB   | 2.35                     | 0.57              |
| 1:F:324:ALA:O    | 1:F:326:ARG:NE   | 2.38                     | 0.57              |
| 1:F:380:ARG:HH11 | 1:F:380:ARG:HG2  | 1.69                     | 0.57              |
| 1:F:5:THR:HG23   | 1:F:8:ASP:OD1    | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:223:ARG:HE   | 1:H:223:ARG:HA   | 1.70                     | 0.57              |
| 1:I:114:ARG:HH12 | 1:I:115:ILE:HD11 | 1.69                     | 0.57              |
| 1:J:96:ILE:HD12  | 1:J:107:ASP:HB2  | 1.86                     | 0.57              |
| 1:C:52:PHE:CE2   | 1:C:54:GLY:HA2   | 2.40                     | 0.56              |
| 1:C:68:MET:HG2   | 1:C:97:TYR:O     | 2.05                     | 0.56              |
| 1:D:111:ASN:ND2  | 1:D:409:LEU:HA   | 2.17                     | 0.56              |
| 1:G:383:ASN:HB2  | 1:G:385:ILE:CG1  | 2.35                     | 0.56              |
| 1:I:58:GLU:HB3   | 1:I:62:ARG:HB2   | 1.86                     | 0.56              |
| 1:J:282:ALA:HA   | 1:J:285:PHE:CE2  | 2.39                     | 0.56              |
| 1:K:83:THR:CB    | 1:K:88:LYS:HA    | 2.34                     | 0.56              |
| 1:E:264:ASP:C    | 1:E:266:GLN:N    | 2.59                     | 0.56              |
| 1:E:74:LEU:H     | 1:E:74:LEU:HD22  | 1.70                     | 0.56              |
| 1:F:23:LEU:HB2   | 1:F:35:VAL:HG13  | 1.86                     | 0.56              |
| 1:F:437:ARG:HB2  | 1:F:437:ARG:NH1  | 2.20                     | 0.56              |
| 1:H:119:MET:SD   | 1:H:127:PHE:HB2  | 2.44                     | 0.56              |
| 1:H:272:LYS:HZ1  | 1:H:276:ALA:HB2  | 1.70                     | 0.56              |
| 1:I:4:TYR:HB3    | 1:I:9:ILE:HD11   | 1.87                     | 0.56              |
| 1:L:136:PHE:HB3  | 1:L:138:PHE:CE1  | 2.41                     | 0.56              |
| 1:L:357:GLY:HA2  | 1:L:362:LEU:HD22 | 1.86                     | 0.56              |
| 1:A:115:ILE:HD11 | 1:A:408:ALA:O    | 2.05                     | 0.56              |
| 1:B:127:PHE:CE2  | 1:B:351:LEU:HG   | 2.41                     | 0.56              |
| 1:C:146:PRO:HG3  | 1:C:228:HIS:CD2  | 2.40                     | 0.56              |
| 1:F:380:ARG:HH11 | 1:F:385:ILE:HG21 | 1.70                     | 0.56              |
| 1:I:100:ASP:OD1  | 1:I:100:ASP:N    | 2.37                     | 0.56              |
| 1:I:173:VAL:HG13 | 1:I:183:ILE:CD1  | 2.22                     | 0.56              |
| 1:J:320:ILE:HG22 | 1:J:321:ARG:N    | 2.20                     | 0.56              |
| 1:E:117:LYS:HD3  | 1:E:117:LYS:O    | 2.05                     | 0.56              |
| 1:G:6:ARG:HG3    | 1:G:10:GLU:OE2   | 2.04                     | 0.56              |
| 1:H:169:ARG:NH2  | 1:H:195:HIS:ND1  | 2.53                     | 0.56              |
| 1:H:64:GLU:OE2   | 1:I:315:ASN:HA   | 2.06                     | 0.56              |
| 1:J:129:LEU:HD22 | 1:J:131:PRO:HG3  | 1.87                     | 0.56              |
| 1:J:131:PRO:HG2  | 1:J:211:ILE:HD11 | 1.87                     | 0.56              |
| 1:L:60:PHE:CE1   | 1:L:423:ILE:HD11 | 2.40                     | 0.56              |
| 1:B:100:ASP:OD1  | 1:B:101:GLY:N    | 2.39                     | 0.56              |
| 1:B:402:ASN:O    | 1:B:406:VAL:HG23 | 2.05                     | 0.56              |
| 1:C:282:ALA:O    | 1:C:284:SER:N    | 2.39                     | 0.56              |
| 1:D:319:LEU:HD12 | 1:D:336:SER:HB3  | 1.86                     | 0.56              |
| 1:E:293:VAL:HG11 | 1:E:428:PHE:CD2  | 2.40                     | 0.56              |
| 1:G:62:ARG:O     | 1:G:63:ILE:HG23  | 2.05                     | 0.56              |
| 1:I:169:ARG:NH2  | 1:I:195:HIS:ND1  | 2.53                     | 0.56              |
| 1:K:345:LEU:O    | 1:K:348:SER:HB2  | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:156:TYR:HE1  | 1:L:189:GLU:OE1  | 1.88                     | 0.56              |
| 1:L:78:VAL:CG1   | 1:L:91:ARG:HG3   | 2.36                     | 0.56              |
| 1:L:57:ILE:CD1   | 1:L:96:ILE:HG12  | 2.34                     | 0.56              |
| 1:B:58:GLU:O     | 1:B:61:VAL:HG22  | 2.05                     | 0.56              |
| 1:A:64:GLU:HG2   | 1:F:316:ARG:HA   | 1.87                     | 0.56              |
| 1:H:52:PHE:HE2   | 1:H:56:SER:HG    | 1.53                     | 0.56              |
| 1:J:116:LEU:O    | 1:J:120:GLU:HG3  | 2.06                     | 0.56              |
| 1:J:46:LEU:HD21  | 1:J:74:LEU:HD11  | 1.87                     | 0.56              |
| 1:K:276:ALA:HB2  | 1:K:364:ALA:HB2  | 1.86                     | 0.56              |
| 1:E:232:MET:CE   | 1:K:437:ARG:HA   | 2.36                     | 0.56              |
| 1:A:186:SER:HB2  | 1:A:197:ILE:HD13 | 1.86                     | 0.56              |
| 1:A:380:ARG:HA   | 1:A:383:ASN:HB2  | 1.86                     | 0.56              |
| 1:A:442:SER:HB3  | 1:H:153:LYS:HD2  | 1.87                     | 0.56              |
| 1:D:100:ASP:OD2  | 1:D:101:GLY:N    | 2.39                     | 0.56              |
| 1:D:309:VAL:HG23 | 1:D:386:VAL:O    | 2.06                     | 0.56              |
| 1:D:418:ILE:O    | 1:D:422:GLU:HG3  | 2.06                     | 0.56              |
| 1:D:6:ARG:NH1    | 1:D:6:ARG:HG3    | 2.21                     | 0.56              |
| 1:E:140:LEU:HD12 | 1:E:226:GLY:HA2  | 1.88                     | 0.56              |
| 1:E:52:PHE:CD1   | 1:E:70:LEU:HD13  | 2.40                     | 0.56              |
| 1:A:37:ILE:HG22  | 1:F:185:ALA:CA   | 2.35                     | 0.56              |
| 1:H:167:ASN:HB3  | 1:H:170:ARG:NH2  | 2.20                     | 0.56              |
| 1:H:74:LEU:H     | 1:H:74:LEU:CD2   | 2.14                     | 0.56              |
| 1:J:319:LEU:HD23 | 1:J:320:ILE:CD1  | 2.35                     | 0.56              |
| 1:L:23:LEU:HB2   | 1:L:35:VAL:CG2   | 2.35                     | 0.56              |
| 1:C:313:ALA:O    | 1:C:314:GLN:HB2  | 2.06                     | 0.56              |
| 1:E:138:PHE:CD2  | 1:E:148:LEU:HA   | 2.41                     | 0.56              |
| 1:F:160:ALA:CB   | 1:F:169:ARG:HH21 | 2.19                     | 0.56              |
| 1:F:319:LEU:HG   | 1:F:320:ILE:HD12 | 1.87                     | 0.56              |
| 1:I:234:LYS:HE3  | 1:I:239:VAL:O    | 2.05                     | 0.56              |
| 1:K:252:LYS:O    | 1:K:253:ASN:HB2  | 2.04                     | 0.56              |
| 1:K:38:PRO:HD2   | 1:K:41:GLN:HG3   | 1.88                     | 0.56              |
| 1:E:204:ALA:HB1  | 1:E:347:LEU:HD13 | 1.86                     | 0.56              |
| 1:E:372:ILE:HD12 | 1:E:373:TYR:H    | 1.71                     | 0.56              |
| 1:F:379:GLU:HG3  | 1:F:385:ILE:HD12 | 1.88                     | 0.56              |
| 1:G:183:ILE:HD13 | 1:L:38:PRO:HG2   | 1.87                     | 0.56              |
| 1:H:28:ILE:HG22  | 1:H:57:ILE:O     | 2.05                     | 0.56              |
| 1:H:328:ILE:H    | 1:H:328:ILE:CD1  | 2.18                     | 0.56              |
| 1:K:135:PHE:HB3  | 1:K:231:PHE:CE1  | 2.41                     | 0.56              |
| 1:K:163:ASP:C    | 1:K:164:LEU:HD23 | 2.26                     | 0.56              |
| 1:K:32:ILE:HD13  | 1:K:216:LEU:HD13 | 1.88                     | 0.56              |
| 1:A:319:LEU:O    | 1:A:319:LEU:HD23 | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:377:LYS:O    | 1:C:381:MET:HG3  | 2.06                     | 0.56              |
| 1:D:377:LYS:HG3  | 1:D:380:ARG:HH21 | 1.69                     | 0.56              |
| 1:G:308:TYR:HE2  | 1:G:380:ARG:HE   | 1.54                     | 0.56              |
| 1:G:325:SER:CB   | 1:G:331:ARG:HH22 | 2.17                     | 0.56              |
| 1:I:175:GLU:HG3  | 1:I:221:ILE:HD11 | 1.88                     | 0.56              |
| 1:K:167:ASN:OD1  | 1:K:170:ARG:HB3  | 2.05                     | 0.56              |
| 1:K:137:LEU:HD23 | 1:K:229:ALA:HA   | 1.88                     | 0.56              |
| 1:K:49:LYS:HD3   | 1:K:69:TYR:CE2   | 2.41                     | 0.56              |
| 1:B:372:ILE:CG2  | 1:B:385:ILE:HG21 | 2.36                     | 0.56              |
| 1:D:323:PRO:HG2  | 1:D:331:ARG:NH2  | 2.21                     | 0.56              |
| 1:D:429:ARG:O    | 1:J:297:LYS:HD3  | 2.06                     | 0.56              |
| 1:E:393:ALA:HB2  | 1:E:425:TRP:CE2  | 2.41                     | 0.56              |
| 1:F:120:GLU:C    | 1:F:122:LEU:H    | 2.09                     | 0.56              |
| 1:I:208:CYS:HA   | 1:I:211:ILE:HG12 | 1.88                     | 0.56              |
| 1:L:83:THR:CG2   | 1:L:89:VAL:HB    | 2.35                     | 0.56              |
| 1:E:35:VAL:CG1   | 1:E:70:LEU:HD21  | 2.36                     | 0.55              |
| 1:F:55:SER:O     | 1:F:62:ARG:HG2   | 2.06                     | 0.55              |
| 1:G:32:ILE:HD13  | 1:G:216:LEU:CD1  | 2.33                     | 0.55              |
| 1:I:236:LEU:HB2  | 1:I:239:VAL:HG22 | 1.88                     | 0.55              |
| 1:I:319:LEU:C    | 1:I:320:ILE:HD12 | 2.27                     | 0.55              |
| 1:I:415:GLU:HG3  | 4:I:620:HOH:O    | 2.05                     | 0.55              |
| 1:K:21:ILE:HD13  | 1:K:39:VAL:HA    | 1.87                     | 0.55              |
| 1:K:82:TRP:HZ3   | 1:K:221:ILE:HD11 | 1.71                     | 0.55              |
| 1:K:50:VAL:O     | 1:K:69:TYR:HA    | 2.05                     | 0.55              |
| 1:D:102:THR:HB   | 1:D:103:PRO:HD2  | 1.87                     | 0.55              |
| 1:I:23:LEU:HB2   | 1:I:35:VAL:CG1   | 2.36                     | 0.55              |
| 1:B:138:PHE:HB3  | 1:B:147:THR:O    | 2.06                     | 0.55              |
| 1:C:261:GLU:HA   | 1:C:266:GLN:HG2  | 1.88                     | 0.55              |
| 1:C:115:ILE:HG22 | 1:C:351:LEU:HD12 | 1.89                     | 0.55              |
| 1:D:129:LEU:HD22 | 1:D:130:GLY:H    | 1.71                     | 0.55              |
| 1:E:402:ASN:OD1  | 1:E:403:GLU:N    | 2.39                     | 0.55              |
| 1:F:260:ASP:O    | 1:F:266:GLN:HA   | 2.06                     | 0.55              |
| 1:J:182:GLU:O    | 1:J:200:LYS:HD3  | 2.07                     | 0.55              |
| 1:J:307:CYS:O    | 1:J:388:LEU:HG   | 2.06                     | 0.55              |
| 1:C:33:LYS:O     | 1:C:34:ASN:HB3   | 2.06                     | 0.55              |
| 1:E:266:GLN:HB2  | 1:E:326:ARG:HD2  | 1.88                     | 0.55              |
| 1:G:306:PRO:HG2  | 1:G:335:ARG:HD3  | 1.88                     | 0.55              |
| 1:G:72:PRO:HA    | 1:G:94:CYS:HA    | 1.88                     | 0.55              |
| 1:A:67:ASP:O     | 1:A:68:MET:HG3   | 2.07                     | 0.55              |
| 1:C:404:VAL:HG13 | 1:C:405:MET:CE   | 2.36                     | 0.55              |
| 1:E:288:VAL:O    | 1:E:291:PRO:HD3  | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:160:ALA:HB3  | 1:F:169:ARG:NH2  | 2.22                     | 0.55              |
| 1:G:370:ARG:HH22 | 1:G:383:ASN:HD22 | 1.52                     | 0.55              |
| 1:K:316:ARG:C    | 1:K:318:PRO:HD3  | 2.27                     | 0.55              |
| 1:K:127:PHE:CE2  | 1:K:351:LEU:HB2  | 2.42                     | 0.55              |
| 1:B:138:PHE:CE2  | 1:B:150:LEU:HD23 | 2.41                     | 0.55              |
| 1:A:314:GLN:HG2  | 1:B:64:GLU:OE1   | 2.07                     | 0.55              |
| 1:C:25:PHE:CE1   | 1:C:33:LYS:HB2   | 2.42                     | 0.55              |
| 1:D:249:SER:HA   | 1:D:258:PHE:CE1  | 2.42                     | 0.55              |
| 1:I:182:GLU:O    | 1:I:200:LYS:HB2  | 2.07                     | 0.55              |
| 1:J:83:THR:HB    | 1:J:89:VAL:HG23  | 1.88                     | 0.55              |
| 1:L:74:LEU:H     | 1:L:74:LEU:CD2   | 2.20                     | 0.55              |
| 1:D:123:GLY:O    | 1:D:252:LYS:HG3  | 2.07                     | 0.55              |
| 1:D:26:THR:HG23  | 1:D:30:GLY:HA2   | 1.88                     | 0.55              |
| 1:F:293:VAL:HG12 | 1:L:440:TYR:OH   | 2.07                     | 0.55              |
| 1:F:40:SER:C     | 1:F:41:GLN:HG2   | 2.27                     | 0.55              |
| 1:F:440:TYR:HB2  | 1:L:232:MET:CE   | 2.35                     | 0.55              |
| 1:G:58:GLU:HB2   | 1:G:62:ARG:HG2   | 1.89                     | 0.55              |
| 1:H:421:LYS:HD3  | 1:H:424:GLU:OE2  | 2.07                     | 0.55              |
| 1:K:98:ASN:HB2   | 1:K:102:THR:O    | 2.07                     | 0.55              |
| 1:K:166:GLU:HB2  | 1:K:227:LEU:HD11 | 1.87                     | 0.55              |
| 1:K:54:GLY:C     | 1:K:56:SER:H     | 2.10                     | 0.55              |
| 1:A:168:CYS:O    | 1:A:169:ARG:C    | 2.45                     | 0.55              |
| 1:C:6:ARG:HG3    | 1:C:10:GLU:OE2   | 2.07                     | 0.55              |
| 1:D:162:THR:C    | 1:D:164:LEU:H    | 2.10                     | 0.55              |
| 1:E:62:ARG:HD3   | 1:E:62:ARG:O     | 2.06                     | 0.55              |
| 1:F:251:PHE:HD2  | 1:F:254:GLY:O    | 1.88                     | 0.55              |
| 1:G:368:ILE:HD13 | 1:G:372:ILE:CG1  | 2.37                     | 0.55              |
| 1:G:380:ARG:HB3  | 1:G:385:ILE:O    | 2.06                     | 0.55              |
| 1:G:45:ALA:HA    | 1:G:50:VAL:HG23  | 1.88                     | 0.55              |
| 1:H:118:GLU:O    | 1:H:122:LEU:HD13 | 2.07                     | 0.55              |
| 1:I:291:PRO:O    | 1:I:392:LEU:HD13 | 2.06                     | 0.55              |
| 1:J:321:ARG:O    | 1:J:323:PRO:HD3  | 2.07                     | 0.55              |
| 1:K:402:ASN:O    | 1:K:406:VAL:HG23 | 2.07                     | 0.55              |
| 1:E:292:THR:HB   | 1:K:440:TYR:CE1  | 2.42                     | 0.55              |
| 1:B:124:PHE:HA   | 1:B:252:LYS:HA   | 1.89                     | 0.55              |
| 1:C:105:GLU:CD   | 1:C:412:HIS:HB2  | 2.27                     | 0.55              |
| 1:F:127:PHE:CZ   | 1:F:248:LEU:HD22 | 2.42                     | 0.55              |
| 1:I:248:LEU:HD11 | 1:I:334:VAL:CG2  | 2.30                     | 0.55              |
| 1:J:114:ARG:HH12 | 1:J:115:ILE:HD11 | 1.71                     | 0.55              |
| 1:J:281:HIS:CE1  | 1:J:404:VAL:HG11 | 2.41                     | 0.55              |
| 1:E:232:MET:CE   | 1:K:440:TYR:HB2  | 2.37                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:33:LYS:CA    | 1:L:158:ASP:HA   | 2.29                     | 0.55              |
| 1:A:310:ALA:HB3  | 1:A:372:ILE:CD1  | 2.33                     | 0.55              |
| 1:C:33:LYS:NZ    | 1:C:56:SER:O     | 2.40                     | 0.55              |
| 1:C:400:LYS:HG3  | 1:C:418:ILE:HD12 | 1.88                     | 0.55              |
| 1:E:126:ASP:OD1  | 1:E:251:PHE:HB2  | 2.07                     | 0.55              |
| 1:E:170:ARG:HG2  | 1:E:170:ARG:HH11 | 1.72                     | 0.55              |
| 1:I:338:ASP:OD2  | 1:I:340:ALA:HB3  | 2.06                     | 0.55              |
| 1:J:173:VAL:HG13 | 1:J:183:ILE:HD12 | 1.87                     | 0.55              |
| 1:J:190:VAL:HG13 | 1:J:191:ALA:N    | 2.17                     | 0.55              |
| 1:J:399:PHE:HZ   | 1:J:409:LEU:HD22 | 1.71                     | 0.55              |
| 1:K:109:ARG:HG2  | 1:K:109:ARG:HH21 | 1.72                     | 0.55              |
| 1:L:150:LEU:CD1  | 1:L:192:PRO:HG2  | 2.37                     | 0.55              |
| 1:D:139:LYS:HE3  | 1:D:149:GLU:CB   | 2.38                     | 0.54              |
| 1:F:319:LEU:HG   | 1:F:320:ILE:CD1  | 2.37                     | 0.54              |
| 1:F:342:ASN:HB3  | 1:F:345:LEU:HD12 | 1.89                     | 0.54              |
| 1:I:122:LEU:HD22 | 1:I:355:LEU:HD22 | 1.88                     | 0.54              |
| 1:A:137:LEU:HA   | 1:A:228:HIS:O    | 2.08                     | 0.54              |
| 1:A:78:VAL:HB    | 1:A:91:ARG:NH1   | 2.22                     | 0.54              |
| 1:B:264:ASP:C    | 1:B:266:GLN:H    | 2.09                     | 0.54              |
| 1:G:119:MET:SD   | 1:G:127:PHE:HB2  | 2.47                     | 0.54              |
| 1:G:306:PRO:CG   | 1:G:335:ARG:HH21 | 2.20                     | 0.54              |
| 1:I:13:VAL:HG13  | 1:I:18:VAL:HB    | 1.88                     | 0.54              |
| 1:I:286:THR:O    | 1:I:290:ASN:N    | 2.40                     | 0.54              |
| 1:I:37:ILE:HG22  | 1:J:185:ALA:HB2  | 1.89                     | 0.54              |
| 1:J:49:LYS:HA    | 1:J:49:LYS:HE3   | 1.89                     | 0.54              |
| 1:L:82:TRP:CH2   | 1:L:217:VAL:HG22 | 2.40                     | 0.54              |
| 1:A:104:PHE:CZ   | 1:A:106:GLY:HA3  | 2.43                     | 0.54              |
| 1:A:41:GLN:NE2   | 1:F:200:LYS:HE2  | 2.18                     | 0.54              |
| 1:B:131:PRO:HG2  | 1:B:199:PHE:HD1  | 1.71                     | 0.54              |
| 1:D:351:LEU:O    | 1:D:351:LEU:HD13 | 2.07                     | 0.54              |
| 1:A:224:LYS:HB2  | 1:F:164:LEU:CD1  | 2.38                     | 0.54              |
| 1:H:67:ASP:O     | 1:H:99:PRO:HG3   | 2.07                     | 0.54              |
| 1:J:211:ILE:O    | 1:J:215:LYS:HG3  | 2.07                     | 0.54              |
| 1:A:115:ILE:HG22 | 1:A:351:LEU:HD23 | 1.90                     | 0.54              |
| 1:A:64:GLU:HG2   | 1:F:316:ARG:CA   | 2.38                     | 0.54              |
| 1:B:207:SER:O    | 1:B:211:ILE:HG13 | 2.08                     | 0.54              |
| 1:B:295:SER:O    | 1:B:299:LEU:HD13 | 2.07                     | 0.54              |
| 1:C:201:TYR:C    | 1:C:201:TYR:HD1  | 2.11                     | 0.54              |
| 1:F:372:ILE:HA   | 1:F:375:MET:HG3  | 1.88                     | 0.54              |
| 1:G:267:LEU:CD2  | 1:G:326:ARG:NH1  | 2.70                     | 0.54              |
| 1:I:114:ARG:CB   | 1:I:114:ARG:HH11 | 2.20                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:383:ASN:HB2  | 1:J:385:ILE:HG12 | 1.90                     | 0.54              |
| 1:K:236:LEU:HB2  | 1:K:239:VAL:HG21 | 1.88                     | 0.54              |
| 1:A:252:LYS:HB2  | 1:A:252:LYS:HZ3  | 1.73                     | 0.54              |
| 1:C:260:ASP:O    | 1:C:266:GLN:HA   | 2.08                     | 0.54              |
| 1:D:127:PHE:CZ   | 1:D:351:LEU:HD23 | 2.42                     | 0.54              |
| 1:F:319:LEU:HD13 | 1:F:388:LEU:HD11 | 1.90                     | 0.54              |
| 1:J:396:LEU:HD11 | 1:J:421:LYS:HB3  | 1.88                     | 0.54              |
| 1:K:270:THR:CG2  | 1:K:358:ILE:HD12 | 2.37                     | 0.54              |
| 1:L:114:ARG:HH21 | 1:L:115:ILE:HG13 | 1.73                     | 0.54              |
| 1:A:170:ARG:NH1  | 1:B:84:ALA:HB1   | 2.23                     | 0.54              |
| 1:G:77:PHE:HZ    | 1:G:79:ILE:HD11  | 1.72                     | 0.54              |
| 1:H:49:LYS:HD3   | 1:H:69:TYR:HE2   | 1.72                     | 0.54              |
| 1:J:33:LYS:HE2   | 1:K:158:ASP:OD1  | 2.07                     | 0.54              |
| 1:K:18:VAL:HA    | 1:K:88:LYS:HB2   | 1.90                     | 0.54              |
| 1:K:310:ALA:CB   | 1:K:372:ILE:HD13 | 2.37                     | 0.54              |
| 1:K:83:THR:HG22  | 1:K:89:VAL:HG23  | 1.90                     | 0.54              |
| 1:C:145:GLU:HA   | 1:C:145:GLU:OE1  | 2.08                     | 0.54              |
| 1:C:244:MET:HB2  | 1:C:339:PRO:HD3  | 1.88                     | 0.54              |
| 1:D:115:ILE:CG2  | 1:D:351:LEU:HD12 | 2.38                     | 0.54              |
| 1:E:170:ARG:O    | 1:E:174:LEU:HG   | 2.08                     | 0.54              |
| 1:E:400:LYS:HA   | 1:E:414:PHE:HZ   | 1.72                     | 0.54              |
| 1:G:160:ALA:CB   | 1:G:188:HIS:HD2  | 2.18                     | 0.54              |
| 1:I:328:ILE:HG12 | 1:I:329:SER:N    | 2.20                     | 0.54              |
| 1:A:272:LYS:NZ   | 1:A:311:TRP:CH2  | 2.76                     | 0.54              |
| 1:B:2:ALA:O      | 1:B:3:LYS:HB2    | 2.08                     | 0.54              |
| 1:B:95:ASP:O     | 1:B:97:TYR:HD1   | 1.90                     | 0.54              |
| 1:D:104:PHE:CE2  | 1:D:106:GLY:HA3  | 2.43                     | 0.54              |
| 1:D:128:ASN:HD22 | 1:D:203:GLY:HA2  | 1.73                     | 0.54              |
| 1:E:368:ILE:HG21 | 1:E:372:ILE:CG2  | 2.38                     | 0.54              |
| 1:F:376:SER:O    | 1:F:380:ARG:HG3  | 2.07                     | 0.54              |
| 1:G:169:ARG:NH2  | 1:G:195:HIS:ND1  | 2.56                     | 0.54              |
| 1:G:325:SER:CB   | 1:G:331:ARG:NH2  | 2.70                     | 0.54              |
| 1:G:204:ALA:HB1  | 1:G:347:LEU:HD23 | 1.90                     | 0.54              |
| 1:H:236:LEU:HB2  | 1:H:239:VAL:HG22 | 1.89                     | 0.54              |
| 1:H:236:LEU:HB2  | 1:H:239:VAL:HG21 | 1.89                     | 0.54              |
| 1:H:384:GLY:O    | 1:H:386:VAL:HG23 | 2.08                     | 0.54              |
| 1:J:281:HIS:HE1  | 1:J:356:ASP:OD1  | 1.90                     | 0.54              |
| 1:J:39:VAL:HG13  | 1:J:40:SER:N     | 2.23                     | 0.54              |
| 1:L:423:ILE:C    | 1:L:423:ILE:HD12 | 2.27                     | 0.54              |
| 1:B:278:ILE:CG2  | 1:B:320:ILE:HD11 | 2.38                     | 0.54              |
| 1:B:129:LEU:HG   | 1:B:347:LEU:CD2  | 2.37                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:256:ASN:ND2  | 1:D:328:ILE:O    | 2.41                     | 0.54              |
| 1:E:393:ALA:HB2  | 1:E:425:TRP:CD2  | 2.43                     | 0.54              |
| 1:E:96:ILE:HD13  | 1:E:107:ASP:CG   | 2.28                     | 0.54              |
| 1:F:409:LEU:O    | 1:F:413:LEU:HB2  | 2.07                     | 0.54              |
| 1:F:96:ILE:H     | 1:F:96:ILE:HD12  | 1.73                     | 0.54              |
| 1:H:258:PHE:HA   | 1:H:271:ALA:HB2  | 1.89                     | 0.54              |
| 1:I:156:TYR:C    | 1:I:158:ASP:H    | 2.11                     | 0.54              |
| 1:J:169:ARG:HG3  | 1:J:195:HIS:HB3  | 1.90                     | 0.54              |
| 1:A:281:HIS:O    | 1:A:284:SER:HB2  | 2.09                     | 0.54              |
| 1:A:323:PRO:HD2  | 1:A:331:ARG:O    | 2.08                     | 0.54              |
| 1:A:316:ARG:HD3  | 1:B:63:ILE:O     | 2.08                     | 0.54              |
| 1:C:252:LYS:NZ   | 1:C:252:LYS:HB2  | 2.23                     | 0.54              |
| 1:C:404:VAL:HG13 | 1:C:405:MET:HE2  | 1.90                     | 0.54              |
| 1:E:199:PHE:HZ   | 1:E:214:PHE:CG   | 2.26                     | 0.54              |
| 1:F:393:ALA:HB2  | 1:F:425:TRP:CE2  | 2.43                     | 0.54              |
| 1:G:127:PHE:N    | 4:G:608:HOH:O    | 2.36                     | 0.54              |
| 1:H:27:ASP:HB2   | 1:H:57:ILE:O     | 2.07                     | 0.54              |
| 1:H:323:PRO:HD2  | 1:H:331:ARG:O    | 2.08                     | 0.54              |
| 1:J:172:ILE:O    | 1:J:176:LEU:HG   | 2.07                     | 0.54              |
| 1:B:211:ILE:CG2  | 1:B:215:LYS:HE3  | 2.37                     | 0.53              |
| 1:B:126:ASP:CB   | 1:B:251:PHE:HB2  | 2.25                     | 0.53              |
| 1:C:51:MET:CE    | 1:C:67:ASP:HB3   | 2.37                     | 0.53              |
| 1:G:256:ASN:ND2  | 1:G:330:THR:HB   | 2.23                     | 0.53              |
| 1:G:325:SER:HB2  | 1:G:331:ARG:HH21 | 1.71                     | 0.53              |
| 1:L:404:VAL:HG13 | 1:L:405:MET:HE2  | 1.90                     | 0.53              |
| 1:C:97:TYR:HD2   | 1:C:101:GLY:O    | 1.91                     | 0.53              |
| 1:E:160:ALA:O    | 1:E:161:PRO:C    | 2.46                     | 0.53              |
| 1:E:201:TYR:O    | 1:E:202:ALA:HB2  | 2.08                     | 0.53              |
| 1:E:55:SER:HB2   | 1:E:62:ARG:HB2   | 1.89                     | 0.53              |
| 1:H:49:LYS:HD3   | 1:H:69:TYR:CE2   | 2.43                     | 0.53              |
| 1:I:206:ARG:O    | 1:I:206:ARG:HD3  | 2.09                     | 0.53              |
| 1:I:328:ILE:N    | 1:I:328:ILE:HD13 | 2.12                     | 0.53              |
| 1:K:85:GLU:CD    | 1:K:85:GLU:H     | 2.10                     | 0.53              |
| 1:L:201:TYR:C    | 1:L:201:TYR:CD1  | 2.81                     | 0.53              |
| 1:L:310:ALA:HB1  | 1:L:368:ILE:HB   | 1.90                     | 0.53              |
| 1:B:178:GLU:CD   | 1:C:86:LYS:HD3   | 2.29                     | 0.53              |
| 1:B:291:PRO:HB2  | 1:B:421:LYS:HE3  | 1.90                     | 0.53              |
| 1:E:345:LEU:HD22 | 1:E:409:LEU:HD22 | 1.88                     | 0.53              |
| 1:F:281:HIS:CE1  | 1:F:404:VAL:HG11 | 2.43                     | 0.53              |
| 1:H:28:ILE:HD11  | 1:H:417:PHE:CA   | 2.39                     | 0.53              |
| 1:I:440:TYR:HD1  | 1:I:444:TYR:CE2  | 2.25                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:81:PRO:HG2   | 1:J:82:TRP:CE3   | 2.44                     | 0.53              |
| 1:K:378:GLU:HA   | 1:K:381:MET:HG2  | 1.91                     | 0.53              |
| 1:L:316:ARG:HG3  | 1:L:316:ARG:HH11 | 1.74                     | 0.53              |
| 1:L:6:ARG:HD2    | 1:L:46:LEU:HD13  | 1.89                     | 0.53              |
| 1:L:96:ILE:N     | 1:L:96:ILE:HD12  | 2.22                     | 0.53              |
| 1:A:223:ARG:HG3  | 1:A:223:ARG:NH1  | 2.23                     | 0.53              |
| 1:A:338:ASP:HB2  | 1:A:339:PRO:CD   | 2.38                     | 0.53              |
| 1:B:201:TYR:CD1  | 1:B:201:TYR:N    | 2.77                     | 0.53              |
| 1:D:275:ILE:O    | 1:D:279:VAL:HG23 | 2.08                     | 0.53              |
| 1:E:319:LEU:CG   | 1:E:320:ILE:HD12 | 2.27                     | 0.53              |
| 1:E:51:MET:SD    | 1:E:67:ASP:HB3   | 2.48                     | 0.53              |
| 1:F:160:ALA:O    | 1:F:161:PRO:C    | 2.47                     | 0.53              |
| 1:G:146:PRO:HG3  | 1:G:228:HIS:CD2  | 2.44                     | 0.53              |
| 1:G:21:ILE:CD1   | 1:G:42:LEU:HD13  | 2.37                     | 0.53              |
| 1:I:116:LEU:O    | 1:I:119:MET:HB3  | 2.09                     | 0.53              |
| 1:J:112:LEU:O    | 1:J:116:LEU:HG   | 2.09                     | 0.53              |
| 1:J:423:ILE:O    | 1:J:427:MET:HG3  | 2.07                     | 0.53              |
| 1:L:231:PHE:HB3  | 1:L:339:PRO:CB   | 2.38                     | 0.53              |
| 1:A:107:ASP:OD2  | 1:A:110:ASN:N    | 2.41                     | 0.53              |
| 1:A:291:PRO:HG3  | 1:A:341:ALA:HA   | 1.90                     | 0.53              |
| 1:B:278:ILE:HG22 | 1:B:320:ILE:HD11 | 1.88                     | 0.53              |
| 1:C:24:GLN:HE21  | 1:C:91:ARG:HB2   | 1.74                     | 0.53              |
| 1:E:160:ALA:HB2  | 1:E:188:HIS:HD2  | 1.73                     | 0.53              |
| 1:E:231:PHE:HB3  | 1:E:339:PRO:HB2  | 1.90                     | 0.53              |
| 1:E:263:ALA:O    | 1:E:266:GLN:HA   | 2.09                     | 0.53              |
| 1:F:182:GLU:HB3  | 1:F:200:LYS:CD   | 2.34                     | 0.53              |
| 1:G:231:PHE:O    | 1:G:339:PRO:HG2  | 2.08                     | 0.53              |
| 1:H:371:ASN:OD1  | 1:H:373:TYR:HD1  | 1.91                     | 0.53              |
| 1:I:418:ILE:HG22 | 1:I:422:GLU:HG3  | 1.89                     | 0.53              |
| 1:J:247:ASN:ND2  | 1:J:331:ARG:HD2  | 2.22                     | 0.53              |
| 1:J:404:VAL:HG13 | 1:J:405:MET:CE   | 2.38                     | 0.53              |
| 1:K:348:SER:O    | 1:K:352:ALA:HB2  | 2.09                     | 0.53              |
| 1:L:201:TYR:C    | 1:L:201:TYR:HD1  | 2.12                     | 0.53              |
| 1:L:215:LYS:O    | 1:L:219:LYS:HG2  | 2.09                     | 0.53              |
| 1:L:368:ILE:HG12 | 1:L:385:ILE:HG23 | 1.90                     | 0.53              |
| 1:E:5:THR:HG23   | 1:E:8:ASP:CG     | 2.29                     | 0.53              |
| 1:G:156:TYR:C    | 1:G:158:ASP:H    | 2.12                     | 0.53              |
| 1:I:28:ILE:HD13  | 1:I:28:ILE:O     | 2.08                     | 0.53              |
| 1:K:399:PHE:CE1  | 1:K:405:MET:HB3  | 2.44                     | 0.53              |
| 1:A:399:PHE:HZ   | 1:A:409:LEU:HD12 | 1.73                     | 0.53              |
| 1:B:265:LEU:O    | 1:B:266:GLN:HB2  | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:19:LYS:HD2   | 1:D:86:LYS:O     | 2.08                     | 0.53              |
| 1:D:375:MET:SD   | 1:D:379:GLU:HB3  | 2.48                     | 0.53              |
| 1:I:123:GLY:O    | 1:I:252:LYS:HG3  | 2.08                     | 0.53              |
| 1:I:96:ILE:N     | 1:I:96:ILE:HD12  | 2.23                     | 0.53              |
| 1:A:146:PRO:HB3  | 1:A:228:HIS:ND1  | 2.23                     | 0.53              |
| 1:A:35:VAL:HG11  | 1:A:70:LEU:CD2   | 2.39                     | 0.53              |
| 1:C:197:ILE:HD12 | 1:C:214:PHE:CZ   | 2.43                     | 0.53              |
| 1:D:349:VAL:HB   | 1:D:405:MET:SD   | 2.49                     | 0.53              |
| 1:F:151:ASN:HD22 | 1:F:166:GLU:CD   | 2.12                     | 0.53              |
| 1:F:175:GLU:HG3  | 1:F:221:ILE:HD11 | 1.91                     | 0.53              |
| 1:F:234:LYS:HB3  | 1:F:294:ASN:HD21 | 1.73                     | 0.53              |
| 1:F:9:ILE:HG13   | 1:F:74:LEU:HD12  | 1.91                     | 0.53              |
| 1:G:182:GLU:O    | 1:G:200:LYS:HG3  | 2.09                     | 0.53              |
| 1:H:20:TYR:CZ    | 1:H:36:GLU:HB3   | 2.44                     | 0.53              |
| 1:I:423:ILE:O    | 1:I:427:MET:HG3  | 2.08                     | 0.53              |
| 1:J:125:SER:HB3  | 1:J:126:ASP:OD1  | 2.09                     | 0.53              |
| 1:L:380:ARG:HH11 | 1:L:380:ARG:CB   | 2.22                     | 0.53              |
| 1:C:332:VAL:HG13 | 1:C:332:VAL:O    | 2.08                     | 0.53              |
| 1:C:368:ILE:HD13 | 1:C:384:GLY:O    | 2.09                     | 0.53              |
| 1:D:249:SER:HB3  | 1:D:331:ARG:CB   | 2.39                     | 0.53              |
| 1:E:326:ARG:HH11 | 1:E:326:ARG:HG2  | 1.74                     | 0.53              |
| 1:F:128:ASN:OD1  | 1:F:201:TYR:CE1  | 2.62                     | 0.53              |
| 1:F:169:ARG:O    | 1:F:172:ILE:HB   | 2.09                     | 0.53              |
| 1:F:419:GLU:O    | 1:F:423:ILE:HG23 | 2.09                     | 0.53              |
| 1:H:282:ALA:HA   | 1:H:285:PHE:CE2  | 2.44                     | 0.53              |
| 1:H:316:ARG:HB2  | 1:H:371:ASN:HD21 | 1.73                     | 0.53              |
| 1:I:34:ASN:C     | 1:I:34:ASN:ND2   | 2.62                     | 0.53              |
| 1:J:288:VAL:O    | 1:J:291:PRO:HD3  | 2.09                     | 0.53              |
| 1:L:261:GLU:HA   | 1:L:266:GLN:HE21 | 1.73                     | 0.53              |
| 1:B:360:ASN:O    | 1:B:361:LYS:C    | 2.47                     | 0.53              |
| 1:D:281:HIS:NE2  | 1:D:404:VAL:HG21 | 2.24                     | 0.53              |
| 1:G:175:GLU:O    | 1:G:178:GLU:HB3  | 2.09                     | 0.53              |
| 1:I:35:VAL:HG13  | 1:I:35:VAL:O     | 2.08                     | 0.53              |
| 1:I:35:VAL:HG11  | 1:I:70:LEU:HD23  | 1.90                     | 0.53              |
| 1:K:82:TRP:CZ3   | 1:K:221:ILE:HD11 | 2.43                     | 0.53              |
| 1:L:278:ILE:O    | 1:L:282:ALA:HB2  | 2.08                     | 0.53              |
| 1:A:281:HIS:HD2  | 1:A:402:ASN:ND2  | 2.07                     | 0.52              |
| 1:B:159:LEU:CD1  | 1:C:22:ARG:NH1   | 2.72                     | 0.52              |
| 1:B:243:GLY:CA   | 1:B:298:ARG:NH1  | 2.72                     | 0.52              |
| 1:C:3:LYS:HG2    | 1:C:4:TYR:HD1    | 1.73                     | 0.52              |
| 1:D:371:ASN:OD1  | 1:D:375:MET:HB2  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:259:PHE:O    | 1:E:268:SER:HB3  | 2.09                     | 0.52              |
| 1:F:24:GLN:NE2   | 1:F:91:ARG:NH1   | 2.57                     | 0.52              |
| 1:H:244:MET:N    | 1:H:338:ASP:HA   | 2.25                     | 0.52              |
| 1:I:168:CYS:O    | 1:I:172:ILE:HG13 | 2.09                     | 0.52              |
| 1:I:371:ASN:ND2  | 1:I:375:MET:HG2  | 2.23                     | 0.52              |
| 1:J:160:ALA:HB2  | 1:J:188:HIS:CD2  | 2.43                     | 0.52              |
| 1:J:377:LYS:H    | 1:J:377:LYS:CD   | 2.13                     | 0.52              |
| 1:K:95:ASP:OD1   | 1:K:109:ARG:HG2  | 2.09                     | 0.52              |
| 1:A:35:VAL:HG13  | 1:A:35:VAL:O     | 2.08                     | 0.52              |
| 1:B:285:PHE:HB2  | 1:B:349:VAL:CG1  | 2.39                     | 0.52              |
| 1:D:399:PHE:CE1  | 1:D:405:MET:HB3  | 2.44                     | 0.52              |
| 1:E:160:ALA:HB1  | 1:E:161:PRO:CD   | 2.38                     | 0.52              |
| 1:E:361:LYS:O    | 1:E:362:LEU:HD23 | 2.09                     | 0.52              |
| 1:F:183:ILE:HD12 | 1:F:197:ILE:CG2  | 2.39                     | 0.52              |
| 1:F:297:LYS:HE3  | 1:L:436:GLU:OE2  | 2.09                     | 0.52              |
| 1:I:114:ARG:NH2  | 1:I:407:LYS:O    | 2.42                     | 0.52              |
| 1:K:152:ASP:CB   | 1:K:161:PRO:HG3  | 2.37                     | 0.52              |
| 1:K:326:ARG:HG3  | 1:K:327:GLY:N    | 2.23                     | 0.52              |
| 1:A:380:ARG:HA   | 1:A:383:ASN:HD22 | 1.73                     | 0.52              |
| 1:C:115:ILE:HD11 | 1:C:408:ALA:O    | 2.09                     | 0.52              |
| 1:D:83:THR:HB    | 1:D:87:GLY:O     | 2.09                     | 0.52              |
| 1:F:133:PRO:HG2  | 1:F:199:PHE:HE1  | 1.75                     | 0.52              |
| 1:G:33:LYS:HD3   | 1:H:158:ASP:OD1  | 2.10                     | 0.52              |
| 1:G:368:ILE:O    | 1:G:369:ASP:HB2  | 2.09                     | 0.52              |
| 1:J:162:THR:O    | 1:J:164:LEU:N    | 2.43                     | 0.52              |
| 1:K:170:ARG:HG2  | 1:K:174:LEU:CD2  | 2.40                     | 0.52              |
| 1:K:232:MET:HB3  | 1:K:235:PRO:HG3  | 1.91                     | 0.52              |
| 1:A:337:VAL:HG12 | 1:A:338:ASP:H    | 1.73                     | 0.52              |
| 1:B:231:PHE:HB3  | 1:B:339:PRO:HB2  | 1.90                     | 0.52              |
| 1:C:435:TRP:CZ2  | 1:C:439:GLN:HG3  | 2.44                     | 0.52              |
| 1:E:234:LYS:HB3  | 1:E:294:ASN:HD21 | 1.74                     | 0.52              |
| 1:G:33:LYS:HE3   | 1:H:156:TYR:O    | 2.10                     | 0.52              |
| 1:H:286:THR:HG23 | 1:H:290:ASN:ND2  | 2.25                     | 0.52              |
| 1:H:276:ALA:HA   | 1:H:364:ALA:HB2  | 1.91                     | 0.52              |
| 1:I:166:GLU:O    | 1:I:168:CYS:N    | 2.42                     | 0.52              |
| 1:I:261:GLU:CA   | 1:I:266:GLN:HG2  | 2.27                     | 0.52              |
| 1:J:272:LYS:CA   | 1:J:275:ILE:HD12 | 2.29                     | 0.52              |
| 1:K:259:PHE:CD1  | 1:K:326:ARG:HD2  | 2.42                     | 0.52              |
| 1:A:53:ASP:OD2   | 1:A:55:SER:HB3   | 2.09                     | 0.52              |
| 1:B:236:LEU:HB2  | 1:B:239:VAL:HG21 | 1.92                     | 0.52              |
| 1:B:248:LEU:O    | 1:B:331:ARG:HB2  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:68:MET:SD    | 1:B:96:ILE:CG2   | 2.98                     | 0.52              |
| 1:D:318:PRO:O    | 1:D:335:ARG:HD2  | 2.10                     | 0.52              |
| 1:F:136:PHE:HB3  | 1:F:138:PHE:HE1  | 1.75                     | 0.52              |
| 1:F:261:GLU:HA   | 1:F:266:GLN:HE21 | 1.74                     | 0.52              |
| 1:F:323:PRO:HD2  | 1:F:331:ARG:O    | 2.09                     | 0.52              |
| 1:E:164:LEU:HG   | 1:F:82:TRP:HB3   | 1.92                     | 0.52              |
| 1:G:315:ASN:HB3  | 1:G:318:PRO:HD3  | 1.92                     | 0.52              |
| 1:K:135:PHE:HB3  | 1:K:231:PHE:CD1  | 2.45                     | 0.52              |
| 1:L:274:PHE:HD1  | 1:L:358:ILE:HD11 | 1.75                     | 0.52              |
| 1:L:5:THR:HG23   | 1:L:8:ASP:OD2    | 2.09                     | 0.52              |
| 1:A:150:LEU:CD1  | 1:A:192:PRO:HB2  | 2.39                     | 0.52              |
| 1:B:160:ALA:O    | 1:B:161:PRO:C    | 2.47                     | 0.52              |
| 1:B:243:GLY:HA3  | 1:B:298:ARG:NH1  | 2.23                     | 0.52              |
| 1:C:297:LYS:HE2  | 1:I:429:ARG:O    | 2.09                     | 0.52              |
| 1:G:333:GLU:HG2  | 1:G:335:ARG:HG2  | 1.90                     | 0.52              |
| 1:H:79:ILE:O     | 1:H:79:ILE:HG22  | 2.08                     | 0.52              |
| 1:K:322:ILE:HG22 | 1:K:322:ILE:O    | 2.10                     | 0.52              |
| 1:L:237:PHE:CD1  | 1:L:238:GLY:N    | 2.78                     | 0.52              |
| 1:L:34:ASN:C     | 1:L:34:ASN:ND2   | 2.63                     | 0.52              |
| 1:L:73:ASP:HB3   | 1:L:76:THR:OG1   | 2.09                     | 0.52              |
| 1:A:274:PHE:HE2  | 1:A:332:VAL:HG21 | 1.74                     | 0.52              |
| 1:A:86:LYS:HD2   | 1:F:178:GLU:OE1  | 2.10                     | 0.52              |
| 1:B:375:MET:HB3  | 1:B:379:GLU:HB2  | 1.92                     | 0.52              |
| 1:B:291:PRO:O    | 1:B:392:LEU:HD13 | 2.09                     | 0.52              |
| 1:E:27:ASP:HA    | 1:E:57:ILE:HG23  | 1.91                     | 0.52              |
| 1:F:206:ARG:HB2  | 4:F:621:HOH:O    | 2.10                     | 0.52              |
| 1:G:157:PHE:CE1  | 1:L:35:VAL:HG12  | 2.45                     | 0.52              |
| 1:G:33:LYS:HD3   | 1:H:158:ASP:HA   | 1.92                     | 0.52              |
| 1:H:309:VAL:HG13 | 1:H:319:LEU:HD23 | 1.92                     | 0.52              |
| 1:L:404:VAL:HG13 | 1:L:405:MET:CE   | 2.40                     | 0.52              |
| 1:A:37:ILE:HD13  | 1:A:37:ILE:H     | 1.74                     | 0.52              |
| 1:B:397:GLU:HA   | 1:B:400:LYS:HE2  | 1.91                     | 0.52              |
| 1:C:244:MET:HE2  | 1:C:337:VAL:HG12 | 1.92                     | 0.52              |
| 1:D:23:LEU:HD13  | 1:D:70:LEU:HD23  | 1.92                     | 0.52              |
| 1:E:278:ILE:HG23 | 1:E:285:PHE:CZ   | 2.45                     | 0.52              |
| 1:E:285:PHE:HB3  | 1:E:405:MET:SD   | 2.50                     | 0.52              |
| 1:G:286:THR:HA   | 1:G:289:THR:OG1  | 2.10                     | 0.52              |
| 1:I:406:VAL:HG22 | 1:I:414:PHE:CZ   | 2.44                     | 0.52              |
| 1:J:150:LEU:HD13 | 1:J:192:PRO:HG2  | 1.91                     | 0.52              |
| 1:I:224:LYS:HD3  | 1:J:164:LEU:HD11 | 1.90                     | 0.52              |
| 1:K:53:ASP:CG    | 1:K:65:GLU:HG2   | 2.30                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:184:GLU:OE1  | 1:L:200:LYS:HG2  | 2.10                     | 0.52              |
| 1:A:379:GLU:HG2  | 1:A:379:GLU:O    | 2.08                     | 0.52              |
| 1:C:143:LYS:HA   | 1:C:143:LYS:HE2  | 1.90                     | 0.52              |
| 1:C:58:GLU:HG2   | 1:C:416:HIS:CD2  | 2.44                     | 0.52              |
| 1:D:306:PRO:O    | 1:D:388:LEU:HD12 | 2.09                     | 0.52              |
| 1:F:160:ALA:HB3  | 1:F:169:ARG:HH21 | 1.74                     | 0.52              |
| 1:F:380:ARG:NH1  | 1:F:385:ILE:HG21 | 2.25                     | 0.52              |
| 1:F:397:GLU:HA   | 1:F:400:LYS:HD3  | 1.91                     | 0.52              |
| 1:G:259:PHE:HB2  | 1:G:330:THR:HG21 | 1.91                     | 0.52              |
| 1:H:372:ILE:HG13 | 1:H:385:ILE:HD12 | 1.90                     | 0.52              |
| 1:I:140:LEU:HD12 | 1:I:226:GLY:C    | 2.30                     | 0.52              |
| 1:I:127:PHE:HZ   | 1:I:248:LEU:HD23 | 1.75                     | 0.52              |
| 1:D:297:LYS:HE3  | 1:J:436:GLU:OE1  | 2.08                     | 0.52              |
| 1:L:82:TRP:HE1   | 1:L:221:ILE:HD11 | 1.74                     | 0.52              |
| 1:L:285:PHE:C    | 1:L:285:PHE:CD1  | 2.84                     | 0.52              |
| 1:C:22:ARG:NH1   | 1:C:36:GLU:OE2   | 2.43                     | 0.52              |
| 1:D:127:PHE:CD2  | 1:D:351:LEU:HD23 | 2.45                     | 0.52              |
| 1:E:281:HIS:HD2  | 1:E:402:ASN:ND2  | 2.00                     | 0.52              |
| 1:E:345:LEU:HD22 | 1:E:409:LEU:CD2  | 2.40                     | 0.52              |
| 1:F:13:VAL:HG21  | 1:F:42:LEU:HD21  | 1.92                     | 0.52              |
| 1:F:375:MET:O    | 1:F:380:ARG:NH2  | 2.43                     | 0.52              |
| 1:F:52:PHE:CZ    | 1:F:54:GLY:HA2   | 2.46                     | 0.52              |
| 1:G:167:ASN:HD22 | 1:G:170:ARG:CZ   | 2.23                     | 0.52              |
| 1:H:129:LEU:C    | 1:H:129:LEU:HD13 | 2.29                     | 0.52              |
| 1:H:8:ASP:O      | 1:H:12:LEU:HG    | 2.10                     | 0.52              |
| 1:H:370:ARG:O    | 1:H:372:ILE:HG23 | 2.10                     | 0.52              |
| 1:H:378:GLU:O    | 1:H:381:MET:HG3  | 2.09                     | 0.52              |
| 1:H:78:VAL:HB    | 1:H:91:ARG:HG3   | 1.92                     | 0.52              |
| 1:A:386:VAL:HG12 | 1:A:387:ASP:N    | 2.24                     | 0.51              |
| 1:D:135:PHE:HB3  | 1:D:231:PHE:CE1  | 2.45                     | 0.51              |
| 1:E:128:ASN:HA   | 1:E:202:ALA:O    | 2.09                     | 0.51              |
| 1:G:120:GLU:HA   | 1:G:124:PHE:O    | 2.10                     | 0.51              |
| 1:G:76:THR:HG21  | 1:G:93:ILE:HB    | 1.92                     | 0.51              |
| 1:H:397:GLU:HA   | 1:H:400:LYS:HZ1  | 1.75                     | 0.51              |
| 1:J:97:TYR:CE2   | 1:J:103:PRO:HG3  | 2.45                     | 0.51              |
| 1:L:131:PRO:HG2  | 1:L:199:PHE:HD2  | 1.75                     | 0.51              |
| 1:L:34:ASN:ND2   | 1:L:34:ASN:O     | 2.43                     | 0.51              |
| 1:A:250:LEU:HD12 | 1:A:258:PHE:CE2  | 2.46                     | 0.51              |
| 1:D:357:GLY:HA2  | 1:D:362:LEU:HD22 | 1.92                     | 0.51              |
| 1:F:244:MET:N    | 1:F:338:ASP:HA   | 2.25                     | 0.51              |
| 1:G:311:TRP:HB3  | 1:G:320:ILE:HB   | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:63:ILE:HG13  | 1:G:64:GLU:H     | 1.75                     | 0.51              |
| 1:H:364:ALA:HB1  | 1:H:365:PRO:HD2  | 1.92                     | 0.51              |
| 1:I:131:PRO:HD2  | 1:I:199:PHE:HB2  | 1.93                     | 0.51              |
| 1:I:402:ASN:OD1  | 1:I:404:VAL:HG12 | 2.10                     | 0.51              |
| 1:J:11:LYS:O     | 1:J:15:GLU:HG3   | 2.10                     | 0.51              |
| 1:K:147:THR:C    | 1:K:149:GLU:H    | 2.13                     | 0.51              |
| 1:K:54:GLY:C     | 1:K:56:SER:N     | 2.63                     | 0.51              |
| 1:L:285:PHE:C    | 1:L:285:PHE:HD1  | 2.12                     | 0.51              |
| 1:L:85:GLU:C     | 1:L:87:GLY:H     | 2.14                     | 0.51              |
| 1:A:343:PRO:O    | 1:A:347:LEU:HB2  | 2.10                     | 0.51              |
| 1:A:35:VAL:HG11  | 1:A:70:LEU:HD23  | 1.93                     | 0.51              |
| 1:E:285:PHE:CB   | 1:E:349:VAL:HG13 | 2.41                     | 0.51              |
| 1:F:325:SER:O    | 1:F:326:ARG:HD3  | 2.10                     | 0.51              |
| 1:H:349:VAL:CG2  | 1:H:405:MET:SD   | 2.99                     | 0.51              |
| 1:I:155:GLY:O    | 1:I:158:ASP:HB2  | 2.11                     | 0.51              |
| 1:I:319:LEU:HB3  | 1:I:320:ILE:HD12 | 1.93                     | 0.51              |
| 1:J:356:ASP:HA   | 1:J:359:LYS:HE2  | 1.92                     | 0.51              |
| 1:J:434:PRO:O    | 1:J:438:GLU:HG3  | 2.11                     | 0.51              |
| 1:K:3:LYS:HE2    | 1:K:4:TYR:OH     | 2.10                     | 0.51              |
| 1:L:344:TYR:O    | 1:L:348:SER:HB2  | 2.09                     | 0.51              |
| 1:L:372:ILE:HG22 | 1:L:385:ILE:HD13 | 1.92                     | 0.51              |
| 1:A:110:ASN:O    | 1:A:113:LYS:HB2  | 2.11                     | 0.51              |
| 1:B:135:PHE:HB3  | 1:B:231:PHE:CD1  | 2.45                     | 0.51              |
| 1:B:286:THR:HG21 | 1:B:388:LEU:HD22 | 1.92                     | 0.51              |
| 1:D:236:LEU:HB2  | 1:D:239:VAL:HG21 | 1.90                     | 0.51              |
| 1:E:91:ARG:NH1   | 1:E:93:ILE:HD11  | 2.25                     | 0.51              |
| 1:F:379:GLU:HG3  | 1:F:385:ILE:CD1  | 2.41                     | 0.51              |
| 1:F:48:ASN:HB3   | 1:F:71:TYR:CE1   | 2.46                     | 0.51              |
| 1:J:349:VAL:HG23 | 1:J:409:LEU:CD1  | 2.40                     | 0.51              |
| 1:L:375:MET:HG3  | 1:L:379:GLU:CG   | 2.38                     | 0.51              |
| 1:A:288:VAL:O    | 1:A:291:PRO:HD3  | 2.10                     | 0.51              |
| 1:A:421:LYS:HD3  | 1:A:424:GLU:OE2  | 2.10                     | 0.51              |
| 1:C:323:PRO:HD2  | 1:C:331:ARG:O    | 2.10                     | 0.51              |
| 1:D:211:ILE:HG22 | 1:D:215:LYS:HE3  | 1.91                     | 0.51              |
| 1:D:52:PHE:CE2   | 1:D:54:GLY:HA2   | 2.45                     | 0.51              |
| 1:D:68:MET:CE    | 1:D:104:PHE:HB2  | 2.40                     | 0.51              |
| 1:E:417:PHE:HD2  | 1:E:418:ILE:HD12 | 1.75                     | 0.51              |
| 1:F:271:ALA:O    | 1:F:275:ILE:HG12 | 2.11                     | 0.51              |
| 1:F:267:LEU:HD21 | 1:F:326:ARG:NH1  | 2.25                     | 0.51              |
| 1:H:162:THR:C    | 1:H:164:LEU:H    | 2.14                     | 0.51              |
| 1:J:207:SER:O    | 1:J:210:ASP:N    | 2.43                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:191:ALA:HB2  | 1:J:240:ASN:HB2  | 1.93                     | 0.51              |
| 1:K:21:ILE:HD12  | 1:K:21:ILE:N     | 2.24                     | 0.51              |
| 1:K:377:LYS:HA   | 1:K:380:ARG:NH2  | 2.25                     | 0.51              |
| 1:D:22:ARG:NH1   | 1:D:36:GLU:OE2   | 2.43                     | 0.51              |
| 1:D:406:VAL:HG22 | 1:D:414:PHE:CZ   | 2.45                     | 0.51              |
| 1:F:114:ARG:NH2  | 1:F:407:LYS:O    | 2.44                     | 0.51              |
| 1:G:203:GLY:O    | 1:G:204:ALA:C    | 2.48                     | 0.51              |
| 1:H:116:LEU:HD22 | 1:H:119:MET:CE   | 2.40                     | 0.51              |
| 1:H:345:LEU:O    | 1:H:349:VAL:HG12 | 2.11                     | 0.51              |
| 1:B:300:VAL:HA   | 1:H:429:ARG:HH22 | 1.75                     | 0.51              |
| 1:I:160:ALA:O    | 1:I:161:PRO:C    | 2.49                     | 0.51              |
| 1:I:150:LEU:HD13 | 1:I:192:PRO:HB2  | 1.93                     | 0.51              |
| 1:K:380:ARG:HB2  | 1:K:380:ARG:NH1  | 2.26                     | 0.51              |
| 1:L:23:LEU:HB2   | 1:L:35:VAL:HG22  | 1.92                     | 0.51              |
| 1:L:383:ASN:HB2  | 1:L:385:ILE:CG1  | 2.40                     | 0.51              |
| 1:A:237:PHE:CD1  | 1:A:238:GLY:N    | 2.79                     | 0.51              |
| 1:B:164:LEU:C    | 1:B:164:LEU:HD23 | 2.31                     | 0.51              |
| 1:B:393:ALA:HB2  | 1:B:425:TRP:CE2  | 2.45                     | 0.51              |
| 1:C:380:ARG:CB   | 1:C:380:ARG:HH11 | 2.23                     | 0.51              |
| 1:D:20:TYR:CZ    | 1:D:36:GLU:HB3   | 2.45                     | 0.51              |
| 1:D:406:VAL:HG22 | 1:D:414:PHE:CE1  | 2.45                     | 0.51              |
| 1:G:281:HIS:CD2  | 1:G:402:ASN:HD21 | 2.28                     | 0.51              |
| 1:H:397:GLU:CD   | 1:H:400:LYS:HZ1  | 2.14                     | 0.51              |
| 1:I:203:GLY:O    | 1:I:207:SER:N    | 2.38                     | 0.51              |
| 1:I:285:PHE:HB2  | 1:I:349:VAL:HG11 | 1.93                     | 0.51              |
| 1:I:37:ILE:HG22  | 1:J:185:ALA:CB   | 2.41                     | 0.51              |
| 1:K:83:THR:CG2   | 1:K:89:VAL:H     | 2.04                     | 0.51              |
| 1:L:242:SER:O    | 1:L:298:ARG:NE   | 2.44                     | 0.51              |
| 1:L:30:GLY:HA2   | 1:L:342:ASN:ND2  | 2.25                     | 0.51              |
| 1:L:311:TRP:NE1  | 1:L:367:PRO:HA   | 2.25                     | 0.51              |
| 1:A:191:ALA:HB3  | 1:A:194:GLN:NE2  | 2.25                     | 0.51              |
| 1:A:300:VAL:HG22 | 1:G:429:ARG:NH2  | 2.26                     | 0.51              |
| 1:A:38:PRO:HD2   | 1:A:41:GLN:HG3   | 1.93                     | 0.51              |
| 1:D:57:ILE:HD11  | 1:D:96:ILE:HG21  | 1.91                     | 0.51              |
| 1:G:37:ILE:HG22  | 1:H:185:ALA:CB   | 2.41                     | 0.51              |
| 1:G:98:ASN:ND2   | 1:G:104:PHE:HA   | 2.25                     | 0.51              |
| 1:J:162:THR:HG22 | 1:J:163:ASP:N    | 2.26                     | 0.51              |
| 1:J:429:ARG:HD3  | 4:J:610:HOH:O    | 2.10                     | 0.51              |
| 1:K:19:LYS:HA    | 1:K:39:VAL:HB    | 1.91                     | 0.51              |
| 1:L:9:ILE:O      | 1:L:13:VAL:HG23  | 2.11                     | 0.51              |
| 1:L:316:ARG:HB2  | 1:L:370:ARG:NH1  | 2.26                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:51:MET:HE3   | 1:L:69:TYR:CE1   | 2.46                     | 0.51              |
| 1:A:158:ASP:OD2  | 1:B:33:LYS:HE2   | 2.11                     | 0.51              |
| 1:A:200:LYS:NZ   | 1:B:41:GLN:NE2   | 2.59                     | 0.51              |
| 1:D:128:ASN:ND2  | 1:D:203:GLY:HA2  | 2.26                     | 0.51              |
| 1:D:315:ASN:ND2  | 1:D:370:ARG:HA   | 2.26                     | 0.51              |
| 1:F:281:HIS:O    | 1:F:284:SER:N    | 2.42                     | 0.51              |
| 1:G:370:ARG:NH2  | 1:G:383:ASN:HD22 | 2.08                     | 0.51              |
| 1:H:34:ASN:ND2   | 1:H:34:ASN:C     | 2.64                     | 0.51              |
| 1:L:109:ARG:HG2  | 1:L:109:ARG:HH21 | 1.76                     | 0.51              |
| 1:L:306:PRO:O    | 1:L:388:LEU:HD12 | 2.11                     | 0.51              |
| 1:B:370:ARG:NH2  | 1:B:375:MET:CG   | 2.71                     | 0.51              |
| 1:C:124:PHE:CE2  | 1:C:250:LEU:HD13 | 2.46                     | 0.51              |
| 1:E:145:GLU:OE1  | 1:E:145:GLU:HA   | 2.11                     | 0.51              |
| 1:E:147:THR:C    | 1:E:149:GLU:H    | 2.15                     | 0.51              |
| 1:E:206:ARG:O    | 1:E:209:ASP:HB2  | 2.11                     | 0.51              |
| 1:D:159:LEU:CD1  | 1:E:22:ARG:HH11  | 2.23                     | 0.51              |
| 1:F:146:PRO:O    | 1:F:147:THR:HG23 | 2.10                     | 0.51              |
| 1:F:205:VAL:CG1  | 1:F:206:ARG:N    | 2.74                     | 0.51              |
| 1:F:223:ARG:C    | 1:F:225:HIS:H    | 2.14                     | 0.51              |
| 1:F:386:VAL:HG23 | 1:F:386:VAL:O    | 2.11                     | 0.51              |
| 1:G:260:ASP:HB3  | 1:G:263:ALA:HB3  | 1.93                     | 0.51              |
| 1:H:223:ARG:O    | 1:H:226:GLY:N    | 2.41                     | 0.51              |
| 1:I:116:LEU:HD23 | 1:I:351:LEU:HD11 | 1.93                     | 0.51              |
| 1:K:107:ASP:OD2  | 1:K:110:ASN:OD1  | 2.29                     | 0.51              |
| 1:K:129:LEU:HD23 | 1:K:207:SER:OG   | 2.10                     | 0.51              |
| 1:B:91:ARG:C     | 1:B:91:ARG:HD2   | 2.32                     | 0.50              |
| 1:D:253:ASN:O    | 1:D:255:VAL:HG13 | 2.11                     | 0.50              |
| 1:D:34:ASN:O     | 1:D:34:ASN:ND2   | 2.44                     | 0.50              |
| 1:D:311:TRP:CD1  | 1:D:365:PRO:HG2  | 2.46                     | 0.50              |
| 1:E:356:ASP:O    | 1:E:360:ASN:HB2  | 2.11                     | 0.50              |
| 1:E:374:VAL:HG23 | 1:E:375:MET:N    | 2.26                     | 0.50              |
| 1:G:406:VAL:HA   | 1:G:414:PHE:CD1  | 2.46                     | 0.50              |
| 1:H:243:GLY:C    | 1:H:339:PRO:HD3  | 2.32                     | 0.50              |
| 1:K:35:VAL:HG13  | 1:K:35:VAL:O     | 2.12                     | 0.50              |
| 1:E:232:MET:HE3  | 1:K:440:TYR:HB2  | 1.93                     | 0.50              |
| 1:F:437:ARG:HD3  | 1:L:148:LEU:CD2  | 2.41                     | 0.50              |
| 1:L:13:VAL:HG13  | 1:L:18:VAL:HB    | 1.93                     | 0.50              |
| 1:L:371:ASN:HD21 | 1:L:374:VAL:HB   | 1.75                     | 0.50              |
| 1:L:23:LEU:HB3   | 1:L:70:LEU:HD23  | 1.93                     | 0.50              |
| 1:L:82:TRP:HE1   | 1:L:221:ILE:HD13 | 1.76                     | 0.50              |
| 1:A:389:PRO:HA   | 1:A:394:GLU:OE1  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:167:ASN:HD22 | 1:D:170:ARG:HB3  | 1.76                     | 0.50              |
| 1:A:36:GLU:OE2   | 1:F:169:ARG:NH1  | 2.41                     | 0.50              |
| 1:F:172:ILE:HD12 | 1:F:218:VAL:HA   | 1.92                     | 0.50              |
| 1:F:3:LYS:HE2    | 1:F:4:TYR:CE2    | 2.46                     | 0.50              |
| 1:F:53:ASP:OD1   | 1:F:62:ARG:NH2   | 2.43                     | 0.50              |
| 1:G:223:ARG:C    | 1:G:225:HIS:H    | 2.15                     | 0.50              |
| 1:G:315:ASN:HB3  | 1:G:318:PRO:HG3  | 1.93                     | 0.50              |
| 1:H:351:LEU:CD2  | 1:H:355:LEU:HG   | 2.42                     | 0.50              |
| 1:H:5:THR:O      | 1:H:7:GLU:N      | 2.44                     | 0.50              |
| 1:I:293:VAL:HG11 | 1:I:428:PHE:CD1  | 2.46                     | 0.50              |
| 1:A:170:ARG:NH1  | 1:A:171:ASP:OD2  | 2.44                     | 0.50              |
| 1:A:437:ARG:O    | 1:A:441:MET:HB2  | 2.11                     | 0.50              |
| 1:D:160:ALA:HB3  | 1:D:169:ARG:HH22 | 1.76                     | 0.50              |
| 1:E:378:GLU:O    | 1:E:382:GLU:HG3  | 2.11                     | 0.50              |
| 1:G:237:PHE:CD2  | 1:G:238:GLY:N    | 2.79                     | 0.50              |
| 1:G:267:LEU:CD2  | 1:G:326:ARG:HH12 | 2.24                     | 0.50              |
| 1:H:372:ILE:HA   | 1:H:375:MET:SD   | 2.51                     | 0.50              |
| 1:I:35:VAL:HG11  | 1:I:70:LEU:HD21  | 1.92                     | 0.50              |
| 1:J:160:ALA:O    | 1:J:161:PRO:O    | 2.30                     | 0.50              |
| 1:L:135:PHE:HB3  | 1:L:231:PHE:CD1  | 2.46                     | 0.50              |
| 1:B:35:VAL:O     | 1:B:35:VAL:HG13  | 2.11                     | 0.50              |
| 1:B:371:ASN:HD22 | 1:B:372:ILE:N    | 2.10                     | 0.50              |
| 1:E:437:ARG:O    | 1:E:441:MET:HB3  | 2.12                     | 0.50              |
| 1:F:60:PHE:CZ    | 1:F:423:ILE:HD11 | 2.46                     | 0.50              |
| 1:G:164:LEU:CD1  | 1:L:224:LYS:HD3  | 2.41                     | 0.50              |
| 1:G:211:ILE:HD13 | 1:G:244:MET:HE3  | 1.93                     | 0.50              |
| 1:G:375:MET:SD   | 1:G:380:ARG:HA   | 2.51                     | 0.50              |
| 1:G:399:PHE:HZ   | 1:G:409:LEU:CD2  | 2.21                     | 0.50              |
| 1:H:203:GLY:O    | 1:H:206:ARG:N    | 2.42                     | 0.50              |
| 1:H:399:PHE:HZ   | 1:H:409:LEU:HD12 | 1.76                     | 0.50              |
| 1:H:52:PHE:HE2   | 1:H:56:SER:OG    | 1.95                     | 0.50              |
| 1:J:169:ARG:HG3  | 1:J:169:ARG:HH21 | 1.76                     | 0.50              |
| 1:J:224:LYS:HB2  | 1:K:164:LEU:HD12 | 1.93                     | 0.50              |
| 1:K:20:TYR:OH    | 1:K:36:GLU:HG3   | 2.11                     | 0.50              |
| 1:K:81:PRO:HG2   | 1:K:82:TRP:CE3   | 2.47                     | 0.50              |
| 1:L:306:PRO:HB3  | 1:L:319:LEU:HA   | 1.93                     | 0.50              |
| 1:L:376:SER:H    | 1:L:379:GLU:CG   | 2.25                     | 0.50              |
| 1:A:253:ASN:O    | 1:A:255:VAL:HG23 | 2.12                     | 0.50              |
| 1:B:165:GLY:HA3  | 1:C:223:ARG:HH21 | 1.77                     | 0.50              |
| 1:F:133:PRO:HD2  | 1:F:197:ILE:O    | 2.11                     | 0.50              |
| 1:G:429:ARG:NH1  | 1:G:430:THR:HG22 | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:199:PHE:N    | 1:I:199:PHE:CD1  | 2.79                     | 0.50              |
| 1:I:267:LEU:HG   | 1:I:326:ARG:HH12 | 1.75                     | 0.50              |
| 1:J:234:LYS:HB3  | 1:J:294:ASN:ND2  | 2.27                     | 0.50              |
| 1:J:351:LEU:CD2  | 1:J:355:LEU:HG   | 2.40                     | 0.50              |
| 1:J:52:PHE:CZ    | 1:J:54:GLY:HA2   | 2.47                     | 0.50              |
| 1:A:133:PRO:O    | 1:A:196:GLU:HG3  | 2.12                     | 0.50              |
| 1:A:91:ARG:NH2   | 1:A:213:THR:OG1  | 2.43                     | 0.50              |
| 1:A:267:LEU:HD21 | 1:A:326:ARG:HH12 | 1.77                     | 0.50              |
| 1:C:127:PHE:CE2  | 1:C:351:LEU:HB2  | 2.47                     | 0.50              |
| 1:D:121:ASP:O    | 1:D:122:LEU:HD23 | 2.12                     | 0.50              |
| 1:F:16:GLU:HG3   | 1:F:88:LYS:HE3   | 1.94                     | 0.50              |
| 1:I:169:ARG:HG3  | 1:I:195:HIS:CG   | 2.47                     | 0.50              |
| 1:I:199:PHE:N    | 1:I:199:PHE:HD1  | 2.10                     | 0.50              |
| 1:I:216:LEU:HD11 | 1:J:159:LEU:HD13 | 1.93                     | 0.50              |
| 1:J:176:LEU:CB   | 1:J:183:ILE:HD11 | 2.40                     | 0.50              |
| 1:J:46:LEU:CD2   | 1:J:74:LEU:HD11  | 2.41                     | 0.50              |
| 1:L:81:PRO:HG2   | 1:L:82:TRP:H     | 1.76                     | 0.50              |
| 1:A:281:HIS:HD2  | 1:A:402:ASN:HD21 | 1.59                     | 0.50              |
| 1:A:321:ARG:HG2  | 1:A:322:ILE:N    | 2.25                     | 0.50              |
| 1:B:97:TYR:CE2   | 1:B:103:PRO:HG3  | 2.47                     | 0.50              |
| 1:C:326:ARG:HA   | 1:C:330:THR:OG1  | 2.11                     | 0.50              |
| 1:G:100:ASP:OD2  | 1:G:101:GLY:N    | 2.41                     | 0.50              |
| 1:G:434:PRO:O    | 1:G:438:GLU:HG3  | 2.12                     | 0.50              |
| 1:I:142:GLU:N    | 1:I:142:GLU:OE2  | 2.38                     | 0.50              |
| 1:I:396:LEU:HD11 | 1:I:421:LYS:HB3  | 1.94                     | 0.50              |
| 1:I:84:ALA:HB3   | 1:I:87:GLY:O     | 2.12                     | 0.50              |
| 1:J:196:GLU:O    | 1:J:197:ILE:HD13 | 2.11                     | 0.50              |
| 1:J:236:LEU:HD12 | 1:J:239:VAL:HG21 | 1.93                     | 0.50              |
| 1:J:257:ALA:O    | 1:J:270:THR:HG23 | 2.12                     | 0.50              |
| 1:J:399:PHE:HE1  | 1:J:405:MET:HB3  | 1.76                     | 0.50              |
| 1:J:64:GLU:HG2   | 1:K:315:ASN:O    | 2.12                     | 0.50              |
| 1:L:286:THR:HG23 | 1:L:290:ASN:HD22 | 1.77                     | 0.50              |
| 1:A:164:LEU:HD11 | 1:B:224:LYS:HD3  | 1.93                     | 0.50              |
| 1:A:275:ILE:O    | 1:A:279:VAL:HG23 | 2.12                     | 0.50              |
| 1:C:338:ASP:HB2  | 1:C:339:PRO:HD2  | 1.94                     | 0.50              |
| 1:E:375:MET:HB3  | 1:E:379:GLU:HG2  | 1.94                     | 0.50              |
| 1:F:22:ARG:HH11  | 1:F:22:ARG:HG2   | 1.76                     | 0.50              |
| 1:F:45:ALA:HA    | 1:F:50:VAL:CG2   | 2.35                     | 0.50              |
| 1:G:132:GLU:OE2  | 4:G:615:HOH:O    | 2.19                     | 0.50              |
| 1:H:160:ALA:HB3  | 1:H:169:ARG:HH12 | 1.77                     | 0.50              |
| 1:H:95:ASP:OD1   | 1:H:109:ARG:HD3  | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:372:ILE:O    | 1:K:373:TYR:HD2  | 1.94                     | 0.50              |
| 1:A:435:TRP:O    | 1:A:439:GLN:HG2  | 2.12                     | 0.50              |
| 1:C:405:MET:HE2  | 1:C:405:MET:N    | 2.27                     | 0.50              |
| 1:D:140:LEU:CD2  | 1:D:228:HIS:HB2  | 2.42                     | 0.50              |
| 1:D:200:LYS:CE   | 1:E:41:GLN:HE22  | 2.25                     | 0.50              |
| 1:E:148:LEU:HD13 | 1:E:148:LEU:N    | 2.26                     | 0.50              |
| 1:F:402:ASN:OD1  | 1:F:404:VAL:HG12 | 2.12                     | 0.50              |
| 1:G:245:HIS:CD2  | 1:G:335:ARG:HB3  | 2.47                     | 0.50              |
| 1:G:404:VAL:HG22 | 1:G:405:MET:HE2  | 1.93                     | 0.50              |
| 1:I:236:LEU:HD12 | 1:I:239:VAL:HG21 | 1.94                     | 0.50              |
| 1:I:355:LEU:C    | 1:I:357:GLY:H    | 2.15                     | 0.50              |
| 1:K:5:THR:HG23   | 1:K:8:ASP:H      | 1.77                     | 0.50              |
| 1:L:156:TYR:CE1  | 1:L:189:GLU:OE1  | 2.64                     | 0.50              |
| 1:L:281:HIS:CE1  | 1:L:404:VAL:HG11 | 2.47                     | 0.50              |
| 1:A:328:ILE:C    | 1:A:328:ILE:HD12 | 2.32                     | 0.49              |
| 1:C:182:GLU:HG2  | 1:C:200:LYS:HD2  | 1.94                     | 0.49              |
| 1:C:3:LYS:HB3    | 1:C:75:ASN:OD1   | 2.12                     | 0.49              |
| 1:D:282:ALA:HA   | 1:D:285:PHE:CZ   | 2.46                     | 0.49              |
| 1:G:112:LEU:HD12 | 1:G:344:TYR:HD2  | 1.77                     | 0.49              |
| 1:H:111:ASN:O    | 1:H:115:ILE:HG12 | 2.11                     | 0.49              |
| 1:H:184:GLU:HB2  | 1:H:199:PHE:O    | 2.12                     | 0.49              |
| 1:H:20:TYR:O     | 1:H:89:VAL:HG13  | 2.11                     | 0.49              |
| 1:H:311:TRP:HB3  | 1:H:320:ILE:HB   | 1.93                     | 0.49              |
| 1:I:156:TYR:O    | 1:I:158:ASP:N    | 2.44                     | 0.49              |
| 1:I:80:PHE:CE1   | 1:I:91:ARG:HG2   | 2.42                     | 0.49              |
| 1:K:115:ILE:HG22 | 1:K:351:LEU:CD1  | 2.38                     | 0.49              |
| 1:L:261:GLU:O    | 1:L:266:GLN:HG2  | 2.12                     | 0.49              |
| 1:B:252:LYS:O    | 1:B:253:ASN:HB2  | 2.12                     | 0.49              |
| 1:B:393:ALA:HB2  | 1:B:425:TRP:CD2  | 2.46                     | 0.49              |
| 1:D:161:PRO:HB2  | 1:D:167:ASN:OD1  | 2.12                     | 0.49              |
| 1:D:174:LEU:HD13 | 1:E:86:LYS:HB2   | 1.94                     | 0.49              |
| 1:G:27:ASP:HB2   | 1:G:57:ILE:HA    | 1.93                     | 0.49              |
| 1:H:189:GLU:OE2  | 1:H:190:VAL:HG23 | 2.12                     | 0.49              |
| 1:H:82:TRP:HE1   | 1:H:221:ILE:HD11 | 1.75                     | 0.49              |
| 1:H:74:LEU:HD22  | 1:H:74:LEU:N     | 2.17                     | 0.49              |
| 1:H:224:LYS:HB2  | 1:I:164:LEU:HD13 | 1.93                     | 0.49              |
| 1:I:368:ILE:HG21 | 1:I:372:ILE:CG2  | 2.42                     | 0.49              |
| 1:J:162:THR:CG2  | 1:J:163:ASP:N    | 2.75                     | 0.49              |
| 1:J:309:VAL:CG2  | 1:J:386:VAL:HB   | 2.42                     | 0.49              |
| 1:J:208:CYS:HA   | 1:J:343:PRO:HB2  | 1.94                     | 0.49              |
| 1:K:338:ASP:C    | 1:K:338:ASP:OD2  | 2.50                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:391:THR:OG1  | 1:K:394:GLU:HB2  | 2.12                     | 0.49              |
| 1:K:48:ASN:HB3   | 1:K:71:TYR:CD1   | 2.47                     | 0.49              |
| 1:B:399:PHE:HZ   | 1:B:409:LEU:HD12 | 1.77                     | 0.49              |
| 1:C:203:GLY:O    | 1:C:205:VAL:N    | 2.45                     | 0.49              |
| 1:C:282:ALA:C    | 1:C:284:SER:N    | 2.66                     | 0.49              |
| 1:C:156:TYR:CE2  | 1:D:62:ARG:NH1   | 2.80                     | 0.49              |
| 1:E:293:VAL:HG11 | 1:E:428:PHE:CE2  | 2.47                     | 0.49              |
| 1:F:309:VAL:O    | 1:F:310:ALA:HB2  | 2.12                     | 0.49              |
| 1:F:24:GLN:HE21  | 1:F:91:ARG:HH11  | 1.59                     | 0.49              |
| 1:G:384:GLY:C    | 1:G:385:ILE:HD13 | 2.31                     | 0.49              |
| 1:H:76:THR:O     | 1:H:78:VAL:HG23  | 2.12                     | 0.49              |
| 1:K:183:ILE:HD12 | 1:K:183:ILE:N    | 2.27                     | 0.49              |
| 1:E:429:ARG:NH2  | 1:K:300:VAL:HG12 | 2.26                     | 0.49              |
| 1:K:115:ILE:HD11 | 1:K:408:ALA:O    | 2.12                     | 0.49              |
| 1:L:58:GLU:O     | 1:L:61:VAL:HG22  | 2.12                     | 0.49              |
| 1:A:52:PHE:CE1   | 1:A:70:LEU:CD1   | 2.95                     | 0.49              |
| 1:B:107:ASP:HB3  | 1:B:110:ASN:HB2  | 1.95                     | 0.49              |
| 1:B:109:ARG:HG3  | 1:B:344:TYR:CE2  | 2.48                     | 0.49              |
| 1:B:409:LEU:O    | 1:B:413:LEU:HB2  | 2.12                     | 0.49              |
| 1:C:402:ASN:ND2  | 1:C:404:VAL:HG12 | 2.28                     | 0.49              |
| 1:D:311:TRP:HA   | 1:D:320:ILE:HB   | 1.94                     | 0.49              |
| 1:E:271:ALA:O    | 1:E:272:LYS:C    | 2.50                     | 0.49              |
| 1:E:45:ALA:HA    | 1:E:50:VAL:HG23  | 1.95                     | 0.49              |
| 1:E:48:ASN:OD1   | 1:E:72:PRO:HD2   | 2.13                     | 0.49              |
| 1:E:74:LEU:H     | 1:E:74:LEU:CD2   | 2.26                     | 0.49              |
| 1:F:129:LEU:HD22 | 1:F:131:PRO:CD   | 2.42                     | 0.49              |
| 1:F:85:GLU:C     | 1:F:87:GLY:H     | 2.15                     | 0.49              |
| 1:G:239:VAL:O    | 1:G:239:VAL:HG23 | 2.11                     | 0.49              |
| 1:G:23:LEU:HB3   | 1:G:70:LEU:HD23  | 1.94                     | 0.49              |
| 1:H:328:ILE:HD13 | 1:H:329:SER:H    | 1.76                     | 0.49              |
| 1:H:6:ARG:O      | 1:H:6:ARG:HG3    | 2.13                     | 0.49              |
| 1:I:256:ASN:ND2  | 1:I:328:ILE:O    | 2.46                     | 0.49              |
| 1:I:273:HIS:O    | 1:I:276:ALA:HB3  | 2.12                     | 0.49              |
| 1:I:399:PHE:HZ   | 1:I:409:LEU:HD11 | 1.76                     | 0.49              |
| 1:J:129:LEU:O    | 1:J:201:TYR:HA   | 2.12                     | 0.49              |
| 1:B:380:ARG:HA   | 1:B:383:ASN:HD22 | 1.77                     | 0.49              |
| 1:C:212:GLN:OE1  | 1:C:212:GLN:HA   | 2.11                     | 0.49              |
| 1:C:297:LYS:N    | 1:C:297:LYS:HD2  | 2.28                     | 0.49              |
| 1:D:264:ASP:C    | 1:D:266:GLN:N    | 2.64                     | 0.49              |
| 1:D:293:VAL:HG23 | 1:J:440:TYR:OH   | 2.12                     | 0.49              |
| 1:E:326:ARG:HH11 | 1:E:326:ARG:CG   | 2.25                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:145:GLU:HA   | 1:G:145:GLU:OE1  | 2.13                     | 0.49              |
| 1:G:402:ASN:OD1  | 1:G:402:ASN:C    | 2.51                     | 0.49              |
| 1:H:161:PRO:O    | 1:H:167:ASN:ND2  | 2.45                     | 0.49              |
| 1:I:133:PRO:CA   | 1:I:244:MET:HG3  | 2.43                     | 0.49              |
| 1:I:308:TYR:OH   | 1:I:380:ARG:HD2  | 2.12                     | 0.49              |
| 1:I:312:SER:OG   | 1:I:369:ASP:HA   | 2.13                     | 0.49              |
| 1:I:320:ILE:HG22 | 1:I:321:ARG:N    | 2.26                     | 0.49              |
| 1:I:52:PHE:CD1   | 1:I:70:LEU:HD22  | 2.48                     | 0.49              |
| 1:K:27:ASP:C     | 1:K:27:ASP:OD2   | 2.51                     | 0.49              |
| 1:A:360:ASN:O    | 1:A:361:LYS:C    | 2.50                     | 0.49              |
| 1:F:119:MET:O    | 1:F:124:PHE:HB2  | 2.12                     | 0.49              |
| 1:F:197:ILE:HD12 | 1:F:214:PHE:CE1  | 2.48                     | 0.49              |
| 1:F:280:LYS:HG3  | 1:F:281:HIS:CD2  | 2.46                     | 0.49              |
| 1:G:309:VAL:HA   | 1:G:319:LEU:HD22 | 1.95                     | 0.49              |
| 1:G:310:ALA:HB3  | 1:G:372:ILE:HD11 | 1.93                     | 0.49              |
| 1:H:235:PRO:O    | 1:H:236:LEU:HD23 | 2.12                     | 0.49              |
| 1:H:286:THR:HG23 | 1:H:290:ASN:HD22 | 1.77                     | 0.49              |
| 1:H:5:THR:C      | 1:H:7:GLU:N      | 2.65                     | 0.49              |
| 1:J:22:ARG:HH11  | 1:J:22:ARG:HG2   | 1.77                     | 0.49              |
| 1:J:85:GLU:C     | 1:J:87:GLY:H     | 2.16                     | 0.49              |
| 1:K:271:ALA:O    | 1:K:275:ILE:HG13 | 2.13                     | 0.49              |
| 1:A:138:PHE:CE2  | 1:A:236:LEU:HD11 | 2.47                     | 0.49              |
| 1:A:232:MET:CE   | 1:A:235:PRO:HA   | 2.42                     | 0.49              |
| 1:D:11:LYS:HG3   | 1:D:15:GLU:OE2   | 2.13                     | 0.49              |
| 1:D:13:VAL:HG21  | 1:D:42:LEU:CD2   | 2.42                     | 0.49              |
| 1:D:443:GLN:CA   | 1:D:443:GLN:HE21 | 2.25                     | 0.49              |
| 1:E:142:GLU:H    | 1:E:142:GLU:CD   | 2.15                     | 0.49              |
| 1:E:223:ARG:C    | 1:E:225:HIS:H    | 2.16                     | 0.49              |
| 1:F:127:PHE:CD2  | 1:F:351:LEU:HG   | 2.47                     | 0.49              |
| 1:K:25:PHE:HB2   | 1:K:96:ILE:HD11  | 1.94                     | 0.49              |
| 1:A:52:PHE:HE1   | 1:A:70:LEU:HD13  | 1.77                     | 0.49              |
| 1:B:419:GLU:O    | 1:B:423:ILE:HG12 | 2.12                     | 0.49              |
| 1:C:54:GLY:O     | 1:C:57:ILE:HG12  | 2.12                     | 0.49              |
| 1:C:18:VAL:CG2   | 1:C:79:ILE:HD12  | 2.42                     | 0.49              |
| 1:C:79:ILE:HD13  | 1:C:90:ALA:HB2   | 1.95                     | 0.49              |
| 1:D:243:GLY:N    | 1:D:298:ARG:NH1  | 2.61                     | 0.49              |
| 1:D:78:VAL:HG21  | 1:D:91:ARG:HH21  | 1.76                     | 0.49              |
| 1:D:80:PHE:CD2   | 1:D:80:PHE:N     | 2.81                     | 0.49              |
| 1:F:187:HIS:CE1  | 1:F:196:GLU:OE1  | 2.62                     | 0.49              |
| 1:F:146:PRO:CG   | 1:F:228:HIS:CD2  | 2.87                     | 0.49              |
| 1:F:322:ILE:HD12 | 1:F:322:ILE:N    | 2.28                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:433:HIS:O    | 1:F:436:GLU:HB2  | 2.13                     | 0.49              |
| 1:G:371:ASN:O    | 1:G:372:ILE:HB   | 2.13                     | 0.49              |
| 1:I:58:GLU:O     | 1:I:61:VAL:HG22  | 2.13                     | 0.49              |
| 1:I:67:ASP:O     | 1:I:99:PRO:HG3   | 2.12                     | 0.49              |
| 1:L:355:LEU:C    | 1:L:357:GLY:H    | 2.15                     | 0.49              |
| 1:A:3:LYS:HB3    | 1:A:3:LYS:HZ3    | 1.74                     | 0.49              |
| 1:B:129:LEU:CD1  | 1:B:207:SER:HB3  | 2.42                     | 0.49              |
| 1:D:200:LYS:HE2  | 1:E:41:GLN:HE22  | 1.78                     | 0.49              |
| 1:G:73:ASP:HA    | 4:G:612:HOH:O    | 2.11                     | 0.49              |
| 1:H:166:GLU:O    | 1:H:166:GLU:OE1  | 2.31                     | 0.49              |
| 1:H:91:ARG:HD2   | 1:H:91:ARG:C     | 2.33                     | 0.49              |
| 1:I:63:ILE:H     | 1:I:63:ILE:HD12  | 1.77                     | 0.49              |
| 1:J:129:LEU:HD22 | 1:J:131:PRO:CD   | 2.43                     | 0.49              |
| 1:J:24:GLN:NE2   | 1:J:32:ILE:HD11  | 2.27                     | 0.49              |
| 1:J:258:PHE:HA   | 1:J:271:ALA:HB2  | 1.93                     | 0.49              |
| 1:K:282:ALA:C    | 1:K:284:SER:H    | 2.16                     | 0.49              |
| 1:A:27:ASP:OD1   | 1:A:31:THR:HB    | 2.12                     | 0.49              |
| 1:C:18:VAL:HG21  | 1:C:79:ILE:CD1   | 2.42                     | 0.49              |
| 1:D:286:THR:HA   | 1:D:289:THR:OG1  | 2.12                     | 0.49              |
| 1:D:351:LEU:O    | 1:D:355:LEU:HG   | 2.13                     | 0.49              |
| 1:E:380:ARG:O    | 1:E:385:ILE:O    | 2.31                     | 0.49              |
| 1:F:283:THR:HG23 | 1:F:309:VAL:HG21 | 1.95                     | 0.49              |
| 1:F:52:PHE:CD1   | 1:F:70:LEU:HD13  | 2.48                     | 0.49              |
| 1:G:174:LEU:HD23 | 1:L:86:LYS:HB3   | 1.95                     | 0.49              |
| 1:J:78:VAL:HB    | 1:J:91:ARG:HG3   | 1.94                     | 0.49              |
| 1:K:317:SER:N    | 1:K:318:PRO:HD3  | 2.28                     | 0.49              |
| 1:L:124:PHE:CZ   | 1:L:358:ILE:HG21 | 2.48                     | 0.49              |
| 1:A:281:HIS:CD2  | 1:A:402:ASN:HD21 | 2.30                     | 0.48              |
| 1:A:23:LEU:HB2   | 1:A:35:VAL:CG1   | 2.43                     | 0.48              |
| 1:A:3:LYS:HB3    | 1:A:3:LYS:HZ2    | 1.76                     | 0.48              |
| 1:B:308:TYR:HE1  | 1:B:373:TYR:CE1  | 2.31                     | 0.48              |
| 1:B:315:ASN:HD22 | 1:B:318:PRO:HD3  | 1.78                     | 0.48              |
| 1:B:370:ARG:HH12 | 1:B:375:MET:HG3  | 1.78                     | 0.48              |
| 1:B:45:ALA:HA    | 1:B:50:VAL:HG23  | 1.95                     | 0.48              |
| 1:D:177:GLU:OE2  | 1:D:177:GLU:HA   | 2.13                     | 0.48              |
| 1:D:199:PHE:HZ   | 1:D:214:PHE:HB2  | 1.78                     | 0.48              |
| 1:F:308:TYR:CD1  | 1:F:372:ILE:HG21 | 2.48                     | 0.48              |
| 1:F:66:SER:O     | 1:F:68:MET:N     | 2.47                     | 0.48              |
| 1:J:160:ALA:O    | 1:J:161:PRO:C    | 2.51                     | 0.48              |
| 1:L:140:LEU:HD12 | 1:L:226:GLY:HA2  | 1.94                     | 0.48              |
| 1:A:206:ARG:NH1  | 1:A:206:ARG:CG   | 2.74                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:300:VAL:HG13 | 1:A:301:PRO:HD2  | 1.94                     | 0.48              |
| 1:A:324:ALA:O    | 1:A:325:SER:O    | 2.31                     | 0.48              |
| 1:C:129:LEU:HD22 | 1:C:131:PRO:CD   | 2.41                     | 0.48              |
| 1:C:160:ALA:HB1  | 1:C:161:PRO:CD   | 2.43                     | 0.48              |
| 1:C:91:ARG:C     | 1:C:91:ARG:HD2   | 2.34                     | 0.48              |
| 1:F:48:ASN:OD1   | 1:F:72:PRO:HD2   | 2.12                     | 0.48              |
| 1:G:203:GLY:O    | 1:G:206:ARG:N    | 2.46                     | 0.48              |
| 1:G:258:PHE:HB3  | 1:G:271:ALA:N    | 2.29                     | 0.48              |
| 1:G:375:MET:HE1  | 1:G:379:GLU:O    | 2.13                     | 0.48              |
| 1:G:281:HIS:CD2  | 1:G:404:VAL:HG11 | 2.47                     | 0.48              |
| 1:H:371:ASN:OD1  | 1:H:374:VAL:HG22 | 2.12                     | 0.48              |
| 1:I:208:CYS:HA   | 1:I:211:ILE:CG1  | 2.43                     | 0.48              |
| 1:J:160:ALA:HB2  | 1:J:188:HIS:HD2  | 1.79                     | 0.48              |
| 1:J:268:SER:OG   | 1:J:270:THR:HG23 | 2.13                     | 0.48              |
| 1:J:76:THR:O     | 1:J:78:VAL:HG23  | 2.13                     | 0.48              |
| 1:C:286:THR:HG22 | 1:C:290:ASN:ND2  | 2.28                     | 0.48              |
| 1:D:273:HIS:CE1  | 1:D:361:LYS:CA   | 2.96                     | 0.48              |
| 1:E:260:ASP:HB2  | 1:E:268:SER:HA   | 1.95                     | 0.48              |
| 1:F:129:LEU:HD23 | 1:F:130:GLY:H    | 1.78                     | 0.48              |
| 1:J:199:PHE:HZ   | 1:J:214:PHE:CG   | 2.31                     | 0.48              |
| 1:J:306:PRO:CG   | 1:J:335:ARG:HB2  | 2.37                     | 0.48              |
| 1:J:30:GLY:CA    | 1:J:342:ASN:ND2  | 2.74                     | 0.48              |
| 1:K:104:PHE:CZ   | 1:K:106:GLY:HA3  | 2.48                     | 0.48              |
| 1:K:138:PHE:HB3  | 1:K:147:THR:O    | 2.13                     | 0.48              |
| 1:K:234:LYS:HB3  | 1:K:294:ASN:HD21 | 1.78                     | 0.48              |
| 1:K:37:ILE:HG22  | 1:L:185:ALA:HA   | 1.94                     | 0.48              |
| 1:L:380:ARG:HB3  | 1:L:380:ARG:HH11 | 1.77                     | 0.48              |
| 1:C:291:PRO:HG2  | 1:C:292:THR:H    | 1.78                     | 0.48              |
| 1:C:402:ASN:C    | 1:C:402:ASN:OD1  | 2.51                     | 0.48              |
| 1:D:173:VAL:HG13 | 1:D:183:ILE:HG13 | 1.96                     | 0.48              |
| 1:E:78:VAL:HB    | 1:E:91:ARG:HG3   | 1.95                     | 0.48              |
| 1:F:375:MET:HE2  | 1:F:385:ILE:HD11 | 1.94                     | 0.48              |
| 4:G:604:HOH:O    | 1:H:157:PHE:HZ   | 1.96                     | 0.48              |
| 1:H:21:ILE:HG12  | 1:H:21:ILE:O     | 2.13                     | 0.48              |
| 1:J:259:PHE:CE1  | 1:J:326:ARG:HB3  | 2.48                     | 0.48              |
| 1:L:310:ALA:HB1  | 1:L:368:ILE:CB   | 2.43                     | 0.48              |
| 1:G:178:GLU:HG2  | 1:L:86:LYS:HE2   | 1.94                     | 0.48              |
| 1:A:27:ASP:CG    | 1:A:31:THR:HB    | 2.34                     | 0.48              |
| 1:C:321:ARG:O    | 1:C:323:PRO:HD3  | 2.13                     | 0.48              |
| 1:E:331:ARG:NH2  | 1:E:331:ARG:HG2  | 2.28                     | 0.48              |
| 1:E:375:MET:HA   | 1:E:379:GLU:OE1  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:160:ALA:HB1  | 1:F:161:PRO:CD   | 2.39                     | 0.48              |
| 1:F:297:LYS:HE3  | 1:L:436:GLU:CD   | 2.34                     | 0.48              |
| 1:I:328:ILE:C    | 1:I:330:THR:H    | 2.16                     | 0.48              |
| 1:I:63:ILE:N     | 1:I:63:ILE:HD12  | 2.28                     | 0.48              |
| 1:K:116:LEU:O    | 1:K:119:MET:HB3  | 2.13                     | 0.48              |
| 1:L:440:TYR:HD1  | 1:L:444:TYR:CE2  | 2.32                     | 0.48              |
| 1:D:325:SER:OG   | 1:D:329:SER:HB2  | 2.14                     | 0.48              |
| 1:E:19:LYS:HA    | 1:E:39:VAL:HB    | 1.94                     | 0.48              |
| 1:H:272:LYS:NZ   | 1:H:364:ALA:H    | 2.09                     | 0.48              |
| 1:H:282:ALA:C    | 1:H:284:SER:H    | 2.17                     | 0.48              |
| 1:H:291:PRO:HG3  | 1:H:341:ALA:HA   | 1.94                     | 0.48              |
| 1:I:282:ALA:HB1  | 1:I:319:LEU:HD21 | 1.96                     | 0.48              |
| 1:I:311:TRP:HB3  | 1:I:320:ILE:HB   | 1.96                     | 0.48              |
| 1:D:437:ARG:HA   | 1:J:232:MET:HE3  | 1.96                     | 0.48              |
| 1:K:129:LEU:HD11 | 1:K:246:CYS:HB3  | 1.95                     | 0.48              |
| 1:K:426:ASP:HA   | 1:K:429:ARG:HG2  | 1.95                     | 0.48              |
| 1:L:176:LEU:O    | 1:L:181:PHE:HB2  | 2.13                     | 0.48              |
| 1:L:310:ALA:HB2  | 1:L:385:ILE:HG22 | 1.96                     | 0.48              |
| 1:L:396:LEU:O    | 1:L:400:LYS:HG3  | 2.12                     | 0.48              |
| 1:A:111:ASN:O    | 1:A:115:ILE:HG12 | 2.14                     | 0.48              |
| 1:A:11:LYS:HZ3   | 1:A:15:GLU:HB2   | 1.79                     | 0.48              |
| 1:A:243:GLY:HA3  | 1:A:298:ARG:NH1  | 2.29                     | 0.48              |
| 1:A:402:ASN:OD1  | 1:A:404:VAL:HG12 | 2.13                     | 0.48              |
| 1:B:380:ARG:HA   | 1:B:383:ASN:ND2  | 2.29                     | 0.48              |
| 1:C:100:ASP:O    | 1:C:102:THR:HG22 | 2.14                     | 0.48              |
| 1:D:208:CYS:SG   | 1:D:347:LEU:HD12 | 2.53                     | 0.48              |
| 1:C:164:LEU:CD1  | 1:D:224:LYS:HD3  | 2.38                     | 0.48              |
| 1:D:242:SER:O    | 1:D:339:PRO:HD2  | 2.13                     | 0.48              |
| 1:D:280:LYS:HD3  | 1:D:281:HIS:CE1  | 2.49                     | 0.48              |
| 1:F:97:TYR:CD1   | 1:F:103:PRO:HA   | 2.48                     | 0.48              |
| 1:F:189:GLU:HB3  | 1:F:194:GLN:NE2  | 2.29                     | 0.48              |
| 1:F:35:VAL:HG13  | 1:F:35:VAL:O     | 2.13                     | 0.48              |
| 1:G:119:MET:HG2  | 1:G:124:PHE:HB2  | 1.95                     | 0.48              |
| 1:G:23:LEU:HB2   | 1:G:35:VAL:CG1   | 2.41                     | 0.48              |
| 1:G:271:ALA:O    | 1:G:275:ILE:HD12 | 2.14                     | 0.48              |
| 1:J:167:ASN:O    | 1:J:171:ASP:OD1  | 2.31                     | 0.48              |
| 1:J:173:VAL:HG13 | 1:J:183:ILE:CD1  | 2.44                     | 0.48              |
| 1:K:236:LEU:HB2  | 1:K:239:VAL:HG23 | 1.96                     | 0.48              |
| 1:K:236:LEU:O    | 1:K:239:VAL:HG23 | 2.13                     | 0.48              |
| 1:K:22:ARG:NH1   | 1:K:36:GLU:OE2   | 2.45                     | 0.48              |
| 1:L:24:GLN:HE22  | 1:L:91:ARG:HH11  | 1.60                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:131:PRO:HG2  | 1:A:211:ILE:HD11 | 1.96                     | 0.48              |
| 1:A:156:TYR:O    | 1:A:158:ASP:N    | 2.46                     | 0.48              |
| 1:D:205:VAL:HG23 | 1:D:206:ARG:N    | 2.26                     | 0.48              |
| 1:G:13:VAL:CG1   | 1:G:18:VAL:HB    | 2.41                     | 0.48              |
| 1:G:20:TYR:OH    | 1:G:36:GLU:HB3   | 2.13                     | 0.48              |
| 1:I:150:LEU:HD12 | 1:I:192:PRO:HB2  | 1.96                     | 0.48              |
| 1:I:6:ARG:NH2    | 1:I:47:ASP:OD1   | 2.46                     | 0.48              |
| 1:K:234:LYS:N    | 1:K:235:PRO:HD3  | 2.29                     | 0.48              |
| 1:L:147:THR:C    | 1:L:149:GLU:H    | 2.16                     | 0.48              |
| 1:C:109:ARG:HD2  | 1:C:344:TYR:CE2  | 2.49                     | 0.48              |
| 1:D:251:PHE:N    | 1:D:251:PHE:CD1  | 2.82                     | 0.48              |
| 1:D:292:THR:OG1  | 1:D:295:SER:HB2  | 2.13                     | 0.48              |
| 1:E:319:LEU:C    | 1:E:320:ILE:HD12 | 2.34                     | 0.48              |
| 1:F:429:ARG:HH21 | 1:L:300:VAL:CG2  | 2.15                     | 0.48              |
| 1:G:261:GLU:O    | 1:G:266:GLN:HG2  | 2.13                     | 0.48              |
| 1:H:41:GLN:NE2   | 1:I:200:LYS:NZ   | 2.56                     | 0.48              |
| 1:I:355:LEU:C    | 1:I:357:GLY:N    | 2.66                     | 0.48              |
| 1:J:207:SER:O    | 1:J:208:CYS:C    | 2.51                     | 0.48              |
| 1:J:51:MET:SD    | 1:J:67:ASP:HB3   | 2.54                     | 0.48              |
| 1:K:22:ARG:NH1   | 1:L:159:LEU:HD13 | 2.28                     | 0.48              |
| 1:E:297:LYS:HE3  | 1:K:436:GLU:CD   | 2.34                     | 0.48              |
| 1:B:55:SER:OG    | 1:B:62:ARG:NE    | 2.46                     | 0.48              |
| 1:C:393:ALA:HB2  | 1:C:425:TRP:CE2  | 2.48                     | 0.48              |
| 1:D:218:VAL:O    | 1:D:222:ALA:HB2  | 2.14                     | 0.48              |
| 1:D:77:PHE:CE1   | 1:D:90:ALA:HB1   | 2.49                     | 0.48              |
| 1:E:32:ILE:CD1   | 1:E:216:LEU:HD13 | 2.44                     | 0.48              |
| 1:E:272:LYS:O    | 1:E:275:ILE:HB   | 2.14                     | 0.48              |
| 1:G:158:ASP:OD1  | 1:G:158:ASP:N    | 2.47                     | 0.48              |
| 1:H:137:LEU:HD12 | 1:H:195:HIS:HE2  | 1.79                     | 0.48              |
| 1:H:250:LEU:HB2  | 1:H:258:PHE:CZ   | 2.48                     | 0.48              |
| 1:H:423:ILE:O    | 1:H:427:MET:HG3  | 2.14                     | 0.48              |
| 1:J:212:GLN:CA   | 1:J:212:GLN:OE1  | 2.58                     | 0.48              |
| 1:J:135:PHE:HB3  | 1:J:231:PHE:CE1  | 2.49                     | 0.48              |
| 1:J:299:LEU:CD1  | 1:J:299:LEU:N    | 2.77                     | 0.48              |
| 1:K:98:ASN:C     | 1:K:100:ASP:H    | 2.16                     | 0.48              |
| 1:L:189:GLU:HB3  | 1:L:194:GLN:NE2  | 2.29                     | 0.48              |
| 1:L:418:ILE:O    | 1:L:422:GLU:HG3  | 2.13                     | 0.48              |
| 1:A:311:TRP:HA   | 1:A:320:ILE:O    | 2.14                     | 0.47              |
| 1:A:315:ASN:OD1  | 1:A:371:ASN:HA   | 2.14                     | 0.47              |
| 1:A:78:VAL:HG12  | 1:A:91:ARG:CG    | 2.44                     | 0.47              |
| 1:B:120:GLU:C    | 1:B:122:LEU:N    | 2.68                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:279:VAL:HG13 | 1:B:309:VAL:HG12 | 1.95                     | 0.47              |
| 1:C:20:TYR:HB3   | 1:C:89:VAL:HG22  | 1.96                     | 0.47              |
| 1:D:413:LEU:HA   | 1:D:413:LEU:HD23 | 1.73                     | 0.47              |
| 1:E:278:ILE:HG23 | 1:E:285:PHE:CE2  | 2.49                     | 0.47              |
| 1:E:294:ASN:HD22 | 1:E:297:LYS:HG3  | 1.79                     | 0.47              |
| 1:F:264:ASP:O    | 1:F:265:LEU:HB2  | 2.14                     | 0.47              |
| 1:F:286:THR:O    | 1:F:290:ASN:N    | 2.45                     | 0.47              |
| 1:F:370:ARG:NH1  | 1:F:375:MET:HE3  | 2.29                     | 0.47              |
| 1:G:360:ASN:O    | 1:G:361:LYS:C    | 2.53                     | 0.47              |
| 1:H:28:ILE:HD11  | 1:H:417:PHE:HA   | 1.96                     | 0.47              |
| 1:I:319:LEU:CB   | 1:I:320:ILE:HD12 | 2.44                     | 0.47              |
| 1:J:121:ASP:C    | 1:J:122:LEU:HD22 | 2.34                     | 0.47              |
| 1:J:138:PHE:CD2  | 1:J:148:LEU:HA   | 2.48                     | 0.47              |
| 1:J:402:ASN:CG   | 1:J:405:MET:HG2  | 2.34                     | 0.47              |
| 1:K:270:THR:HG22 | 1:K:358:ILE:CD1  | 2.40                     | 0.47              |
| 1:K:311:TRP:HA   | 1:K:320:ILE:HB   | 1.96                     | 0.47              |
| 1:K:326:ARG:HD3  | 1:K:330:THR:OG1  | 2.14                     | 0.47              |
| 1:L:156:TYR:HB2  | 1:L:190:VAL:HA   | 1.96                     | 0.47              |
| 1:C:295:SER:O    | 1:C:299:LEU:HD13 | 2.15                     | 0.47              |
| 1:C:316:ARG:HG2  | 1:C:373:TYR:CG   | 2.49                     | 0.47              |
| 1:D:134:GLU:HG3  | 1:D:243:GLY:O    | 2.13                     | 0.47              |
| 1:E:402:ASN:CG   | 1:E:405:MET:HG2  | 2.35                     | 0.47              |
| 1:F:342:ASN:HD21 | 1:F:344:TYR:HD1  | 1.62                     | 0.47              |
| 1:F:347:LEU:HD22 | 1:F:347:LEU:N    | 2.29                     | 0.47              |
| 1:G:160:ALA:HB3  | 1:G:169:ARG:HH12 | 1.79                     | 0.47              |
| 1:G:370:ARG:HG3  | 1:G:370:ARG:HH11 | 1.79                     | 0.47              |
| 1:G:309:VAL:HB   | 1:G:386:VAL:HG23 | 1.95                     | 0.47              |
| 1:G:79:ILE:HD13  | 1:G:90:ALA:HB2   | 1.96                     | 0.47              |
| 1:H:140:LEU:HD12 | 1:H:226:GLY:HA2  | 1.96                     | 0.47              |
| 1:H:349:VAL:HG23 | 1:H:405:MET:SD   | 2.53                     | 0.47              |
| 1:I:116:LEU:HD23 | 1:I:351:LEU:CD1  | 2.44                     | 0.47              |
| 1:K:404:VAL:HG23 | 1:K:405:MET:HE2  | 1.96                     | 0.47              |
| 1:L:291:PRO:HG2  | 1:L:292:THR:HG23 | 1.96                     | 0.47              |
| 1:B:231:PHE:O    | 1:B:339:PRO:HG2  | 2.14                     | 0.47              |
| 1:B:262:ASN:HD22 | 1:B:262:ASN:N    | 2.08                     | 0.47              |
| 1:B:315:ASN:HD22 | 1:B:318:PRO:CD   | 2.27                     | 0.47              |
| 1:C:114:ARG:HH21 | 1:C:115:ILE:HD11 | 1.78                     | 0.47              |
| 1:D:167:ASN:ND2  | 1:D:170:ARG:HB2  | 2.29                     | 0.47              |
| 1:D:176:LEU:HD11 | 1:D:214:PHE:CD1  | 2.49                     | 0.47              |
| 1:D:55:SER:HB2   | 1:D:62:ARG:HB2   | 1.95                     | 0.47              |
| 1:E:80:PHE:CE1   | 1:E:91:ARG:HB3   | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:148:LEU:N    | 1:G:148:LEU:HD22 | 2.29                     | 0.47              |
| 1:G:306:PRO:HA   | 1:G:317:SER:HB2  | 1.96                     | 0.47              |
| 1:G:368:ILE:HD13 | 1:G:372:ILE:HG13 | 1.96                     | 0.47              |
| 1:H:168:CYS:O    | 1:H:169:ARG:C    | 2.53                     | 0.47              |
| 1:B:300:VAL:HG11 | 1:H:430:THR:CG2  | 2.44                     | 0.47              |
| 1:I:126:ASP:HB2  | 1:I:251:PHE:HB2  | 1.96                     | 0.47              |
| 1:C:228:HIS:HE1  | 1:I:441:MET:O    | 1.96                     | 0.47              |
| 1:J:36:GLU:HG2   | 1:K:186:SER:O    | 2.14                     | 0.47              |
| 1:J:48:ASN:HB3   | 1:J:71:TYR:CD1   | 2.49                     | 0.47              |
| 1:K:129:LEU:HB3  | 1:K:207:SER:OG   | 2.15                     | 0.47              |
| 1:L:325:SER:HB2  | 1:L:329:SER:HB3  | 1.96                     | 0.47              |
| 1:B:147:THR:HG22 | 1:B:149:GLU:HG3  | 1.94                     | 0.47              |
| 1:B:203:GLY:O    | 1:B:206:ARG:N    | 2.47                     | 0.47              |
| 1:B:261:GLU:HA   | 1:B:266:GLN:HE22 | 1.80                     | 0.47              |
| 1:B:308:TYR:HE1  | 1:B:373:TYR:CD1  | 2.32                     | 0.47              |
| 1:C:244:MET:O    | 1:C:337:VAL:HB   | 2.13                     | 0.47              |
| 1:C:127:PHE:CE2  | 1:C:347:LEU:HD22 | 2.49                     | 0.47              |
| 1:D:160:ALA:HB2  | 1:D:188:HIS:CD2  | 2.49                     | 0.47              |
| 1:D:168:CYS:O    | 1:D:169:ARG:C    | 2.52                     | 0.47              |
| 1:D:156:TYR:HB2  | 1:D:190:VAL:HA   | 1.96                     | 0.47              |
| 1:E:140:LEU:HD12 | 1:E:227:LEU:N    | 2.29                     | 0.47              |
| 1:F:172:ILE:O    | 1:F:176:LEU:HG   | 2.14                     | 0.47              |
| 1:F:91:ARG:C     | 1:F:91:ARG:HD2   | 2.34                     | 0.47              |
| 1:G:245:HIS:NE2  | 1:G:335:ARG:HB3  | 2.29                     | 0.47              |
| 1:G:52:PHE:CD1   | 1:G:70:LEU:HD13  | 2.48                     | 0.47              |
| 1:H:131:PRO:C    | 1:H:133:PRO:HD3  | 2.34                     | 0.47              |
| 1:I:114:ARG:HH12 | 1:I:115:ILE:CD1  | 2.26                     | 0.47              |
| 1:L:203:GLY:O    | 1:L:204:ALA:C    | 2.52                     | 0.47              |
| 1:A:105:GLU:H    | 1:A:105:GLU:CD   | 2.18                     | 0.47              |
| 1:A:11:LYS:HD2   | 1:A:15:GLU:OE1   | 2.14                     | 0.47              |
| 1:A:48:ASN:OD1   | 1:A:71:TYR:HA    | 2.14                     | 0.47              |
| 1:B:25:PHE:CE1   | 1:B:33:LYS:HB2   | 2.49                     | 0.47              |
| 1:C:375:MET:HA   | 1:C:379:GLU:OE1  | 2.14                     | 0.47              |
| 1:D:345:LEU:HD22 | 1:D:409:LEU:CD2  | 2.44                     | 0.47              |
| 1:D:34:ASN:C     | 1:D:34:ASN:HD22  | 2.17                     | 0.47              |
| 1:E:399:PHE:CE2  | 1:E:418:ILE:HD11 | 2.49                     | 0.47              |
| 1:E:74:LEU:N     | 1:E:74:LEU:HD22  | 2.29                     | 0.47              |
| 1:F:353:ALA:HB2  | 1:F:405:MET:HE3  | 1.96                     | 0.47              |
| 1:F:309:VAL:HG23 | 1:F:386:VAL:O    | 2.14                     | 0.47              |
| 1:H:271:ALA:O    | 1:H:275:ILE:HG12 | 2.14                     | 0.47              |
| 1:H:347:LEU:O    | 1:H:348:SER:C    | 2.52                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:63:ILE:O     | 1:J:316:ARG:NH1  | 2.47                     | 0.47              |
| 1:J:129:LEU:CD2  | 1:J:130:GLY:N    | 2.74                     | 0.47              |
| 1:K:5:THR:H      | 1:K:8:ASP:HB2    | 1.80                     | 0.47              |
| 1:L:58:GLU:HG3   | 1:L:416:HIS:ND1  | 2.29                     | 0.47              |
| 1:C:203:GLY:O    | 1:C:204:ALA:C    | 2.53                     | 0.47              |
| 1:C:274:PHE:CE2  | 1:C:332:VAL:HG11 | 2.49                     | 0.47              |
| 1:C:435:TRP:CE2  | 1:C:439:GLN:HG3  | 2.49                     | 0.47              |
| 1:D:84:ALA:C     | 1:D:86:LYS:H     | 2.18                     | 0.47              |
| 1:F:23:LEU:HB3   | 1:F:70:LEU:HD23  | 1.95                     | 0.47              |
| 1:G:151:ASN:HD22 | 1:G:166:GLU:CD   | 2.17                     | 0.47              |
| 1:G:208:CYS:O    | 1:G:212:GLN:HG2  | 2.15                     | 0.47              |
| 1:H:360:ASN:O    | 1:H:361:LYS:C    | 2.51                     | 0.47              |
| 1:I:5:THR:H      | 1:I:8:ASP:HB2    | 1.80                     | 0.47              |
| 1:K:168:CYS:SG   | 1:K:227:LEU:HD12 | 2.54                     | 0.47              |
| 1:K:291:PRO:CG   | 1:K:341:ALA:HA   | 2.40                     | 0.47              |
| 1:A:337:VAL:HG12 | 1:A:338:ASP:N    | 2.30                     | 0.47              |
| 1:A:5:THR:O      | 1:A:9:ILE:HG12   | 2.15                     | 0.47              |
| 1:B:243:GLY:HA3  | 1:B:298:ARG:HH12 | 1.79                     | 0.47              |
| 1:B:440:TYR:O    | 1:B:444:TYR:HB2  | 2.14                     | 0.47              |
| 1:C:185:ALA:CB   | 1:D:37:ILE:HG22  | 2.45                     | 0.47              |
| 1:C:124:PHE:CZ   | 1:C:358:ILE:HD13 | 2.50                     | 0.47              |
| 1:E:5:THR:O      | 1:E:8:ASP:HB2    | 2.15                     | 0.47              |
| 1:F:215:LYS:O    | 1:F:219:LYS:HB2  | 2.14                     | 0.47              |
| 1:G:211:ILE:HD13 | 1:G:244:MET:CE   | 2.45                     | 0.47              |
| 1:H:135:PHE:HB3  | 1:H:231:PHE:CD1  | 2.50                     | 0.47              |
| 1:H:139:LYS:HA   | 1:H:227:LEU:HD23 | 1.96                     | 0.47              |
| 1:J:289:THR:HB   | 1:J:337:VAL:HG22 | 1.96                     | 0.47              |
| 1:K:351:LEU:O    | 1:K:351:LEU:HD13 | 2.14                     | 0.47              |
| 1:K:405:MET:HE2  | 1:K:405:MET:HA   | 1.96                     | 0.47              |
| 1:L:355:LEU:C    | 1:L:357:GLY:N    | 2.67                     | 0.47              |
| 1:L:396:LEU:HD22 | 1:L:418:ILE:HD13 | 1.97                     | 0.47              |
| 1:B:380:ARG:NH1  | 1:B:387:ASP:OD1  | 2.47                     | 0.47              |
| 1:C:321:ARG:O    | 1:C:333:GLU:HB3  | 2.14                     | 0.47              |
| 1:C:402:ASN:HD21 | 1:C:404:VAL:HG12 | 1.78                     | 0.47              |
| 1:D:4:TYR:CE2    | 1:D:12:LEU:HD11  | 2.50                     | 0.47              |
| 1:D:167:ASN:HD22 | 1:D:170:ARG:CB   | 2.28                     | 0.47              |
| 1:D:375:MET:HG2  | 1:D:376:SER:N    | 2.29                     | 0.47              |
| 1:E:170:ARG:HG2  | 1:E:170:ARG:NH1  | 2.29                     | 0.47              |
| 1:E:247:ASN:HD22 | 1:E:331:ARG:NE   | 2.12                     | 0.47              |
| 1:F:326:ARG:HD2  | 1:F:330:THR:HG23 | 1.96                     | 0.47              |
| 1:G:3:LYS:HB3    | 1:G:75:ASN:ND2   | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:125:SER:OG   | 1:H:253:ASN:N    | 2.48                     | 0.47              |
| 1:H:175:GLU:O    | 1:H:179:MET:HG3  | 2.15                     | 0.47              |
| 1:H:183:ILE:HG23 | 1:H:198:ASP:O    | 2.14                     | 0.47              |
| 1:H:5:THR:H      | 1:H:8:ASP:CB     | 2.17                     | 0.47              |
| 1:I:370:ARG:N    | 1:I:370:ARG:HD3  | 2.29                     | 0.47              |
| 1:J:151:ASN:HD22 | 1:J:166:GLU:CD   | 2.17                     | 0.47              |
| 1:J:176:LEU:HD12 | 1:J:183:ILE:HD11 | 1.95                     | 0.47              |
| 1:J:17:ASN:ND2   | 1:J:87:GLY:HA2   | 2.30                     | 0.47              |
| 1:L:309:VAL:HG21 | 1:L:386:VAL:HB   | 1.96                     | 0.47              |
| 1:A:150:LEU:HD12 | 1:A:192:PRO:HB2  | 1.96                     | 0.47              |
| 1:A:306:PRO:HB3  | 1:A:319:LEU:CA   | 2.37                     | 0.47              |
| 1:B:277:GLY:HA3  | 1:B:353:ALA:O    | 2.14                     | 0.47              |
| 1:B:159:LEU:HD13 | 1:C:34:ASN:CG    | 2.34                     | 0.47              |
| 1:D:159:LEU:HD13 | 1:E:22:ARG:HH11  | 1.80                     | 0.47              |
| 1:E:421:LYS:HD3  | 1:E:424:GLU:OE1  | 2.15                     | 0.47              |
| 1:F:221:ILE:O    | 1:F:225:HIS:HD2  | 1.98                     | 0.47              |
| 1:J:24:GLN:HE21  | 1:J:32:ILE:HD11  | 1.80                     | 0.47              |
| 1:A:160:ALA:HB2  | 1:A:188:HIS:CD2  | 2.50                     | 0.47              |
| 1:B:119:MET:SD   | 1:B:127:PHE:HB2  | 2.54                     | 0.47              |
| 1:B:142:GLU:HG3  | 1:B:143:LYS:H    | 1.80                     | 0.47              |
| 1:B:167:ASN:HD22 | 1:B:170:ARG:CZ   | 2.28                     | 0.47              |
| 1:B:283:THR:HB   | 1:B:398:GLU:OE1  | 2.15                     | 0.47              |
| 1:C:159:LEU:HD12 | 1:D:34:ASN:CG    | 2.35                     | 0.47              |
| 1:E:208:CYS:SG   | 1:E:347:LEU:HD12 | 2.55                     | 0.47              |
| 1:E:32:ILE:HD13  | 1:E:216:LEU:HB2  | 1.96                     | 0.47              |
| 1:E:322:ILE:CD1  | 1:E:322:ILE:N    | 2.77                     | 0.47              |
| 1:E:440:TYR:HB2  | 1:K:232:MET:HE3  | 1.97                     | 0.47              |
| 1:F:109:ARG:NH2  | 1:F:109:ARG:HG2  | 2.29                     | 0.47              |
| 1:G:17:ASN:ND2   | 1:G:87:GLY:HA2   | 2.30                     | 0.47              |
| 1:G:291:PRO:HG3  | 1:G:341:ALA:HA   | 1.96                     | 0.47              |
| 1:G:57:ILE:O     | 1:G:59:GLY:N     | 2.47                     | 0.47              |
| 1:I:216:LEU:HD21 | 1:J:162:THR:OG1  | 2.15                     | 0.47              |
| 1:J:285:PHE:HB2  | 1:J:349:VAL:CG1  | 2.45                     | 0.47              |
| 1:L:383:ASN:HB2  | 1:L:385:ILE:HD11 | 1.96                     | 0.47              |
| 1:G:156:TYR:CE2  | 1:L:62:ARG:NH1   | 2.83                     | 0.47              |
| 1:A:160:ALA:CB   | 1:A:188:HIS:CD2  | 2.98                     | 0.47              |
| 1:B:258:PHE:HZ   | 1:B:274:PHE:CG   | 2.33                     | 0.47              |
| 1:C:174:LEU:O    | 1:C:178:GLU:HG2  | 2.14                     | 0.47              |
| 1:C:27:ASP:OD1   | 1:C:33:LYS:HE3   | 2.15                     | 0.47              |
| 1:C:369:ASP:CG   | 1:C:370:ARG:H    | 2.18                     | 0.47              |
| 1:C:9:ILE:O      | 1:C:12:LEU:N     | 2.47                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:153:LYS:NZ   | 1:D:145:GLU:OE1  | 2.45                     | 0.47              |
| 1:D:21:ILE:CD1   | 1:D:39:VAL:HA    | 2.45                     | 0.47              |
| 1:D:23:LEU:HB3   | 1:D:94:CYS:SG    | 2.55                     | 0.47              |
| 1:E:131:PRO:HG2  | 1:E:199:PHE:CD1  | 2.49                     | 0.47              |
| 1:E:48:ASN:O     | 1:E:69:TYR:HD2   | 1.97                     | 0.47              |
| 1:H:325:SER:HB2  | 1:H:331:ARG:HH22 | 1.80                     | 0.47              |
| 1:H:58:GLU:HG2   | 1:H:416:HIS:CD2  | 2.50                     | 0.47              |
| 1:J:325:SER:HB3  | 1:J:329:SER:CB   | 2.45                     | 0.47              |
| 1:K:319:LEU:HG   | 1:K:320:ILE:CD1  | 2.45                     | 0.47              |
| 1:L:226:GLY:O    | 1:L:227:LEU:HD23 | 2.15                     | 0.47              |
| 1:B:41:GLN:NE2   | 1:B:44:LYS:HD2   | 2.29                     | 0.46              |
| 1:B:49:LYS:HE2   | 1:B:49:LYS:HA    | 1.98                     | 0.46              |
| 1:C:23:LEU:HB3   | 1:C:94:CYS:SG    | 2.55                     | 0.46              |
| 1:C:429:ARG:HH11 | 1:C:429:ARG:HG3  | 1.80                     | 0.46              |
| 1:C:45:ALA:O     | 1:C:72:PRO:HG3   | 2.15                     | 0.46              |
| 1:E:200:LYS:HG2  | 1:E:201:TYR:H    | 1.80                     | 0.46              |
| 1:E:236:LEU:HB2  | 1:E:239:VAL:HG21 | 1.97                     | 0.46              |
| 1:F:203:GLY:O    | 1:F:204:ALA:C    | 2.52                     | 0.46              |
| 1:F:4:TYR:HB3    | 1:F:9:ILE:CD1    | 2.45                     | 0.46              |
| 1:G:143:LYS:HD3  | 1:G:143:LYS:N    | 2.29                     | 0.46              |
| 1:H:281:HIS:CE1  | 1:H:404:VAL:HG11 | 2.51                     | 0.46              |
| 1:H:37:ILE:HG22  | 1:I:185:ALA:CB   | 2.45                     | 0.46              |
| 1:H:409:LEU:O    | 1:H:413:LEU:HB2  | 2.15                     | 0.46              |
| 1:J:127:PHE:CE2  | 1:J:351:LEU:HG   | 2.50                     | 0.46              |
| 1:J:322:ILE:CD1  | 1:J:332:VAL:HG13 | 2.45                     | 0.46              |
| 1:K:215:LYS:HG2  | 1:K:231:PHE:CE2  | 2.50                     | 0.46              |
| 1:K:351:LEU:O    | 1:K:351:LEU:HD22 | 2.14                     | 0.46              |
| 1:L:311:TRP:HA   | 1:L:320:ILE:HB   | 1.97                     | 0.46              |
| 1:A:368:ILE:HD12 | 1:A:385:ILE:HD11 | 1.96                     | 0.46              |
| 1:A:310:ALA:CB   | 1:A:372:ILE:HD13 | 2.40                     | 0.46              |
| 1:A:57:ILE:HD13  | 1:A:96:ILE:HG13  | 1.96                     | 0.46              |
| 1:B:146:PRO:HG3  | 1:B:228:HIS:CD2  | 2.50                     | 0.46              |
| 1:C:270:THR:O    | 1:C:274:PHE:HB2  | 2.15                     | 0.46              |
| 1:C:371:ASN:OD1  | 1:C:374:VAL:HG22 | 2.15                     | 0.46              |
| 1:D:4:TYR:HB3    | 1:D:9:ILE:HD11   | 1.97                     | 0.46              |
| 1:E:315:ASN:OD1  | 1:E:372:ILE:HG12 | 2.16                     | 0.46              |
| 1:F:170:ARG:NH1  | 1:F:171:ASP:OD2  | 2.48                     | 0.46              |
| 1:F:368:ILE:HG21 | 1:F:372:ILE:HD11 | 1.94                     | 0.46              |
| 1:G:48:ASN:OD1   | 1:G:72:PRO:HD2   | 2.14                     | 0.46              |
| 1:H:236:LEU:O    | 1:H:239:VAL:HG22 | 2.15                     | 0.46              |
| 1:H:4:TYR:CB     | 1:H:9:ILE:HG13   | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:96:ILE:HD13  | 1:H:107:ASP:CG   | 2.36                     | 0.46              |
| 1:I:160:ALA:CB   | 1:I:169:ARG:HH12 | 2.26                     | 0.46              |
| 1:I:207:SER:O    | 1:I:211:ILE:HG12 | 2.16                     | 0.46              |
| 1:J:100:ASP:OD1  | 1:J:101:GLY:N    | 2.48                     | 0.46              |
| 1:J:163:ASP:HA   | 1:J:170:ARG:NH1  | 2.31                     | 0.46              |
| 1:J:310:ALA:CA   | 1:J:368:ILE:HG13 | 2.43                     | 0.46              |
| 1:K:296:TYR:CD1  | 1:K:296:TYR:N    | 2.84                     | 0.46              |
| 1:K:54:GLY:O     | 1:K:56:SER:N     | 2.48                     | 0.46              |
| 1:K:49:LYS:HD3   | 1:K:69:TYR:HE2   | 1.78                     | 0.46              |
| 1:K:48:ASN:HB3   | 1:K:71:TYR:CE1   | 2.50                     | 0.46              |
| 1:L:183:ILE:H    | 1:L:183:ILE:HD12 | 1.81                     | 0.46              |
| 1:A:166:GLU:CD   | 1:A:167:ASN:H    | 2.19                     | 0.46              |
| 1:A:271:ALA:O    | 1:A:275:ILE:HG13 | 2.15                     | 0.46              |
| 1:B:402:ASN:OD1  | 1:B:405:MET:HG2  | 2.15                     | 0.46              |
| 1:C:114:ARG:NH2  | 1:C:115:ILE:HD11 | 2.30                     | 0.46              |
| 1:C:114:ARG:HH21 | 1:C:115:ILE:CD1  | 2.28                     | 0.46              |
| 1:B:162:THR:HG21 | 1:C:220:THR:OG1  | 2.15                     | 0.46              |
| 1:C:85:GLU:OE2   | 1:C:86:LYS:N     | 2.48                     | 0.46              |
| 1:D:176:LEU:HD11 | 1:D:214:PHE:HD1  | 1.78                     | 0.46              |
| 1:E:139:LYS:HB2  | 1:E:149:GLU:HB3  | 1.97                     | 0.46              |
| 1:A:36:GLU:CD    | 1:F:169:ARG:HH12 | 2.18                     | 0.46              |
| 1:F:319:LEU:C    | 1:F:320:ILE:HD12 | 2.34                     | 0.46              |
| 1:F:310:ALA:HB1  | 1:F:368:ILE:HG12 | 1.98                     | 0.46              |
| 1:G:46:LEU:HD22  | 1:G:74:LEU:HD11  | 1.97                     | 0.46              |
| 1:H:160:ALA:CB   | 1:H:169:ARG:HH12 | 2.28                     | 0.46              |
| 1:H:172:ILE:HD13 | 1:H:221:ILE:HB   | 1.97                     | 0.46              |
| 1:H:318:PRO:HB2  | 1:H:320:ILE:O    | 2.15                     | 0.46              |
| 1:I:392:LEU:HD21 | 1:I:421:LYS:HB3  | 1.97                     | 0.46              |
| 1:J:17:ASN:HD21  | 1:J:87:GLY:HA2   | 1.81                     | 0.46              |
| 1:J:140:LEU:HD12 | 1:J:226:GLY:C    | 2.36                     | 0.46              |
| 1:J:328:ILE:C    | 1:J:328:ILE:HD12 | 2.35                     | 0.46              |
| 1:K:360:ASN:HB2  | 1:K:362:LEU:CD1  | 2.45                     | 0.46              |
| 1:C:444:TYR:OH   | 1:I:29:LEU:HD22  | 2.16                     | 0.46              |
| 1:D:168:CYS:SG   | 1:D:227:LEU:HD12 | 2.55                     | 0.46              |
| 1:D:5:THR:O      | 1:D:8:ASP:N      | 2.48                     | 0.46              |
| 1:E:115:ILE:O    | 1:E:118:GLU:HB3  | 2.15                     | 0.46              |
| 1:D:164:LEU:HD23 | 1:E:220:THR:CG2  | 2.46                     | 0.46              |
| 1:F:131:PRO:HG2  | 1:F:199:PHE:CD1  | 2.50                     | 0.46              |
| 1:F:188:HIS:HE1  | 1:F:191:ALA:O    | 1.97                     | 0.46              |
| 1:F:420:ALA:O    | 1:F:423:ILE:HG13 | 2.15                     | 0.46              |
| 1:H:116:LEU:O    | 1:H:119:MET:HB3  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:208:CYS:N    | 1:J:211:ILE:HD12 | 2.30                     | 0.46              |
| 1:J:282:ALA:C    | 1:J:284:SER:H    | 2.18                     | 0.46              |
| 1:D:294:ASN:HB2  | 1:J:436:GLU:HB3  | 1.97                     | 0.46              |
| 1:J:72:PRO:N     | 1:J:94:CYS:HB3   | 2.31                     | 0.46              |
| 1:J:82:TRP:HE1   | 1:K:163:ASP:HB2  | 1.81                     | 0.46              |
| 1:K:311:TRP:O    | 1:K:312:SER:HB3  | 2.14                     | 0.46              |
| 1:K:115:ILE:CG2  | 1:K:351:LEU:HD12 | 2.39                     | 0.46              |
| 1:K:83:THR:OG1   | 1:K:88:LYS:HD3   | 2.15                     | 0.46              |
| 1:L:124:PHE:HZ   | 1:L:358:ILE:HG21 | 1.80                     | 0.46              |
| 1:L:386:VAL:CG1  | 1:L:387:ASP:H    | 2.12                     | 0.46              |
| 1:B:239:VAL:HG23 | 1:B:239:VAL:O    | 2.14                     | 0.46              |
| 1:C:116:LEU:HD11 | 1:C:204:ALA:HB3  | 1.97                     | 0.46              |
| 1:D:310:ALA:CB   | 1:D:368:ILE:HG21 | 2.42                     | 0.46              |
| 1:E:119:MET:HG2  | 1:E:124:PHE:HB2  | 1.98                     | 0.46              |
| 1:F:370:ARG:HH21 | 1:F:372:ILE:CD1  | 2.29                     | 0.46              |
| 1:H:116:LEU:HD22 | 1:H:119:MET:HE2  | 1.96                     | 0.46              |
| 1:H:272:LYS:NZ   | 1:H:276:ALA:HB2  | 2.31                     | 0.46              |
| 1:H:278:ILE:O    | 1:H:282:ALA:HB2  | 2.15                     | 0.46              |
| 1:H:315:ASN:ND2  | 1:H:371:ASN:HA   | 2.31                     | 0.46              |
| 1:H:63:ILE:HG22  | 1:H:64:GLU:HG3   | 1.97                     | 0.46              |
| 1:I:201:TYR:C    | 1:I:201:TYR:CD1  | 2.88                     | 0.46              |
| 1:I:285:PHE:HB2  | 1:I:349:VAL:HG13 | 1.96                     | 0.46              |
| 1:I:371:ASN:HB2  | 1:I:374:VAL:HG22 | 1.97                     | 0.46              |
| 1:J:82:TRP:HE1   | 1:K:163:ASP:CB   | 2.29                     | 0.46              |
| 1:F:430:THR:HG22 | 1:L:300:VAL:HG21 | 1.97                     | 0.46              |
| 1:L:91:ARG:HD2   | 1:L:92:PHE:N     | 2.29                     | 0.46              |
| 1:A:259:PHE:HE2  | 1:A:261:GLU:OE2  | 1.99                     | 0.46              |
| 1:A:108:PRO:O    | 1:A:344:TYR:HB3  | 2.16                     | 0.46              |
| 1:A:80:PHE:HA    | 1:A:81:PRO:HD3   | 1.78                     | 0.46              |
| 1:C:267:LEU:CD2  | 1:C:326:ARG:NH1  | 2.78                     | 0.46              |
| 1:D:443:GLN:HA   | 1:D:443:GLN:HE21 | 1.81                     | 0.46              |
| 1:E:234:LYS:HB3  | 1:E:294:ASN:ND2  | 2.30                     | 0.46              |
| 1:H:182:GLU:HB3  | 1:H:200:LYS:CD   | 2.31                     | 0.46              |
| 1:I:160:ALA:HB3  | 1:I:169:ARG:HH12 | 1.79                     | 0.46              |
| 1:I:27:ASP:C     | 1:I:27:ASP:OD2   | 2.53                     | 0.46              |
| 1:J:91:ARG:CD    | 1:J:91:ARG:C     | 2.82                     | 0.46              |
| 1:K:312:SER:HB2  | 1:K:369:ASP:OD1  | 2.16                     | 0.46              |
| 1:B:287:ALA:HB2  | 1:B:395:ALA:HB1  | 1.98                     | 0.46              |
| 1:C:111:ASN:OD1  | 1:C:409:LEU:HA   | 2.15                     | 0.46              |
| 1:C:274:PHE:HE2  | 1:C:332:VAL:HG11 | 1.80                     | 0.46              |
| 1:C:431:GLN:O    | 1:I:297:LYS:HD2  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:342:ASN:HB3  | 1:D:345:LEU:HB2  | 1.96                     | 0.46              |
| 1:E:376:SER:O    | 1:E:380:ARG:HG3  | 2.16                     | 0.46              |
| 1:F:129:LEU:CD2  | 1:F:130:GLY:N    | 2.78                     | 0.46              |
| 1:F:345:LEU:CD2  | 1:F:409:LEU:HD22 | 2.45                     | 0.46              |
| 1:H:370:ARG:HH22 | 1:H:375:MET:CE   | 2.28                     | 0.46              |
| 1:I:267:LEU:HG   | 1:I:326:ARG:NH1  | 2.31                     | 0.46              |
| 1:J:273:HIS:CE1  | 1:J:361:LYS:CA   | 2.99                     | 0.46              |
| 1:L:232:MET:SD   | 1:L:235:PRO:HA   | 2.56                     | 0.46              |
| 1:B:138:PHE:CE2  | 1:B:150:LEU:CD2  | 2.99                     | 0.46              |
| 1:C:21:ILE:HD13  | 1:C:39:VAL:HA    | 1.97                     | 0.46              |
| 1:C:380:ARG:HA   | 1:C:385:ILE:HD12 | 1.97                     | 0.46              |
| 1:C:433:HIS:N    | 1:C:436:GLU:OE1  | 2.48                     | 0.46              |
| 1:D:288:VAL:O    | 1:D:291:PRO:HD3  | 2.15                     | 0.46              |
| 1:E:189:GLU:HB3  | 1:E:194:GLN:OE1  | 2.15                     | 0.46              |
| 1:E:211:ILE:HG22 | 1:E:215:LYS:HE2  | 1.98                     | 0.46              |
| 1:A:300:VAL:CG2  | 1:G:429:ARG:HH12 | 2.28                     | 0.46              |
| 1:H:282:ALA:HB1  | 1:H:319:LEU:HD21 | 1.97                     | 0.46              |
| 1:H:332:VAL:HG13 | 1:H:332:VAL:O    | 2.16                     | 0.46              |
| 1:I:27:ASP:OD2   | 1:I:29:LEU:N     | 2.48                     | 0.46              |
| 1:I:124:PHE:CE1  | 1:I:358:ILE:HD13 | 2.51                     | 0.46              |
| 1:I:357:GLY:HA2  | 1:I:362:LEU:HD13 | 1.98                     | 0.46              |
| 1:I:418:ILE:HG22 | 1:I:422:GLU:CG   | 2.45                     | 0.46              |
| 1:J:33:LYS:HB3   | 1:K:157:PHE:O    | 2.16                     | 0.46              |
| 1:K:98:ASN:O     | 1:K:100:ASP:N    | 2.49                     | 0.46              |
| 1:A:372:ILE:O    | 1:A:380:ARG:NH2  | 2.48                     | 0.46              |
| 1:A:58:GLU:O     | 1:A:61:VAL:HG22  | 2.16                     | 0.46              |
| 1:B:159:LEU:HB2  | 1:C:32:ILE:O     | 2.15                     | 0.46              |
| 1:C:127:PHE:HE2  | 1:C:347:LEU:HD22 | 1.80                     | 0.46              |
| 1:C:160:ALA:O    | 1:C:161:PRO:C    | 2.54                     | 0.46              |
| 1:B:159:LEU:HD12 | 1:C:22:ARG:NH1   | 2.27                     | 0.46              |
| 1:C:62:ARG:HH21  | 1:C:65:GLU:HB3   | 1.81                     | 0.46              |
| 1:D:232:MET:HE2  | 1:D:234:LYS:O    | 2.16                     | 0.46              |
| 1:F:309:VAL:HB   | 1:F:386:VAL:CG2  | 2.41                     | 0.46              |
| 1:F:231:PHE:HB3  | 1:F:339:PRO:HB2  | 1.97                     | 0.46              |
| 1:F:355:LEU:HD23 | 1:F:355:LEU:HA   | 1.67                     | 0.46              |
| 1:G:315:ASN:HB3  | 1:G:318:PRO:CG   | 2.46                     | 0.46              |
| 1:G:402:ASN:CG   | 1:G:405:MET:HG2  | 2.36                     | 0.46              |
| 1:I:25:PHE:CE1   | 1:I:33:LYS:HB2   | 2.50                     | 0.46              |
| 1:I:282:ALA:O    | 1:I:284:SER:N    | 2.49                     | 0.46              |
| 1:J:206:ARG:HG3  | 1:J:206:ARG:NH1  | 2.31                     | 0.46              |
| 1:J:23:LEU:HB3   | 1:J:70:LEU:HD23  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:33:LYS:O     | 1:L:34:ASN:HB3   | 2.16                     | 0.46              |
| 1:L:73:ASP:O     | 1:L:75:ASN:N     | 2.49                     | 0.46              |
| 1:A:252:LYS:CE   | 1:A:253:ASN:ND2  | 2.78                     | 0.46              |
| 1:A:306:PRO:O    | 1:A:388:LEU:HD12 | 2.16                     | 0.46              |
| 1:A:309:VAL:HG23 | 1:A:386:VAL:O    | 2.16                     | 0.46              |
| 1:B:300:VAL:HG11 | 1:H:430:THR:HG22 | 1.98                     | 0.46              |
| 1:C:142:GLU:H    | 1:C:142:GLU:CD   | 2.20                     | 0.46              |
| 1:C:296:TYR:CE1  | 1:C:392:LEU:HA   | 2.51                     | 0.46              |
| 1:C:399:PHE:HZ   | 1:C:409:LEU:HD11 | 1.81                     | 0.46              |
| 1:E:201:TYR:HD2  | 1:E:201:TYR:H    | 1.63                     | 0.46              |
| 1:E:436:GLU:HG2  | 1:K:294:ASN:HB2  | 1.98                     | 0.46              |
| 1:G:406:VAL:HG22 | 1:G:414:PHE:CZ   | 2.50                     | 0.46              |
| 1:I:127:PHE:CZ   | 1:I:248:LEU:HD23 | 2.50                     | 0.46              |
| 1:I:272:LYS:HA   | 1:I:275:ILE:HD12 | 1.97                     | 0.46              |
| 1:J:167:ASN:HA   | 1:J:167:ASN:HD22 | 1.51                     | 0.46              |
| 1:J:320:ILE:HG22 | 1:J:321:ARG:H    | 1.81                     | 0.46              |
| 1:J:368:ILE:CD1  | 1:J:385:ILE:HG23 | 2.46                     | 0.46              |
| 1:K:151:ASN:HB2  | 1:K:166:GLU:OE2  | 2.16                     | 0.46              |
| 1:L:287:ALA:HB2  | 1:L:395:ALA:C    | 2.36                     | 0.46              |
| 1:A:259:PHE:CE2  | 1:A:261:GLU:OE2  | 2.69                     | 0.45              |
| 1:A:306:PRO:CB   | 1:A:319:LEU:HA   | 2.37                     | 0.45              |
| 1:B:261:GLU:HA   | 1:B:266:GLN:NE2  | 2.31                     | 0.45              |
| 1:C:429:ARG:O    | 1:I:297:LYS:HD3  | 2.16                     | 0.45              |
| 1:D:9:ILE:O      | 1:D:13:VAL:HG23  | 2.16                     | 0.45              |
| 1:E:100:ASP:OD2  | 1:E:102:THR:HG23 | 2.16                     | 0.45              |
| 1:F:140:LEU:HD12 | 1:F:226:GLY:C    | 2.37                     | 0.45              |
| 1:G:13:VAL:HG21  | 1:G:42:LEU:HD21  | 1.97                     | 0.45              |
| 1:G:166:GLU:HG2  | 1:G:168:CYS:H    | 1.81                     | 0.45              |
| 1:G:423:ILE:O    | 1:G:424:GLU:C    | 2.54                     | 0.45              |
| 1:G:86:LYS:HG3   | 1:H:174:LEU:CB   | 2.43                     | 0.45              |
| 1:H:166:GLU:O    | 1:H:166:GLU:CD   | 2.54                     | 0.45              |
| 1:H:242:SER:O    | 1:H:339:PRO:CD   | 2.61                     | 0.45              |
| 1:J:19:LYS:HG3   | 1:J:87:GLY:HA3   | 1.97                     | 0.45              |
| 1:J:140:LEU:HD11 | 1:J:227:LEU:O    | 2.16                     | 0.45              |
| 1:D:436:GLU:OE2  | 1:J:297:LYS:HG3  | 2.15                     | 0.45              |
| 1:J:371:ASN:HD21 | 1:J:373:TYR:HB2  | 1.79                     | 0.45              |
| 1:K:309:VAL:HG13 | 1:K:319:LEU:CD2  | 2.43                     | 0.45              |
| 1:K:51:MET:HA    | 1:K:68:MET:O     | 2.16                     | 0.45              |
| 1:K:35:VAL:CG1   | 1:K:70:LEU:HD11  | 2.46                     | 0.45              |
| 1:L:114:ARG:NH2  | 1:L:115:ILE:CD1  | 2.78                     | 0.45              |
| 1:L:275:ILE:O    | 1:L:279:VAL:HG23 | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:116:LEU:HA   | 1:A:116:LEU:HD23 | 1.75                     | 0.45              |
| 1:A:356:ASP:O    | 1:A:360:ASN:HB2  | 2.16                     | 0.45              |
| 1:B:381:MET:C    | 1:B:382:GLU:HG3  | 2.37                     | 0.45              |
| 1:C:159:LEU:O    | 1:C:160:ALA:O    | 2.33                     | 0.45              |
| 1:D:138:PHE:HA   | 1:D:149:GLU:O    | 2.16                     | 0.45              |
| 1:D:26:THR:OG1   | 1:D:212:GLN:NE2  | 2.47                     | 0.45              |
| 1:D:308:TYR:HA   | 1:D:387:ASP:HA   | 1.98                     | 0.45              |
| 1:A:33:LYS:HE2   | 1:F:158:ASP:OD2  | 2.16                     | 0.45              |
| 1:I:80:PHE:HB2   | 1:I:89:VAL:O     | 2.15                     | 0.45              |
| 1:J:112:LEU:HD11 | 1:J:208:CYS:SG   | 2.56                     | 0.45              |
| 1:A:326:ARG:HD3  | 1:A:326:ARG:HA   | 1.82                     | 0.45              |
| 1:A:9:ILE:HG21   | 1:A:92:PHE:HZ    | 1.81                     | 0.45              |
| 1:D:4:TYR:HB3    | 1:D:9:ILE:CD1    | 2.47                     | 0.45              |
| 1:E:252:LYS:O    | 1:E:255:VAL:HG22 | 2.16                     | 0.45              |
| 1:D:184:GLU:HG3  | 1:E:44:LYS:NZ    | 2.31                     | 0.45              |
| 1:F:345:LEU:HD22 | 1:F:409:LEU:HD22 | 1.98                     | 0.45              |
| 1:G:147:THR:C    | 1:G:149:GLU:H    | 2.20                     | 0.45              |
| 1:H:273:HIS:NE2  | 1:H:361:LYS:HA   | 2.32                     | 0.45              |
| 1:H:20:TYR:OH    | 1:H:36:GLU:HB3   | 2.16                     | 0.45              |
| 1:I:236:LEU:HB2  | 1:I:239:VAL:CG2  | 2.46                     | 0.45              |
| 1:I:282:ALA:C    | 1:I:284:SER:N    | 2.70                     | 0.45              |
| 1:J:37:ILE:HG13  | 1:J:41:GLN:HB2   | 1.97                     | 0.45              |
| 1:K:234:LYS:HB3  | 1:K:294:ASN:ND2  | 2.32                     | 0.45              |
| 1:L:130:GLY:O    | 1:L:247:ASN:ND2  | 2.49                     | 0.45              |
| 1:A:211:ILE:O    | 1:A:214:PHE:HB3  | 2.16                     | 0.45              |
| 1:A:376:SER:HB3  | 1:A:378:GLU:OE1  | 2.17                     | 0.45              |
| 1:B:110:ASN:O    | 1:B:113:LYS:HB2  | 2.17                     | 0.45              |
| 1:C:127:PHE:CZ   | 1:C:248:LEU:HD22 | 2.51                     | 0.45              |
| 1:C:18:VAL:HG21  | 1:C:79:ILE:HD12  | 1.98                     | 0.45              |
| 1:C:347:LEU:HD23 | 1:C:347:LEU:HA   | 1.80                     | 0.45              |
| 1:C:402:ASN:CG   | 1:C:404:VAL:HG12 | 2.36                     | 0.45              |
| 1:D:184:GLU:OE1  | 1:D:200:LYS:HG2  | 2.16                     | 0.45              |
| 1:E:134:GLU:HG2  | 1:E:196:GLU:HG3  | 1.99                     | 0.45              |
| 1:F:175:GLU:HG3  | 1:F:221:ILE:CD1  | 2.46                     | 0.45              |
| 1:E:169:ARG:NH2  | 1:F:36:GLU:OE2   | 2.45                     | 0.45              |
| 1:F:56:SER:HA    | 1:F:62:ARG:HD2   | 1.98                     | 0.45              |
| 1:G:172:ILE:O    | 1:G:176:LEU:HG   | 2.16                     | 0.45              |
| 1:H:79:ILE:O     | 1:H:80:PHE:C     | 2.55                     | 0.45              |
| 1:J:308:TYR:CD1  | 1:J:372:ILE:HG21 | 2.51                     | 0.45              |
| 1:K:290:ASN:HB3  | 1:K:295:SER:HB3  | 1.99                     | 0.45              |
| 1:K:309:VAL:HG22 | 1:K:319:LEU:HD22 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:85:GLU:HG2   | 1:L:170:ARG:NH1  | 2.27                     | 0.45              |
| 1:L:132:GLU:HB3  | 1:L:196:GLU:OE1  | 2.16                     | 0.45              |
| 1:L:345:LEU:HD22 | 1:L:409:LEU:CD1  | 2.47                     | 0.45              |
| 1:A:20:TYR:OH    | 1:A:36:GLU:HG3   | 2.17                     | 0.45              |
| 1:B:176:LEU:HD11 | 1:B:214:PHE:CE1  | 2.51                     | 0.45              |
| 1:D:166:GLU:HA   | 1:D:225:HIS:CD2  | 2.52                     | 0.45              |
| 1:E:247:ASN:ND2  | 1:E:331:ARG:HE   | 2.14                     | 0.45              |
| 1:F:119:MET:HA   | 1:F:355:LEU:CD1  | 2.46                     | 0.45              |
| 1:F:84:ALA:HB3   | 1:F:87:GLY:O     | 2.16                     | 0.45              |
| 1:G:237:PHE:O    | 1:G:239:VAL:N    | 2.49                     | 0.45              |
| 1:G:440:TYR:O    | 1:G:441:MET:C    | 2.55                     | 0.45              |
| 1:G:45:ALA:HA    | 1:G:50:VAL:CG2   | 2.46                     | 0.45              |
| 1:I:68:MET:HE2   | 1:I:104:PHE:HB2  | 1.98                     | 0.45              |
| 1:I:106:GLY:HA2  | 1:I:413:LEU:HG   | 1.98                     | 0.45              |
| 1:J:322:ILE:HD11 | 1:J:332:VAL:HG13 | 1.98                     | 0.45              |
| 1:E:429:ARG:NH1  | 1:K:300:VAL:HG12 | 2.32                     | 0.45              |
| 1:K:244:MET:H    | 1:K:338:ASP:HA   | 1.80                     | 0.45              |
| 1:A:169:ARG:NH2  | 1:A:195:HIS:ND1  | 2.64                     | 0.45              |
| 1:A:280:LYS:HD2  | 1:A:362:LEU:HD21 | 1.98                     | 0.45              |
| 1:C:255:VAL:HG12 | 1:C:256:ASN:H    | 1.81                     | 0.45              |
| 1:C:315:ASN:HD21 | 1:C:369:ASP:CB   | 2.29                     | 0.45              |
| 1:C:321:ARG:HD3  | 1:C:333:GLU:OE1  | 2.17                     | 0.45              |
| 1:G:204:ALA:HB1  | 1:G:347:LEU:CD2  | 2.47                     | 0.45              |
| 1:G:95:ASP:OD1   | 1:G:109:ARG:NH2  | 2.49                     | 0.45              |
| 1:I:368:ILE:HG22 | 1:I:368:ILE:O    | 2.17                     | 0.45              |
| 1:K:127:PHE:HZ   | 1:K:248:LEU:HD22 | 1.73                     | 0.45              |
| 1:K:258:PHE:CA   | 1:K:271:ALA:HB2  | 2.47                     | 0.45              |
| 1:A:276:ALA:HB2  | 1:A:364:ALA:HB2  | 1.97                     | 0.45              |
| 1:A:320:ILE:N    | 1:A:320:ILE:HD12 | 2.32                     | 0.45              |
| 1:A:380:ARG:HD3  | 1:A:387:ASP:OD1  | 2.17                     | 0.45              |
| 1:B:30:GLY:N     | 1:B:342:ASN:HD22 | 2.15                     | 0.45              |
| 1:B:364:ALA:HB1  | 1:B:365:PRO:HD2  | 1.99                     | 0.45              |
| 1:E:260:ASP:O    | 1:E:266:GLN:HA   | 2.17                     | 0.45              |
| 1:E:406:VAL:HG22 | 1:E:414:PHE:CZ   | 2.51                     | 0.45              |
| 1:E:96:ILE:H     | 1:E:96:ILE:CD1   | 2.22                     | 0.45              |
| 1:F:230:THR:HG23 | 1:F:230:THR:O    | 2.17                     | 0.45              |
| 1:E:170:ARG:NH1  | 1:F:84:ALA:HB1   | 2.31                     | 0.45              |
| 1:H:78:VAL:HG12  | 1:H:79:ILE:N     | 2.32                     | 0.45              |
| 1:I:426:ASP:HA   | 1:I:429:ARG:HG2  | 1.98                     | 0.45              |
| 1:J:163:ASP:O    | 1:J:164:LEU:HB2  | 2.17                     | 0.45              |
| 1:K:396:LEU:HD22 | 1:K:418:ILE:HD13 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:35:VAL:HG13  | 1:C:35:VAL:O     | 2.17                     | 0.45              |
| 1:C:383:ASN:N    | 1:C:383:ASN:HD22 | 2.14                     | 0.45              |
| 1:C:383:ASN:ND2  | 1:C:383:ASN:N    | 2.64                     | 0.45              |
| 1:D:145:GLU:OE2  | 1:D:146:PRO:HD2  | 2.17                     | 0.45              |
| 1:D:259:PHE:HZ   | 1:D:261:GLU:HG3  | 1.82                     | 0.45              |
| 1:D:96:ILE:HD13  | 1:D:96:ILE:N     | 2.32                     | 0.45              |
| 1:F:298:ARG:HD2  | 1:F:298:ARG:O    | 2.17                     | 0.45              |
| 1:F:399:PHE:HE1  | 1:F:405:MET:HB3  | 1.80                     | 0.45              |
| 1:H:368:ILE:HG21 | 1:H:372:ILE:HD12 | 1.98                     | 0.45              |
| 1:H:404:VAL:HG13 | 1:H:405:MET:CE   | 2.47                     | 0.45              |
| 1:B:297:LYS:HD3  | 1:H:429:ARG:O    | 2.17                     | 0.45              |
| 1:H:86:LYS:HB2   | 1:I:174:LEU:HD23 | 1.99                     | 0.45              |
| 1:K:282:ALA:HA   | 1:K:285:PHE:CE1  | 2.51                     | 0.45              |
| 1:K:419:GLU:O    | 1:K:423:ILE:HG12 | 2.16                     | 0.45              |
| 1:L:83:THR:C     | 1:L:85:GLU:OE2   | 2.55                     | 0.45              |
| 1:A:129:LEU:HD13 | 1:A:131:PRO:HG3  | 1.99                     | 0.45              |
| 1:B:213:THR:O    | 1:B:217:VAL:HG23 | 2.17                     | 0.45              |
| 1:B:260:ASP:HB2  | 1:B:268:SER:CA   | 2.47                     | 0.45              |
| 1:C:316:ARG:HG2  | 1:C:373:TYR:CD2  | 2.52                     | 0.45              |
| 1:D:183:ILE:HD13 | 1:D:183:ILE:N    | 2.31                     | 0.45              |
| 1:E:169:ARG:HH21 | 1:F:36:GLU:CD    | 2.19                     | 0.45              |
| 1:E:201:TYR:C    | 1:E:201:TYR:CD2  | 2.88                     | 0.45              |
| 1:D:158:ASP:OD2  | 1:E:33:LYS:HE2   | 2.17                     | 0.45              |
| 1:G:35:VAL:O     | 1:G:35:VAL:HG13  | 2.17                     | 0.45              |
| 1:B:430:THR:CG2  | 1:H:300:VAL:HG21 | 2.47                     | 0.45              |
| 1:H:248:LEU:O    | 1:H:331:ARG:HB2  | 2.16                     | 0.45              |
| 1:B:148:LEU:CD2  | 1:H:437:ARG:HD3  | 2.44                     | 0.45              |
| 1:I:402:ASN:CG   | 1:I:405:MET:HG2  | 2.37                     | 0.45              |
| 1:J:296:TYR:HE2  | 1:J:389:PRO:HG2  | 1.82                     | 0.45              |
| 1:J:406:VAL:HG22 | 1:J:414:PHE:CE1  | 2.51                     | 0.45              |
| 1:J:6:ARG:HG3    | 1:J:46:LEU:HD13  | 1.99                     | 0.45              |
| 1:K:129:LEU:CD1  | 1:K:246:CYS:HB3  | 2.46                     | 0.45              |
| 1:B:312:SER:HB3  | 1:B:315:ASN:HB2  | 1.99                     | 0.45              |
| 1:B:48:ASN:HB3   | 1:B:71:TYR:CD1   | 2.51                     | 0.45              |
| 1:C:9:ILE:CD1    | 1:C:74:LEU:HB3   | 2.46                     | 0.45              |
| 1:D:322:ILE:N    | 1:D:322:ILE:HD12 | 2.32                     | 0.45              |
| 1:D:346:ALA:O    | 1:D:347:LEU:C    | 2.56                     | 0.45              |
| 1:D:6:ARG:NE     | 1:D:46:LEU:HD13  | 2.32                     | 0.45              |
| 1:D:58:GLU:O     | 1:D:61:VAL:HG22  | 2.17                     | 0.45              |
| 1:E:175:GLU:O    | 1:E:179:MET:HB2  | 2.17                     | 0.45              |
| 1:E:70:LEU:O     | 1:E:72:PRO:HD3   | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:100:ASP:CG   | 1:H:101:GLY:H    | 2.21                     | 0.45              |
| 1:H:309:VAL:HG13 | 1:H:319:LEU:CD2  | 2.47                     | 0.45              |
| 1:I:280:LYS:HG2  | 1:I:281:HIS:CD2  | 2.51                     | 0.45              |
| 1:I:410:GLY:O    | 1:I:411:GLU:C    | 2.55                     | 0.45              |
| 1:K:316:ARG:HE   | 1:K:370:ARG:NH1  | 2.14                     | 0.45              |
| 1:K:48:ASN:OD1   | 1:K:71:TYR:HA    | 2.17                     | 0.45              |
| 1:L:18:VAL:HG21  | 1:L:79:ILE:HD12  | 1.98                     | 0.45              |
| 1:L:325:SER:HB2  | 1:L:329:SER:CB   | 2.48                     | 0.45              |
| 1:L:129:LEU:CG   | 1:L:347:LEU:HD21 | 2.46                     | 0.45              |
| 1:A:166:GLU:CD   | 1:A:167:ASN:N    | 2.71                     | 0.44              |
| 1:B:309:VAL:HB   | 1:B:386:VAL:HG13 | 1.99                     | 0.44              |
| 1:B:68:MET:HE3   | 1:B:96:ILE:HG21  | 1.99                     | 0.44              |
| 1:C:100:ASP:O    | 1:C:102:THR:N    | 2.50                     | 0.44              |
| 1:C:114:ARG:O    | 1:C:117:LYS:HB2  | 2.17                     | 0.44              |
| 1:C:217:VAL:HG12 | 1:C:221:ILE:HD12 | 1.99                     | 0.44              |
| 1:C:74:LEU:HD23  | 1:C:74:LEU:N     | 2.32                     | 0.44              |
| 1:D:150:LEU:CD1  | 1:D:192:PRO:HB2  | 2.37                     | 0.44              |
| 1:D:211:ILE:O    | 1:D:215:LYS:HG3  | 2.17                     | 0.44              |
| 1:D:390:ALA:HB1  | 1:J:429:ARG:NE   | 2.29                     | 0.44              |
| 1:F:321:ARG:HD3  | 1:F:335:ARG:HD2  | 1.98                     | 0.44              |
| 1:F:375:MET:HE2  | 1:F:385:ILE:CD1  | 2.47                     | 0.44              |
| 1:F:402:ASN:OD1  | 1:F:404:VAL:CG1  | 2.65                     | 0.44              |
| 1:G:223:ARG:O    | 1:G:226:GLY:N    | 2.50                     | 0.44              |
| 1:G:328:ILE:C    | 1:G:330:THR:H    | 2.20                     | 0.44              |
| 1:I:286:THR:HG23 | 1:I:290:ASN:ND2  | 2.31                     | 0.44              |
| 1:D:437:ARG:NH1  | 1:J:235:PRO:O    | 2.45                     | 0.44              |
| 1:J:260:ASP:CG   | 1:J:263:ALA:HB2  | 2.38                     | 0.44              |
| 1:E:429:ARG:HH12 | 1:K:300:VAL:CG1  | 2.30                     | 0.44              |
| 1:A:160:ALA:O    | 1:A:161:PRO:O    | 2.35                     | 0.44              |
| 1:B:134:GLU:HG3  | 1:B:243:GLY:O    | 2.16                     | 0.44              |
| 1:B:150:LEU:HD13 | 1:B:192:PRO:HB2  | 1.98                     | 0.44              |
| 1:C:97:TYR:CD2   | 1:C:101:GLY:O    | 2.70                     | 0.44              |
| 1:E:169:ARG:HH11 | 1:E:195:HIS:CD2  | 2.32                     | 0.44              |
| 1:F:189:GLU:HB3  | 1:F:194:GLN:HE21 | 1.82                     | 0.44              |
| 1:F:35:VAL:HG11  | 1:F:70:LEU:HD22  | 1.99                     | 0.44              |
| 1:G:223:ARG:CB   | 1:G:223:ARG:HH11 | 2.31                     | 0.44              |
| 1:H:311:TRP:HA   | 1:H:320:ILE:O    | 2.17                     | 0.44              |
| 1:D:440:TYR:CE1  | 1:J:292:THR:HB   | 2.53                     | 0.44              |
| 1:K:83:THR:O     | 1:K:84:ALA:HB3   | 2.16                     | 0.44              |
| 1:K:91:ARG:HD2   | 1:K:91:ARG:C     | 2.37                     | 0.44              |
| 1:L:375:MET:HG2  | 1:L:380:ARG:CG   | 2.46                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:73:ASP:O     | 1:L:76:THR:N     | 2.37                     | 0.44              |
| 1:A:163:ASP:O    | 1:A:165:GLY:N    | 2.50                     | 0.44              |
| 1:A:27:ASP:OD2   | 1:A:27:ASP:C     | 2.55                     | 0.44              |
| 1:A:319:LEU:HD22 | 1:A:320:ILE:HD11 | 1.99                     | 0.44              |
| 1:A:55:SER:CB    | 1:A:62:ARG:HE    | 2.31                     | 0.44              |
| 1:C:286:THR:O    | 1:C:290:ASN:N    | 2.50                     | 0.44              |
| 1:C:418:ILE:O    | 1:C:422:GLU:HG3  | 2.17                     | 0.44              |
| 1:D:167:ASN:ND2  | 1:D:170:ARG:CB   | 2.79                     | 0.44              |
| 1:D:293:VAL:HG11 | 1:D:428:PHE:CG   | 2.52                     | 0.44              |
| 1:D:435:TRP:CE2  | 1:D:439:GLN:HG3  | 2.52                     | 0.44              |
| 1:E:400:LYS:HA   | 1:E:414:PHE:CZ   | 2.52                     | 0.44              |
| 1:E:5:THR:O      | 1:E:9:ILE:HG12   | 2.17                     | 0.44              |
| 1:H:308:TYR:HA   | 1:H:387:ASP:HA   | 1.99                     | 0.44              |
| 1:J:120:GLU:C    | 1:J:122:LEU:H    | 2.21                     | 0.44              |
| 1:J:383:ASN:HB2  | 1:J:385:ILE:CG1  | 2.48                     | 0.44              |
| 1:K:281:HIS:CE1  | 1:K:404:VAL:HG21 | 2.52                     | 0.44              |
| 1:L:166:GLU:OE2  | 1:L:166:GLU:O    | 2.35                     | 0.44              |
| 1:L:253:ASN:O    | 1:L:255:VAL:HG23 | 2.18                     | 0.44              |
| 1:L:423:ILE:O    | 1:L:427:MET:HG3  | 2.17                     | 0.44              |
| 1:A:319:LEU:C    | 1:A:319:LEU:HD23 | 2.38                     | 0.44              |
| 1:A:2:ALA:O      | 1:A:3:LYS:HB2    | 2.17                     | 0.44              |
| 1:C:248:LEU:HB2  | 1:C:332:VAL:HG13 | 1.99                     | 0.44              |
| 1:C:25:PHE:CE1   | 1:C:33:LYS:CB    | 3.00                     | 0.44              |
| 1:C:96:ILE:CD1   | 1:C:96:ILE:N     | 2.81                     | 0.44              |
| 1:D:372:ILE:HG13 | 1:D:373:TYR:N    | 2.33                     | 0.44              |
| 1:E:138:PHE:HD2  | 1:E:148:LEU:HA   | 1.81                     | 0.44              |
| 1:F:151:ASN:ND2  | 1:F:166:GLU:OE2  | 2.50                     | 0.44              |
| 1:F:326:ARG:HA   | 1:F:326:ARG:HD3  | 1.79                     | 0.44              |
| 1:G:311:TRP:O    | 1:G:368:ILE:HG13 | 2.17                     | 0.44              |
| 1:G:32:ILE:HG22  | 1:H:159:LEU:HD12 | 1.98                     | 0.44              |
| 1:I:86:LYS:CB    | 1:J:174:LEU:HD13 | 2.38                     | 0.44              |
| 1:J:48:ASN:O     | 1:J:69:TYR:HD2   | 1.99                     | 0.44              |
| 1:K:34:ASN:C     | 1:K:34:ASN:ND2   | 2.69                     | 0.44              |
| 1:L:256:ASN:OD1  | 1:L:258:PHE:N    | 2.50                     | 0.44              |
| 1:L:355:LEU:O    | 1:L:357:GLY:N    | 2.51                     | 0.44              |
| 1:A:138:PHE:HZ   | 1:A:236:LEU:HD11 | 1.82                     | 0.44              |
| 1:B:360:ASN:HB2  | 1:B:362:LEU:HD13 | 1.99                     | 0.44              |
| 1:C:315:ASN:HD21 | 1:C:369:ASP:HA   | 1.82                     | 0.44              |
| 1:D:308:TYR:CD1  | 1:D:372:ILE:HB   | 2.53                     | 0.44              |
| 1:D:115:ILE:HG23 | 1:D:351:LEU:HD12 | 2.00                     | 0.44              |
| 1:E:374:VAL:HG23 | 1:E:375:MET:H    | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:237:PHE:CD2  | 1:F:238:GLY:N    | 2.85                     | 0.44              |
| 1:F:418:ILE:HG22 | 1:F:422:GLU:OE1  | 2.17                     | 0.44              |
| 1:H:252:LYS:O    | 1:H:253:ASN:HB2  | 2.17                     | 0.44              |
| 1:H:294:ASN:HA   | 1:H:297:LYS:HD3  | 1.99                     | 0.44              |
| 1:H:370:ARG:HH11 | 1:H:370:ARG:CG   | 2.28                     | 0.44              |
| 1:J:349:VAL:HG22 | 1:J:405:MET:SD   | 2.58                     | 0.44              |
| 1:A:397:GLU:O    | 1:A:401:SER:HB3  | 2.17                     | 0.44              |
| 1:C:45:ALA:HA    | 1:C:50:VAL:HG23  | 2.00                     | 0.44              |
| 1:D:28:ILE:HG22  | 1:D:29:LEU:HG    | 1.99                     | 0.44              |
| 1:E:298:ARG:HG2  | 1:E:298:ARG:O    | 2.18                     | 0.44              |
| 1:E:370:ARG:NH1  | 1:E:370:ARG:HG3  | 2.32                     | 0.44              |
| 1:E:443:GLN:O    | 1:E:443:GLN:HG2  | 2.16                     | 0.44              |
| 1:F:440:TYR:HD1  | 1:F:444:TYR:HE2  | 1.65                     | 0.44              |
| 1:G:162:THR:HG21 | 1:L:220:THR:OG1  | 2.17                     | 0.44              |
| 1:G:323:PRO:HD2  | 1:G:331:ARG:O    | 2.18                     | 0.44              |
| 1:I:250:LEU:HB2  | 1:I:258:PHE:CE2  | 2.53                     | 0.44              |
| 1:I:279:VAL:HG13 | 1:I:309:VAL:CG1  | 2.45                     | 0.44              |
| 1:J:138:PHE:HB3  | 1:J:147:THR:O    | 2.18                     | 0.44              |
| 1:A:300:VAL:CG1  | 1:A:301:PRO:HD2  | 2.48                     | 0.44              |
| 1:B:224:LYS:HE2  | 1:B:225:HIS:CE1  | 2.53                     | 0.44              |
| 1:B:297:LYS:HE3  | 1:H:436:GLU:OE1  | 2.17                     | 0.44              |
| 1:B:371:ASN:HD22 | 1:B:372:ILE:H    | 1.64                     | 0.44              |
| 1:B:406:VAL:HG22 | 1:B:414:PHE:CE1  | 2.52                     | 0.44              |
| 1:D:137:LEU:HD13 | 1:D:227:LEU:HD13 | 2.00                     | 0.44              |
| 1:D:300:VAL:HG21 | 1:J:430:THR:HG22 | 1.99                     | 0.44              |
| 1:E:70:LEU:HG    | 1:E:94:CYS:HB2   | 1.99                     | 0.44              |
| 1:F:280:LYS:HE2  | 1:F:281:HIS:NE2  | 2.33                     | 0.44              |
| 1:F:282:ALA:HA   | 1:F:285:PHE:CE2  | 2.52                     | 0.44              |
| 1:F:440:TYR:HD1  | 1:F:444:TYR:CE2  | 2.35                     | 0.44              |
| 1:G:9:ILE:O      | 1:G:13:VAL:HG23  | 2.17                     | 0.44              |
| 1:I:251:PHE:CD1  | 1:I:256:ASN:HA   | 2.53                     | 0.44              |
| 1:I:5:THR:HG22   | 1:I:8:ASP:CG     | 2.38                     | 0.44              |
| 1:K:360:ASN:HB2  | 1:K:362:LEU:HD11 | 2.00                     | 0.44              |
| 1:L:316:ARG:NH1  | 1:L:316:ARG:HG3  | 2.33                     | 0.44              |
| 1:B:285:PHE:HB2  | 1:B:349:VAL:HG11 | 2.00                     | 0.44              |
| 1:C:6:ARG:CD     | 1:C:46:LEU:HD13  | 2.48                     | 0.44              |
| 1:D:23:LEU:HB2   | 1:D:35:VAL:HG13  | 2.00                     | 0.44              |
| 1:E:314:GLN:NE2  | 1:E:321:ARG:NH2  | 2.55                     | 0.44              |
| 1:E:309:VAL:CG2  | 1:E:386:VAL:HG23 | 2.46                     | 0.44              |
| 1:E:392:LEU:O    | 1:E:392:LEU:HG   | 2.18                     | 0.44              |
| 1:E:418:ILE:N    | 1:E:418:ILE:HD12 | 2.33                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:286:THR:HA   | 1:F:289:THR:OG1  | 2.18                     | 0.44              |
| 1:G:140:LEU:HD12 | 1:G:226:GLY:C    | 2.37                     | 0.44              |
| 1:G:250:LEU:O    | 1:G:257:ALA:HB3  | 2.18                     | 0.44              |
| 1:G:286:THR:HG23 | 1:G:290:ASN:OD1  | 2.18                     | 0.44              |
| 1:G:370:ARG:NH2  | 1:G:383:ASN:ND2  | 2.66                     | 0.44              |
| 1:H:380:ARG:HH11 | 1:H:380:ARG:CB   | 2.28                     | 0.44              |
| 1:H:16:GLU:O     | 1:H:88:LYS:HG3   | 2.18                     | 0.44              |
| 1:I:22:ARG:NH1   | 1:J:159:LEU:CD2  | 2.81                     | 0.44              |
| 1:I:282:ALA:CB   | 1:I:319:LEU:HD21 | 2.47                     | 0.44              |
| 1:J:129:LEU:HD22 | 1:J:131:PRO:CG   | 2.48                     | 0.44              |
| 1:J:399:PHE:CD1  | 1:J:405:MET:HB3  | 2.52                     | 0.44              |
| 1:J:54:GLY:O     | 1:J:56:SER:N     | 2.51                     | 0.44              |
| 1:A:31:THR:HG22  | 1:A:33:LYS:HG3   | 1.98                     | 0.44              |
| 1:A:36:GLU:HG2   | 1:A:36:GLU:H     | 1.67                     | 0.44              |
| 1:A:39:VAL:HG22  | 1:A:39:VAL:O     | 2.17                     | 0.44              |
| 1:E:185:ALA:HB2  | 1:F:37:ILE:HG22  | 1.99                     | 0.44              |
| 1:E:80:PHE:HE1   | 1:E:91:ARG:HB3   | 1.82                     | 0.44              |
| 1:G:115:ILE:N    | 1:G:115:ILE:HD12 | 2.32                     | 0.44              |
| 1:A:102:THR:HG22 | 1:A:103:PRO:HD2  | 2.00                     | 0.43              |
| 1:A:37:ILE:HG22  | 1:F:185:ALA:HB2  | 1.97                     | 0.43              |
| 1:A:69:TYR:O     | 1:A:70:LEU:HD13  | 2.18                     | 0.43              |
| 1:B:158:ASP:HA   | 1:C:33:LYS:HA    | 1.98                     | 0.43              |
| 1:B:124:PHE:CZ   | 1:B:358:ILE:HD13 | 2.53                     | 0.43              |
| 1:B:55:SER:HB2   | 1:B:62:ARG:HB2   | 2.00                     | 0.43              |
| 1:B:18:VAL:HG11  | 1:B:90:ALA:HB2   | 1.99                     | 0.43              |
| 1:C:117:LYS:O    | 1:C:120:GLU:N    | 2.51                     | 0.43              |
| 1:C:32:ILE:N     | 1:C:32:ILE:CD1   | 2.79                     | 0.43              |
| 1:C:377:LYS:C    | 1:C:381:MET:HE2  | 2.38                     | 0.43              |
| 1:D:376:SER:O    | 1:D:380:ARG:HG3  | 2.18                     | 0.43              |
| 1:D:76:THR:O     | 1:D:78:VAL:HG23  | 2.17                     | 0.43              |
| 1:F:372:ILE:HG23 | 1:F:375:MET:SD   | 2.58                     | 0.43              |
| 1:G:312:SER:CB   | 1:G:315:ASN:HB2  | 2.47                     | 0.43              |
| 1:I:200:LYS:O    | 1:I:201:TYR:C    | 2.56                     | 0.43              |
| 1:J:211:ILE:HG22 | 1:J:215:LYS:HE3  | 2.00                     | 0.43              |
| 1:J:386:VAL:CG1  | 1:J:387:ASP:H    | 2.14                     | 0.43              |
| 1:J:396:LEU:HD11 | 1:J:421:LYS:CB   | 2.48                     | 0.43              |
| 1:L:259:PHE:CE1  | 1:L:326:ARG:HB3  | 2.53                     | 0.43              |
| 1:A:44:LYS:HE2   | 1:A:49:LYS:O     | 2.18                     | 0.43              |
| 1:B:273:HIS:O    | 1:B:276:ALA:HB3  | 2.18                     | 0.43              |
| 1:B:368:ILE:CG2  | 1:B:370:ARG:HG3  | 2.48                     | 0.43              |
| 1:C:213:THR:O    | 1:C:217:VAL:HG23 | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:46:LEU:HD22  | 1:D:74:LEU:HD21  | 2.00                     | 0.43              |
| 1:D:45:ALA:CA    | 1:D:50:VAL:HG23  | 2.46                     | 0.43              |
| 1:F:153:LYS:HG2  | 1:F:153:LYS:O    | 2.18                     | 0.43              |
| 1:F:380:ARG:NH1  | 1:F:385:ILE:CG2  | 2.80                     | 0.43              |
| 1:I:271:ALA:O    | 1:I:275:ILE:HD12 | 2.17                     | 0.43              |
| 1:I:34:ASN:HD22  | 1:I:34:ASN:C     | 2.20                     | 0.43              |
| 1:I:51:MET:SD    | 1:I:67:ASP:HB3   | 2.57                     | 0.43              |
| 1:J:285:PHE:HB2  | 1:J:349:VAL:HG13 | 2.00                     | 0.43              |
| 1:K:189:GLU:HB3  | 1:K:194:GLN:NE2  | 2.33                     | 0.43              |
| 1:K:406:VAL:HG13 | 1:K:414:PHE:CD2  | 2.54                     | 0.43              |
| 1:K:28:ILE:HD11  | 1:K:417:PHE:HA   | 1.99                     | 0.43              |
| 1:L:316:ARG:HG2  | 1:L:373:TYR:HB2  | 2.00                     | 0.43              |
| 1:L:383:ASN:HB2  | 1:L:385:ILE:HG12 | 1.99                     | 0.43              |
| 1:A:252:LYS:NZ   | 1:A:253:ASN:ND2  | 2.65                     | 0.43              |
| 1:A:80:PHE:HB3   | 1:A:82:TRP:CE3   | 2.53                     | 0.43              |
| 1:B:129:LEU:HD22 | 1:B:130:GLY:H    | 1.80                     | 0.43              |
| 1:B:4:TYR:HB3    | 1:B:9:ILE:HD11   | 1.98                     | 0.43              |
| 1:C:402:ASN:OD1  | 1:C:404:VAL:CG1  | 2.65                     | 0.43              |
| 1:C:48:ASN:O     | 1:C:69:TYR:HD2   | 2.01                     | 0.43              |
| 1:C:55:SER:CB    | 1:C:62:ARG:HG2   | 2.46                     | 0.43              |
| 1:D:388:LEU:HB3  | 1:D:389:PRO:HD2  | 2.00                     | 0.43              |
| 1:D:6:ARG:HE     | 1:D:46:LEU:HD13  | 1.83                     | 0.43              |
| 1:D:23:LEU:HB3   | 1:D:70:LEU:HD23  | 2.00                     | 0.43              |
| 1:D:78:VAL:O     | 1:D:90:ALA:HA    | 2.18                     | 0.43              |
| 1:D:72:PRO:HA    | 1:D:94:CYS:HA    | 2.01                     | 0.43              |
| 1:E:184:GLU:OE2  | 1:F:44:LYS:HE3   | 2.18                     | 0.43              |
| 1:E:407:LYS:HA   | 1:E:407:LYS:HE2  | 2.01                     | 0.43              |
| 1:G:308:TYR:CD2  | 1:G:380:ARG:HD3  | 2.52                     | 0.43              |
| 1:H:206:ARG:O    | 1:H:206:ARG:HD3  | 2.19                     | 0.43              |
| 1:H:223:ARG:O    | 1:H:225:HIS:N    | 2.52                     | 0.43              |
| 1:I:133:PRO:HA   | 1:I:244:MET:HG3  | 2.00                     | 0.43              |
| 1:I:287:ALA:HB2  | 1:I:395:ALA:CB   | 2.46                     | 0.43              |
| 1:J:183:ILE:HG22 | 1:J:184:GLU:N    | 2.32                     | 0.43              |
| 1:J:82:TRP:HH2   | 1:J:217:VAL:HG22 | 1.83                     | 0.43              |
| 1:J:256:ASN:ND2  | 1:J:330:THR:HB   | 2.33                     | 0.43              |
| 1:K:262:ASN:O    | 1:K:263:ALA:HB2  | 2.18                     | 0.43              |
| 1:K:351:LEU:O    | 1:K:355:LEU:HG   | 2.19                     | 0.43              |
| 1:A:245:HIS:CD2  | 1:A:335:ARG:HA   | 2.54                     | 0.43              |
| 1:B:115:ILE:O    | 1:B:118:GLU:HB2  | 2.17                     | 0.43              |
| 1:B:139:LYS:HA   | 1:B:227:LEU:HD23 | 2.00                     | 0.43              |
| 1:B:290:ASN:OD1  | 1:B:338:ASP:OD1  | 2.37                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:162:THR:O    | 1:C:164:LEU:N    | 2.51                     | 0.43              |
| 1:D:8:ASP:O      | 1:D:11:LYS:HB3   | 2.19                     | 0.43              |
| 1:D:321:ARG:O    | 1:D:333:GLU:HB3  | 2.18                     | 0.43              |
| 1:D:45:ALA:HB2   | 1:D:50:VAL:HG21  | 2.01                     | 0.43              |
| 1:F:359:LYS:C    | 1:F:360:ASN:HD22 | 2.21                     | 0.43              |
| 1:G:162:THR:HG22 | 1:G:163:ASP:N    | 2.34                     | 0.43              |
| 1:G:112:LEU:HD11 | 1:G:208:CYS:SG   | 2.59                     | 0.43              |
| 1:H:240:ASN:HA   | 1:H:240:ASN:HD22 | 1.58                     | 0.43              |
| 1:H:307:CYS:O    | 1:H:387:ASP:HA   | 2.18                     | 0.43              |
| 1:J:285:PHE:C    | 1:J:285:PHE:CD1  | 2.92                     | 0.43              |
| 1:J:406:VAL:HG22 | 1:J:414:PHE:CZ   | 2.54                     | 0.43              |
| 1:L:137:LEU:HD23 | 1:L:229:ALA:HA   | 2.01                     | 0.43              |
| 1:L:311:TRP:H    | 1:L:368:ILE:HD13 | 1.84                     | 0.43              |
| 1:L:333:GLU:HG2  | 1:L:335:ARG:HG2  | 2.01                     | 0.43              |
| 1:A:319:LEU:HD22 | 1:A:320:ILE:HD12 | 1.98                     | 0.43              |
| 1:A:376:SER:O    | 1:A:380:ARG:HB2  | 2.19                     | 0.43              |
| 1:A:402:ASN:C    | 1:A:402:ASN:OD1  | 2.56                     | 0.43              |
| 1:B:201:TYR:OH   | 1:B:331:ARG:NE   | 2.49                     | 0.43              |
| 1:B:28:ILE:O     | 1:B:28:ILE:HG12  | 2.18                     | 0.43              |
| 1:C:239:VAL:O    | 1:C:240:ASN:C    | 2.57                     | 0.43              |
| 1:C:252:LYS:C    | 1:C:254:GLY:H    | 2.20                     | 0.43              |
| 1:C:414:PHE:CE2  | 1:C:418:ILE:HG13 | 2.53                     | 0.43              |
| 1:C:74:LEU:HA    | 1:C:92:PHE:HE2   | 1.82                     | 0.43              |
| 1:D:161:PRO:HD3  | 4:D:620:HOH:O    | 2.18                     | 0.43              |
| 1:D:233:PRO:HG3  | 1:D:338:ASP:OD2  | 2.19                     | 0.43              |
| 1:D:360:ASN:O    | 1:D:361:LYS:C    | 2.56                     | 0.43              |
| 1:E:328:ILE:C    | 1:E:330:THR:H    | 2.21                     | 0.43              |
| 1:F:163:ASP:HA   | 1:F:167:ASN:HD22 | 1.83                     | 0.43              |
| 1:G:132:GLU:HB3  | 1:G:196:GLU:OE1  | 2.19                     | 0.43              |
| 1:G:152:ASP:OD1  | 1:G:193:GLY:HA2  | 2.18                     | 0.43              |
| 1:G:426:ASP:HA   | 1:G:429:ARG:HG2  | 2.00                     | 0.43              |
| 1:G:429:ARG:HG3  | 1:G:430:THR:N    | 2.33                     | 0.43              |
| 1:I:321:ARG:O    | 1:I:333:GLU:HB3  | 2.18                     | 0.43              |
| 1:I:5:THR:HG22   | 1:I:8:ASP:OD1    | 2.18                     | 0.43              |
| 1:I:9:ILE:HG13   | 1:I:74:LEU:CD1   | 2.48                     | 0.43              |
| 1:J:353:ALA:HB2  | 1:J:405:MET:HE1  | 2.01                     | 0.43              |
| 1:J:389:PRO:CB   | 1:J:394:GLU:HB3  | 2.41                     | 0.43              |
| 1:J:28:ILE:HG12  | 1:J:57:ILE:O     | 2.19                     | 0.43              |
| 1:K:58:GLU:OE1   | 1:K:416:HIS:CD2  | 2.72                     | 0.43              |
| 1:L:205:VAL:O    | 1:L:206:ARG:C    | 2.57                     | 0.43              |
| 1:L:258:PHE:O    | 1:L:330:THR:HG21 | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:115:ILE:HD11 | 1:L:408:ALA:O    | 2.19                     | 0.43              |
| 1:A:116:LEU:O    | 1:A:120:GLU:HG3  | 2.19                     | 0.43              |
| 1:A:259:PHE:CE1  | 1:A:266:GLN:HB3  | 2.54                     | 0.43              |
| 1:A:297:LYS:HD3  | 1:G:429:ARG:O    | 2.18                     | 0.43              |
| 1:A:313:ALA:HA   | 1:A:321:ARG:HG3  | 2.00                     | 0.43              |
| 1:B:127:PHE:CD2  | 1:B:351:LEU:HG   | 2.54                     | 0.43              |
| 1:B:300:VAL:HG22 | 1:H:429:ARG:NH2  | 2.33                     | 0.43              |
| 1:C:271:ALA:O    | 1:C:275:ILE:HG13 | 2.18                     | 0.43              |
| 1:C:300:VAL:HG13 | 1:C:300:VAL:O    | 2.19                     | 0.43              |
| 1:C:325:SER:HB2  | 1:C:331:ARG:HH22 | 1.83                     | 0.43              |
| 1:D:250:LEU:O    | 1:D:257:ALA:HB3  | 2.19                     | 0.43              |
| 1:E:278:ILE:O    | 1:E:282:ALA:N    | 2.52                     | 0.43              |
| 1:E:329:SER:O    | 1:E:331:ARG:NH2  | 2.51                     | 0.43              |
| 1:E:37:ILE:O     | 1:E:37:ILE:HG13  | 2.18                     | 0.43              |
| 1:E:67:ASP:O     | 1:E:68:MET:HG2   | 2.19                     | 0.43              |
| 1:F:223:ARG:C    | 1:F:225:HIS:N    | 2.71                     | 0.43              |
| 1:F:37:ILE:O     | 1:F:37:ILE:HG13  | 2.17                     | 0.43              |
| 1:F:430:THR:HG22 | 1:L:300:VAL:HG11 | 2.00                     | 0.43              |
| 1:F:440:TYR:CD1  | 1:F:444:TYR:HE2  | 2.35                     | 0.43              |
| 1:G:322:ILE:HA   | 1:G:323:PRO:HD2  | 1.84                     | 0.43              |
| 1:G:346:ALA:O    | 1:G:350:LEU:HB2  | 2.19                     | 0.43              |
| 1:H:370:ARG:HH22 | 1:H:375:MET:HE3  | 1.84                     | 0.43              |
| 1:I:212:GLN:O    | 1:I:213:THR:C    | 2.57                     | 0.43              |
| 1:I:175:GLU:HG3  | 1:I:221:ILE:CD1  | 2.48                     | 0.43              |
| 1:I:249:SER:HB3  | 1:I:331:ARG:HB3  | 2.01                     | 0.43              |
| 1:I:68:MET:HB3   | 1:I:97:TYR:O     | 2.19                     | 0.43              |
| 1:K:261:GLU:HG3  | 1:K:262:ASN:ND2  | 2.34                     | 0.43              |
| 1:K:74:LEU:CD2   | 1:K:74:LEU:H     | 2.32                     | 0.43              |
| 1:L:316:ARG:HG2  | 1:L:373:TYR:CB   | 2.48                     | 0.43              |
| 1:G:178:GLU:OE1  | 1:L:86:LYS:HE3   | 2.19                     | 0.43              |
| 1:A:402:ASN:OD1  | 1:A:405:MET:HG2  | 2.19                     | 0.43              |
| 1:B:160:ALA:HB3  | 1:B:169:ARG:NH1  | 2.34                     | 0.43              |
| 1:B:203:GLY:O    | 1:B:204:ALA:C    | 2.57                     | 0.43              |
| 1:B:351:LEU:CD2  | 1:B:355:LEU:HG   | 2.49                     | 0.43              |
| 1:D:160:ALA:O    | 1:D:161:PRO:C    | 2.57                     | 0.43              |
| 1:D:306:PRO:HB3  | 1:D:319:LEU:HA   | 2.01                     | 0.43              |
| 1:D:430:THR:HG22 | 1:J:300:VAL:HG22 | 2.01                     | 0.43              |
| 1:E:53:ASP:CG    | 1:E:65:GLU:HG3   | 2.39                     | 0.43              |
| 1:F:181:PHE:CE2  | 1:F:210:ASP:HB3  | 2.53                     | 0.43              |
| 1:F:97:TYR:C     | 1:F:98:ASN:HD22  | 2.22                     | 0.43              |
| 1:G:66:SER:HA    | 1:H:314:GLN:OE1  | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:2:ALA:HB1    | 1:G:75:ASN:OD1   | 2.19                     | 0.43              |
| 1:I:100:ASP:HB2  | 1:I:101:GLY:H    | 1.32                     | 0.43              |
| 1:I:259:PHE:HA   | 1:I:330:THR:HG21 | 2.00                     | 0.43              |
| 1:I:317:SER:C    | 1:I:373:TYR:OH   | 2.57                     | 0.43              |
| 1:L:360:ASN:HB2  | 1:L:362:LEU:HD13 | 2.01                     | 0.43              |
| 1:L:73:ASP:O     | 1:L:76:THR:OG1   | 2.31                     | 0.43              |
| 1:A:156:TYR:C    | 1:A:158:ASP:H    | 2.22                     | 0.43              |
| 1:A:232:MET:HE1  | 1:A:235:PRO:HA   | 1.99                     | 0.43              |
| 1:D:244:MET:H    | 1:D:338:ASP:HA   | 1.83                     | 0.43              |
| 1:E:183:ILE:HG22 | 1:E:198:ASP:O    | 2.19                     | 0.43              |
| 1:F:20:TYR:CZ    | 1:F:36:GLU:HB2   | 2.54                     | 0.43              |
| 1:F:432:VAL:HB   | 1:L:237:PHE:HB2  | 2.00                     | 0.43              |
| 1:G:162:THR:O    | 1:G:164:LEU:O    | 2.36                     | 0.43              |
| 1:A:436:GLU:OE1  | 1:G:297:LYS:NZ   | 2.52                     | 0.43              |
| 1:H:113:LYS:O    | 1:H:116:LEU:HB2  | 2.19                     | 0.43              |
| 1:H:143:LYS:HA   | 1:H:143:LYS:HE2  | 2.00                     | 0.43              |
| 1:H:162:THR:O    | 1:H:164:LEU:N    | 2.51                     | 0.43              |
| 1:H:282:ALA:HA   | 1:H:285:PHE:CZ   | 2.53                     | 0.43              |
| 1:H:376:SER:HB3  | 1:H:379:GLU:HB2  | 2.00                     | 0.43              |
| 1:H:23:LEU:HD11  | 1:H:37:ILE:HD13  | 2.01                     | 0.43              |
| 1:H:372:ILE:O    | 1:H:380:ARG:HD3  | 2.19                     | 0.43              |
| 1:I:128:ASN:HB2  | 1:I:249:SER:OG   | 2.18                     | 0.43              |
| 1:I:28:ILE:HD11  | 1:I:417:PHE:HB2  | 2.01                     | 0.43              |
| 1:I:418:ILE:O    | 1:I:420:ALA:N    | 2.52                     | 0.43              |
| 1:J:196:GLU:HG2  | 1:J:198:ASP:OD2  | 2.19                     | 0.43              |
| 1:J:319:LEU:HD23 | 1:J:320:ILE:HD11 | 1.99                     | 0.43              |
| 1:J:354:GLY:O    | 1:J:358:ILE:HG12 | 2.18                     | 0.43              |
| 1:K:224:LYS:HG3  | 1:L:164:LEU:HD11 | 2.00                     | 0.43              |
| 1:K:28:ILE:HG12  | 1:K:28:ILE:O     | 2.18                     | 0.43              |
| 1:K:326:ARG:NH1  | 1:K:326:ARG:HB2  | 2.33                     | 0.43              |
| 1:K:375:MET:HB2  | 1:K:379:GLU:HB2  | 2.01                     | 0.43              |
| 1:K:78:VAL:HB    | 1:K:91:ARG:CG    | 2.45                     | 0.43              |
| 1:L:100:ASP:O    | 1:L:102:THR:N    | 2.51                     | 0.43              |
| 1:F:232:MET:CE   | 1:L:437:ARG:HA   | 2.48                     | 0.43              |
| 1:A:145:GLU:OE1  | 1:A:146:PRO:HD2  | 2.19                     | 0.43              |
| 1:A:58:GLU:HB3   | 1:A:61:VAL:HG23  | 2.00                     | 0.43              |
| 1:B:160:ALA:HB1  | 1:B:161:PRO:CD   | 2.44                     | 0.43              |
| 1:B:374:VAL:HG23 | 1:B:375:MET:N    | 2.34                     | 0.43              |
| 1:B:418:ILE:HG22 | 1:B:419:GLU:N    | 2.33                     | 0.43              |
| 1:D:26:THR:HG1   | 1:D:212:GLN:HE21 | 1.66                     | 0.43              |
| 1:D:260:ASP:HB2  | 1:D:268:SER:HB3  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:360:ASN:O    | 1:E:361:LYS:O    | 2.37                     | 0.43              |
| 1:F:369:ASP:OD1  | 1:F:369:ASP:N    | 2.52                     | 0.43              |
| 1:F:376:SER:O    | 1:F:379:GLU:HG2  | 2.19                     | 0.43              |
| 1:G:393:ALA:HB2  | 1:G:425:TRP:CE2  | 2.54                     | 0.43              |
| 1:H:9:ILE:O      | 1:H:13:VAL:HG23  | 2.18                     | 0.43              |
| 1:H:183:ILE:HD12 | 1:H:183:ILE:H    | 1.83                     | 0.43              |
| 1:H:96:ILE:HD12  | 1:H:96:ILE:H     | 1.82                     | 0.43              |
| 1:I:200:LYS:O    | 1:I:201:TYR:O    | 2.37                     | 0.43              |
| 1:J:141:ASP:OD2  | 1:J:141:ASP:C    | 2.57                     | 0.43              |
| 1:J:371:ASN:O    | 1:J:375:MET:HG3  | 2.19                     | 0.43              |
| 1:D:297:LYS:HE3  | 1:J:436:GLU:CD   | 2.39                     | 0.43              |
| 1:J:91:ARG:HD2   | 1:J:92:PHE:N     | 2.34                     | 0.43              |
| 1:K:172:ILE:HG22 | 1:K:173:VAL:N    | 2.33                     | 0.43              |
| 1:K:83:THR:HA    | 1:K:85:GLU:OE2   | 2.18                     | 0.43              |
| 1:A:102:THR:HG21 | 4:A:610:HOH:O    | 2.18                     | 0.43              |
| 1:A:37:ILE:N     | 1:A:37:ILE:HD13  | 2.33                     | 0.43              |
| 1:B:285:PHE:HB2  | 1:B:349:VAL:HG13 | 2.00                     | 0.43              |
| 1:B:306:PRO:HB3  | 1:B:319:LEU:HA   | 2.01                     | 0.43              |
| 1:C:337:VAL:CG1  | 1:C:338:ASP:N    | 2.82                     | 0.43              |
| 1:E:136:PHE:CE1  | 1:E:235:PRO:HG2  | 2.53                     | 0.43              |
| 1:E:273:HIS:NE2  | 1:E:361:LYS:CA   | 2.82                     | 0.43              |
| 1:F:201:TYR:CD1  | 1:F:201:TYR:C    | 2.93                     | 0.43              |
| 1:G:160:ALA:CB   | 1:G:169:ARG:HH12 | 2.32                     | 0.43              |
| 1:G:151:ASN:ND2  | 1:G:166:GLU:OE1  | 2.52                     | 0.43              |
| 1:G:131:PRO:HG2  | 1:G:199:PHE:HE1  | 1.84                     | 0.43              |
| 1:G:32:ILE:O     | 1:H:159:LEU:HB2  | 2.19                     | 0.43              |
| 1:H:21:ILE:HD12  | 1:H:39:VAL:HA    | 2.01                     | 0.43              |
| 1:J:409:LEU:O    | 1:J:413:LEU:HB2  | 2.19                     | 0.43              |
| 1:J:52:PHE:CD1   | 1:J:70:LEU:HD13  | 2.53                     | 0.43              |
| 1:K:63:ILE:HG22  | 1:K:64:GLU:HG3   | 2.01                     | 0.43              |
| 1:L:156:TYR:O    | 1:L:158:ASP:N    | 2.52                     | 0.43              |
| 1:L:225:HIS:O    | 1:L:227:LEU:HG   | 2.19                     | 0.43              |
| 1:L:34:ASN:C     | 1:L:34:ASN:HD22  | 2.18                     | 0.43              |
| 1:B:18:VAL:HG12  | 1:B:21:ILE:HD12  | 2.00                     | 0.42              |
| 1:C:315:ASN:HD21 | 1:C:369:ASP:CA   | 2.32                     | 0.42              |
| 1:C:388:LEU:HA   | 1:C:388:LEU:HD23 | 1.85                     | 0.42              |
| 1:E:112:LEU:O    | 1:E:116:LEU:HG   | 2.19                     | 0.42              |
| 1:E:274:PHE:CE1  | 1:E:354:GLY:HA3  | 2.54                     | 0.42              |
| 1:E:28:ILE:HD11  | 1:E:417:PHE:HB2  | 2.01                     | 0.42              |
| 1:F:104:PHE:HD2  | 1:F:107:ASP:HB2  | 1.84                     | 0.42              |
| 1:F:172:ILE:CD1  | 1:F:221:ILE:HB   | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:274:PHE:HD2  | 1:F:332:VAL:HG21 | 1.84                     | 0.42              |
| 1:F:28:ILE:HD11  | 1:F:417:PHE:HB2  | 2.00                     | 0.42              |
| 1:G:314:GLN:HE22 | 1:L:66:SER:CA    | 2.31                     | 0.42              |
| 1:G:338:ASP:CB   | 1:G:339:PRO:HD2  | 2.47                     | 0.42              |
| 1:H:437:ARG:O    | 1:H:441:MET:CB   | 2.67                     | 0.42              |
| 1:I:140:LEU:HA   | 1:I:145:GLU:O    | 2.18                     | 0.42              |
| 1:I:20:TYR:HB2   | 1:J:174:LEU:HD21 | 2.01                     | 0.42              |
| 1:I:371:ASN:O    | 1:I:372:ILE:HG23 | 2.18                     | 0.42              |
| 1:I:19:LYS:HA    | 1:I:39:VAL:HB    | 1.99                     | 0.42              |
| 1:J:16:GLU:O     | 1:J:17:ASN:HB3   | 2.18                     | 0.42              |
| 1:J:17:ASN:O     | 1:J:17:ASN:CG    | 2.57                     | 0.42              |
| 1:J:45:ALA:HA    | 1:J:50:VAL:HG23  | 2.00                     | 0.42              |
| 1:K:224:LYS:HG3  | 1:L:164:LEU:CD1  | 2.48                     | 0.42              |
| 1:A:186:SER:HB2  | 1:A:196:GLU:O    | 2.19                     | 0.42              |
| 1:A:191:ALA:H    | 1:A:194:GLN:NE2  | 2.17                     | 0.42              |
| 1:A:402:ASN:CG   | 1:A:405:MET:HG2  | 2.40                     | 0.42              |
| 1:B:6:ARG:HG2    | 1:B:10:GLU:OE1   | 2.18                     | 0.42              |
| 1:C:133:PRO:HG3  | 1:C:199:PHE:HE1  | 1.83                     | 0.42              |
| 1:C:169:ARG:HD3  | 1:C:186:SER:OG   | 2.19                     | 0.42              |
| 1:D:12:LEU:O     | 1:D:16:GLU:HB2   | 2.19                     | 0.42              |
| 1:D:194:GLN:HE22 | 1:D:240:ASN:HB3  | 1.84                     | 0.42              |
| 1:E:236:LEU:HB2  | 1:E:239:VAL:CG2  | 2.49                     | 0.42              |
| 1:E:354:GLY:O    | 1:E:358:ILE:HG13 | 2.19                     | 0.42              |
| 1:G:325:SER:HB3  | 1:G:329:SER:HB2  | 2.00                     | 0.42              |
| 1:G:287:ALA:HB2  | 1:G:395:ALA:HB1  | 2.00                     | 0.42              |
| 1:G:35:VAL:HG11  | 1:G:70:LEU:CD2   | 2.49                     | 0.42              |
| 1:H:328:ILE:HG12 | 1:H:329:SER:N    | 2.35                     | 0.42              |
| 1:H:370:ARG:O    | 1:H:372:ILE:N    | 2.52                     | 0.42              |
| 1:I:116:LEU:O    | 1:I:120:GLU:HG2  | 2.19                     | 0.42              |
| 1:I:129:LEU:CD2  | 1:I:131:PRO:HG3  | 2.35                     | 0.42              |
| 1:J:349:VAL:HG23 | 1:J:409:LEU:HD13 | 2.00                     | 0.42              |
| 1:J:402:ASN:C    | 1:J:402:ASN:OD1  | 2.58                     | 0.42              |
| 1:L:282:ALA:HA   | 1:L:285:PHE:CZ   | 2.54                     | 0.42              |
| 1:L:411:GLU:O    | 1:L:415:GLU:HB2  | 2.19                     | 0.42              |
| 1:L:423:ILE:HD12 | 1:L:424:GLU:N    | 2.34                     | 0.42              |
| 1:A:126:ASP:HB2  | 1:A:251:PHE:HB2  | 1.99                     | 0.42              |
| 1:A:259:PHE:CE1  | 1:A:326:ARG:HB3  | 2.54                     | 0.42              |
| 1:A:265:LEU:HD12 | 1:A:265:LEU:N    | 2.34                     | 0.42              |
| 1:B:147:THR:C    | 1:B:149:GLU:H    | 2.21                     | 0.42              |
| 1:B:276:ALA:HB2  | 1:B:364:ALA:HB2  | 2.01                     | 0.42              |
| 1:B:73:ASP:O     | 1:B:76:THR:OG1   | 2.30                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:281:HIS:NE2  | 1:C:404:VAL:HG11 | 2.33                     | 0.42              |
| 1:E:107:ASP:OD1  | 1:E:108:PRO:HD2  | 2.20                     | 0.42              |
| 1:F:289:THR:O    | 1:F:341:ALA:HB2  | 2.19                     | 0.42              |
| 1:G:409:LEU:O    | 1:G:413:LEU:HB2  | 2.19                     | 0.42              |
| 1:H:316:ARG:HD2  | 1:H:316:ARG:HA   | 1.90                     | 0.42              |
| 1:I:399:PHE:CZ   | 1:I:409:LEU:HD11 | 2.54                     | 0.42              |
| 1:J:328:ILE:C    | 1:J:330:THR:H    | 2.22                     | 0.42              |
| 1:J:351:LEU:HD23 | 1:J:355:LEU:HG   | 2.01                     | 0.42              |
| 1:K:216:LEU:HA   | 1:K:216:LEU:HD12 | 1.88                     | 0.42              |
| 1:K:84:ALA:O     | 1:K:85:GLU:C     | 2.58                     | 0.42              |
| 1:L:272:LYS:HZ3  | 1:L:311:TRP:HH2  | 1.58                     | 0.42              |
| 1:L:55:SER:HA    | 1:L:58:GLU:OE2   | 2.19                     | 0.42              |
| 1:A:317:SER:N    | 1:A:318:PRO:CD   | 2.83                     | 0.42              |
| 1:B:374:VAL:HG23 | 1:B:375:MET:HG3  | 2.02                     | 0.42              |
| 1:B:37:ILE:CD1   | 1:B:45:ALA:HB2   | 2.50                     | 0.42              |
| 1:C:114:ARG:HH12 | 1:C:410:GLY:CA   | 2.32                     | 0.42              |
| 1:D:320:ILE:HG22 | 1:D:321:ARG:N    | 2.34                     | 0.42              |
| 1:E:124:PHE:HD2  | 1:E:252:LYS:HB2  | 1.84                     | 0.42              |
| 1:E:131:PRO:HG3  | 1:E:211:ILE:HD11 | 2.01                     | 0.42              |
| 1:E:80:PHE:CD1   | 1:E:80:PHE:N     | 2.88                     | 0.42              |
| 1:E:80:PHE:HA    | 1:E:81:PRO:HD3   | 1.85                     | 0.42              |
| 1:F:430:THR:CG2  | 1:L:300:VAL:HG11 | 2.48                     | 0.42              |
| 1:F:54:GLY:HA3   | 1:F:68:MET:HE2   | 2.02                     | 0.42              |
| 1:F:9:ILE:HG13   | 1:F:74:LEU:CD1   | 2.50                     | 0.42              |
| 1:E:163:ASP:OD1  | 1:F:89:VAL:HG21  | 2.19                     | 0.42              |
| 1:G:191:ALA:HB3  | 1:G:194:GLN:NE2  | 2.33                     | 0.42              |
| 1:G:256:ASN:O    | 1:G:258:PHE:N    | 2.52                     | 0.42              |
| 1:G:402:ASN:OD1  | 1:G:405:MET:HG2  | 2.19                     | 0.42              |
| 1:G:54:GLY:HA3   | 1:G:68:MET:CE    | 2.49                     | 0.42              |
| 1:H:267:LEU:HD21 | 1:H:326:ARG:HH12 | 1.82                     | 0.42              |
| 1:I:156:TYR:C    | 1:I:158:ASP:N    | 2.72                     | 0.42              |
| 1:I:208:CYS:CA   | 1:I:211:ILE:HG12 | 2.49                     | 0.42              |
| 1:J:115:ILE:HG22 | 1:J:115:ILE:O    | 2.19                     | 0.42              |
| 1:E:297:LYS:HD2  | 1:K:431:GLN:O    | 2.19                     | 0.42              |
| 1:F:436:GLU:CD   | 1:L:297:LYS:HE3  | 2.40                     | 0.42              |
| 1:L:58:GLU:HB3   | 1:L:61:VAL:HG23  | 2.01                     | 0.42              |
| 1:A:140:LEU:HD12 | 1:A:226:GLY:HA2  | 2.01                     | 0.42              |
| 1:A:168:CYS:O    | 1:A:170:ARG:N    | 2.53                     | 0.42              |
| 1:A:256:ASN:OD1  | 1:A:258:PHE:HB2  | 2.19                     | 0.42              |
| 1:A:381:MET:CE   | 1:A:381:MET:HA   | 2.49                     | 0.42              |
| 1:B:264:ASP:C    | 1:B:266:GLN:N    | 2.73                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:275:ILE:O    | 1:B:279:VAL:HG23 | 2.20                     | 0.42              |
| 1:B:76:THR:O     | 1:B:78:VAL:HG23  | 2.20                     | 0.42              |
| 1:B:18:VAL:HG11  | 1:B:90:ALA:CB    | 2.49                     | 0.42              |
| 1:C:281:HIS:ND1  | 1:C:353:ALA:HA   | 2.35                     | 0.42              |
| 1:C:70:LEU:HA    | 1:C:70:LEU:HD12  | 1.88                     | 0.42              |
| 1:D:110:ASN:O    | 1:D:113:LYS:HB2  | 2.19                     | 0.42              |
| 1:D:319:LEU:HD12 | 1:D:336:SER:CB   | 2.48                     | 0.42              |
| 1:D:412:HIS:O    | 1:D:413:LEU:C    | 2.58                     | 0.42              |
| 1:E:396:LEU:O    | 1:E:400:LYS:HG3  | 2.19                     | 0.42              |
| 1:E:20:TYR:HB3   | 1:E:89:VAL:HG22  | 2.01                     | 0.42              |
| 1:F:281:HIS:O    | 1:F:282:ALA:C    | 2.58                     | 0.42              |
| 1:F:285:PHE:C    | 1:F:285:PHE:CD1  | 2.93                     | 0.42              |
| 1:F:410:GLY:O    | 1:F:411:GLU:C    | 2.57                     | 0.42              |
| 1:G:138:PHE:HB3  | 1:G:147:THR:O    | 2.18                     | 0.42              |
| 1:G:148:LEU:HD22 | 1:G:148:LEU:H    | 1.84                     | 0.42              |
| 1:G:267:LEU:O    | 1:G:268:SER:O    | 2.38                     | 0.42              |
| 1:G:57:ILE:C     | 1:G:59:GLY:N     | 2.72                     | 0.42              |
| 1:H:41:GLN:HE22  | 1:I:200:LYS:HZ3  | 1.66                     | 0.42              |
| 1:J:37:ILE:HG13  | 1:J:41:GLN:CB    | 2.49                     | 0.42              |
| 1:L:173:VAL:HG22 | 1:L:197:ILE:HD13 | 2.02                     | 0.42              |
| 1:L:85:GLU:N     | 1:L:85:GLU:CD    | 2.73                     | 0.42              |
| 1:C:76:THR:O     | 1:C:78:VAL:HG23  | 2.19                     | 0.42              |
| 1:D:260:ASP:OD1  | 1:D:263:ALA:HB2  | 2.20                     | 0.42              |
| 1:E:162:THR:HG22 | 1:E:163:ASP:N    | 2.35                     | 0.42              |
| 1:E:172:ILE:O    | 1:E:176:LEU:HG   | 2.19                     | 0.42              |
| 1:E:296:TYR:HB3  | 1:E:390:ALA:O    | 2.19                     | 0.42              |
| 1:F:280:LYS:HE2  | 1:F:281:HIS:HE2  | 1.84                     | 0.42              |
| 1:F:426:ASP:O    | 1:F:430:THR:HG23 | 2.19                     | 0.42              |
| 1:F:434:PRO:HD2  | 4:L:607:HOH:O    | 2.19                     | 0.42              |
| 1:G:410:GLY:O    | 1:G:412:HIS:N    | 2.53                     | 0.42              |
| 1:H:3:LYS:HG2    | 1:H:4:TYR:CE1    | 2.54                     | 0.42              |
| 1:J:310:ALA:HB2  | 1:J:385:ILE:HG22 | 2.01                     | 0.42              |
| 1:J:326:ARG:HB3  | 1:J:327:GLY:H    | 1.67                     | 0.42              |
| 1:J:9:ILE:HG13   | 1:J:74:LEU:CD1   | 2.41                     | 0.42              |
| 1:K:258:PHE:HA   | 1:K:271:ALA:HB2  | 2.01                     | 0.42              |
| 1:L:126:ASP:HB2  | 1:L:251:PHE:HB2  | 2.00                     | 0.42              |
| 1:L:399:PHE:CD2  | 1:L:418:ILE:HD11 | 2.50                     | 0.42              |
| 1:A:264:ASP:C    | 1:A:266:GLN:N    | 2.73                     | 0.42              |
| 1:B:168:CYS:O    | 1:B:172:ILE:HG13 | 2.19                     | 0.42              |
| 1:B:18:VAL:HG12  | 1:B:21:ILE:CD1   | 2.49                     | 0.42              |
| 1:B:400:LYS:HB2  | 1:B:400:LYS:HE3  | 1.80                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:142:GLU:N    | 1:E:142:GLU:CD   | 2.73                     | 0.42              |
| 1:E:306:PRO:HB3  | 1:E:319:LEU:CA   | 2.48                     | 0.42              |
| 1:H:264:ASP:N    | 1:H:264:ASP:OD2  | 2.52                     | 0.42              |
| 1:I:257:ALA:O    | 1:I:270:THR:HB   | 2.20                     | 0.42              |
| 1:J:282:ALA:HA   | 1:J:285:PHE:CE1  | 2.54                     | 0.42              |
| 1:J:291:PRO:HG2  | 1:J:292:THR:H    | 1.84                     | 0.42              |
| 1:K:163:ASP:O    | 1:K:164:LEU:HD23 | 2.20                     | 0.42              |
| 1:L:146:PRO:HB3  | 1:L:228:HIS:CD2  | 2.55                     | 0.42              |
| 1:A:13:VAL:HG11  | 1:A:42:LEU:HD22  | 2.01                     | 0.42              |
| 1:A:216:LEU:HA   | 1:A:216:LEU:HD12 | 1.75                     | 0.42              |
| 1:A:264:ASP:C    | 1:A:265:LEU:HD12 | 2.40                     | 0.42              |
| 1:A:341:ALA:HB1  | 1:A:346:ALA:HB2  | 2.02                     | 0.42              |
| 1:A:273:HIS:NE2  | 1:A:361:LYS:HA   | 2.33                     | 0.42              |
| 1:B:137:LEU:HD23 | 1:B:229:ALA:HA   | 2.02                     | 0.42              |
| 1:B:274:PHE:O    | 1:B:278:ILE:HD13 | 2.20                     | 0.42              |
| 1:C:430:THR:HG22 | 1:I:300:VAL:HG11 | 2.01                     | 0.42              |
| 1:D:318:PRO:HG2  | 1:D:320:ILE:O    | 2.19                     | 0.42              |
| 1:E:136:PHE:HE2  | 1:E:194:GLN:HB2  | 1.81                     | 0.42              |
| 1:E:30:GLY:CA    | 1:E:342:ASN:ND2  | 2.83                     | 0.42              |
| 1:F:224:LYS:HD2  | 1:F:225:HIS:CD2  | 2.55                     | 0.42              |
| 1:G:20:TYR:HB3   | 1:G:89:VAL:HG22  | 2.01                     | 0.42              |
| 1:G:32:ILE:HG21  | 1:G:216:LEU:HD13 | 2.01                     | 0.42              |
| 1:G:417:PHE:O    | 1:G:418:ILE:C    | 2.58                     | 0.42              |
| 1:G:421:LYS:CD   | 1:G:424:GLU:OE2  | 2.66                     | 0.42              |
| 1:H:248:LEU:HD21 | 1:H:347:LEU:HD11 | 2.00                     | 0.42              |
| 1:I:426:ASP:OD1  | 1:I:429:ARG:NH1  | 2.52                     | 0.42              |
| 1:J:258:PHE:HZ   | 1:J:274:PHE:CD1  | 2.37                     | 0.42              |
| 1:J:400:LYS:HA   | 1:J:414:PHE:CZ   | 2.55                     | 0.42              |
| 1:K:115:ILE:O    | 1:K:118:GLU:HB2  | 2.20                     | 0.42              |
| 1:L:19:LYS:HA    | 1:L:39:VAL:CG1   | 2.49                     | 0.42              |
| 1:L:355:LEU:HD23 | 1:L:355:LEU:HA   | 1.77                     | 0.42              |
| 1:B:150:LEU:CD1  | 1:B:192:PRO:HB2  | 2.50                     | 0.42              |
| 1:B:253:ASN:O    | 1:B:255:VAL:HG23 | 2.20                     | 0.42              |
| 1:B:282:ALA:HA   | 1:B:285:PHE:CE1  | 2.55                     | 0.42              |
| 1:B:317:SER:HB2  | 1:B:335:ARG:HH22 | 1.84                     | 0.42              |
| 1:B:28:ILE:HD11  | 1:B:417:PHE:HB2  | 2.02                     | 0.42              |
| 1:B:62:ARG:O     | 1:B:62:ARG:HG3   | 2.20                     | 0.42              |
| 1:C:206:ARG:HG3  | 4:C:604:HOH:O    | 2.19                     | 0.42              |
| 1:C:209:ASP:O    | 1:C:212:GLN:HB2  | 2.20                     | 0.42              |
| 1:C:372:ILE:O    | 1:C:380:ARG:HD3  | 2.20                     | 0.42              |
| 1:E:12:LEU:HA    | 1:E:15:GLU:OE1   | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:53:ASP:OD1   | 1:E:65:GLU:HG3   | 2.20                     | 0.42              |
| 1:E:9:ILE:HG13   | 1:E:74:LEU:CD1   | 2.29                     | 0.42              |
| 1:F:22:ARG:NH1   | 1:F:22:ARG:HG2   | 2.34                     | 0.42              |
| 1:F:9:ILE:HD12   | 1:F:77:PHE:CG    | 2.55                     | 0.42              |
| 1:H:258:PHE:CA   | 1:H:271:ALA:HB2  | 2.50                     | 0.42              |
| 1:I:137:LEU:HD23 | 1:I:229:ALA:HA   | 2.02                     | 0.42              |
| 1:J:208:CYS:HA   | 1:J:211:ILE:HD12 | 2.01                     | 0.42              |
| 1:J:267:LEU:CD2  | 1:J:326:ARG:HH12 | 2.33                     | 0.42              |
| 1:J:368:ILE:HD11 | 1:J:384:GLY:O    | 2.20                     | 0.42              |
| 1:K:169:ARG:HG3  | 1:K:169:ARG:NH2  | 2.34                     | 0.42              |
| 1:E:431:GLN:HG2  | 1:K:435:TRP:CD1  | 2.54                     | 0.42              |
| 1:L:32:ILE:CD1   | 1:L:216:LEU:HD22 | 2.50                     | 0.42              |
| 1:L:35:VAL:O     | 1:L:35:VAL:HG23  | 2.20                     | 0.42              |
| 1:L:399:PHE:CE1  | 1:L:405:MET:HB3  | 2.55                     | 0.42              |
| 1:A:129:LEU:HD22 | 1:A:130:GLY:N    | 2.34                     | 0.42              |
| 1:A:167:ASN:C    | 1:A:167:ASN:HD22 | 2.22                     | 0.42              |
| 1:A:383:ASN:C    | 1:A:385:ILE:H    | 2.22                     | 0.42              |
| 1:A:52:PHE:HZ    | 1:A:57:ILE:HD11  | 1.85                     | 0.42              |
| 1:B:141:ASP:OD2  | 1:B:141:ASP:C    | 2.59                     | 0.42              |
| 1:B:52:PHE:CD1   | 1:B:70:LEU:HD13  | 2.55                     | 0.42              |
| 1:C:39:VAL:C     | 1:C:41:GLN:H     | 2.23                     | 0.42              |
| 1:C:52:PHE:CZ    | 1:C:54:GLY:HA2   | 2.54                     | 0.42              |
| 1:D:11:LYS:CG    | 1:D:15:GLU:OE2   | 2.67                     | 0.42              |
| 1:E:259:PHE:CE2  | 1:E:326:ARG:HD3  | 2.55                     | 0.42              |
| 1:E:441:MET:HG3  | 1:E:441:MET:O    | 2.19                     | 0.42              |
| 1:E:67:ASP:C     | 1:E:68:MET:HG2   | 2.40                     | 0.42              |
| 1:F:108:PRO:O    | 1:F:111:ASN:N    | 2.53                     | 0.42              |
| 1:G:137:LEU:O    | 1:G:151:ASN:HB3  | 2.19                     | 0.42              |
| 1:H:380:ARG:CZ   | 1:H:380:ARG:HB2  | 2.50                     | 0.42              |
| 1:I:223:ARG:O    | 1:I:226:GLY:N    | 2.53                     | 0.42              |
| 1:C:300:VAL:HG21 | 1:I:430:THR:HG22 | 2.01                     | 0.42              |
| 1:J:191:ALA:HB3  | 1:J:194:GLN:NE2  | 2.34                     | 0.42              |
| 1:J:260:ASP:OD1  | 1:J:263:ALA:HB2  | 2.20                     | 0.42              |
| 1:K:112:LEU:HD12 | 1:K:205:VAL:HG22 | 2.02                     | 0.42              |
| 1:K:264:ASP:C    | 1:K:266:GLN:N    | 2.74                     | 0.42              |
| 1:K:315:ASN:HD22 | 1:K:315:ASN:HA   | 1.58                     | 0.42              |
| 1:K:37:ILE:HD12  | 1:K:38:PRO:O     | 2.20                     | 0.42              |
| 1:L:163:ASP:HA   | 1:L:167:ASN:HD22 | 1.85                     | 0.42              |
| 1:L:437:ARG:HD2  | 4:L:622:HOH:O    | 2.18                     | 0.42              |
| 1:A:354:GLY:O    | 1:A:358:ILE:HG12 | 2.20                     | 0.41              |
| 1:A:58:GLU:H     | 1:A:58:GLU:HG2   | 1.66                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:83:THR:HG23  | 1:A:83:THR:O     | 2.20                     | 0.41              |
| 1:B:155:GLY:H    | 1:B:158:ASP:CG   | 2.23                     | 0.41              |
| 1:B:373:TYR:N    | 1:B:373:TYR:CD2  | 2.88                     | 0.41              |
| 1:C:137:LEU:HD12 | 1:C:195:HIS:HE2  | 1.85                     | 0.41              |
| 1:C:283:THR:HG21 | 1:C:386:VAL:HG12 | 2.02                     | 0.41              |
| 1:C:9:ILE:HD11   | 1:C:74:LEU:HB3   | 2.01                     | 0.41              |
| 1:C:78:VAL:HB    | 1:C:91:ARG:HG3   | 2.02                     | 0.41              |
| 1:D:146:PRO:CG   | 1:D:228:HIS:CD2  | 3.03                     | 0.41              |
| 1:E:141:ASP:OD2  | 1:E:144:GLY:N    | 2.53                     | 0.41              |
| 1:E:34:ASN:OD1   | 1:E:35:VAL:N     | 2.53                     | 0.41              |
| 1:E:380:ARG:HB3  | 1:E:380:ARG:HH11 | 1.85                     | 0.41              |
| 1:F:143:LYS:HE3  | 1:F:143:LYS:HB2  | 1.88                     | 0.41              |
| 1:F:175:GLU:O    | 1:F:179:MET:HG3  | 2.20                     | 0.41              |
| 1:F:282:ALA:HA   | 1:F:285:PHE:CZ   | 2.55                     | 0.41              |
| 1:F:296:TYR:HB3  | 1:F:390:ALA:O    | 2.19                     | 0.41              |
| 1:F:52:PHE:CE2   | 1:F:54:GLY:HA2   | 2.54                     | 0.41              |
| 1:F:4:TYR:CB     | 1:F:9:ILE:HD11   | 2.47                     | 0.41              |
| 1:G:250:LEU:HB3  | 1:G:257:ALA:HB3  | 2.02                     | 0.41              |
| 1:H:3:LYS:HB2    | 1:H:75:ASN:OD1   | 2.20                     | 0.41              |
| 1:I:183:ILE:HD13 | 1:I:197:ILE:CG2  | 2.50                     | 0.41              |
| 1:I:285:PHE:HB3  | 1:I:405:MET:SD   | 2.60                     | 0.41              |
| 1:J:131:PRO:HG2  | 1:J:211:ILE:CG1  | 2.50                     | 0.41              |
| 1:J:312:SER:HB3  | 1:J:315:ASN:HB2  | 2.02                     | 0.41              |
| 1:K:360:ASN:N    | 1:K:360:ASN:ND2  | 2.68                     | 0.41              |
| 1:K:380:ARG:CB   | 1:K:385:ILE:HD12 | 2.48                     | 0.41              |
| 1:K:98:ASN:HB3   | 1:K:100:ASP:OD2  | 2.19                     | 0.41              |
| 1:L:175:GLU:HA   | 1:L:175:GLU:OE2  | 2.20                     | 0.41              |
| 1:L:311:TRP:CG   | 1:L:311:TRP:O    | 2.73                     | 0.41              |
| 1:B:103:PRO:HB3  | 1:B:110:ASN:ND2  | 2.35                     | 0.41              |
| 1:B:309:VAL:CG2  | 1:B:386:VAL:HG13 | 2.50                     | 0.41              |
| 1:C:164:LEU:HD23 | 1:C:164:LEU:C    | 2.40                     | 0.41              |
| 1:C:360:ASN:O    | 1:C:361:LYS:C    | 2.57                     | 0.41              |
| 1:C:370:ARG:HB3  | 1:C:371:ASN:H    | 1.63                     | 0.41              |
| 1:D:259:PHE:HB2  | 1:D:330:THR:OG1  | 2.20                     | 0.41              |
| 1:E:85:GLU:H     | 1:E:85:GLU:CD    | 2.16                     | 0.41              |
| 1:F:133:PRO:HG2  | 1:F:199:PHE:CE1  | 2.55                     | 0.41              |
| 1:F:342:ASN:CB   | 1:F:345:LEU:HD12 | 2.50                     | 0.41              |
| 1:H:112:LEU:HD12 | 1:H:344:TYR:HA   | 2.02                     | 0.41              |
| 1:H:328:ILE:N    | 1:H:328:ILE:CD1  | 2.81                     | 0.41              |
| 1:I:116:LEU:HA   | 1:I:116:LEU:HD23 | 1.93                     | 0.41              |
| 1:H:86:LYS:HG3   | 1:I:174:LEU:HB3  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:293:VAL:HG11 | 1:I:428:PHE:CG   | 2.54                     | 0.41              |
| 1:J:9:ILE:O      | 1:J:13:VAL:HG23  | 2.19                     | 0.41              |
| 1:J:16:GLU:HA    | 1:J:16:GLU:OE2   | 2.20                     | 0.41              |
| 1:J:139:LYS:HA   | 1:J:227:LEU:HD23 | 2.02                     | 0.41              |
| 1:J:291:PRO:O    | 1:J:392:LEU:HD13 | 2.20                     | 0.41              |
| 1:J:393:ALA:HB2  | 1:J:425:TRP:CE2  | 2.56                     | 0.41              |
| 1:K:27:ASP:HA    | 1:K:57:ILE:HG23  | 2.02                     | 0.41              |
| 1:L:276:ALA:O    | 1:L:279:VAL:HB   | 2.20                     | 0.41              |
| 1:L:368:ILE:HG21 | 1:L:372:ILE:HG21 | 2.01                     | 0.41              |
| 1:A:119:MET:CE   | 1:A:127:PHE:HB2  | 2.50                     | 0.41              |
| 1:A:230:THR:OG1  | 1:A:232:MET:HB2  | 2.20                     | 0.41              |
| 1:A:234:LYS:HE3  | 1:A:239:VAL:O    | 2.20                     | 0.41              |
| 1:A:274:PHE:CE2  | 1:A:278:ILE:HD11 | 2.55                     | 0.41              |
| 1:B:405:MET:O    | 1:B:406:VAL:C    | 2.58                     | 0.41              |
| 1:C:338:ASP:OD2  | 1:C:340:ALA:HB3  | 2.20                     | 0.41              |
| 1:C:364:ALA:HB1  | 1:C:365:PRO:HD2  | 2.03                     | 0.41              |
| 1:D:289:THR:C    | 1:D:290:ASN:ND2  | 2.73                     | 0.41              |
| 1:D:248:LEU:HD11 | 1:D:350:LEU:HD13 | 2.02                     | 0.41              |
| 1:D:378:GLU:OE2  | 1:D:381:MET:HE3  | 2.21                     | 0.41              |
| 1:E:150:LEU:HD13 | 1:E:192:PRO:HG2  | 2.02                     | 0.41              |
| 1:E:80:PHE:HD2   | 1:E:82:TRP:CZ3   | 2.38                     | 0.41              |
| 1:A:86:LYS:HG3   | 1:F:174:LEU:HB3  | 2.01                     | 0.41              |
| 1:F:133:PRO:CG   | 1:F:199:PHE:HE1  | 2.33                     | 0.41              |
| 1:F:200:LYS:O    | 1:F:201:TYR:C    | 2.58                     | 0.41              |
| 1:F:129:LEU:O    | 1:F:201:TYR:HA   | 2.21                     | 0.41              |
| 1:F:36:GLU:H     | 1:F:36:GLU:HG2   | 1.67                     | 0.41              |
| 1:G:211:ILE:HG22 | 1:G:215:LYS:HE3  | 2.03                     | 0.41              |
| 1:K:116:LEU:HD23 | 1:K:116:LEU:HA   | 1.90                     | 0.41              |
| 1:L:172:ILE:O    | 1:L:176:LEU:HG   | 2.20                     | 0.41              |
| 1:L:282:ALA:HA   | 1:L:285:PHE:CE1  | 2.56                     | 0.41              |
| 1:L:314:GLN:HA   | 1:L:314:GLN:HE21 | 1.85                     | 0.41              |
| 1:A:286:THR:HG21 | 1:A:389:PRO:HD2  | 2.03                     | 0.41              |
| 1:A:300:VAL:HG22 | 1:G:429:ARG:NH1  | 2.33                     | 0.41              |
| 1:B:309:VAL:HG21 | 1:B:386:VAL:HG13 | 2.02                     | 0.41              |
| 1:C:135:PHE:HB3  | 1:C:231:PHE:CE1  | 2.55                     | 0.41              |
| 1:C:189:GLU:HA   | 1:C:189:GLU:OE2  | 2.18                     | 0.41              |
| 1:D:381:MET:HG2  | 4:D:605:HOH:O    | 2.20                     | 0.41              |
| 1:E:297:LYS:HD3  | 1:K:429:ARG:O    | 2.19                     | 0.41              |
| 1:E:405:MET:O    | 1:E:408:ALA:N    | 2.47                     | 0.41              |
| 1:E:23:LEU:HB3   | 1:E:70:LEU:HD23  | 2.02                     | 0.41              |
| 1:E:73:ASP:OD2   | 1:E:76:THR:HG23  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:319:LEU:CD1  | 1:F:336:SER:HB3  | 2.47                     | 0.41              |
| 1:F:80:PHE:HB3   | 1:F:82:TRP:CE3   | 2.55                     | 0.41              |
| 1:A:440:TYR:OH   | 1:G:293:VAL:HG23 | 2.21                     | 0.41              |
| 1:H:137:LEU:HD12 | 1:H:195:HIS:NE2  | 2.35                     | 0.41              |
| 1:B:436:GLU:CD   | 1:H:297:LYS:HE3  | 2.40                     | 0.41              |
| 1:H:310:ALA:HB1  | 1:H:368:ILE:CG1  | 2.47                     | 0.41              |
| 1:H:418:ILE:O    | 1:H:422:GLU:HG3  | 2.21                     | 0.41              |
| 1:J:271:ALA:O    | 1:J:274:PHE:HB3  | 2.21                     | 0.41              |
| 1:K:289:THR:C    | 1:K:290:ASN:ND2  | 2.74                     | 0.41              |
| 1:L:105:GLU:OE1  | 1:L:105:GLU:O    | 2.37                     | 0.41              |
| 1:L:141:ASP:OD2  | 1:L:144:GLY:N    | 2.53                     | 0.41              |
| 1:A:234:LYS:HB3  | 1:A:294:ASN:ND2  | 2.35                     | 0.41              |
| 1:A:296:TYR:HB3  | 1:A:390:ALA:O    | 2.20                     | 0.41              |
| 1:B:260:ASP:HB2  | 1:B:268:SER:HA   | 2.01                     | 0.41              |
| 1:B:30:GLY:H     | 1:B:342:ASN:HD22 | 1.69                     | 0.41              |
| 1:B:280:LYS:HD2  | 1:B:362:LEU:CD2  | 2.51                     | 0.41              |
| 1:C:232:MET:HA   | 1:C:233:PRO:HD3  | 1.86                     | 0.41              |
| 1:C:291:PRO:O    | 1:C:392:LEU:HD13 | 2.20                     | 0.41              |
| 1:C:321:ARG:HB2  | 1:C:335:ARG:HD2  | 2.03                     | 0.41              |
| 1:C:345:LEU:CD2  | 1:C:413:LEU:HD13 | 2.50                     | 0.41              |
| 1:D:163:ASP:OD1  | 1:E:89:VAL:HG21  | 2.20                     | 0.41              |
| 1:D:164:LEU:HD11 | 1:E:224:LYS:NZ   | 2.35                     | 0.41              |
| 1:D:169:ARG:O    | 1:D:170:ARG:C    | 2.58                     | 0.41              |
| 1:D:6:ARG:O      | 1:D:6:ARG:HD3    | 2.21                     | 0.41              |
| 1:D:71:TYR:C     | 1:D:94:CYS:HB3   | 2.41                     | 0.41              |
| 1:E:439:GLN:HB2  | 1:E:440:TYR:H    | 1.72                     | 0.41              |
| 1:F:279:VAL:HG13 | 1:F:309:VAL:HG12 | 2.02                     | 0.41              |
| 1:F:281:HIS:HE1  | 1:F:356:ASP:OD2  | 2.04                     | 0.41              |
| 1:G:23:LEU:O     | 1:G:35:VAL:HG12  | 2.20                     | 0.41              |
| 1:J:250:LEU:HB2  | 1:J:258:PHE:CZ   | 2.56                     | 0.41              |
| 1:J:319:LEU:HD23 | 1:J:320:ILE:HG12 | 2.02                     | 0.41              |
| 1:J:404:VAL:O    | 1:J:408:ALA:N    | 2.52                     | 0.41              |
| 1:K:143:LYS:O    | 1:K:144:GLY:C    | 2.57                     | 0.41              |
| 1:K:247:ASN:HB3  | 1:K:331:ARG:CG   | 2.47                     | 0.41              |
| 1:K:252:LYS:O    | 1:K:252:LYS:HD2  | 2.20                     | 0.41              |
| 1:K:33:LYS:HA    | 1:L:158:ASP:CA   | 2.38                     | 0.41              |
| 1:K:73:ASP:O     | 1:K:74:LEU:C     | 2.58                     | 0.41              |
| 1:K:72:PRO:HA    | 1:K:94:CYS:HB3   | 2.03                     | 0.41              |
| 1:L:186:SER:O    | 1:L:187:HIS:HB3  | 2.20                     | 0.41              |
| 1:A:119:MET:HG2  | 1:A:124:PHE:HB2  | 2.01                     | 0.41              |
| 1:A:327:GLY:C    | 1:A:329:SER:H    | 2.23                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:351:LEU:HD22 | 1:B:355:LEU:HG   | 2.02                     | 0.41              |
| 1:C:129:LEU:HD23 | 1:C:130:GLY:N    | 2.36                     | 0.41              |
| 1:C:377:LYS:O    | 1:C:381:MET:HE2  | 2.20                     | 0.41              |
| 1:D:65:GLU:HG3   | 1:D:65:GLU:O     | 2.20                     | 0.41              |
| 1:F:146:PRO:HG3  | 1:F:228:HIS:HD2  | 1.75                     | 0.41              |
| 1:F:170:ARG:HG2  | 1:F:170:ARG:HH11 | 1.85                     | 0.41              |
| 1:F:150:LEU:HD22 | 1:F:192:PRO:O    | 2.21                     | 0.41              |
| 1:F:221:ILE:O    | 1:F:225:HIS:CD2  | 2.73                     | 0.41              |
| 1:F:41:GLN:HB3   | 1:F:41:GLN:HE21  | 1.59                     | 0.41              |
| 1:F:82:TRP:HH2   | 1:F:217:VAL:HG22 | 1.85                     | 0.41              |
| 1:G:131:PRO:HG2  | 1:G:199:PHE:CE1  | 2.55                     | 0.41              |
| 1:G:32:ILE:HG21  | 1:G:216:LEU:CD1  | 2.51                     | 0.41              |
| 1:I:212:GLN:OE1  | 1:I:212:GLN:HA   | 2.21                     | 0.41              |
| 1:I:9:ILE:CG1    | 1:I:74:LEU:HD12  | 2.50                     | 0.41              |
| 1:J:102:THR:HA   | 1:J:103:PRO:HD3  | 1.92                     | 0.41              |
| 1:J:135:PHE:N    | 1:J:135:PHE:CD1  | 2.88                     | 0.41              |
| 1:J:319:LEU:O    | 1:J:320:ILE:HD13 | 2.20                     | 0.41              |
| 1:J:85:GLU:O     | 1:J:87:GLY:N     | 2.43                     | 0.41              |
| 1:K:58:GLU:OE1   | 1:K:416:HIS:NE2  | 2.53                     | 0.41              |
| 1:K:67:ASP:N     | 1:K:67:ASP:OD2   | 2.53                     | 0.41              |
| 1:L:320:ILE:HG22 | 1:L:321:ARG:N    | 2.35                     | 0.41              |
| 1:A:117:LYS:C    | 1:A:119:MET:N    | 2.74                     | 0.41              |
| 1:D:383:ASN:HD22 | 1:D:383:ASN:HA   | 1.60                     | 0.41              |
| 1:E:151:ASN:HD22 | 1:E:166:GLU:CD   | 2.24                     | 0.41              |
| 1:E:91:ARG:CZ    | 1:E:93:ILE:HD11  | 2.51                     | 0.41              |
| 1:E:96:ILE:HD13  | 1:E:107:ASP:OD1  | 2.21                     | 0.41              |
| 1:G:306:PRO:HG2  | 1:G:335:ARG:HB2  | 2.02                     | 0.41              |
| 1:I:248:LEU:HD13 | 1:I:332:VAL:HG23 | 2.02                     | 0.41              |
| 1:J:114:ARG:NH1  | 1:J:115:ILE:HD11 | 2.35                     | 0.41              |
| 1:K:423:ILE:O    | 1:K:427:MET:HG3  | 2.20                     | 0.41              |
| 1:K:46:LEU:C     | 1:K:48:ASN:H     | 2.24                     | 0.41              |
| 1:L:129:LEU:HD22 | 1:L:131:PRO:HD3  | 2.02                     | 0.41              |
| 1:B:214:PHE:O    | 1:B:218:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:315:ASN:OD1  | 1:B:371:ASN:HA   | 2.21                     | 0.41              |
| 1:C:232:MET:CG   | 1:C:294:ASN:HD22 | 2.34                     | 0.41              |
| 1:C:378:GLU:OE1  | 1:C:378:GLU:N    | 2.48                     | 0.41              |
| 1:C:24:GLN:HE22  | 1:C:91:ARG:HH11  | 1.64                     | 0.41              |
| 1:E:169:ARG:O    | 1:E:171:ASP:N    | 2.54                     | 0.41              |
| 1:E:176:LEU:HD11 | 1:E:214:PHE:CD1  | 2.56                     | 0.41              |
| 1:F:205:VAL:HG13 | 1:F:206:ARG:H    | 1.85                     | 0.41              |
| 1:G:112:LEU:HD12 | 1:G:344:TYR:CD2  | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:199:PHE:N    | 1:G:199:PHE:CD1  | 2.85                     | 0.41              |
| 1:G:116:LEU:CD1  | 1:G:205:VAL:HG23 | 2.50                     | 0.41              |
| 1:G:44:LYS:HE3   | 1:G:49:LYS:O     | 2.21                     | 0.41              |
| 1:G:55:SER:CB    | 1:G:62:ARG:HE    | 2.33                     | 0.41              |
| 1:H:186:SER:HB2  | 1:H:197:ILE:HG12 | 2.02                     | 0.41              |
| 1:H:346:ALA:O    | 1:H:350:LEU:HB2  | 2.20                     | 0.41              |
| 1:I:140:LEU:HD12 | 1:I:227:LEU:N    | 2.36                     | 0.41              |
| 1:I:223:ARG:O    | 1:I:225:HIS:N    | 2.54                     | 0.41              |
| 1:I:321:ARG:HE   | 1:I:321:ARG:HB3  | 1.75                     | 0.41              |
| 1:J:134:GLU:HG2  | 1:J:196:GLU:HB2  | 2.01                     | 0.41              |
| 1:J:4:TYR:HB3    | 1:J:9:ILE:HD11   | 2.02                     | 0.41              |
| 1:J:58:GLU:O     | 1:J:59:GLY:C     | 2.58                     | 0.41              |
| 1:K:120:GLU:HA   | 1:K:124:PHE:O    | 2.19                     | 0.41              |
| 1:A:399:PHE:HZ   | 1:A:409:LEU:CD1  | 2.33                     | 0.41              |
| 1:A:429:ARG:HG3  | 1:A:429:ARG:HH11 | 1.86                     | 0.41              |
| 1:B:32:ILE:HD13  | 1:B:216:LEU:HD12 | 2.02                     | 0.41              |
| 1:D:296:TYR:N    | 1:D:296:TYR:CD1  | 2.89                     | 0.41              |
| 1:D:288:VAL:HG22 | 1:D:417:PHE:CE2  | 2.56                     | 0.41              |
| 1:E:225:HIS:O    | 1:E:227:LEU:HG   | 2.21                     | 0.41              |
| 1:E:399:PHE:CE1  | 1:E:405:MET:HB3  | 2.56                     | 0.41              |
| 1:F:275:ILE:O    | 1:F:279:VAL:HG23 | 2.20                     | 0.41              |
| 1:F:241:GLY:HA3  | 1:F:298:ARG:CG   | 2.50                     | 0.41              |
| 1:G:13:VAL:HG21  | 1:G:42:LEU:CD2   | 2.51                     | 0.41              |
| 1:H:124:PHE:CD2  | 1:H:250:LEU:HD13 | 2.56                     | 0.41              |
| 1:H:135:PHE:HB3  | 1:H:231:PHE:CE1  | 2.54                     | 0.41              |
| 1:H:397:GLU:HA   | 1:H:400:LYS:NZ   | 2.36                     | 0.41              |
| 1:I:152:ASP:OD2  | 1:I:188:HIS:NE2  | 2.39                     | 0.41              |
| 1:I:151:ASN:HD22 | 1:I:166:GLU:CD   | 2.23                     | 0.41              |
| 1:I:20:TYR:OH    | 1:I:36:GLU:HG3   | 2.20                     | 0.41              |
| 1:I:396:LEU:HD11 | 1:I:421:LYS:CB   | 2.51                     | 0.41              |
| 1:J:207:SER:O    | 1:J:209:ASP:N    | 2.53                     | 0.41              |
| 1:J:27:ASP:C     | 1:J:27:ASP:OD2   | 2.59                     | 0.41              |
| 1:J:36:GLU:H     | 1:J:36:GLU:HG2   | 1.67                     | 0.41              |
| 1:J:19:LYS:HD2   | 1:J:86:LYS:O     | 2.21                     | 0.41              |
| 1:K:141:ASP:HB3  | 1:K:147:THR:CG2  | 2.51                     | 0.41              |
| 1:K:186:SER:HB2  | 1:K:196:GLU:O    | 2.21                     | 0.41              |
| 1:K:28:ILE:HD11  | 1:K:417:PHE:N    | 2.36                     | 0.41              |
| 1:L:185:ALA:O    | 1:L:186:SER:HB2  | 2.19                     | 0.41              |
| 1:L:132:GLU:HG2  | 1:L:198:ASP:OD1  | 2.20                     | 0.41              |
| 1:L:20:TYR:CZ    | 1:L:36:GLU:HB3   | 2.56                     | 0.41              |
| 1:A:407:LYS:O    | 1:A:408:ALA:C    | 2.59                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:421:LYS:HD3  | 1:A:421:LYS:HA   | 1.89                     | 0.41              |
| 1:B:109:ARG:O    | 1:B:112:LEU:HB3  | 2.21                     | 0.41              |
| 1:B:112:LEU:O    | 1:B:116:LEU:HG   | 2.21                     | 0.41              |
| 1:B:175:GLU:O    | 1:B:179:MET:HG3  | 2.21                     | 0.41              |
| 1:B:68:MET:SD    | 1:B:96:ILE:HG22  | 2.60                     | 0.41              |
| 1:C:248:LEU:HB2  | 1:C:332:VAL:CG1  | 2.51                     | 0.41              |
| 1:D:170:ARG:O    | 1:D:174:LEU:HG   | 2.21                     | 0.41              |
| 1:D:203:GLY:O    | 1:D:205:VAL:N    | 2.54                     | 0.41              |
| 1:D:21:ILE:HD11  | 1:D:39:VAL:HA    | 2.03                     | 0.41              |
| 1:D:350:LEU:HD23 | 1:D:350:LEU:HA   | 1.87                     | 0.41              |
| 1:E:182:GLU:HA   | 1:E:182:GLU:OE1  | 2.21                     | 0.41              |
| 1:E:306:PRO:CB   | 1:E:319:LEU:HA   | 2.47                     | 0.41              |
| 1:E:371:ASN:HB3  | 1:E:375:MET:CG   | 2.51                     | 0.41              |
| 1:F:112:LEU:O    | 1:F:116:LEU:HG   | 2.21                     | 0.41              |
| 1:F:245:HIS:CD2  | 1:F:335:ARG:HA   | 2.56                     | 0.41              |
| 1:F:343:PRO:O    | 1:F:347:LEU:HD23 | 2.21                     | 0.41              |
| 1:F:378:GLU:O    | 1:F:381:MET:HG2  | 2.21                     | 0.41              |
| 1:G:20:TYR:OH    | 1:G:36:GLU:CB    | 2.69                     | 0.41              |
| 1:G:41:GLN:NE2   | 1:G:44:LYS:HD3   | 2.36                     | 0.41              |
| 1:H:393:ALA:HB2  | 1:H:425:TRP:CD2  | 2.55                     | 0.41              |
| 1:H:3:LYS:HD3    | 1:H:4:TYR:HE1    | 1.86                     | 0.41              |
| 1:I:283:THR:HG22 | 1:I:388:LEU:HD23 | 2.02                     | 0.41              |
| 1:I:418:ILE:O    | 1:I:419:GLU:C    | 2.59                     | 0.41              |
| 1:I:393:ALA:HB2  | 1:I:425:TRP:CE2  | 2.56                     | 0.41              |
| 1:J:343:PRO:O    | 1:J:347:LEU:HB2  | 2.21                     | 0.41              |
| 1:K:20:TYR:C     | 1:K:21:ILE:HD12  | 2.40                     | 0.41              |
| 1:J:64:GLU:HG2   | 1:K:315:ASN:C    | 2.42                     | 0.41              |
| 1:L:152:ASP:OD2  | 1:L:188:HIS:NE2  | 2.40                     | 0.41              |
| 1:L:91:ARG:CD    | 1:L:91:ARG:C     | 2.83                     | 0.41              |
| 1:A:28:ILE:CG2   | 1:A:29:LEU:N     | 2.83                     | 0.41              |
| 1:B:256:ASN:O    | 1:B:258:PHE:N    | 2.53                     | 0.41              |
| 1:A:156:TYR:CE2  | 1:B:62:ARG:NH1   | 2.89                     | 0.41              |
| 1:C:129:LEU:HD23 | 1:C:130:GLY:H    | 1.86                     | 0.41              |
| 1:C:169:ARG:O    | 1:C:172:ILE:HB   | 2.21                     | 0.41              |
| 1:C:286:THR:O    | 1:C:290:ASN:HB2  | 2.21                     | 0.41              |
| 1:C:301:PRO:HB3  | 1:C:308:TYR:OH   | 2.21                     | 0.41              |
| 1:C:74:LEU:HA    | 1:C:92:PHE:CE2   | 2.56                     | 0.41              |
| 1:D:443:GLN:HA   | 1:D:443:GLN:NE2  | 2.36                     | 0.41              |
| 1:E:172:ILE:HD11 | 1:E:221:ILE:HB   | 2.03                     | 0.41              |
| 1:E:436:GLU:OE1  | 1:K:297:LYS:NZ   | 2.54                     | 0.41              |
| 1:F:113:LYS:O    | 1:F:116:LEU:HB2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:262:ASN:O    | 1:F:263:ALA:HB2  | 2.21                     | 0.41              |
| 1:G:98:ASN:HD21  | 1:G:104:PHE:HA   | 1.86                     | 0.41              |
| 1:G:410:GLY:O    | 1:G:411:GLU:C    | 2.59                     | 0.41              |
| 1:H:125:SER:HB2  | 1:H:251:PHE:HB3  | 2.03                     | 0.41              |
| 1:H:355:LEU:HA   | 1:H:355:LEU:HD23 | 1.86                     | 0.41              |
| 1:I:97:TYR:HE2   | 1:I:101:GLY:O    | 2.04                     | 0.41              |
| 1:I:170:ARG:NH1  | 1:I:171:ASP:OD2  | 2.54                     | 0.41              |
| 1:I:58:GLU:CB    | 1:I:62:ARG:HB2   | 2.51                     | 0.41              |
| 1:J:306:PRO:HB3  | 1:J:319:LEU:HA   | 2.02                     | 0.41              |
| 1:J:78:VAL:HG11  | 1:J:179:MET:CE   | 2.51                     | 0.41              |
| 1:K:141:ASP:OD1  | 1:K:145:GLU:HB2  | 2.21                     | 0.41              |
| 1:K:60:PHE:HZ    | 1:K:420:ALA:O    | 2.03                     | 0.41              |
| 1:L:138:PHE:CZ   | 1:L:150:LEU:HD23 | 2.55                     | 0.41              |
| 1:L:214:PHE:O    | 1:L:215:LYS:C    | 2.57                     | 0.41              |
| 1:L:282:ALA:C    | 1:L:284:SER:H    | 2.25                     | 0.41              |
| 1:L:331:ARG:HH11 | 1:L:331:ARG:HG2  | 1.86                     | 0.41              |
| 1:A:234:LYS:HB3  | 1:A:294:ASN:HD21 | 1.86                     | 0.40              |
| 1:B:115:ILE:HD11 | 1:B:408:ALA:HA   | 2.04                     | 0.40              |
| 1:B:371:ASN:O    | 1:B:374:VAL:HG22 | 2.21                     | 0.40              |
| 1:B:281:HIS:CD2  | 1:B:404:VAL:HG21 | 2.56                     | 0.40              |
| 1:B:441:MET:O    | 1:H:228:HIS:CE1  | 2.66                     | 0.40              |
| 1:C:52:PHE:HE1   | 1:C:70:LEU:HD13  | 1.79                     | 0.40              |
| 1:D:139:LYS:O    | 1:D:147:THR:HG23 | 2.21                     | 0.40              |
| 1:D:184:GLU:OE2  | 1:D:200:LYS:NZ   | 2.50                     | 0.40              |
| 1:D:81:PRO:HA    | 4:D:619:HOH:O    | 2.21                     | 0.40              |
| 1:E:110:ASN:HA   | 1:E:110:ASN:HD22 | 1.71                     | 0.40              |
| 1:E:262:ASN:HA   | 1:E:262:ASN:HD22 | 1.55                     | 0.40              |
| 1:E:338:ASP:HB2  | 1:E:339:PRO:CD   | 2.50                     | 0.40              |
| 1:G:150:LEU:HD13 | 1:G:192:PRO:O    | 2.21                     | 0.40              |
| 1:G:156:TYR:O    | 1:G:158:ASP:N    | 2.54                     | 0.40              |
| 1:A:231:PHE:HB2  | 1:G:444:TYR:OXT  | 2.21                     | 0.40              |
| 1:H:370:ARG:NH1  | 1:H:370:ARG:CG   | 2.84                     | 0.40              |
| 1:I:258:PHE:HA   | 1:I:271:ALA:HB2  | 2.03                     | 0.40              |
| 1:I:53:ASP:C     | 1:I:53:ASP:OD2   | 2.60                     | 0.40              |
| 1:J:116:LEU:HD23 | 1:J:351:LEU:CD1  | 2.51                     | 0.40              |
| 1:J:37:ILE:HG22  | 1:K:185:ALA:HB2  | 2.03                     | 0.40              |
| 1:K:264:ASP:C    | 1:K:266:GLN:H    | 2.25                     | 0.40              |
| 1:K:258:PHE:CB   | 1:K:271:ALA:HB2  | 2.51                     | 0.40              |
| 1:K:320:ILE:HG22 | 1:K:321:ARG:N    | 2.36                     | 0.40              |
| 1:K:322:ILE:HA   | 1:K:323:PRO:HD2  | 1.95                     | 0.40              |
| 1:K:33:LYS:HA    | 1:L:159:LEU:H    | 1.86                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:203:GLY:O    | 1:L:205:VAL:N    | 2.54                     | 0.40              |
| 1:A:260:ASP:O    | 1:A:266:GLN:HA   | 2.20                     | 0.40              |
| 1:B:274:PHE:CE1  | 1:B:354:GLY:HA3  | 2.56                     | 0.40              |
| 1:B:377:LYS:HD3  | 1:B:387:ASP:OD2  | 2.20                     | 0.40              |
| 1:C:106:GLY:O    | 1:C:413:LEU:HD21 | 2.21                     | 0.40              |
| 1:C:112:LEU:HD12 | 1:C:344:TYR:CD2  | 2.51                     | 0.40              |
| 1:D:293:VAL:HG11 | 1:D:428:PHE:CD2  | 2.56                     | 0.40              |
| 1:D:45:ALA:HA    | 1:D:50:VAL:CG2   | 2.50                     | 0.40              |
| 1:D:54:GLY:C     | 1:D:56:SER:N     | 2.74                     | 0.40              |
| 1:E:273:HIS:NE2  | 1:E:361:LYS:CB   | 2.85                     | 0.40              |
| 1:E:409:LEU:HB3  | 1:E:413:LEU:HB2  | 2.03                     | 0.40              |
| 1:E:440:TYR:HD1  | 1:E:444:TYR:CE2  | 2.38                     | 0.40              |
| 1:G:167:ASN:HD22 | 1:G:170:ARG:NH1  | 2.18                     | 0.40              |
| 1:G:183:ILE:HG21 | 1:G:197:ILE:HG22 | 2.03                     | 0.40              |
| 1:G:250:LEU:CB   | 1:G:258:PHE:CZ   | 2.98                     | 0.40              |
| 1:G:375:MET:CE   | 1:G:385:ILE:HG13 | 2.51                     | 0.40              |
| 1:G:78:VAL:HG11  | 1:G:91:ARG:NH2   | 2.36                     | 0.40              |
| 1:H:404:VAL:HG13 | 1:H:405:MET:HE2  | 2.02                     | 0.40              |
| 1:I:127:PHE:CE2  | 1:I:347:LEU:HD11 | 2.56                     | 0.40              |
| 1:J:129:LEU:HD22 | 1:J:131:PRO:HD3  | 2.02                     | 0.40              |
| 1:J:389:PRO:HG3  | 1:J:395:ALA:HB2  | 2.03                     | 0.40              |
| 1:K:133:PRO:HD2  | 1:K:197:ILE:O    | 2.21                     | 0.40              |
| 1:K:377:LYS:HA   | 1:K:380:ARG:CZ   | 2.52                     | 0.40              |
| 1:K:60:PHE:CD1   | 1:K:60:PHE:C     | 2.93                     | 0.40              |
| 1:L:110:ASN:HA   | 1:L:110:ASN:HD22 | 1.66                     | 0.40              |
| 1:L:374:VAL:HG12 | 1:L:374:VAL:O    | 2.21                     | 0.40              |
| 1:B:338:ASP:HB2  | 1:B:339:PRO:CD   | 2.47                     | 0.40              |
| 1:C:159:LEU:HA   | 1:C:159:LEU:HD12 | 1.95                     | 0.40              |
| 1:C:416:HIS:O    | 1:C:417:PHE:C    | 2.60                     | 0.40              |
| 1:D:103:PRO:HB2  | 1:D:110:ASN:OD1  | 2.22                     | 0.40              |
| 1:D:347:LEU:HD23 | 1:D:347:LEU:HA   | 1.90                     | 0.40              |
| 1:D:378:GLU:OE1  | 1:D:382:GLU:HG3  | 2.21                     | 0.40              |
| 1:E:274:PHE:CE2  | 1:E:278:ILE:HD11 | 2.56                     | 0.40              |
| 1:F:122:LEU:HD12 | 1:F:355:LEU:HD13 | 2.02                     | 0.40              |
| 1:F:351:LEU:CD2  | 1:F:355:LEU:HG   | 2.51                     | 0.40              |
| 1:G:285:PHE:CD1  | 1:G:285:PHE:C    | 2.95                     | 0.40              |
| 1:G:34:ASN:CG    | 1:H:159:LEU:HG   | 2.41                     | 0.40              |
| 1:H:243:GLY:HA2  | 1:H:338:ASP:HA   | 2.03                     | 0.40              |
| 1:I:129:LEU:HD23 | 1:I:130:GLY:N    | 2.36                     | 0.40              |
| 1:I:203:GLY:O    | 1:I:204:ALA:C    | 2.60                     | 0.40              |
| 1:L:156:TYR:C    | 1:L:158:ASP:H    | 2.24                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:296:TYR:CE1  | 1:L:392:LEU:HA   | 2.56                     | 0.40              |
| 1:L:380:ARG:NH1  | 1:L:380:ARG:CB   | 2.85                     | 0.40              |
| 1:A:402:ASN:HD21 | 1:A:404:VAL:HG12 | 1.87                     | 0.40              |
| 1:B:18:VAL:HG22  | 1:B:88:LYS:HB2   | 2.04                     | 0.40              |
| 1:C:155:GLY:O    | 1:C:158:ASP:HB2  | 2.21                     | 0.40              |
| 1:C:232:MET:HG3  | 1:C:294:ASN:HD22 | 1.87                     | 0.40              |
| 1:D:289:THR:HG22 | 1:D:337:VAL:HG13 | 2.03                     | 0.40              |
| 1:E:282:ALA:C    | 1:E:284:SER:N    | 2.73                     | 0.40              |
| 1:F:109:ARG:HE   | 1:F:205:VAL:CG2  | 2.34                     | 0.40              |
| 1:F:82:TRP:CH2   | 1:F:217:VAL:HG22 | 2.56                     | 0.40              |
| 1:G:258:PHE:O    | 1:G:330:THR:HG21 | 2.22                     | 0.40              |
| 1:G:351:LEU:CD2  | 1:G:355:LEU:HG   | 2.51                     | 0.40              |
| 1:G:370:ARG:HH22 | 1:G:383:ASN:ND2  | 2.19                     | 0.40              |
| 1:H:83:THR:O     | 1:H:83:THR:HG23  | 2.22                     | 0.40              |
| 1:I:129:LEU:O    | 1:I:131:PRO:HD3  | 2.21                     | 0.40              |
| 1:I:174:LEU:HD12 | 1:I:174:LEU:HA   | 1.90                     | 0.40              |
| 1:I:259:PHE:CD1  | 1:I:260:ASP:N    | 2.89                     | 0.40              |
| 1:J:273:HIS:CE1  | 1:J:361:LYS:HB3  | 2.57                     | 0.40              |
| 1:J:274:PHE:C    | 1:J:274:PHE:CD2  | 2.95                     | 0.40              |
| 1:K:207:SER:O    | 1:K:211:ILE:HG13 | 2.21                     | 0.40              |
| 1:K:124:PHE:CZ   | 1:K:358:ILE:HG21 | 2.56                     | 0.40              |
| 1:L:115:ILE:H    | 1:L:115:ILE:HD12 | 1.87                     | 0.40              |
| 1:L:337:VAL:HG12 | 1:L:338:ASP:N    | 2.36                     | 0.40              |
| 1:L:351:LEU:O    | 1:L:355:LEU:N    | 2.43                     | 0.40              |
| 1:A:129:LEU:CD2  | 1:A:130:GLY:N    | 2.85                     | 0.40              |
| 1:A:142:GLU:N    | 1:A:142:GLU:CD   | 2.74                     | 0.40              |
| 1:A:203:GLY:O    | 1:A:204:ALA:C    | 2.60                     | 0.40              |
| 1:A:252:LYS:O    | 1:A:253:ASN:HB2  | 2.21                     | 0.40              |
| 1:B:159:LEU:HD11 | 1:C:22:ARG:NH1   | 2.34                     | 0.40              |
| 1:B:343:PRO:O    | 1:B:347:LEU:HB2  | 2.21                     | 0.40              |
| 1:B:116:LEU:HD23 | 1:B:351:LEU:HD11 | 2.03                     | 0.40              |
| 1:C:22:ARG:HB3   | 1:C:34:ASN:HD22  | 1.86                     | 0.40              |
| 1:C:282:ALA:HA   | 1:C:285:PHE:CZ   | 2.57                     | 0.40              |
| 1:D:13:VAL:HG21  | 1:D:42:LEU:HD22  | 2.02                     | 0.40              |
| 1:E:324:ALA:O    | 1:E:325:SER:C    | 2.60                     | 0.40              |
| 1:E:429:ARG:HH11 | 1:E:429:ARG:HG3  | 1.87                     | 0.40              |
| 1:F:288:VAL:O    | 1:F:291:PRO:HD3  | 2.22                     | 0.40              |
| 1:G:183:ILE:CG2  | 1:G:197:ILE:HG22 | 2.52                     | 0.40              |
| 1:G:258:PHE:HA   | 1:G:268:SER:OG   | 2.22                     | 0.40              |
| 1:H:20:TYR:OH    | 1:H:36:GLU:CB    | 2.69                     | 0.40              |
| 1:I:355:LEU:O    | 1:I:357:GLY:N    | 2.54                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:360:ASN:O    | 1:I:361:LYS:C    | 2.60                     | 0.40              |
| 1:I:68:MET:CE    | 1:I:104:PHE:HB2  | 2.51                     | 0.40              |
| 1:J:19:LYS:HA    | 1:J:39:VAL:HB    | 2.02                     | 0.40              |
| 1:K:345:LEU:O    | 1:K:349:VAL:HG22 | 2.21                     | 0.40              |
| 1:K:406:VAL:HG22 | 1:K:414:PHE:CZ   | 2.56                     | 0.40              |
| 1:L:308:TYR:OH   | 1:L:373:TYR:HA   | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 435/443 (98%)   | 358 (82%)  | 63 (14%)  | 14 (3%)  | 5           | 25 |
| 1   | B     | 435/443 (98%)   | 367 (84%)  | 52 (12%)  | 16 (4%)  | 4           | 22 |
| 1   | C     | 434/443 (98%)   | 341 (79%)  | 67 (15%)  | 26 (6%)  | 2           | 11 |
| 1   | D     | 435/443 (98%)   | 347 (80%)  | 72 (17%)  | 16 (4%)  | 4           | 22 |
| 1   | E     | 434/443 (98%)   | 344 (79%)  | 66 (15%)  | 24 (6%)  | 2           | 13 |
| 1   | F     | 433/443 (98%)   | 345 (80%)  | 69 (16%)  | 19 (4%)  | 3           | 18 |
| 1   | G     | 434/443 (98%)   | 353 (81%)  | 58 (13%)  | 23 (5%)  | 2           | 14 |
| 1   | H     | 433/443 (98%)   | 356 (82%)  | 58 (13%)  | 19 (4%)  | 3           | 18 |
| 1   | I     | 432/443 (98%)   | 364 (84%)  | 45 (10%)  | 23 (5%)  | 2           | 14 |
| 1   | J     | 434/443 (98%)   | 342 (79%)  | 69 (16%)  | 23 (5%)  | 2           | 14 |
| 1   | K     | 434/443 (98%)   | 356 (82%)  | 56 (13%)  | 22 (5%)  | 2           | 15 |
| 1   | L     | 436/443 (98%)   | 346 (79%)  | 66 (15%)  | 24 (6%)  | 2           | 13 |
| All | All   | 5209/5316 (98%) | 4219 (81%) | 741 (14%) | 249 (5%) | 2           | 16 |

All (249) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | LYS  |
| 1   | A     | 161 | PRO  |
| 1   | A     | 166 | GLU  |
| 1   | A     | 325 | SER  |
| 1   | A     | 411 | GLU  |
| 1   | B     | 3   | LYS  |
| 1   | B     | 166 | GLU  |
| 1   | B     | 325 | SER  |
| 1   | C     | 101 | GLY  |
| 1   | C     | 166 | GLU  |
| 1   | C     | 314 | GLN  |
| 1   | C     | 369 | ASP  |
| 1   | D     | 161 | PRO  |
| 1   | D     | 163 | ASP  |
| 1   | D     | 371 | ASN  |
| 1   | E     | 166 | GLU  |
| 1   | E     | 361 | LYS  |
| 1   | E     | 369 | ASP  |
| 1   | E     | 411 | GLU  |
| 1   | F     | 84  | ALA  |
| 1   | F     | 101 | GLY  |
| 1   | F     | 161 | PRO  |
| 1   | F     | 166 | GLU  |
| 1   | F     | 190 | VAL  |
| 1   | F     | 316 | ARG  |
| 1   | G     | 3   | LYS  |
| 1   | G     | 63  | ILE  |
| 1   | G     | 78  | VAL  |
| 1   | G     | 156 | TYR  |
| 1   | G     | 166 | GLU  |
| 1   | G     | 325 | SER  |
| 1   | G     | 369 | ASP  |
| 1   | G     | 411 | GLU  |
| 1   | G     | 441 | MET  |
| 1   | H     | 125 | SER  |
| 1   | H     | 167 | ASN  |
| 1   | H     | 190 | VAL  |
| 1   | I     | 100 | ASP  |
| 1   | I     | 158 | ASP  |
| 1   | I     | 201 | TYR  |
| 1   | I     | 325 | SER  |
| 1   | J     | 3   | LYS  |
| 1   | J     | 161 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 163 | ASP  |
| 1   | J     | 325 | SER  |
| 1   | J     | 368 | ILE  |
| 1   | K     | 156 | TYR  |
| 1   | K     | 161 | PRO  |
| 1   | K     | 162 | THR  |
| 1   | K     | 166 | GLU  |
| 1   | K     | 312 | SER  |
| 1   | L     | 82  | TRP  |
| 1   | L     | 167 | ASN  |
| 1   | L     | 386 | VAL  |
| 1   | A     | 101 | GLY  |
| 1   | A     | 157 | PHE  |
| 1   | A     | 164 | LEU  |
| 1   | A     | 201 | TYR  |
| 1   | A     | 204 | ALA  |
| 1   | A     | 314 | GLN  |
| 1   | A     | 410 | GLY  |
| 1   | B     | 256 | ASN  |
| 1   | B     | 292 | THR  |
| 1   | C     | 161 | PRO  |
| 1   | C     | 163 | ASP  |
| 1   | C     | 283 | THR  |
| 1   | C     | 365 | PRO  |
| 1   | D     | 85  | GLU  |
| 1   | D     | 204 | ALA  |
| 1   | D     | 412 | HIS  |
| 1   | E     | 161 | PRO  |
| 1   | E     | 163 | ASP  |
| 1   | E     | 170 | ARG  |
| 1   | E     | 325 | SER  |
| 1   | E     | 329 | SER  |
| 1   | F     | 67  | ASP  |
| 1   | F     | 157 | PHE  |
| 1   | F     | 260 | ASP  |
| 1   | G     | 58  | GLU  |
| 1   | G     | 157 | PHE  |
| 1   | G     | 161 | PRO  |
| 1   | G     | 256 | ASN  |
| 1   | G     | 257 | ALA  |
| 1   | G     | 268 | SER  |
| 1   | G     | 361 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 163 | ASP  |
| 1   | H     | 260 | ASP  |
| 1   | H     | 325 | SER  |
| 1   | H     | 371 | ASN  |
| 1   | I     | 3   | LYS  |
| 1   | I     | 157 | PHE  |
| 1   | I     | 161 | PRO  |
| 1   | I     | 166 | GLU  |
| 1   | I     | 167 | ASN  |
| 1   | I     | 260 | ASP  |
| 1   | I     | 283 | THR  |
| 1   | I     | 361 | LYS  |
| 1   | I     | 372 | ILE  |
| 1   | I     | 376 | SER  |
| 1   | I     | 441 | MET  |
| 1   | J     | 81  | PRO  |
| 1   | J     | 190 | VAL  |
| 1   | J     | 268 | SER  |
| 1   | J     | 291 | PRO  |
| 1   | J     | 292 | THR  |
| 1   | K     | 85  | GLU  |
| 1   | K     | 368 | ILE  |
| 1   | L     | 74  | LEU  |
| 1   | L     | 83  | THR  |
| 1   | L     | 101 | GLY  |
| 1   | L     | 157 | PHE  |
| 1   | L     | 166 | GLU  |
| 1   | L     | 204 | ALA  |
| 1   | L     | 325 | SER  |
| 1   | L     | 368 | ILE  |
| 1   | B     | 121 | ASP  |
| 1   | B     | 124 | PHE  |
| 1   | B     | 161 | PRO  |
| 1   | B     | 204 | ALA  |
| 1   | B     | 257 | ALA  |
| 1   | B     | 291 | PRO  |
| 1   | C     | 3   | LYS  |
| 1   | C     | 86  | LYS  |
| 1   | C     | 204 | ALA  |
| 1   | C     | 312 | SER  |
| 1   | C     | 348 | SER  |
| 1   | D     | 158 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 360 | ASN  |
| 1   | D     | 361 | LYS  |
| 1   | E     | 143 | LYS  |
| 1   | E     | 148 | LEU  |
| 1   | E     | 224 | LYS  |
| 1   | F     | 310 | ALA  |
| 1   | F     | 361 | LYS  |
| 1   | G     | 329 | SER  |
| 1   | H     | 3   | LYS  |
| 1   | H     | 6   | ARG  |
| 1   | H     | 101 | GLY  |
| 1   | H     | 161 | PRO  |
| 1   | H     | 261 | GLU  |
| 1   | J     | 55  | SER  |
| 1   | J     | 164 | LEU  |
| 1   | J     | 207 | SER  |
| 1   | J     | 283 | THR  |
| 1   | J     | 376 | SER  |
| 1   | K     | 148 | LEU  |
| 1   | K     | 169 | ARG  |
| 1   | K     | 313 | ALA  |
| 1   | L     | 13  | VAL  |
| 1   | L     | 159 | LEU  |
| 1   | L     | 163 | ASP  |
| 1   | L     | 220 | THR  |
| 1   | L     | 371 | ASN  |
| 1   | B     | 39  | VAL  |
| 1   | C     | 6   | ARG  |
| 1   | C     | 139 | LYS  |
| 1   | C     | 160 | ALA  |
| 1   | C     | 261 | GLU  |
| 1   | C     | 325 | SER  |
| 1   | C     | 368 | ILE  |
| 1   | D     | 74  | LEU  |
| 1   | D     | 166 | GLU  |
| 1   | D     | 315 | ASN  |
| 1   | D     | 370 | ARG  |
| 1   | D     | 411 | GLU  |
| 1   | E     | 57  | ILE  |
| 1   | E     | 157 | PHE  |
| 1   | E     | 200 | LYS  |
| 1   | E     | 202 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 262 | ASN  |
| 1   | E     | 268 | SER  |
| 1   | E     | 291 | PRO  |
| 1   | E     | 412 | HIS  |
| 1   | F     | 58  | GLU  |
| 1   | F     | 348 | SER  |
| 1   | F     | 412 | HIS  |
| 1   | G     | 85  | GLU  |
| 1   | G     | 163 | ASP  |
| 1   | G     | 224 | LYS  |
| 1   | G     | 238 | GLY  |
| 1   | H     | 100 | ASP  |
| 1   | H     | 160 | ALA  |
| 1   | H     | 224 | LYS  |
| 1   | H     | 372 | ILE  |
| 1   | H     | 375 | MET  |
| 1   | I     | 17  | ASN  |
| 1   | I     | 268 | SER  |
| 1   | I     | 329 | SER  |
| 1   | I     | 419 | GLU  |
| 1   | J     | 181 | PHE  |
| 1   | J     | 208 | CYS  |
| 1   | J     | 361 | LYS  |
| 1   | K     | 74  | LEU  |
| 1   | K     | 99  | PRO  |
| 1   | L     | 148 | LEU  |
| 1   | L     | 291 | PRO  |
| 1   | L     | 412 | HIS  |
| 1   | A     | 169 | ARG  |
| 1   | B     | 282 | ALA  |
| 1   | C     | 220 | THR  |
| 1   | D     | 169 | ARG  |
| 1   | E     | 144 | GLY  |
| 1   | E     | 376 | SER  |
| 1   | F     | 3   | LYS  |
| 1   | F     | 201 | TYR  |
| 1   | G     | 101 | GLY  |
| 1   | G     | 204 | ALA  |
| 1   | H     | 58  | GLU  |
| 1   | H     | 283 | THR  |
| 1   | I     | 162 | THR  |
| 1   | I     | 204 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 85  | GLU  |
| 1   | J     | 261 | GLU  |
| 1   | J     | 329 | SER  |
| 1   | K     | 75  | ASN  |
| 1   | K     | 83  | THR  |
| 1   | K     | 373 | TYR  |
| 1   | K     | 376 | SER  |
| 1   | K     | 411 | GLU  |
| 1   | L     | 29  | LEU  |
| 1   | L     | 190 | VAL  |
| 1   | L     | 276 | ALA  |
| 1   | L     | 369 | ASP  |
| 1   | A     | 17  | ASN  |
| 1   | B     | 283 | THR  |
| 1   | B     | 368 | ILE  |
| 1   | C     | 157 | PHE  |
| 1   | C     | 291 | PRO  |
| 1   | C     | 349 | VAL  |
| 1   | C     | 370 | ARG  |
| 1   | F     | 220 | THR  |
| 1   | J     | 58  | GLU  |
| 1   | L     | 324 | ALA  |
| 1   | B     | 101 | GLY  |
| 1   | F     | 386 | VAL  |
| 1   | C     | 337 | VAL  |
| 1   | E     | 101 | GLY  |
| 1   | I     | 368 | ILE  |
| 1   | K     | 367 | PRO  |
| 1   | K     | 374 | VAL  |
| 1   | C     | 190 | VAL  |
| 1   | F     | 160 | ALA  |
| 1   | K     | 160 | ALA  |
| 1   | K     | 337 | VAL  |
| 1   | J     | 101 | GLY  |
| 1   | D     | 385 | ILE  |
| 1   | E     | 372 | ILE  |
| 1   | I     | 160 | ALA  |
| 1   | K     | 190 | 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     | 380/382 (100%)  | 341 (90%)  | 39 (10%)  | 8           | 32 |
| 1   | B     | 380/382 (100%)  | 353 (93%)  | 27 (7%)   | 17          | 52 |
| 1   | C     | 379/382 (99%)   | 345 (91%)  | 34 (9%)   | 11          | 40 |
| 1   | D     | 380/382 (100%)  | 347 (91%)  | 33 (9%)   | 12          | 43 |
| 1   | E     | 379/382 (99%)   | 340 (90%)  | 39 (10%)  | 8           | 32 |
| 1   | F     | 378/382 (99%)   | 338 (89%)  | 40 (11%)  | 8           | 30 |
| 1   | G     | 379/382 (99%)   | 340 (90%)  | 39 (10%)  | 8           | 32 |
| 1   | H     | 378/382 (99%)   | 344 (91%)  | 34 (9%)   | 11          | 40 |
| 1   | I     | 377/382 (99%)   | 334 (89%)  | 43 (11%)  | 7           | 27 |
| 1   | J     | 379/382 (99%)   | 338 (89%)  | 41 (11%)  | 7           | 30 |
| 1   | K     | 379/382 (99%)   | 338 (89%)  | 41 (11%)  | 7           | 30 |
| 1   | L     | 380/382 (100%)  | 347 (91%)  | 33 (9%)   | 12          | 43 |
| All | All   | 4548/4584 (99%) | 4105 (90%) | 443 (10%) | 9           | 35 |

All (443) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | LEU  |
| 1   | A     | 34  | ASN  |
| 1   | A     | 36  | GLU  |
| 1   | A     | 37  | ILE  |
| 1   | A     | 70  | LEU  |
| 1   | A     | 78  | VAL  |
| 1   | A     | 85  | GLU  |
| 1   | A     | 91  | ARG  |
| 1   | A     | 94  | CYS  |
| 1   | A     | 102 | THR  |
| 1   | A     | 105 | GLU  |
| 1   | A     | 112 | LEU  |
| 1   | A     | 129 | LEU  |
| 1   | A     | 151 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 159 | LEU  |
| 1   | A     | 161 | PRO  |
| 1   | A     | 164 | LEU  |
| 1   | A     | 167 | ASN  |
| 1   | A     | 169 | ARG  |
| 1   | A     | 186 | SER  |
| 1   | A     | 206 | ARG  |
| 1   | A     | 252 | LYS  |
| 1   | A     | 262 | ASN  |
| 1   | A     | 273 | HIS  |
| 1   | A     | 285 | PHE  |
| 1   | A     | 294 | ASN  |
| 1   | A     | 308 | TYR  |
| 1   | A     | 314 | GLN  |
| 1   | A     | 347 | LEU  |
| 1   | A     | 359 | LYS  |
| 1   | A     | 363 | GLU  |
| 1   | A     | 369 | ASP  |
| 1   | A     | 371 | ASN  |
| 1   | A     | 373 | TYR  |
| 1   | A     | 375 | MET  |
| 1   | A     | 380 | ARG  |
| 1   | A     | 401 | SER  |
| 1   | A     | 431 | GLN  |
| 1   | A     | 441 | MET  |
| 1   | B     | 7   | GLU  |
| 1   | B     | 12  | LEU  |
| 1   | B     | 32  | ILE  |
| 1   | B     | 49  | LYS  |
| 1   | B     | 67  | ASP  |
| 1   | B     | 82  | TRP  |
| 1   | B     | 91  | ARG  |
| 1   | B     | 122 | LEU  |
| 1   | B     | 124 | PHE  |
| 1   | B     | 129 | LEU  |
| 1   | B     | 153 | LYS  |
| 1   | B     | 186 | SER  |
| 1   | B     | 201 | TYR  |
| 1   | B     | 236 | LEU  |
| 1   | B     | 285 | PHE  |
| 1   | B     | 286 | THR  |
| 1   | B     | 294 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 331 | ARG  |
| 1   | B     | 347 | LEU  |
| 1   | B     | 349 | VAL  |
| 1   | B     | 369 | ASP  |
| 1   | B     | 370 | ARG  |
| 1   | B     | 371 | ASN  |
| 1   | B     | 372 | ILE  |
| 1   | B     | 380 | ARG  |
| 1   | B     | 387 | ASP  |
| 1   | B     | 429 | ARG  |
| 1   | C     | 34  | ASN  |
| 1   | C     | 36  | GLU  |
| 1   | C     | 41  | GLN  |
| 1   | C     | 48  | ASN  |
| 1   | C     | 49  | LYS  |
| 1   | C     | 61  | VAL  |
| 1   | C     | 73  | ASP  |
| 1   | C     | 75  | ASN  |
| 1   | C     | 91  | ARG  |
| 1   | C     | 105 | GLU  |
| 1   | C     | 112 | LEU  |
| 1   | C     | 120 | GLU  |
| 1   | C     | 129 | LEU  |
| 1   | C     | 153 | LYS  |
| 1   | C     | 161 | PRO  |
| 1   | C     | 163 | ASP  |
| 1   | C     | 183 | ILE  |
| 1   | C     | 194 | GLN  |
| 1   | C     | 201 | TYR  |
| 1   | C     | 206 | ARG  |
| 1   | C     | 252 | LYS  |
| 1   | C     | 264 | ASP  |
| 1   | C     | 286 | THR  |
| 1   | C     | 297 | LYS  |
| 1   | C     | 308 | TYR  |
| 1   | C     | 312 | SER  |
| 1   | C     | 347 | LEU  |
| 1   | C     | 371 | ASN  |
| 1   | C     | 373 | TYR  |
| 1   | C     | 382 | GLU  |
| 1   | C     | 409 | LEU  |
| 1   | C     | 429 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 431 | GLN  |
| 1   | C     | 441 | MET  |
| 1   | D     | 5   | THR  |
| 1   | D     | 6   | ARG  |
| 1   | D     | 28  | ILE  |
| 1   | D     | 34  | ASN  |
| 1   | D     | 35  | VAL  |
| 1   | D     | 40  | SER  |
| 1   | D     | 70  | LEU  |
| 1   | D     | 82  | TRP  |
| 1   | D     | 91  | ARG  |
| 1   | D     | 94  | CYS  |
| 1   | D     | 112 | LEU  |
| 1   | D     | 129 | LEU  |
| 1   | D     | 145 | GLU  |
| 1   | D     | 151 | ASN  |
| 1   | D     | 159 | LEU  |
| 1   | D     | 161 | PRO  |
| 1   | D     | 163 | ASP  |
| 1   | D     | 164 | LEU  |
| 1   | D     | 177 | GLU  |
| 1   | D     | 183 | ILE  |
| 1   | D     | 207 | SER  |
| 1   | D     | 295 | SER  |
| 1   | D     | 308 | TYR  |
| 1   | D     | 314 | GLN  |
| 1   | D     | 319 | LEU  |
| 1   | D     | 326 | ARG  |
| 1   | D     | 328 | ILE  |
| 1   | D     | 331 | ARG  |
| 1   | D     | 338 | ASP  |
| 1   | D     | 383 | ASN  |
| 1   | D     | 387 | ASP  |
| 1   | D     | 394 | GLU  |
| 1   | D     | 443 | GLN  |
| 1   | E     | 5   | THR  |
| 1   | E     | 7   | GLU  |
| 1   | E     | 8   | ASP  |
| 1   | E     | 11  | LYS  |
| 1   | E     | 16  | GLU  |
| 1   | E     | 51  | MET  |
| 1   | E     | 61  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 62  | ARG  |
| 1   | E     | 82  | TRP  |
| 1   | E     | 91  | ARG  |
| 1   | E     | 105 | GLU  |
| 1   | E     | 109 | ARG  |
| 1   | E     | 110 | ASN  |
| 1   | E     | 126 | ASP  |
| 1   | E     | 129 | LEU  |
| 1   | E     | 148 | LEU  |
| 1   | E     | 149 | GLU  |
| 1   | E     | 161 | PRO  |
| 1   | E     | 164 | LEU  |
| 1   | E     | 183 | ILE  |
| 1   | E     | 201 | TYR  |
| 1   | E     | 223 | ARG  |
| 1   | E     | 230 | THR  |
| 1   | E     | 262 | ASN  |
| 1   | E     | 264 | ASP  |
| 1   | E     | 273 | HIS  |
| 1   | E     | 285 | PHE  |
| 1   | E     | 289 | THR  |
| 1   | E     | 294 | ASN  |
| 1   | E     | 326 | ARG  |
| 1   | E     | 328 | ILE  |
| 1   | E     | 349 | VAL  |
| 1   | E     | 369 | ASP  |
| 1   | E     | 370 | ARG  |
| 1   | E     | 373 | TYR  |
| 1   | E     | 381 | MET  |
| 1   | E     | 391 | THR  |
| 1   | E     | 412 | HIS  |
| 1   | E     | 436 | GLU  |
| 1   | F     | 14  | LYS  |
| 1   | F     | 28  | ILE  |
| 1   | F     | 29  | LEU  |
| 1   | F     | 31  | THR  |
| 1   | F     | 34  | ASN  |
| 1   | F     | 36  | GLU  |
| 1   | F     | 40  | SER  |
| 1   | F     | 41  | GLN  |
| 1   | F     | 61  | VAL  |
| 1   | F     | 70  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 82  | TRP  |
| 1   | F     | 91  | ARG  |
| 1   | F     | 98  | ASN  |
| 1   | F     | 100 | ASP  |
| 1   | F     | 105 | GLU  |
| 1   | F     | 112 | LEU  |
| 1   | F     | 126 | ASP  |
| 1   | F     | 129 | LEU  |
| 1   | F     | 148 | LEU  |
| 1   | F     | 150 | LEU  |
| 1   | F     | 159 | LEU  |
| 1   | F     | 161 | PRO  |
| 1   | F     | 189 | GLU  |
| 1   | F     | 201 | TYR  |
| 1   | F     | 206 | ARG  |
| 1   | F     | 219 | LYS  |
| 1   | F     | 236 | LEU  |
| 1   | F     | 285 | PHE  |
| 1   | F     | 308 | TYR  |
| 1   | F     | 328 | ILE  |
| 1   | F     | 342 | ASN  |
| 1   | F     | 349 | VAL  |
| 1   | F     | 351 | LEU  |
| 1   | F     | 370 | ARG  |
| 1   | F     | 378 | GLU  |
| 1   | F     | 387 | ASP  |
| 1   | F     | 398 | GLU  |
| 1   | F     | 423 | ILE  |
| 1   | F     | 437 | ARG  |
| 1   | F     | 439 | GLN  |
| 1   | G     | 6   | ARG  |
| 1   | G     | 25  | PHE  |
| 1   | G     | 34  | ASN  |
| 1   | G     | 41  | GLN  |
| 1   | G     | 63  | ILE  |
| 1   | G     | 64  | GLU  |
| 1   | G     | 70  | LEU  |
| 1   | G     | 91  | ARG  |
| 1   | G     | 95  | ASP  |
| 1   | G     | 117 | LYS  |
| 1   | G     | 122 | LEU  |
| 1   | G     | 152 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 156 | TYR  |
| 1   | G     | 158 | ASP  |
| 1   | G     | 161 | PRO  |
| 1   | G     | 168 | CYS  |
| 1   | G     | 169 | ARG  |
| 1   | G     | 177 | GLU  |
| 1   | G     | 183 | ILE  |
| 1   | G     | 198 | ASP  |
| 1   | G     | 199 | PHE  |
| 1   | G     | 201 | TYR  |
| 1   | G     | 216 | LEU  |
| 1   | G     | 223 | ARG  |
| 1   | G     | 250 | LEU  |
| 1   | G     | 251 | PHE  |
| 1   | G     | 258 | PHE  |
| 1   | G     | 285 | PHE  |
| 1   | G     | 316 | ARG  |
| 1   | G     | 331 | ARG  |
| 1   | G     | 335 | ARG  |
| 1   | G     | 342 | ASN  |
| 1   | G     | 350 | LEU  |
| 1   | G     | 351 | LEU  |
| 1   | G     | 370 | ARG  |
| 1   | G     | 373 | TYR  |
| 1   | G     | 385 | ILE  |
| 1   | G     | 409 | LEU  |
| 1   | G     | 442 | SER  |
| 1   | H     | 7   | GLU  |
| 1   | H     | 19  | LYS  |
| 1   | H     | 21  | ILE  |
| 1   | H     | 34  | ASN  |
| 1   | H     | 74  | LEU  |
| 1   | H     | 82  | TRP  |
| 1   | H     | 91  | ARG  |
| 1   | H     | 94  | CYS  |
| 1   | H     | 105 | GLU  |
| 1   | H     | 112 | LEU  |
| 1   | H     | 126 | ASP  |
| 1   | H     | 143 | LYS  |
| 1   | H     | 158 | ASP  |
| 1   | H     | 159 | LEU  |
| 1   | H     | 161 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 166 | GLU  |
| 1   | H     | 171 | ASP  |
| 1   | H     | 201 | TYR  |
| 1   | H     | 223 | ARG  |
| 1   | H     | 240 | ASN  |
| 1   | H     | 264 | ASP  |
| 1   | H     | 273 | HIS  |
| 1   | H     | 321 | ARG  |
| 1   | H     | 328 | ILE  |
| 1   | H     | 351 | LEU  |
| 1   | H     | 359 | LYS  |
| 1   | H     | 362 | LEU  |
| 1   | H     | 370 | ARG  |
| 1   | H     | 372 | ILE  |
| 1   | H     | 378 | GLU  |
| 1   | H     | 381 | MET  |
| 1   | H     | 387 | ASP  |
| 1   | H     | 401 | SER  |
| 1   | H     | 419 | GLU  |
| 1   | I     | 7   | GLU  |
| 1   | I     | 8   | ASP  |
| 1   | I     | 28  | ILE  |
| 1   | I     | 34  | ASN  |
| 1   | I     | 40  | SER  |
| 1   | I     | 58  | GLU  |
| 1   | I     | 62  | ARG  |
| 1   | I     | 70  | LEU  |
| 1   | I     | 86  | LYS  |
| 1   | I     | 91  | ARG  |
| 1   | I     | 94  | CYS  |
| 1   | I     | 100 | ASP  |
| 1   | I     | 109 | ARG  |
| 1   | I     | 110 | ASN  |
| 1   | I     | 112 | LEU  |
| 1   | I     | 114 | ARG  |
| 1   | I     | 129 | LEU  |
| 1   | I     | 158 | ASP  |
| 1   | I     | 159 | LEU  |
| 1   | I     | 161 | PRO  |
| 1   | I     | 164 | LEU  |
| 1   | I     | 169 | ARG  |
| 1   | I     | 174 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 199 | PHE  |
| 1   | I     | 201 | TYR  |
| 1   | I     | 206 | ARG  |
| 1   | I     | 207 | SER  |
| 1   | I     | 216 | LEU  |
| 1   | I     | 239 | VAL  |
| 1   | I     | 248 | LEU  |
| 1   | I     | 261 | GLU  |
| 1   | I     | 285 | PHE  |
| 1   | I     | 328 | ILE  |
| 1   | I     | 331 | ARG  |
| 1   | I     | 349 | VAL  |
| 1   | I     | 351 | LEU  |
| 1   | I     | 370 | ARG  |
| 1   | I     | 372 | ILE  |
| 1   | I     | 373 | TYR  |
| 1   | I     | 391 | THR  |
| 1   | I     | 409 | LEU  |
| 1   | I     | 434 | PRO  |
| 1   | I     | 441 | MET  |
| 1   | J     | 5   | THR  |
| 1   | J     | 12  | LEU  |
| 1   | J     | 34  | ASN  |
| 1   | J     | 36  | GLU  |
| 1   | J     | 37  | ILE  |
| 1   | J     | 49  | LYS  |
| 1   | J     | 66  | SER  |
| 1   | J     | 85  | GLU  |
| 1   | J     | 91  | ARG  |
| 1   | J     | 94  | CYS  |
| 1   | J     | 112 | LEU  |
| 1   | J     | 117 | LYS  |
| 1   | J     | 125 | SER  |
| 1   | J     | 126 | ASP  |
| 1   | J     | 129 | LEU  |
| 1   | J     | 142 | GLU  |
| 1   | J     | 161 | PRO  |
| 1   | J     | 167 | ASN  |
| 1   | J     | 169 | ARG  |
| 1   | J     | 200 | LYS  |
| 1   | J     | 201 | TYR  |
| 1   | J     | 206 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 212 | GLN  |
| 1   | J     | 216 | LEU  |
| 1   | J     | 223 | ARG  |
| 1   | J     | 250 | LEU  |
| 1   | J     | 262 | ASN  |
| 1   | J     | 265 | LEU  |
| 1   | J     | 270 | THR  |
| 1   | J     | 272 | LYS  |
| 1   | J     | 285 | PHE  |
| 1   | J     | 286 | THR  |
| 1   | J     | 294 | ASN  |
| 1   | J     | 308 | TYR  |
| 1   | J     | 326 | ARG  |
| 1   | J     | 331 | ARG  |
| 1   | J     | 347 | LEU  |
| 1   | J     | 349 | VAL  |
| 1   | J     | 363 | GLU  |
| 1   | J     | 373 | TYR  |
| 1   | J     | 387 | ASP  |
| 1   | K     | 7   | GLU  |
| 1   | K     | 24  | GLN  |
| 1   | K     | 34  | ASN  |
| 1   | K     | 36  | GLU  |
| 1   | K     | 65  | GLU  |
| 1   | K     | 91  | ARG  |
| 1   | K     | 94  | CYS  |
| 1   | K     | 109 | ARG  |
| 1   | K     | 142 | GLU  |
| 1   | K     | 153 | LYS  |
| 1   | K     | 156 | TYR  |
| 1   | K     | 159 | LEU  |
| 1   | K     | 166 | GLU  |
| 1   | K     | 169 | ARG  |
| 1   | K     | 174 | LEU  |
| 1   | K     | 197 | ILE  |
| 1   | K     | 199 | PHE  |
| 1   | K     | 223 | ARG  |
| 1   | K     | 239 | VAL  |
| 1   | K     | 252 | LYS  |
| 1   | K     | 270 | THR  |
| 1   | K     | 273 | HIS  |
| 1   | K     | 283 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 285 | PHE  |
| 1   | K     | 298 | ARG  |
| 1   | K     | 315 | ASN  |
| 1   | K     | 316 | ARG  |
| 1   | K     | 326 | ARG  |
| 1   | K     | 331 | ARG  |
| 1   | K     | 337 | VAL  |
| 1   | K     | 360 | ASN  |
| 1   | K     | 363 | GLU  |
| 1   | K     | 373 | TYR  |
| 1   | K     | 374 | VAL  |
| 1   | K     | 375 | MET  |
| 1   | K     | 382 | GLU  |
| 1   | K     | 391 | THR  |
| 1   | K     | 411 | GLU  |
| 1   | K     | 426 | ASP  |
| 1   | K     | 439 | GLN  |
| 1   | K     | 442 | SER  |
| 1   | L     | 11  | LYS  |
| 1   | L     | 14  | LYS  |
| 1   | L     | 21  | ILE  |
| 1   | L     | 34  | ASN  |
| 1   | L     | 40  | SER  |
| 1   | L     | 75  | ASN  |
| 1   | L     | 91  | ARG  |
| 1   | L     | 102 | THR  |
| 1   | L     | 105 | GLU  |
| 1   | L     | 109 | ARG  |
| 1   | L     | 122 | LEU  |
| 1   | L     | 129 | LEU  |
| 1   | L     | 149 | GLU  |
| 1   | L     | 162 | THR  |
| 1   | L     | 164 | LEU  |
| 1   | L     | 167 | ASN  |
| 1   | L     | 174 | LEU  |
| 1   | L     | 183 | ILE  |
| 1   | L     | 189 | GLU  |
| 1   | L     | 194 | GLN  |
| 1   | L     | 201 | TYR  |
| 1   | L     | 236 | LEU  |
| 1   | L     | 262 | ASN  |
| 1   | L     | 285 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 321 | ARG  |
| 1   | L     | 325 | SER  |
| 1   | L     | 349 | VAL  |
| 1   | L     | 351 | LEU  |
| 1   | L     | 363 | GLU  |
| 1   | L     | 372 | ILE  |
| 1   | L     | 378 | GLU  |
| 1   | L     | 402 | ASN  |
| 1   | L     | 443 | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (170) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 41  | GLN  |
| 1   | A     | 98  | ASN  |
| 1   | A     | 128 | ASN  |
| 1   | A     | 167 | ASN  |
| 1   | A     | 194 | GLN  |
| 1   | A     | 253 | ASN  |
| 1   | A     | 281 | HIS  |
| 1   | A     | 315 | ASN  |
| 1   | A     | 383 | ASN  |
| 1   | A     | 431 | GLN  |
| 1   | A     | 443 | GLN  |
| 1   | B     | 41  | GLN  |
| 1   | B     | 128 | ASN  |
| 1   | B     | 167 | ASN  |
| 1   | B     | 194 | GLN  |
| 1   | B     | 225 | HIS  |
| 1   | B     | 245 | HIS  |
| 1   | B     | 262 | ASN  |
| 1   | B     | 266 | GLN  |
| 1   | B     | 281 | HIS  |
| 1   | B     | 290 | ASN  |
| 1   | B     | 294 | ASN  |
| 1   | B     | 315 | ASN  |
| 1   | B     | 342 | ASN  |
| 1   | B     | 371 | ASN  |
| 1   | B     | 383 | ASN  |
| 1   | B     | 431 | GLN  |
| 1   | C     | 17  | ASN  |
| 1   | C     | 24  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 34  | ASN  |
| 1   | C     | 98  | ASN  |
| 1   | C     | 110 | ASN  |
| 1   | C     | 225 | HIS  |
| 1   | C     | 228 | HIS  |
| 1   | C     | 245 | HIS  |
| 1   | C     | 266 | GLN  |
| 1   | C     | 290 | ASN  |
| 1   | C     | 294 | ASN  |
| 1   | C     | 314 | GLN  |
| 1   | C     | 416 | HIS  |
| 1   | C     | 431 | GLN  |
| 1   | C     | 439 | GLN  |
| 1   | C     | 443 | GLN  |
| 1   | D     | 110 | ASN  |
| 1   | D     | 111 | ASN  |
| 1   | D     | 128 | ASN  |
| 1   | D     | 187 | HIS  |
| 1   | D     | 194 | GLN  |
| 1   | D     | 225 | HIS  |
| 1   | D     | 228 | HIS  |
| 1   | D     | 262 | ASN  |
| 1   | D     | 273 | HIS  |
| 1   | D     | 281 | HIS  |
| 1   | D     | 290 | ASN  |
| 1   | D     | 314 | GLN  |
| 1   | D     | 383 | ASN  |
| 1   | D     | 433 | HIS  |
| 1   | D     | 443 | GLN  |
| 1   | E     | 41  | GLN  |
| 1   | E     | 110 | ASN  |
| 1   | E     | 151 | ASN  |
| 1   | E     | 187 | HIS  |
| 1   | E     | 195 | HIS  |
| 1   | E     | 225 | HIS  |
| 1   | E     | 228 | HIS  |
| 1   | E     | 247 | ASN  |
| 1   | E     | 262 | ASN  |
| 1   | E     | 281 | HIS  |
| 1   | E     | 290 | ASN  |
| 1   | E     | 314 | GLN  |
| 1   | E     | 342 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 431 | GLN  |
| 1   | F     | 17  | ASN  |
| 1   | F     | 24  | GLN  |
| 1   | F     | 41  | GLN  |
| 1   | F     | 98  | ASN  |
| 1   | F     | 151 | ASN  |
| 1   | F     | 167 | ASN  |
| 1   | F     | 187 | HIS  |
| 1   | F     | 194 | GLN  |
| 1   | F     | 225 | HIS  |
| 1   | F     | 228 | HIS  |
| 1   | F     | 266 | GLN  |
| 1   | F     | 290 | ASN  |
| 1   | F     | 314 | GLN  |
| 1   | F     | 360 | ASN  |
| 1   | F     | 371 | ASN  |
| 1   | F     | 383 | ASN  |
| 1   | F     | 439 | GLN  |
| 1   | F     | 443 | GLN  |
| 1   | G     | 98  | ASN  |
| 1   | G     | 151 | ASN  |
| 1   | G     | 167 | ASN  |
| 1   | G     | 194 | GLN  |
| 1   | G     | 225 | HIS  |
| 1   | G     | 228 | HIS  |
| 1   | G     | 247 | ASN  |
| 1   | G     | 253 | ASN  |
| 1   | G     | 266 | GLN  |
| 1   | G     | 281 | HIS  |
| 1   | G     | 314 | GLN  |
| 1   | G     | 342 | ASN  |
| 1   | G     | 360 | ASN  |
| 1   | G     | 383 | ASN  |
| 1   | G     | 431 | GLN  |
| 1   | G     | 443 | GLN  |
| 1   | H     | 17  | ASN  |
| 1   | H     | 41  | GLN  |
| 1   | H     | 98  | ASN  |
| 1   | H     | 128 | ASN  |
| 1   | H     | 194 | GLN  |
| 1   | H     | 228 | HIS  |
| 1   | H     | 240 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 245 | HIS  |
| 1   | H     | 281 | HIS  |
| 1   | H     | 290 | ASN  |
| 1   | H     | 315 | ASN  |
| 1   | H     | 383 | ASN  |
| 1   | H     | 431 | GLN  |
| 1   | I     | 110 | ASN  |
| 1   | I     | 128 | ASN  |
| 1   | I     | 151 | ASN  |
| 1   | I     | 194 | GLN  |
| 1   | I     | 240 | ASN  |
| 1   | I     | 253 | ASN  |
| 1   | I     | 266 | GLN  |
| 1   | I     | 290 | ASN  |
| 1   | I     | 416 | HIS  |
| 1   | I     | 431 | GLN  |
| 1   | I     | 433 | HIS  |
| 1   | I     | 439 | GLN  |
| 1   | J     | 17  | ASN  |
| 1   | J     | 34  | ASN  |
| 1   | J     | 98  | ASN  |
| 1   | J     | 110 | ASN  |
| 1   | J     | 111 | ASN  |
| 1   | J     | 128 | ASN  |
| 1   | J     | 194 | GLN  |
| 1   | J     | 225 | HIS  |
| 1   | J     | 245 | HIS  |
| 1   | J     | 281 | HIS  |
| 1   | J     | 371 | ASN  |
| 1   | K     | 17  | ASN  |
| 1   | K     | 98  | ASN  |
| 1   | K     | 128 | ASN  |
| 1   | K     | 194 | GLN  |
| 1   | K     | 212 | GLN  |
| 1   | K     | 245 | HIS  |
| 1   | K     | 262 | ASN  |
| 1   | K     | 281 | HIS  |
| 1   | K     | 290 | ASN  |
| 1   | K     | 315 | ASN  |
| 1   | K     | 360 | ASN  |
| 1   | K     | 383 | ASN  |
| 1   | K     | 431 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 443 | GLN  |
| 1   | L     | 24  | GLN  |
| 1   | L     | 98  | ASN  |
| 1   | L     | 110 | ASN  |
| 1   | L     | 111 | ASN  |
| 1   | L     | 128 | ASN  |
| 1   | L     | 151 | ASN  |
| 1   | L     | 167 | ASN  |
| 1   | L     | 194 | GLN  |
| 1   | L     | 228 | HIS  |
| 1   | L     | 266 | GLN  |
| 1   | L     | 281 | HIS  |
| 1   | L     | 290 | ASN  |
| 1   | L     | 402 | ASN  |
| 1   | L     | 431 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 25 are monoatomic - leaving 5 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | SO4  | D     | 501 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.09 | 0        |
| 3   | SO4  | D     | 504 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.06 | 0        |
| 3   | SO4  | E     | 503 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.06 | 0        |
| 3   | SO4  | F     | 503 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.09 | 0        |
| 3   | SO4  | H     | 501 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.05 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 3   | SO4  | D     | 501 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 3   | SO4  | D     | 504 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 3   | SO4  | E     | 503 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 3   | SO4  | F     | 503 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 3   | SO4  | H     | 501 | -    | -       | 0/0/0/0  | 0/0/0/0 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [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(Å²)         | Q<0.9 |
|-----|-------|-----------------|--------|---------|----|----|------------------|-------|
| 1   | A     | 439/443 (99%)   | -0.35  | 5 (1%)  | 80 | 65 | 38, 61, 115, 125 | 0     |
| 1   | B     | 439/443 (99%)   | -0.33  | 6 (1%)  | 75 | 57 | 34, 61, 114, 124 | 0     |
| 1   | C     | 438/443 (98%)   | -0.37  | 6 (1%)  | 75 | 57 | 31, 61, 114, 126 | 0     |
| 1   | D     | 439/443 (99%)   | -0.32  | 6 (1%)  | 75 | 57 | 38, 63, 116, 130 | 0     |
| 1   | E     | 438/443 (98%)   | -0.36  | 5 (1%)  | 80 | 65 | 39, 64, 118, 126 | 0     |
| 1   | F     | 437/443 (98%)   | -0.38  | 7 (1%)  | 72 | 51 | 40, 60, 114, 130 | 0     |
| 1   | G     | 438/443 (98%)   | -0.42  | 2 (0%)  | 90 | 80 | 35, 60, 116, 124 | 0     |
| 1   | H     | 437/443 (98%)   | -0.39  | 3 (0%)  | 87 | 75 | 35, 60, 115, 127 | 0     |
| 1   | I     | 436/443 (98%)   | -0.35  | 6 (1%)  | 75 | 57 | 39, 62, 118, 132 | 0     |
| 1   | J     | 438/443 (98%)   | -0.34  | 5 (1%)  | 80 | 65 | 40, 63, 118, 126 | 0     |
| 1   | K     | 438/443 (98%)   | -0.39  | 4 (0%)  | 84 | 69 | 39, 63, 116, 127 | 0     |
| 1   | L     | 440/443 (99%)   | -0.36  | 6 (1%)  | 75 | 57 | 32, 59, 116, 126 | 0     |
| All | All   | 5257/5316 (98%) | -0.36  | 61 (1%) | 79 | 61 | 31, 62, 116, 132 | 0     |

All (61) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 307 | CYS  | 7.4  |
| 1   | J     | 306 | PRO  | 7.2  |
| 1   | C     | 307 | CYS  | 6.0  |
| 1   | I     | 2   | ALA  | 5.3  |
| 1   | A     | 306 | PRO  | 5.0  |
| 1   | H     | 312 | SER  | 4.9  |
| 1   | C     | 312 | SER  | 4.8  |
| 1   | H     | 307 | CYS  | 4.6  |
| 1   | H     | 369 | ASP  | 4.3  |
| 1   | F     | 312 | SER  | 4.1  |
| 1   | D     | 315 | ASN  | 4.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 312 | SER  | 4.0  |
| 1   | B     | 313 | ALA  | 3.9  |
| 1   | B     | 312 | SER  | 3.7  |
| 1   | K     | 371 | ASN  | 3.6  |
| 1   | F     | 307 | CYS  | 3.6  |
| 1   | D     | 385 | ILE  | 3.4  |
| 1   | D     | 314 | GLN  | 3.4  |
| 1   | L     | 306 | PRO  | 3.3  |
| 1   | F     | 315 | ASN  | 3.2  |
| 1   | A     | 307 | CYS  | 3.1  |
| 1   | D     | 306 | PRO  | 3.1  |
| 1   | B     | 307 | CYS  | 3.1  |
| 1   | E     | 311 | TRP  | 3.1  |
| 1   | J     | 371 | ASN  | 3.0  |
| 1   | G     | 307 | CYS  | 3.0  |
| 1   | K     | 365 | PRO  | 2.9  |
| 1   | I     | 315 | ASN  | 2.9  |
| 1   | C     | 315 | ASN  | 2.9  |
| 1   | J     | 312 | SER  | 2.9  |
| 1   | C     | 311 | TRP  | 2.8  |
| 1   | F     | 369 | ASP  | 2.8  |
| 1   | A     | 312 | SER  | 2.7  |
| 1   | L     | 307 | CYS  | 2.7  |
| 1   | F     | 368 | ILE  | 2.7  |
| 1   | I     | 312 | SER  | 2.6  |
| 1   | E     | 369 | ASP  | 2.6  |
| 1   | L     | 315 | ASN  | 2.6  |
| 1   | L     | 365 | PRO  | 2.4  |
| 1   | E     | 367 | PRO  | 2.4  |
| 1   | C     | 313 | ALA  | 2.3  |
| 1   | A     | 311 | TRP  | 2.3  |
| 1   | B     | 306 | PRO  | 2.3  |
| 1   | E     | 306 | PRO  | 2.3  |
| 1   | B     | 61  | VAL  | 2.3  |
| 1   | L     | 314 | GLN  | 2.2  |
| 1   | F     | 370 | ARG  | 2.2  |
| 1   | K     | 306 | PRO  | 2.2  |
| 1   | D     | 316 | ARG  | 2.2  |
| 1   | C     | 372 | ILE  | 2.1  |
| 1   | F     | 366 | ALA  | 2.1  |
| 1   | J     | 61  | VAL  | 2.1  |
| 1   | B     | 314 | GLN  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 380 | ARG  | 2.1  |
| 1   | G     | 314 | GLN  | 2.1  |
| 1   | I     | 313 | ALA  | 2.1  |
| 1   | I     | 370 | ARG  | 2.1  |
| 1   | K     | 311 | TRP  | 2.0  |
| 1   | A     | 301 | PRO  | 2.0  |
| 1   | I     | 372 | ILE  | 2.0  |
| 1   | E     | 307 | CYS  | 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 3   | SO4  | D     | 501 | 5/5   | 0.76 | 0.33 | 3.07 | 131,131,132,132            | 0     |
| 3   | SO4  | F     | 503 | 5/5   | 0.79 | 0.24 | 2.92 | 181,181,182,182            | 0     |
| 2   | MG   | C     | 501 | 1/1   | 0.96 | 0.22 | 2.18 | 27,27,27,27                | 0     |
| 2   | MG   | H     | 502 | 1/1   | 0.96 | 0.20 | 1.91 | 16,16,16,16                | 0     |
| 2   | MG   | L     | 501 | 1/1   | 0.88 | 0.22 | 1.87 | 30,30,30,30                | 0     |
| 3   | SO4  | E     | 503 | 5/5   | 0.81 | 0.19 | 1.72 | 158,159,159,159            | 0     |
| 2   | MG   | B     | 501 | 1/1   | 0.99 | 0.20 | 1.14 | 21,21,21,21                | 0     |
| 3   | SO4  | H     | 501 | 5/5   | 0.84 | 0.21 | 1.03 | 169,169,169,169            | 0     |
| 2   | MG   | I     | 501 | 1/1   | 0.95 | 0.20 | 0.92 | 18,18,18,18                | 0     |
| 2   | MG   | H     | 503 | 1/1   | 0.97 | 0.19 | 0.84 | 35,35,35,35                | 0     |
| 2   | MG   | K     | 501 | 1/1   | 0.96 | 0.20 | 0.69 | 13,13,13,13                | 0     |
| 2   | MG   | K     | 502 | 1/1   | 0.96 | 0.19 | 0.30 | 39,39,39,39                | 0     |
| 2   | MG   | J     | 501 | 1/1   | 0.95 | 0.19 | 0.26 | 30,30,30,30                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 2   | MG   | F     | 501 | 1/1   | 0.88 | 0.19 | 0.01  | 32,32,32,32                 | 0     |
| 2   | MG   | D     | 503 | 1/1   | 0.94 | 0.18 | -0.38 | 32,32,32,32                 | 0     |
| 2   | MG   | L     | 502 | 1/1   | 0.97 | 0.17 | -0.82 | 29,29,29,29                 | 0     |
| 2   | MG   | I     | 502 | 1/1   | 0.95 | 0.13 | -1.47 | 39,39,39,39                 | 0     |
| 2   | MG   | E     | 502 | 1/1   | 0.93 | 0.14 | -1.55 | 39,39,39,39                 | 0     |
| 2   | MG   | A     | 501 | 1/1   | 0.96 | 0.15 | -1.80 | 10,10,10,10                 | 0     |
| 2   | MG   | F     | 502 | 1/1   | 0.92 | 0.14 | -5.90 | 22,22,22,22                 | 0     |
| 2   | MG   | B     | 503 | 1/1   | 0.51 | 0.39 | -     | 92,92,92,92                 | 0     |
| 2   | MG   | E     | 501 | 1/1   | 0.95 | 0.22 | -     | 22,22,22,22                 | 0     |
| 2   | MG   | G     | 501 | 1/1   | 0.97 | 0.17 | -     | 24,24,24,24                 | 0     |
| 2   | MG   | C     | 502 | 1/1   | 0.98 | 0.27 | -     | 34,34,34,34                 | 0     |
| 2   | MG   | B     | 502 | 1/1   | 0.96 | 0.19 | -     | 23,23,23,23                 | 0     |
| 2   | MG   | A     | 502 | 1/1   | 0.97 | 0.15 | -     | 19,19,19,19                 | 0     |
| 2   | MG   | D     | 502 | 1/1   | 1.00 | 0.16 | -     | 7,7,7,7                     | 0     |
| 3   | SO4  | D     | 504 | 5/5   | 0.90 | 0.13 | -     | 154,154,154,155             | 0     |
| 2   | MG   | J     | 502 | 1/1   | 0.98 | 0.34 | -     | 27,27,27,27                 | 0     |
| 2   | MG   | G     | 502 | 1/1   | 0.97 | 0.22 | -     | 19,19,19,19                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.