



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:58 PM UTC

PDB ID : 5JJ3 / pdb\_00005jj3  
Title : Refined Structure of the Mature Virion Conformation of P22 Portal Protein  
Authors : Lokareddy, R.K.; Sankhala, R.S.; Cingolani, G.  
Deposited on : 2016-04-22  
Resolution : 7.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

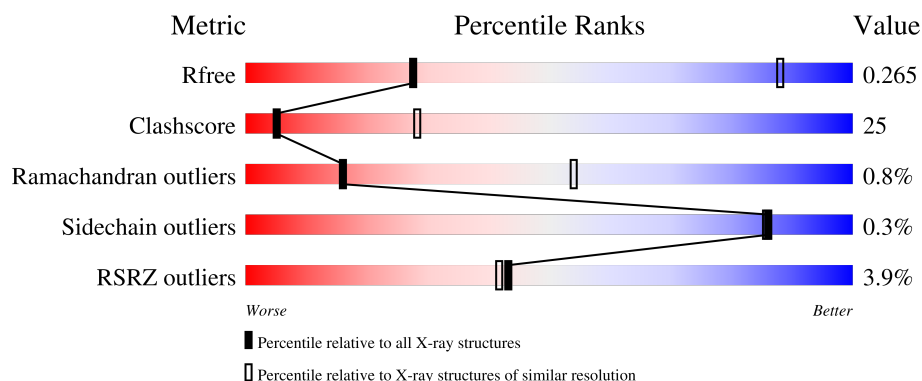
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 7.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1167 (10.00-4.00)                                     |
| Clashscore            | 190562                      | 1007 (9.70-4.04)                                      |
| Ramachandran outliers | 187476                      | 1054 (10.00-4.00)                                     |
| Sidechain outliers    | 187428                      | 1017 (10.00-4.00)                                     |
| RSRZ outliers         | 180081                      | 1161 (10.00-4.00)                                     |

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

| Mol | Chain | Length | Quality of chain                                                       |
|-----|-------|--------|------------------------------------------------------------------------|
| 1   | A     | 725    | <div> <div>2%</div> <div>48%</div> <div>44%</div> <div>7%</div> </div> |
| 1   | B     | 725    | <div> <div>5%</div> <div>48%</div> <div>44%</div> <div>7%</div> </div> |
| 1   | C     | 725    | <div> <div>3%</div> <div>47%</div> <div>45%</div> <div>7%</div> </div> |
| 1   | D     | 725    | <div> <div>4%</div> <div>49%</div> <div>43%</div> <div>7%</div> </div> |
| 1   | E     | 725    | <div> <div>4%</div> <div>48%</div> <div>44%</div> <div>7%</div> </div> |

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| Mol | Chain | Length | Quality of chain     |
|-----|-------|--------|----------------------|
| 1   | F     | 725    | <p>2% 49% 43% 7%</p> |
| 1   | G     | 725    | <p>5% 48% 43% 7%</p> |
| 1   | H     | 725    | <p>3% 49% 43% 7%</p> |
| 1   | I     | 725    | <p>4% 49% 43% 7%</p> |
| 1   | J     | 725    | <p>3% 49% 43% 7%</p> |
| 1   | K     | 725    | <p>3% 48% 44% 7%</p> |
| 1   | L     | 725    | <p>4% 48% 44% 7%</p> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 64536 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.

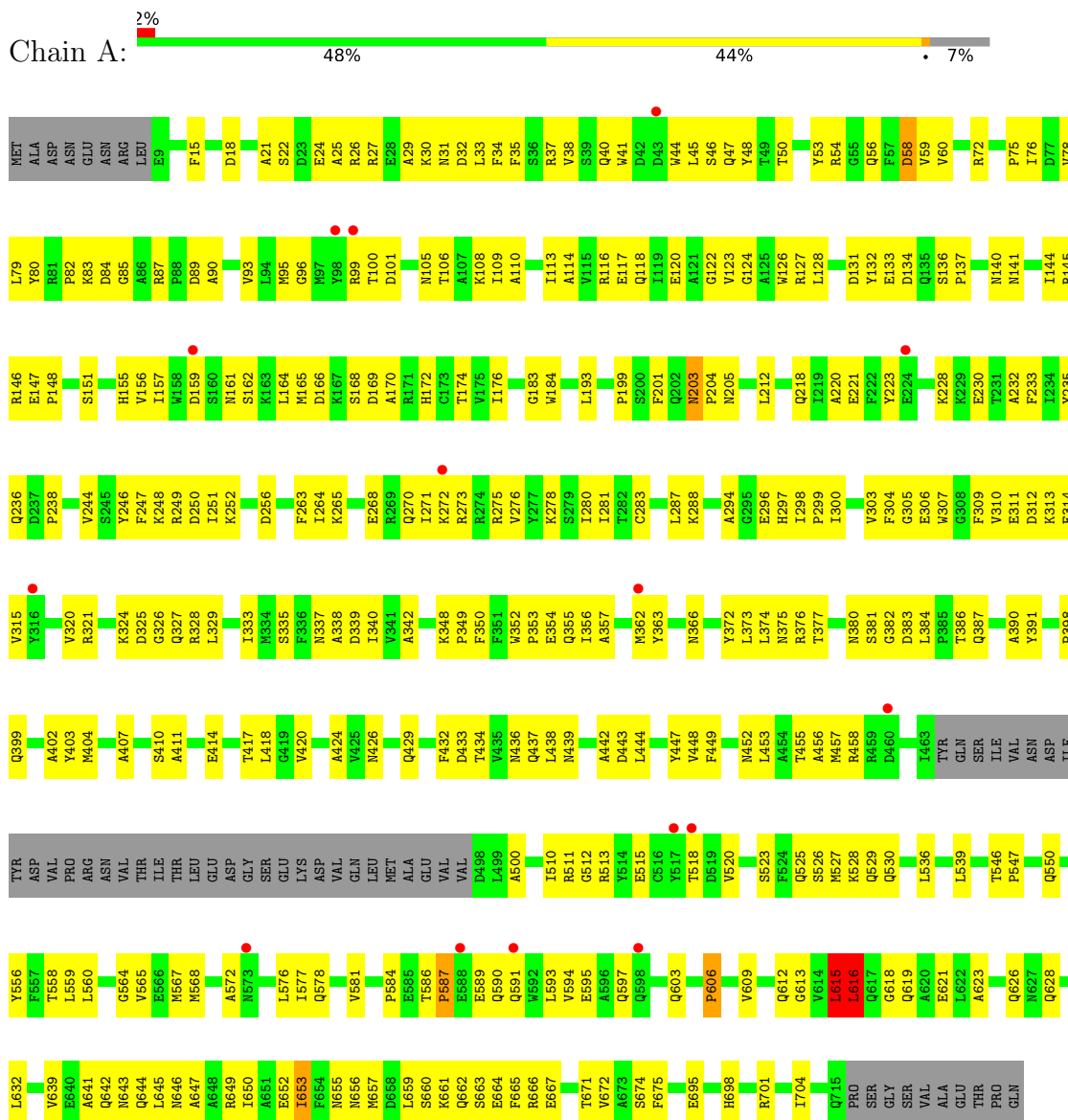
- Molecule 1 is a protein called Portal protein.

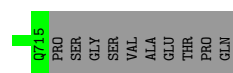
| Mol | Chain | Residues | Atoms |      |     |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| 1   | A     | 673      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5378  | 3367 | 937 | 1051 | 23 |         |         |       |
| 1   | B     | 673      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5378  | 3367 | 937 | 1051 | 23 |         |         |       |
| 1   | C     | 673      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5378  | 3367 | 937 | 1051 | 23 |         |         |       |
| 1   | D     | 673      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5378  | 3367 | 937 | 1051 | 23 |         |         |       |
| 1   | E     | 673      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5378  | 3367 | 937 | 1051 | 23 |         |         |       |
| 1   | F     | 673      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5378  | 3367 | 937 | 1051 | 23 |         |         |       |
| 1   | G     | 673      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5378  | 3367 | 937 | 1051 | 23 |         |         |       |
| 1   | H     | 673      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5378  | 3367 | 937 | 1051 | 23 |         |         |       |
| 1   | I     | 673      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5378  | 3367 | 937 | 1051 | 23 |         |         |       |
| 1   | J     | 673      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5378  | 3367 | 937 | 1051 | 23 |         |         |       |
| 1   | K     | 673      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5378  | 3367 | 937 | 1051 | 23 |         |         |       |
| 1   | L     | 673      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5378  | 3367 | 937 | 1051 | 23 |         |         |       |

### 3 Residue-property plots

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

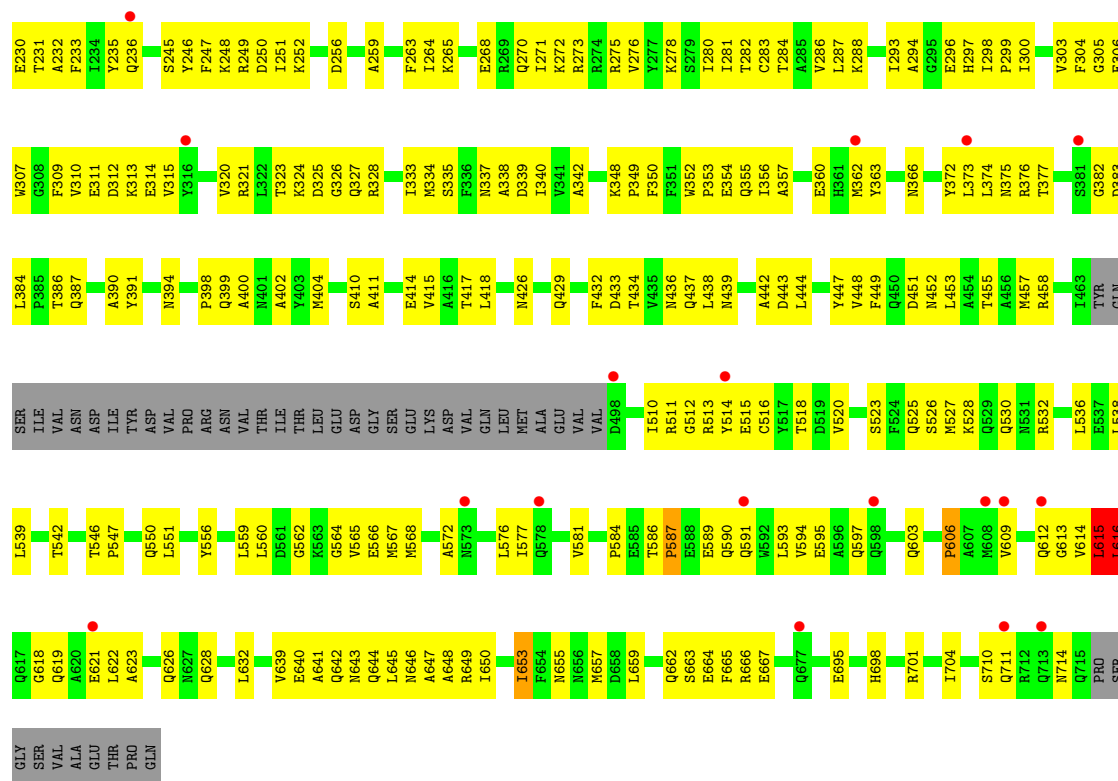
#### • Molecule 1: Portal protein



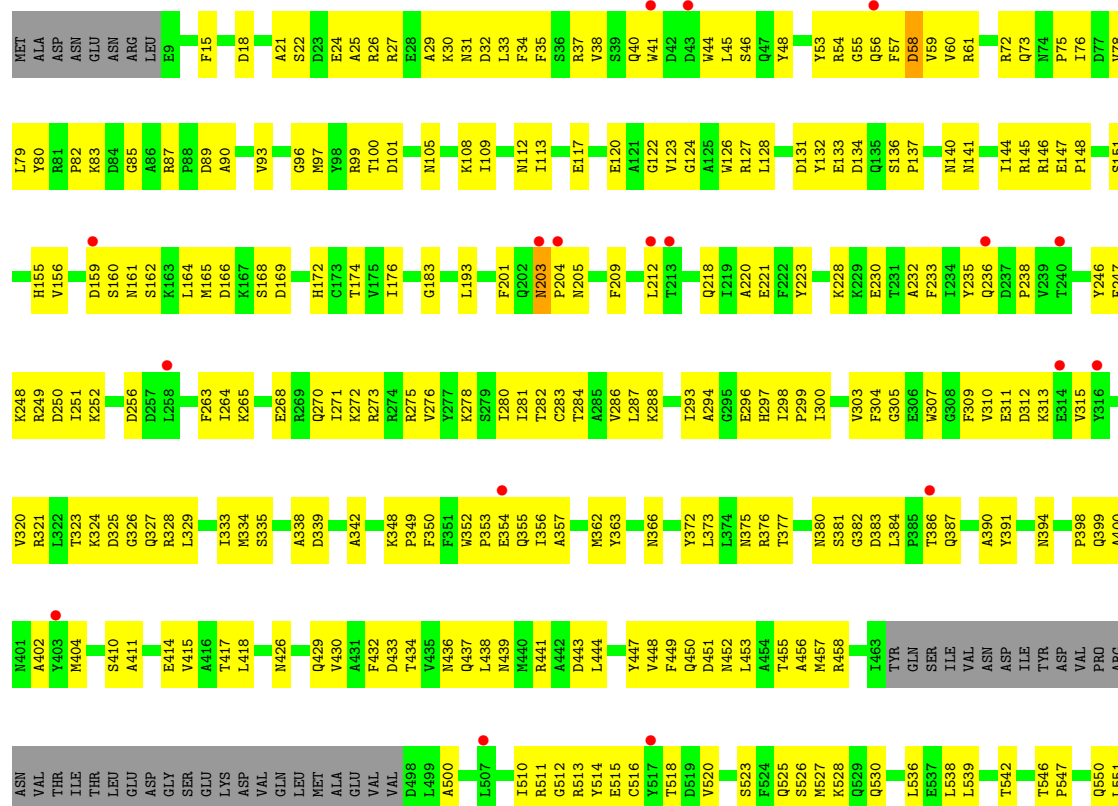


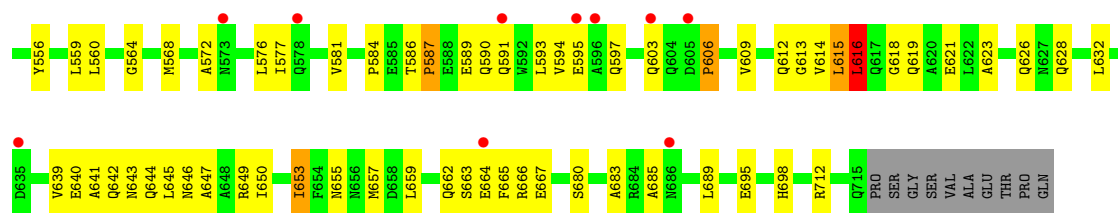
Chain C:  3% 47% 45% 7%



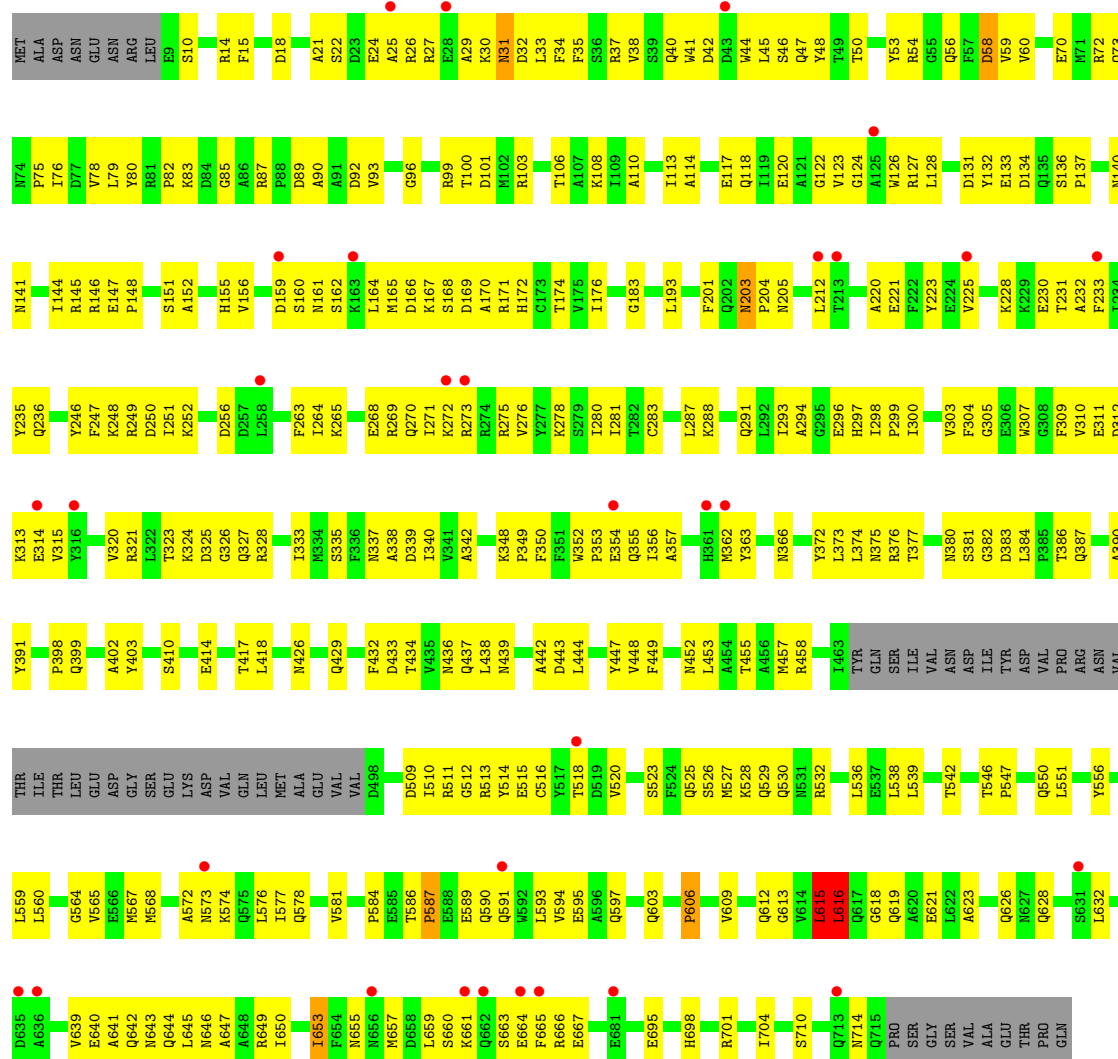


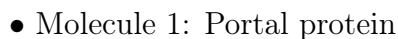
• Molecule 1: Portal protein

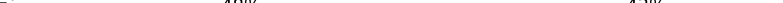




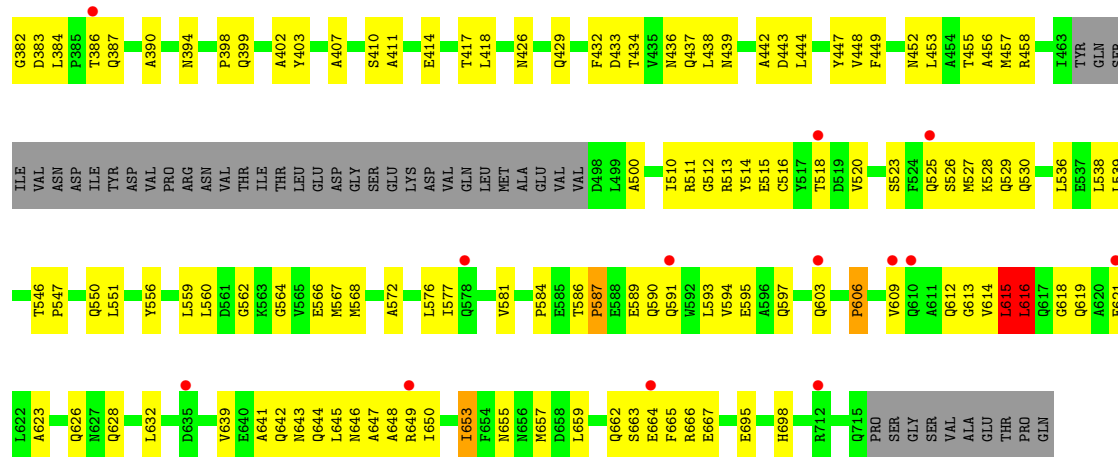
• Molecule 1: Portal protein



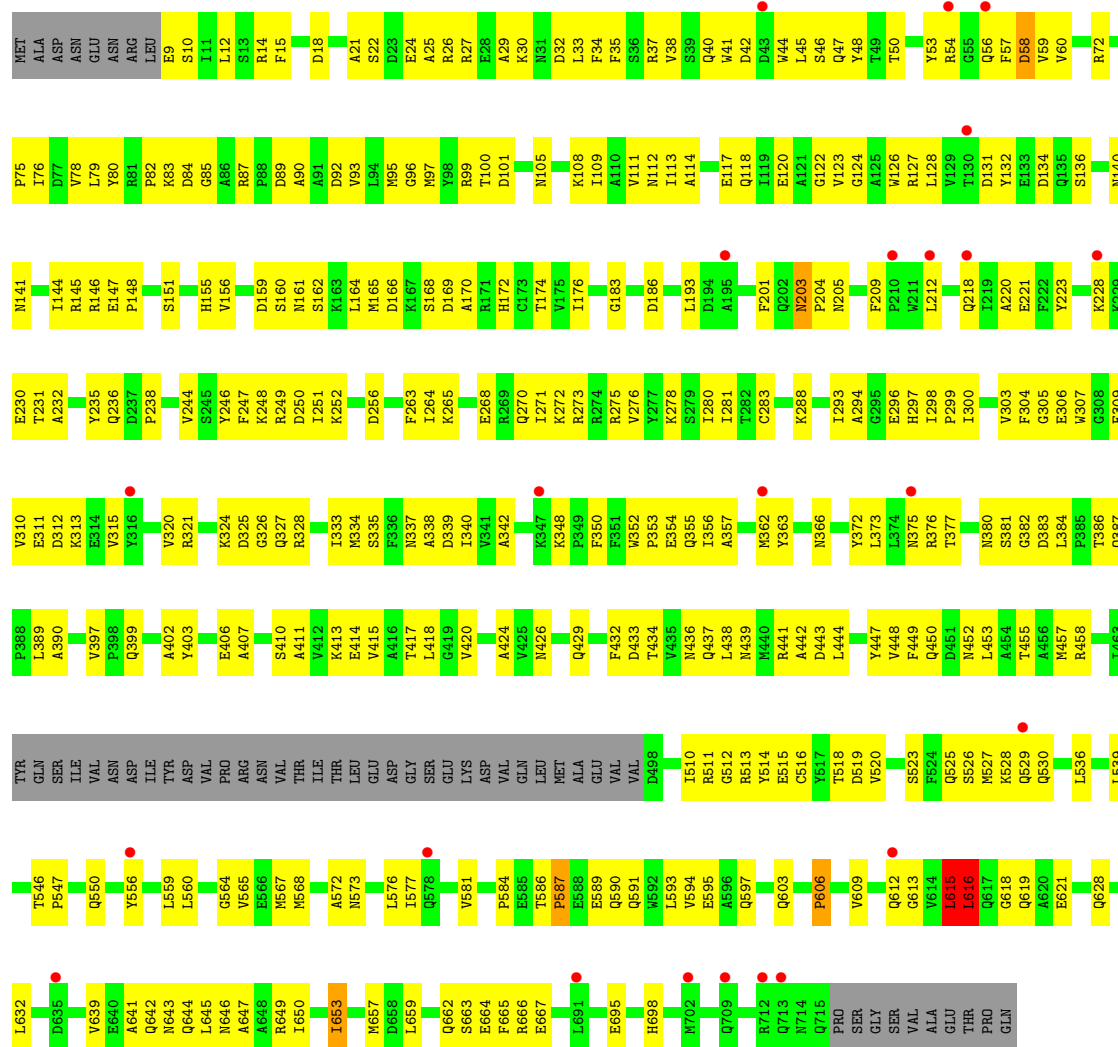


Chain G:  5% 48% 43% 7%

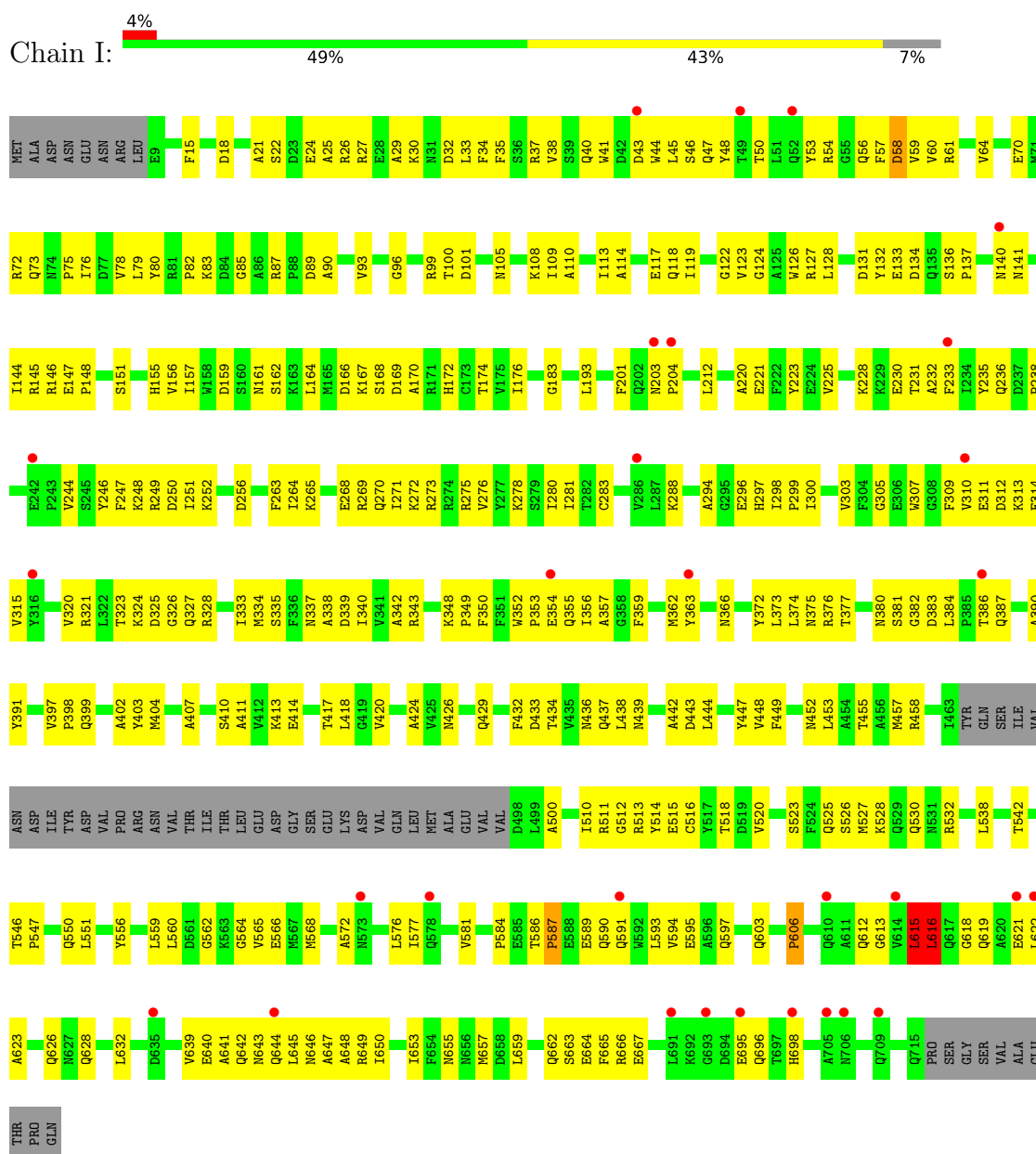




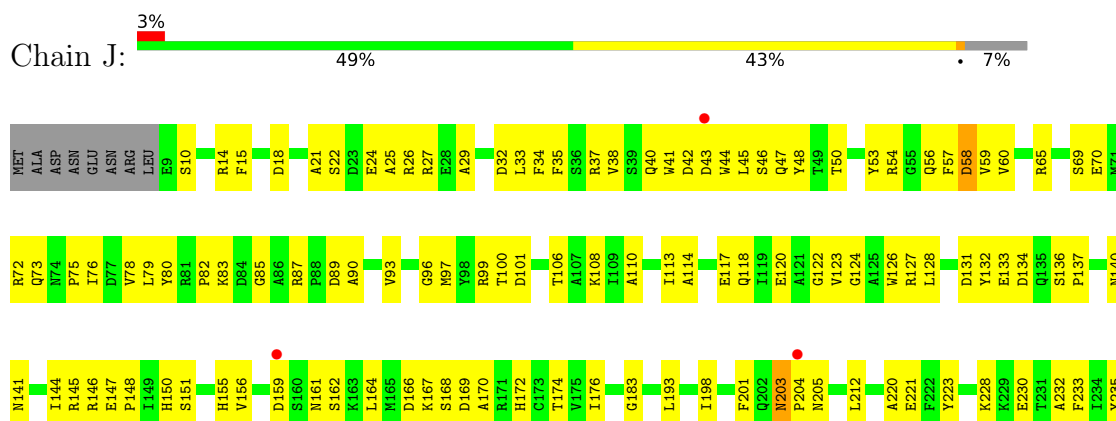
• Molecule 1: Portal protein



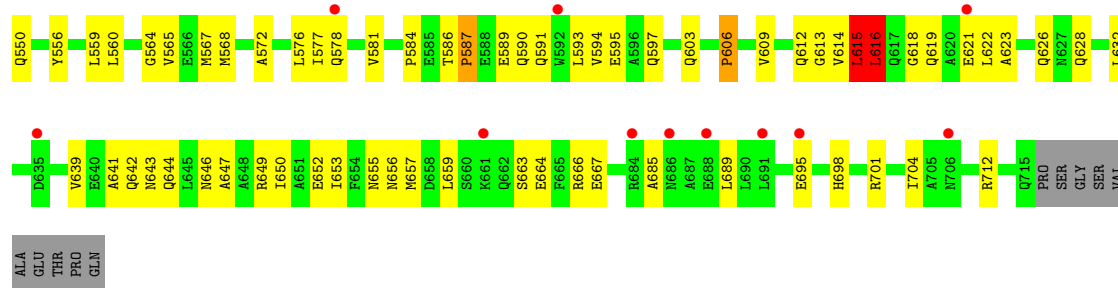
• Molecule 1: Portal protein



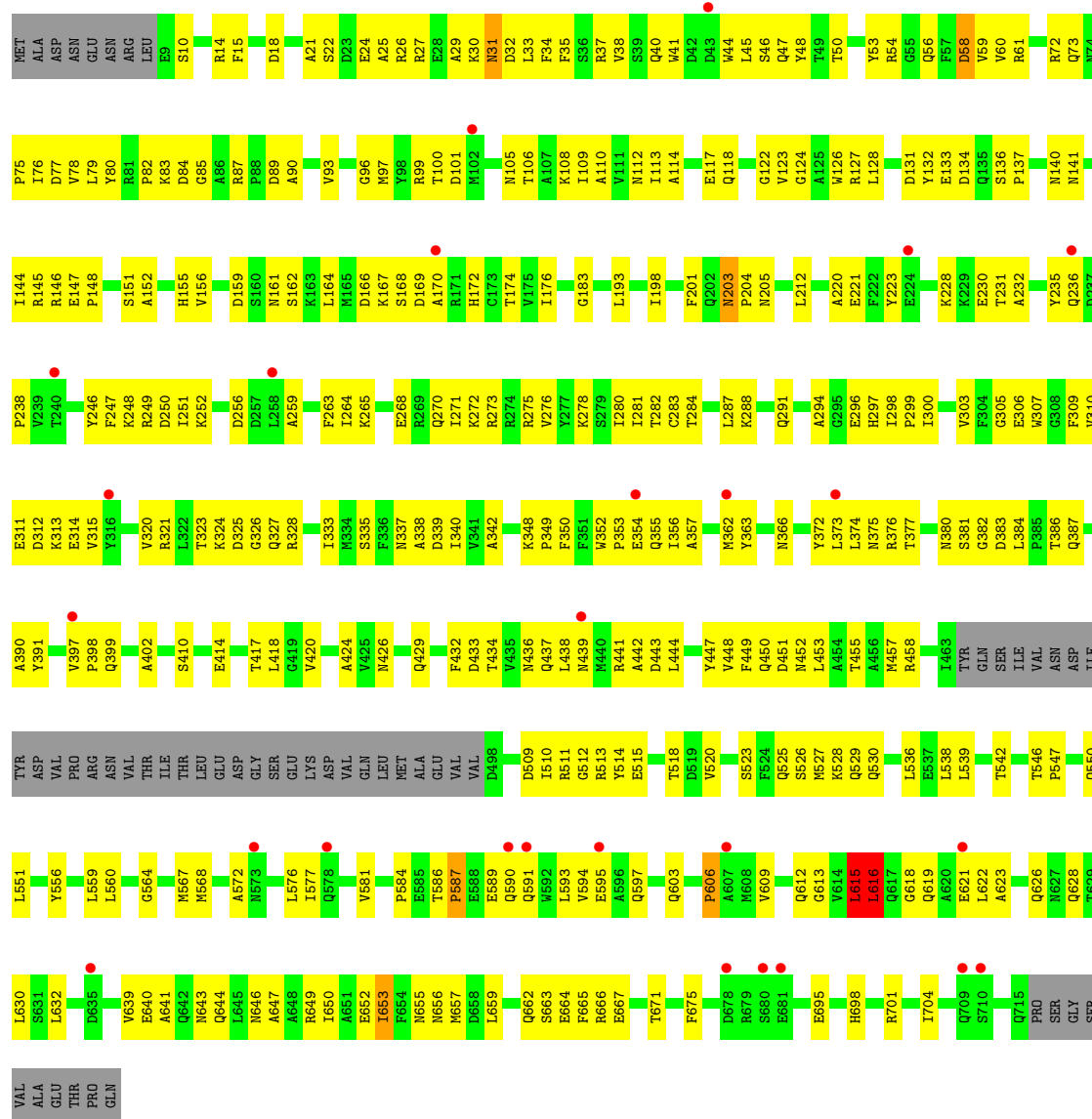
• Molecule 1: Portal protein







• Molecule 1: Portal protein



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | I 4                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 409.04Å 409.04Å 260.00Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 14.99 – 7.00<br>14.99 – 7.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.0 (14.99-7.00)<br>88.7 (14.99-7.00)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.07 (at 7.36Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (1.10.1_2155: ???)                                   | Depositor        |
| R, $R_{free}$                                                           | 0.239 , 0.260<br>0.242 , 0.265                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1689 reflections (4.96%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 214.7                                                       | Xtriage          |
| Anisotropy                                                              | 0.009                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.13 , 0.0                                                  | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | 0.045 for -k,-h,-l                                          | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.88                                                        | EDS              |
| Total number of atoms                                                   | 64536                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 118.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 0.19         | 0/5482         | 0.58        | 2/7429 (0.0%)   |
| 1   | B     | 0.19         | 0/5482         | 0.59        | 2/7429 (0.0%)   |
| 1   | C     | 0.19         | 0/5482         | 0.59        | 2/7429 (0.0%)   |
| 1   | D     | 0.19         | 0/5482         | 0.57        | 2/7429 (0.0%)   |
| 1   | E     | 0.19         | 0/5482         | 0.59        | 2/7429 (0.0%)   |
| 1   | F     | 0.19         | 0/5482         | 0.58        | 2/7429 (0.0%)   |
| 1   | G     | 0.18         | 0/5482         | 0.59        | 2/7429 (0.0%)   |
| 1   | H     | 0.18         | 0/5482         | 0.58        | 2/7429 (0.0%)   |
| 1   | I     | 0.19         | 0/5482         | 0.58        | 2/7429 (0.0%)   |
| 1   | J     | 0.20         | 1/5482 (0.0%)  | 0.58        | 2/7429 (0.0%)   |
| 1   | K     | 0.21         | 1/5482 (0.0%)  | 0.59        | 3/7429 (0.0%)   |
| 1   | L     | 0.20         | 1/5482 (0.0%)  | 0.58        | 2/7429 (0.0%)   |
| All | All   | 0.19         | 3/65784 (0.0%) | 0.58        | 25/89148 (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   | A     | 0                   | 4                   |
| 1   | B     | 0                   | 4                   |
| 1   | C     | 0                   | 3                   |
| 1   | D     | 0                   | 4                   |
| 1   | E     | 0                   | 3                   |
| 1   | F     | 0                   | 4                   |
| 1   | G     | 0                   | 4                   |
| 1   | H     | 0                   | 3                   |
| 1   | I     | 0                   | 3                   |
| 1   | J     | 0                   | 3                   |
| 1   | K     | 0                   | 4                   |
| 1   | L     | 0                   | 3                   |
| All | All   | 0                   | 42                  |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | K     | 198 | ILE  | C-N   | 7.11 | 1.50        | 1.33     |
| 1   | J     | 198 | ILE  | C-N   | 6.69 | 1.49        | 1.33     |
| 1   | L     | 198 | ILE  | C-N   | 5.70 | 1.47        | 1.33     |

All (25) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1   | I     | 616 | LEU  | CA-CB-CG | 8.58 | 146.32      | 116.30   |
| 1   | J     | 616 | LEU  | CA-CB-CG | 8.46 | 145.92      | 116.30   |
| 1   | C     | 615 | LEU  | CA-CB-CG | 8.15 | 144.83      | 116.30   |
| 1   | B     | 616 | LEU  | CA-CB-CG | 7.97 | 144.21      | 116.30   |
| 1   | I     | 615 | LEU  | CA-CB-CG | 7.97 | 144.19      | 116.30   |
| 1   | B     | 615 | LEU  | CA-CB-CG | 7.90 | 143.96      | 116.30   |
| 1   | F     | 615 | LEU  | CA-CB-CG | 7.89 | 143.93      | 116.30   |
| 1   | E     | 615 | LEU  | CA-CB-CG | 7.83 | 143.72      | 116.30   |
| 1   | K     | 615 | LEU  | CA-CB-CG | 7.83 | 143.69      | 116.30   |
| 1   | J     | 615 | LEU  | CA-CB-CG | 7.77 | 143.49      | 116.30   |
| 1   | K     | 616 | LEU  | CA-CB-CG | 7.73 | 143.35      | 116.30   |
| 1   | A     | 615 | LEU  | CA-CB-CG | 7.68 | 143.17      | 116.30   |
| 1   | A     | 616 | LEU  | CA-CB-CG | 7.67 | 143.16      | 116.30   |
| 1   | G     | 615 | LEU  | CA-CB-CG | 7.63 | 143.02      | 116.30   |
| 1   | C     | 616 | LEU  | CA-CB-CG | 7.57 | 142.81      | 116.30   |
| 1   | E     | 616 | LEU  | CA-CB-CG | 7.49 | 142.52      | 116.30   |
| 1   | L     | 615 | LEU  | CA-CB-CG | 7.49 | 142.51      | 116.30   |
| 1   | F     | 616 | LEU  | CA-CB-CG | 7.37 | 142.10      | 116.30   |
| 1   | H     | 615 | LEU  | CA-CB-CG | 7.24 | 141.65      | 116.30   |
| 1   | G     | 616 | LEU  | CA-CB-CG | 7.01 | 140.82      | 116.30   |
| 1   | H     | 616 | LEU  | CA-CB-CG | 6.98 | 140.73      | 116.30   |
| 1   | D     | 616 | LEU  | CA-CB-CG | 6.81 | 140.13      | 116.30   |
| 1   | L     | 616 | LEU  | CA-CB-CG | 6.48 | 138.98      | 116.30   |
| 1   | D     | 615 | LEU  | CA-CB-CG | 5.74 | 136.41      | 116.30   |
| 1   | K     | 616 | LEU  | N-CA-CB  | 5.08 | 117.58      | 110.12   |

There are no chirality outliers.

All (42) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 212 | LEU  | Peptide |
| 1   | A     | 456 | ALA  | Peptide |
| 1   | A     | 59  | VAL  | Peptide |
| 1   | A     | 606 | PRO  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | B     | 212 | LEU  | Peptide |
| 1   | B     | 456 | ALA  | Peptide |
| 1   | B     | 59  | VAL  | Peptide |
| 1   | B     | 606 | PRO  | Peptide |
| 1   | C     | 212 | LEU  | Peptide |
| 1   | C     | 59  | VAL  | Peptide |
| 1   | C     | 606 | PRO  | Peptide |
| 1   | D     | 212 | LEU  | Peptide |
| 1   | D     | 456 | ALA  | Peptide |
| 1   | D     | 59  | VAL  | Peptide |
| 1   | D     | 606 | PRO  | Peptide |
| 1   | E     | 212 | LEU  | Peptide |
| 1   | E     | 59  | VAL  | Peptide |
| 1   | E     | 606 | PRO  | Peptide |
| 1   | F     | 212 | LEU  | Peptide |
| 1   | F     | 456 | ALA  | Peptide |
| 1   | F     | 59  | VAL  | Peptide |
| 1   | F     | 606 | PRO  | Peptide |
| 1   | G     | 212 | LEU  | Peptide |
| 1   | G     | 456 | ALA  | Peptide |
| 1   | G     | 59  | VAL  | Peptide |
| 1   | G     | 606 | PRO  | Peptide |
| 1   | H     | 212 | LEU  | Peptide |
| 1   | H     | 59  | VAL  | Peptide |
| 1   | H     | 606 | PRO  | Peptide |
| 1   | I     | 212 | LEU  | Peptide |
| 1   | I     | 59  | VAL  | Peptide |
| 1   | I     | 606 | PRO  | Peptide |
| 1   | J     | 212 | LEU  | Peptide |
| 1   | J     | 59  | VAL  | Peptide |
| 1   | J     | 606 | PRO  | Peptide |
| 1   | K     | 212 | LEU  | Peptide |
| 1   | K     | 456 | ALA  | Peptide |
| 1   | K     | 59  | VAL  | Peptide |
| 1   | K     | 606 | PRO  | Peptide |
| 1   | L     | 212 | LEU  | Peptide |
| 1   | L     | 59  | VAL  | Peptide |
| 1   | L     | 606 | PRO  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5378  | 0        | 5178     | 287     | 0            |
| 1   | B     | 5378  | 0        | 5178     | 292     | 0            |
| 1   | C     | 5378  | 0        | 5178     | 302     | 0            |
| 1   | D     | 5378  | 0        | 5178     | 284     | 0            |
| 1   | E     | 5378  | 0        | 5178     | 295     | 0            |
| 1   | F     | 5378  | 0        | 5178     | 282     | 0            |
| 1   | G     | 5378  | 0        | 5178     | 282     | 0            |
| 1   | H     | 5378  | 0        | 5178     | 286     | 0            |
| 1   | I     | 5378  | 0        | 5178     | 282     | 0            |
| 1   | J     | 5378  | 0        | 5178     | 286     | 0            |
| 1   | K     | 5378  | 0        | 5178     | 293     | 0            |
| 1   | L     | 5378  | 0        | 5178     | 291     | 0            |
| All | All   | 64536 | 0        | 62136    | 3132    | 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 25.

All (3132) 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:J:220:ALA:HB3 | 1:J:281:ILE:O    | 1.55                     | 1.05              |
| 1:B:220:ALA:HB3 | 1:B:281:ILE:O    | 1.58                     | 1.03              |
| 1:E:220:ALA:HB3 | 1:E:281:ILE:O    | 1.58                     | 1.02              |
| 1:I:220:ALA:HB3 | 1:I:281:ILE:O    | 1.59                     | 1.02              |
| 1:K:220:ALA:HB3 | 1:K:281:ILE:O    | 1.59                     | 1.01              |
| 1:H:220:ALA:HB3 | 1:H:281:ILE:O    | 1.60                     | 1.01              |
| 1:C:220:ALA:HB3 | 1:C:281:ILE:O    | 1.61                     | 1.01              |
| 1:A:220:ALA:HB3 | 1:A:281:ILE:O    | 1.60                     | 1.00              |
| 1:L:220:ALA:HB3 | 1:L:281:ILE:O    | 1.61                     | 0.99              |
| 1:G:220:ALA:HB3 | 1:G:281:ILE:O    | 1.61                     | 0.99              |
| 1:A:613:GLY:HA2 | 1:A:616:LEU:HD12 | 1.47                     | 0.97              |
| 1:F:220:ALA:HB3 | 1:F:281:ILE:O    | 1.63                     | 0.97              |
| 1:D:220:ALA:HB3 | 1:D:281:ILE:O    | 1.66                     | 0.95              |
| 1:H:613:GLY:HA2 | 1:H:616:LEU:HD13 | 1.49                     | 0.94              |
| 1:B:613:GLY:HA2 | 1:B:616:LEU:HD13 | 1.49                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:613:GLY:HA2  | 1:G:616:LEU:HD13 | 1.53                     | 0.91              |
| 1:D:577:ILE:HG12 | 1:D:597:GLN:HE22 | 1.36                     | 0.91              |
| 1:L:577:ILE:HG12 | 1:L:597:GLN:HE22 | 1.36                     | 0.90              |
| 1:A:352:TRP:HB3  | 1:B:376:ARG:HD2  | 1.53                     | 0.89              |
| 1:H:352:TRP:HB3  | 1:I:376:ARG:HD2  | 1.55                     | 0.89              |
| 1:A:376:ARG:HD2  | 1:L:352:TRP:HB3  | 1.55                     | 0.89              |
| 1:C:577:ILE:HG12 | 1:C:597:GLN:HE22 | 1.37                     | 0.89              |
| 1:I:577:ILE:HG12 | 1:I:597:GLN:HE22 | 1.37                     | 0.88              |
| 1:B:352:TRP:HB3  | 1:C:376:ARG:HD2  | 1.54                     | 0.88              |
| 1:I:352:TRP:HB3  | 1:J:376:ARG:HD2  | 1.57                     | 0.87              |
| 1:G:352:TRP:HB3  | 1:H:376:ARG:HD2  | 1.54                     | 0.86              |
| 1:I:434:THR:O    | 1:I:437:GLN:HB3  | 1.75                     | 0.86              |
| 1:D:352:TRP:HB3  | 1:E:376:ARG:HD2  | 1.57                     | 0.86              |
| 1:K:352:TRP:HB3  | 1:L:376:ARG:HD2  | 1.57                     | 0.86              |
| 1:B:577:ILE:HG12 | 1:B:597:GLN:HE22 | 1.39                     | 0.86              |
| 1:G:577:ILE:HG12 | 1:G:597:GLN:HE22 | 1.39                     | 0.85              |
| 1:C:352:TRP:HB3  | 1:D:376:ARG:HD2  | 1.58                     | 0.85              |
| 1:F:352:TRP:HB3  | 1:G:376:ARG:HD2  | 1.59                     | 0.85              |
| 1:J:352:TRP:HB3  | 1:K:376:ARG:HD2  | 1.59                     | 0.85              |
| 1:D:355:GLN:HG2  | 1:E:376:ARG:HH12 | 1.39                     | 0.85              |
| 1:E:352:TRP:HB3  | 1:F:376:ARG:HD2  | 1.57                     | 0.85              |
| 1:A:353:PRO:HD2  | 1:B:376:ARG:HB2  | 1.60                     | 0.84              |
| 1:B:353:PRO:HD2  | 1:C:376:ARG:HB2  | 1.60                     | 0.84              |
| 1:E:577:ILE:HG12 | 1:E:597:GLN:HE22 | 1.42                     | 0.84              |
| 1:B:307:TRP:HA   | 1:B:315:VAL:O    | 1.78                     | 0.83              |
| 1:B:621:GLU:OE2  | 1:C:619:GLN:NE2  | 2.11                     | 0.83              |
| 1:H:248:LYS:HD2  | 1:H:251:ILE:HB   | 1.61                     | 0.83              |
| 1:H:612:GLN:HA   | 1:H:615:LEU:HD13 | 1.61                     | 0.83              |
| 1:J:577:ILE:HG12 | 1:J:597:GLN:HE22 | 1.44                     | 0.83              |
| 1:A:577:ILE:HG12 | 1:A:597:GLN:HE22 | 1.44                     | 0.83              |
| 1:F:577:ILE:HG12 | 1:F:597:GLN:HE22 | 1.43                     | 0.83              |
| 1:K:577:ILE:HG12 | 1:K:597:GLN:HE22 | 1.44                     | 0.83              |
| 1:H:72:ARG:HD2   | 1:H:108:LYS:HE2  | 1.60                     | 0.82              |
| 1:A:621:GLU:OE2  | 1:B:619:GLN:NE2  | 2.11                     | 0.82              |
| 1:L:296:GLU:HB2  | 1:L:449:PHE:HD2  | 1.44                     | 0.82              |
| 1:E:621:GLU:OE2  | 1:F:619:GLN:NE2  | 2.13                     | 0.81              |
| 1:C:613:GLY:HA2  | 1:C:616:LEU:CD1  | 2.10                     | 0.81              |
| 1:F:621:GLU:OE2  | 1:G:619:GLN:NE2  | 2.13                     | 0.81              |
| 1:H:621:GLU:OE2  | 1:I:619:GLN:NE2  | 2.14                     | 0.81              |
| 1:J:621:GLU:OE2  | 1:K:619:GLN:NE2  | 2.12                     | 0.81              |
| 1:I:353:PRO:HD2  | 1:J:376:ARG:HB2  | 1.62                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:619:GLN:NE2  | 1:L:621:GLU:OE2  | 2.13                     | 0.81              |
| 1:F:248:LYS:HD2  | 1:F:251:ILE:HB   | 1.63                     | 0.81              |
| 1:D:72:ARG:HD2   | 1:D:108:LYS:HE2  | 1.61                     | 0.81              |
| 1:I:72:ARG:HD2   | 1:I:108:LYS:HE2  | 1.62                     | 0.81              |
| 1:C:546:THR:HB   | 1:C:550:GLN:HE22 | 1.45                     | 0.80              |
| 1:H:577:ILE:HG12 | 1:H:597:GLN:HE22 | 1.43                     | 0.80              |
| 1:L:307:TRP:HA   | 1:L:315:VAL:O    | 1.80                     | 0.80              |
| 1:H:613:GLY:HA2  | 1:H:616:LEU:CD1  | 2.10                     | 0.80              |
| 1:B:72:ARG:HD2   | 1:B:108:LYS:HE2  | 1.61                     | 0.80              |
| 1:D:128:LEU:HA   | 1:D:145:ARG:O    | 1.81                     | 0.80              |
| 1:D:251:ILE:HD11 | 1:D:273:ARG:HH22 | 1.47                     | 0.80              |
| 1:D:621:GLU:OE2  | 1:E:619:GLN:NE2  | 2.14                     | 0.80              |
| 1:G:25:ALA:O     | 1:G:29:ALA:HB2   | 1.81                     | 0.80              |
| 1:I:621:GLU:OE2  | 1:J:619:GLN:NE2  | 2.14                     | 0.80              |
| 1:K:621:GLU:OE2  | 1:L:619:GLN:NE2  | 2.14                     | 0.80              |
| 1:I:127:ARG:O    | 1:I:146:ARG:HA   | 1.82                     | 0.80              |
| 1:G:307:TRP:HA   | 1:G:315:VAL:O    | 1.82                     | 0.80              |
| 1:G:621:GLU:OE2  | 1:H:619:GLN:NE2  | 2.14                     | 0.80              |
| 1:H:353:PRO:HD2  | 1:I:376:ARG:HB2  | 1.63                     | 0.79              |
| 1:B:248:LYS:HD2  | 1:B:251:ILE:HB   | 1.65                     | 0.79              |
| 1:I:248:LYS:HD2  | 1:I:251:ILE:HB   | 1.64                     | 0.79              |
| 1:J:353:PRO:HD2  | 1:K:376:ARG:HB2  | 1.64                     | 0.79              |
| 1:J:355:GLN:HG2  | 1:K:376:ARG:HH12 | 1.47                     | 0.79              |
| 1:D:296:GLU:HB2  | 1:D:449:PHE:HD2  | 1.47                     | 0.79              |
| 1:F:546:THR:HB   | 1:F:550:GLN:HE22 | 1.48                     | 0.79              |
| 1:H:434:THR:O    | 1:H:437:GLN:HB3  | 1.82                     | 0.79              |
| 1:K:546:THR:HB   | 1:K:550:GLN:HE22 | 1.48                     | 0.79              |
| 1:C:621:GLU:OE2  | 1:D:619:GLN:NE2  | 2.16                     | 0.79              |
| 1:B:128:LEU:HA   | 1:B:145:ARG:O    | 1.83                     | 0.78              |
| 1:J:127:ARG:O    | 1:J:146:ARG:HA   | 1.83                     | 0.78              |
| 1:L:72:ARG:HD2   | 1:L:108:LYS:HE2  | 1.65                     | 0.78              |
| 1:E:353:PRO:HD2  | 1:F:376:ARG:HB2  | 1.63                     | 0.78              |
| 1:A:296:GLU:HB2  | 1:A:449:PHE:HD2  | 1.48                     | 0.78              |
| 1:G:612:GLN:HA   | 1:G:615:LEU:HD13 | 1.66                     | 0.78              |
| 1:H:127:ARG:O    | 1:H:146:ARG:HA   | 1.84                     | 0.78              |
| 1:K:127:ARG:O    | 1:K:146:ARG:HA   | 1.84                     | 0.78              |
| 1:D:25:ALA:O     | 1:D:29:ALA:HB2   | 1.84                     | 0.78              |
| 1:I:355:GLN:HG2  | 1:J:376:ARG:HH12 | 1.48                     | 0.78              |
| 1:G:72:ARG:HD2   | 1:G:108:LYS:HE2  | 1.66                     | 0.77              |
| 1:B:127:ARG:O    | 1:B:146:ARG:HA   | 1.83                     | 0.77              |
| 1:D:546:THR:HB   | 1:D:550:GLN:HE22 | 1.47                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:72:ARG:HD2   | 1:E:108:LYS:HE2  | 1.66                     | 0.77              |
| 1:H:355:GLN:HG2  | 1:I:376:ARG:HH12 | 1.47                     | 0.77              |
| 1:I:25:ALA:O     | 1:I:29:ALA:HB2   | 1.84                     | 0.77              |
| 1:J:248:LYS:HD2  | 1:J:251:ILE:HB   | 1.65                     | 0.77              |
| 1:A:248:LYS:HD2  | 1:A:251:ILE:HB   | 1.64                     | 0.77              |
| 1:D:127:ARG:O    | 1:D:146:ARG:HA   | 1.84                     | 0.77              |
| 1:A:546:THR:HB   | 1:A:550:GLN:HE22 | 1.50                     | 0.77              |
| 1:B:355:GLN:HG2  | 1:C:376:ARG:HH12 | 1.48                     | 0.77              |
| 1:L:128:LEU:HA   | 1:L:145:ARG:O    | 1.85                     | 0.77              |
| 1:I:546:THR:HB   | 1:I:550:GLN:HE22 | 1.48                     | 0.77              |
| 1:A:376:ARG:HH12 | 1:L:355:GLN:HG2  | 1.50                     | 0.77              |
| 1:C:307:TRP:HA   | 1:C:315:VAL:O    | 1.83                     | 0.77              |
| 1:E:25:ALA:O     | 1:E:29:ALA:HB2   | 1.85                     | 0.77              |
| 1:C:248:LYS:HD2  | 1:C:251:ILE:HB   | 1.66                     | 0.77              |
| 1:F:72:ARG:HD2   | 1:F:108:LYS:HE2  | 1.67                     | 0.77              |
| 1:L:127:ARG:O    | 1:L:146:ARG:HA   | 1.85                     | 0.77              |
| 1:K:307:TRP:HA   | 1:K:315:VAL:O    | 1.85                     | 0.76              |
| 1:K:353:PRO:HD2  | 1:L:376:ARG:HB2  | 1.65                     | 0.76              |
| 1:A:72:ARG:HD2   | 1:A:108:LYS:HE2  | 1.67                     | 0.76              |
| 1:D:434:THR:O    | 1:D:437:GLN:HB3  | 1.86                     | 0.76              |
| 1:F:355:GLN:HG2  | 1:G:376:ARG:HH12 | 1.50                     | 0.76              |
| 1:G:546:THR:HB   | 1:G:550:GLN:HE22 | 1.51                     | 0.76              |
| 1:E:546:THR:HB   | 1:E:550:GLN:HE22 | 1.50                     | 0.76              |
| 1:I:128:LEU:HA   | 1:I:145:ARG:O    | 1.85                     | 0.76              |
| 1:F:296:GLU:HB2  | 1:F:449:PHE:HD2  | 1.49                     | 0.76              |
| 1:K:248:LYS:HD2  | 1:K:251:ILE:HB   | 1.65                     | 0.76              |
| 1:A:25:ALA:O     | 1:A:29:ALA:HB2   | 1.85                     | 0.76              |
| 1:D:248:LYS:HD2  | 1:D:251:ILE:HB   | 1.68                     | 0.76              |
| 1:F:127:ARG:O    | 1:F:146:ARG:HA   | 1.85                     | 0.76              |
| 1:G:248:LYS:HD2  | 1:G:251:ILE:HB   | 1.66                     | 0.76              |
| 1:F:128:LEU:HA   | 1:F:145:ARG:O    | 1.86                     | 0.76              |
| 1:E:355:GLN:HG2  | 1:F:376:ARG:HH12 | 1.50                     | 0.76              |
| 1:B:546:THR:HB   | 1:B:550:GLN:HE22 | 1.50                     | 0.76              |
| 1:H:296:GLU:HB2  | 1:H:449:PHE:HD2  | 1.48                     | 0.76              |
| 1:L:248:LYS:HD2  | 1:L:251:ILE:HB   | 1.67                     | 0.76              |
| 1:L:546:THR:HB   | 1:L:550:GLN:HE22 | 1.50                     | 0.76              |
| 1:E:310:VAL:HG22 | 1:F:40:GLN:HG3   | 1.68                     | 0.76              |
| 1:J:25:ALA:O     | 1:J:29:ALA:HB2   | 1.86                     | 0.76              |
| 1:F:251:ILE:HD11 | 1:F:273:ARG:HH22 | 1.49                     | 0.75              |
| 1:E:296:GLU:HB2  | 1:E:449:PHE:HD2  | 1.50                     | 0.75              |
| 1:H:546:THR:HB   | 1:H:550:GLN:HE22 | 1.49                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:127:ARG:O    | 1:A:146:ARG:HA   | 1.86                     | 0.75              |
| 1:I:296:GLU:HB2  | 1:I:449:PHE:HD2  | 1.50                     | 0.75              |
| 1:B:122:GLY:O    | 1:B:305:GLY:N    | 2.18                     | 0.75              |
| 1:F:25:ALA:O     | 1:F:29:ALA:HB2   | 1.86                     | 0.75              |
| 1:J:546:THR:HB   | 1:J:550:GLN:HE22 | 1.50                     | 0.75              |
| 1:E:248:LYS:HD2  | 1:E:251:ILE:HB   | 1.68                     | 0.75              |
| 1:K:613:GLY:HA2  | 1:K:616:LEU:HD13 | 1.68                     | 0.75              |
| 1:A:663:SER:HA   | 1:A:666:ARG:HE   | 1.52                     | 0.75              |
| 1:A:355:GLN:HG2  | 1:B:376:ARG:HH12 | 1.51                     | 0.75              |
| 1:C:25:ALA:O     | 1:C:29:ALA:HB2   | 1.86                     | 0.75              |
| 1:B:25:ALA:O     | 1:B:29:ALA:HB2   | 1.86                     | 0.74              |
| 1:D:122:GLY:O    | 1:D:305:GLY:N    | 2.19                     | 0.74              |
| 1:J:613:GLY:HA2  | 1:J:616:LEU:HD12 | 1.68                     | 0.74              |
| 1:J:251:ILE:HD11 | 1:J:273:ARG:HH22 | 1.51                     | 0.74              |
| 1:K:128:LEU:HA   | 1:K:145:ARG:O    | 1.87                     | 0.74              |
| 1:B:296:GLU:HB2  | 1:B:449:PHE:HD2  | 1.52                     | 0.74              |
| 1:G:127:ARG:O    | 1:G:146:ARG:HA   | 1.86                     | 0.74              |
| 1:G:353:PRO:HD2  | 1:H:376:ARG:HB2  | 1.68                     | 0.74              |
| 1:I:251:ILE:HD11 | 1:I:273:ARG:HH22 | 1.53                     | 0.74              |
| 1:L:25:ALA:O     | 1:L:29:ALA:HB2   | 1.86                     | 0.74              |
| 1:A:325:ASP:OD2  | 1:B:56:GLN:N     | 2.21                     | 0.74              |
| 1:C:663:SER:HA   | 1:C:666:ARG:HE   | 1.52                     | 0.74              |
| 1:E:663:SER:HA   | 1:E:666:ARG:HE   | 1.51                     | 0.74              |
| 1:K:296:GLU:HB2  | 1:K:449:PHE:HD2  | 1.50                     | 0.74              |
| 1:C:251:ILE:HD11 | 1:C:273:ARG:HH22 | 1.53                     | 0.74              |
| 1:C:296:GLU:HB2  | 1:C:449:PHE:HD2  | 1.53                     | 0.74              |
| 1:J:434:THR:O    | 1:J:437:GLN:HB3  | 1.87                     | 0.74              |
| 1:L:122:GLY:O    | 1:L:305:GLY:N    | 2.19                     | 0.74              |
| 1:F:307:TRP:HA   | 1:F:315:VAL:O    | 1.88                     | 0.74              |
| 1:A:307:TRP:HA   | 1:A:315:VAL:O    | 1.86                     | 0.74              |
| 1:E:122:GLY:O    | 1:E:305:GLY:N    | 2.19                     | 0.74              |
| 1:E:127:ARG:O    | 1:E:146:ARG:HA   | 1.87                     | 0.74              |
| 1:J:307:TRP:HA   | 1:J:315:VAL:O    | 1.86                     | 0.74              |
| 1:K:25:ALA:O     | 1:K:29:ALA:HB2   | 1.87                     | 0.74              |
| 1:C:122:GLY:O    | 1:C:305:GLY:N    | 2.20                     | 0.73              |
| 1:C:356:ILE:HG13 | 1:C:357:ALA:H    | 1.53                     | 0.73              |
| 1:F:37:ARG:NH1   | 1:F:48:TYR:OH    | 2.22                     | 0.73              |
| 1:F:122:GLY:O    | 1:F:305:GLY:N    | 2.19                     | 0.73              |
| 1:F:511:ARG:HD3  | 1:F:513:ARG:HH22 | 1.54                     | 0.73              |
| 1:G:296:GLU:HB2  | 1:G:449:PHE:HD2  | 1.53                     | 0.73              |
| 1:J:663:SER:HA   | 1:J:666:ARG:HE   | 1.53                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:663:SER:HA   | 1:B:666:ARG:HE   | 1.54                     | 0.73              |
| 1:D:353:PRO:HD2  | 1:E:376:ARG:HB2  | 1.68                     | 0.73              |
| 1:G:251:ILE:HD11 | 1:G:273:ARG:HH22 | 1.54                     | 0.73              |
| 1:H:38:VAL:HG21  | 1:H:324:LYS:HD2  | 1.69                     | 0.73              |
| 1:L:356:ILE:HG13 | 1:L:357:ALA:H    | 1.53                     | 0.73              |
| 1:G:128:LEU:HA   | 1:G:145:ARG:O    | 1.88                     | 0.73              |
| 1:E:294:ALA:HA   | 1:E:453:LEU:HD23 | 1.71                     | 0.73              |
| 1:K:663:SER:HA   | 1:K:666:ARG:HE   | 1.54                     | 0.73              |
| 1:L:294:ALA:HA   | 1:L:453:LEU:HD23 | 1.71                     | 0.73              |
| 1:B:612:GLN:HA   | 1:B:615:LEU:HD13 | 1.71                     | 0.72              |
| 1:C:127:ARG:O    | 1:C:146:ARG:HA   | 1.89                     | 0.72              |
| 1:D:307:TRP:HA   | 1:D:315:VAL:O    | 1.89                     | 0.72              |
| 1:H:128:LEU:HA   | 1:H:145:ARG:O    | 1.89                     | 0.72              |
| 1:J:296:GLU:HB2  | 1:J:449:PHE:HD2  | 1.53                     | 0.72              |
| 1:E:307:TRP:HA   | 1:E:315:VAL:O    | 1.88                     | 0.72              |
| 1:F:294:ALA:HA   | 1:F:453:LEU:HD23 | 1.71                     | 0.72              |
| 1:F:663:SER:HA   | 1:F:666:ARG:HE   | 1.52                     | 0.72              |
| 1:K:72:ARG:HD2   | 1:K:108:LYS:HE2  | 1.70                     | 0.72              |
| 1:G:294:ALA:HA   | 1:G:453:LEU:HD23 | 1.71                     | 0.72              |
| 1:H:25:ALA:O     | 1:H:29:ALA:HB2   | 1.88                     | 0.72              |
| 1:I:58:ASP:HA    | 1:I:327:GLN:OE1  | 1.90                     | 0.72              |
| 1:K:434:THR:O    | 1:K:437:GLN:HB3  | 1.90                     | 0.72              |
| 1:H:586:THR:HG22 | 1:H:590:GLN:HE22 | 1.53                     | 0.72              |
| 1:I:325:ASP:OD2  | 1:J:56:GLN:N     | 2.22                     | 0.72              |
| 1:J:122:GLY:O    | 1:J:305:GLY:N    | 2.20                     | 0.72              |
| 1:E:128:LEU:HA   | 1:E:145:ARG:O    | 1.90                     | 0.72              |
| 1:C:434:THR:O    | 1:C:437:GLN:HB3  | 1.90                     | 0.72              |
| 1:D:663:SER:HA   | 1:D:666:ARG:HE   | 1.52                     | 0.72              |
| 1:L:663:SER:HA   | 1:L:666:ARG:HE   | 1.54                     | 0.72              |
| 1:H:294:ALA:HA   | 1:H:453:LEU:HD23 | 1.72                     | 0.72              |
| 1:I:122:GLY:O    | 1:I:305:GLY:N    | 2.20                     | 0.72              |
| 1:K:355:GLN:HG2  | 1:L:376:ARG:HH12 | 1.55                     | 0.72              |
| 1:C:128:LEU:HA   | 1:C:145:ARG:O    | 1.88                     | 0.72              |
| 1:F:612:GLN:HA   | 1:F:615:LEU:HD13 | 1.72                     | 0.72              |
| 1:D:325:ASP:OD2  | 1:E:56:GLN:N     | 2.23                     | 0.71              |
| 1:F:356:ILE:HG13 | 1:F:357:ALA:H    | 1.55                     | 0.71              |
| 1:K:612:GLN:HA   | 1:K:615:LEU:HD13 | 1.72                     | 0.71              |
| 1:C:353:PRO:HD2  | 1:D:376:ARG:HB2  | 1.72                     | 0.71              |
| 1:F:586:THR:HG22 | 1:F:590:GLN:HE22 | 1.54                     | 0.71              |
| 1:H:650:ILE:HA   | 1:H:653:ILE:HD12 | 1.73                     | 0.71              |
| 1:B:434:THR:O    | 1:B:437:GLN:HB3  | 1.89                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:307:TRP:HA   | 1:I:315:VAL:O    | 1.90                     | 0.71              |
| 1:C:38:VAL:HG21  | 1:C:324:LYS:HD2  | 1.70                     | 0.71              |
| 1:F:434:THR:O    | 1:F:437:GLN:HB3  | 1.89                     | 0.71              |
| 1:L:251:ILE:HD11 | 1:L:273:ARG:HH22 | 1.56                     | 0.71              |
| 1:C:325:ASP:OD2  | 1:D:56:GLN:N     | 2.24                     | 0.71              |
| 1:A:122:GLY:O    | 1:A:305:GLY:N    | 2.21                     | 0.71              |
| 1:K:586:THR:HG22 | 1:K:590:GLN:HE22 | 1.56                     | 0.71              |
| 1:A:128:LEU:HA   | 1:A:145:ARG:O    | 1.90                     | 0.71              |
| 1:C:58:ASP:HA    | 1:C:327:GLN:OE1  | 1.91                     | 0.71              |
| 1:G:270:GLN:NE2  | 1:G:271:ILE:O    | 2.24                     | 0.71              |
| 1:J:612:GLN:HA   | 1:J:615:LEU:HD13 | 1.73                     | 0.71              |
| 1:K:294:ALA:HA   | 1:K:453:LEU:HD23 | 1.70                     | 0.71              |
| 1:E:251:ILE:HD11 | 1:E:273:ARG:HH22 | 1.55                     | 0.70              |
| 1:A:164:LEU:HD12 | 1:A:166:ASP:HB3  | 1.73                     | 0.70              |
| 1:H:96:GLY:O     | 1:H:100:THR:OG1  | 2.08                     | 0.70              |
| 1:G:663:SER:HA   | 1:G:666:ARG:HE   | 1.55                     | 0.70              |
| 1:A:356:ILE:HG13 | 1:A:357:ALA:H    | 1.57                     | 0.70              |
| 1:K:356:ILE:HG13 | 1:K:357:ALA:H    | 1.56                     | 0.70              |
| 1:C:72:ARG:HD2   | 1:C:108:LYS:HE2  | 1.71                     | 0.70              |
| 1:I:612:GLN:HA   | 1:I:615:LEU:HD13 | 1.74                     | 0.70              |
| 1:E:356:ILE:HG13 | 1:E:357:ALA:H    | 1.56                     | 0.70              |
| 1:B:325:ASP:OD2  | 1:C:56:GLN:N     | 2.24                     | 0.70              |
| 1:F:650:ILE:HA   | 1:F:653:ILE:HD12 | 1.73                     | 0.70              |
| 1:G:434:THR:O    | 1:G:437:GLN:HB3  | 1.90                     | 0.70              |
| 1:A:294:ALA:HA   | 1:A:453:LEU:HD23 | 1.71                     | 0.70              |
| 1:D:356:ILE:HG13 | 1:D:357:ALA:H    | 1.57                     | 0.70              |
| 1:H:663:SER:HA   | 1:H:666:ARG:HE   | 1.55                     | 0.70              |
| 1:K:122:GLY:O    | 1:K:305:GLY:N    | 2.22                     | 0.70              |
| 1:L:339:ASP:HA   | 1:L:342:ALA:HB3  | 1.74                     | 0.70              |
| 1:A:251:ILE:HD11 | 1:A:273:ARG:HH22 | 1.57                     | 0.70              |
| 1:H:122:GLY:O    | 1:H:305:GLY:N    | 2.22                     | 0.70              |
| 1:J:128:LEU:HA   | 1:J:145:ARG:O    | 1.90                     | 0.70              |
| 1:F:613:GLY:HA2  | 1:F:616:LEU:HD12 | 1.73                     | 0.70              |
| 1:L:434:THR:O    | 1:L:437:GLN:HB3  | 1.92                     | 0.70              |
| 1:A:434:THR:O    | 1:A:437:GLN:HB3  | 1.91                     | 0.69              |
| 1:C:612:GLN:HA   | 1:C:615:LEU:HD13 | 1.72                     | 0.69              |
| 1:E:325:ASP:OD2  | 1:F:56:GLN:N     | 2.25                     | 0.69              |
| 1:F:325:ASP:OD2  | 1:G:56:GLN:N     | 2.25                     | 0.69              |
| 1:F:353:PRO:HD2  | 1:G:376:ARG:HB2  | 1.73                     | 0.69              |
| 1:J:38:VAL:HG21  | 1:J:324:LYS:HD2  | 1.74                     | 0.69              |
| 1:E:613:GLY:HA2  | 1:E:616:LEU:HD13 | 1.73                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:58:ASP:HA    | 1:B:327:GLN:OE1  | 1.91                     | 0.69              |
| 1:C:134:ASP:OD1  | 1:C:141:ASN:ND2  | 2.21                     | 0.69              |
| 1:G:38:VAL:HG21  | 1:G:324:LYS:HD2  | 1.74                     | 0.69              |
| 1:I:294:ALA:HA   | 1:I:453:LEU:HD23 | 1.72                     | 0.69              |
| 1:J:72:ARG:HD2   | 1:J:108:LYS:HE2  | 1.73                     | 0.69              |
| 1:I:356:ILE:HG13 | 1:I:357:ALA:H    | 1.57                     | 0.69              |
| 1:C:113:ILE:HG13 | 1:C:148:PRO:HB2  | 1.74                     | 0.69              |
| 1:H:325:ASP:OD2  | 1:I:56:GLN:N     | 2.24                     | 0.69              |
| 1:B:586:THR:HG22 | 1:B:590:GLN:HE22 | 1.56                     | 0.69              |
| 1:D:160:SER:OG   | 1:D:172:HIS:ND1  | 2.21                     | 0.69              |
| 1:D:294:ALA:HA   | 1:D:453:LEU:HD23 | 1.74                     | 0.69              |
| 1:I:663:SER:HA   | 1:I:666:ARG:HE   | 1.55                     | 0.69              |
| 1:A:87:ARG:HG2   | 1:A:89:ASP:H     | 1.57                     | 0.69              |
| 1:A:376:ARG:HB2  | 1:L:353:PRO:HD2  | 1.72                     | 0.69              |
| 1:A:650:ILE:HA   | 1:A:653:ILE:HD12 | 1.74                     | 0.69              |
| 1:D:58:ASP:HA    | 1:D:327:GLN:OE1  | 1.92                     | 0.69              |
| 1:D:586:THR:HG22 | 1:D:590:GLN:HE22 | 1.55                     | 0.69              |
| 1:E:58:ASP:HA    | 1:E:327:GLN:OE1  | 1.92                     | 0.69              |
| 1:F:160:SER:OG   | 1:F:172:HIS:ND1  | 2.23                     | 0.69              |
| 1:G:511:ARG:HD3  | 1:G:513:ARG:HH22 | 1.58                     | 0.69              |
| 1:J:325:ASP:OD2  | 1:K:56:GLN:N     | 2.26                     | 0.69              |
| 1:K:251:ILE:HD11 | 1:K:273:ARG:HH22 | 1.57                     | 0.69              |
| 1:A:586:THR:HG22 | 1:A:590:GLN:HE22 | 1.58                     | 0.69              |
| 1:C:613:GLY:O    | 1:C:616:LEU:HD13 | 1.93                     | 0.69              |
| 1:G:356:ILE:HG13 | 1:G:357:ALA:H    | 1.58                     | 0.69              |
| 1:B:251:ILE:HD11 | 1:B:273:ARG:HH22 | 1.59                     | 0.68              |
| 1:H:37:ARG:NH1   | 1:H:48:TYR:OH    | 2.26                     | 0.68              |
| 1:H:356:ILE:HG13 | 1:H:357:ALA:H    | 1.56                     | 0.68              |
| 1:I:613:GLY:HA2  | 1:I:616:LEU:HD12 | 1.75                     | 0.68              |
| 1:J:356:ILE:HG13 | 1:J:357:ALA:H    | 1.56                     | 0.68              |
| 1:A:612:GLN:HA   | 1:A:615:LEU:HD13 | 1.75                     | 0.68              |
| 1:C:711:GLN:OE1  | 1:D:712:ARG:NH1  | 2.26                     | 0.68              |
| 1:G:122:GLY:O    | 1:G:305:GLY:N    | 2.23                     | 0.68              |
| 1:H:134:ASP:OD1  | 1:H:141:ASN:ND2  | 2.22                     | 0.68              |
| 1:B:356:ILE:HG13 | 1:B:357:ALA:H    | 1.58                     | 0.68              |
| 1:C:613:GLY:HA2  | 1:C:616:LEU:HD12 | 1.74                     | 0.68              |
| 1:C:58:ASP:HB3   | 1:C:60:VAL:HG23  | 1.75                     | 0.68              |
| 1:J:586:THR:HG22 | 1:J:590:GLN:HE22 | 1.59                     | 0.68              |
| 1:L:58:ASP:HA    | 1:L:327:GLN:OE1  | 1.93                     | 0.68              |
| 1:C:270:GLN:NE2  | 1:C:271:ILE:O    | 2.26                     | 0.68              |
| 1:D:270:GLN:NE2  | 1:D:271:ILE:O    | 2.26                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:160:SER:OG   | 1:G:172:HIS:ND1  | 2.19                     | 0.68              |
| 1:A:56:GLN:N     | 1:L:325:ASP:OD2  | 2.26                     | 0.68              |
| 1:B:650:ILE:HA   | 1:B:653:ILE:HD12 | 1.74                     | 0.68              |
| 1:G:510:ILE:HG12 | 1:G:512:GLY:H    | 1.58                     | 0.68              |
| 1:J:294:ALA:HA   | 1:J:453:LEU:HD23 | 1.75                     | 0.68              |
| 1:E:80:TYR:HD1   | 1:E:518:THR:HA   | 1.60                     | 0.68              |
| 1:E:93:VAL:O     | 1:E:96:GLY:N     | 2.27                     | 0.68              |
| 1:K:325:ASP:OD2  | 1:L:56:GLN:N     | 2.27                     | 0.68              |
| 1:B:339:ASP:HA   | 1:B:342:ALA:HB3  | 1.76                     | 0.67              |
| 1:G:25:ALA:O     | 1:G:29:ALA:CB    | 2.42                     | 0.67              |
| 1:H:164:LEU:HD12 | 1:H:166:ASP:HB3  | 1.76                     | 0.67              |
| 1:B:25:ALA:O     | 1:B:29:ALA:CB    | 2.41                     | 0.67              |
| 1:B:294:ALA:HA   | 1:B:453:LEU:HD23 | 1.74                     | 0.67              |
| 1:H:307:TRP:HA   | 1:H:315:VAL:O    | 1.93                     | 0.67              |
| 1:K:510:ILE:HG12 | 1:K:512:GLY:H    | 1.59                     | 0.67              |
| 1:L:93:VAL:O     | 1:L:96:GLY:N     | 2.28                     | 0.67              |
| 1:D:339:ASP:HA   | 1:D:342:ALA:HB3  | 1.75                     | 0.67              |
| 1:F:58:ASP:HB3   | 1:F:60:VAL:HG23  | 1.77                     | 0.67              |
| 1:F:164:LEU:HD12 | 1:F:166:ASP:HB3  | 1.75                     | 0.67              |
| 1:A:25:ALA:O     | 1:A:29:ALA:CB    | 2.42                     | 0.67              |
| 1:B:58:ASP:HB3   | 1:B:60:VAL:HG23  | 1.77                     | 0.67              |
| 1:H:25:ALA:O     | 1:H:29:ALA:CB    | 2.42                     | 0.67              |
| 1:C:294:ALA:HA   | 1:C:453:LEU:HD23 | 1.76                     | 0.67              |
| 1:F:58:ASP:HA    | 1:F:327:GLN:OE1  | 1.93                     | 0.67              |
| 1:G:355:GLN:HG2  | 1:H:376:ARG:HH12 | 1.59                     | 0.67              |
| 1:H:251:ILE:HD11 | 1:H:273:ARG:HH22 | 1.59                     | 0.67              |
| 1:J:22:SER:O     | 1:J:26:ARG:HG2   | 1.95                     | 0.67              |
| 1:B:22:SER:O     | 1:B:26:ARG:HG2   | 1.94                     | 0.67              |
| 1:F:38:VAL:HG21  | 1:F:324:LYS:HD2  | 1.77                     | 0.67              |
| 1:J:161:ASN:HD21 | 1:K:183:GLY:HA3  | 1.59                     | 0.67              |
| 1:J:650:ILE:HA   | 1:J:653:ILE:HD12 | 1.77                     | 0.67              |
| 1:K:58:ASP:HB3   | 1:K:60:VAL:HG23  | 1.76                     | 0.67              |
| 1:D:58:ASP:HB3   | 1:D:60:VAL:HG23  | 1.77                     | 0.67              |
| 1:H:87:ARG:HG2   | 1:H:89:ASP:H     | 1.60                     | 0.67              |
| 1:A:40:GLN:HG3   | 1:L:310:VAL:HG22 | 1.76                     | 0.66              |
| 1:B:270:GLN:NE2  | 1:B:271:ILE:O    | 2.27                     | 0.66              |
| 1:L:38:VAL:HG21  | 1:L:324:LYS:HD2  | 1.77                     | 0.66              |
| 1:C:79:LEU:H     | 1:C:520:VAL:HA   | 1.60                     | 0.66              |
| 1:E:25:ALA:O     | 1:E:29:ALA:CB    | 2.43                     | 0.66              |
| 1:G:93:VAL:O     | 1:G:96:GLY:N     | 2.29                     | 0.66              |
| 1:C:556:TYR:HB3  | 1:C:572:ALA:HB2  | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:58:ASP:HA    | 1:G:327:GLN:OE1  | 1.95                     | 0.66              |
| 1:J:134:ASP:OD1  | 1:J:141:ASN:ND2  | 2.23                     | 0.66              |
| 1:L:556:TYR:HB3  | 1:L:572:ALA:HB2  | 1.78                     | 0.66              |
| 1:A:270:GLN:NE2  | 1:A:271:ILE:O    | 2.28                     | 0.66              |
| 1:D:164:LEU:HD12 | 1:D:166:ASP:HB3  | 1.77                     | 0.66              |
| 1:E:586:THR:HG22 | 1:E:590:GLN:HE22 | 1.59                     | 0.66              |
| 1:I:25:ALA:O     | 1:I:29:ALA:CB    | 2.42                     | 0.66              |
| 1:J:37:ARG:NH1   | 1:J:48:TYR:OH    | 2.28                     | 0.66              |
| 1:K:310:VAL:HG22 | 1:L:40:GLN:HG3   | 1.77                     | 0.66              |
| 1:B:310:VAL:HG22 | 1:C:40:GLN:HG3   | 1.77                     | 0.66              |
| 1:B:613:GLY:HA2  | 1:B:616:LEU:CD1  | 2.22                     | 0.66              |
| 1:C:164:LEU:HD12 | 1:C:166:ASP:HB3  | 1.76                     | 0.66              |
| 1:D:25:ALA:O     | 1:D:29:ALA:CB    | 2.42                     | 0.66              |
| 1:E:510:ILE:HG12 | 1:E:512:GLY:H    | 1.60                     | 0.66              |
| 1:F:22:SER:O     | 1:F:26:ARG:HG2   | 1.96                     | 0.66              |
| 1:H:457:MET:O    | 1:H:458:ARG:HG2  | 1.96                     | 0.66              |
| 1:K:339:ASP:HA   | 1:K:342:ALA:HB3  | 1.78                     | 0.66              |
| 1:I:586:THR:HG22 | 1:I:590:GLN:HE22 | 1.60                     | 0.66              |
| 1:J:457:MET:O    | 1:J:458:ARG:HG2  | 1.96                     | 0.66              |
| 1:K:134:ASP:OD1  | 1:K:141:ASN:ND2  | 2.26                     | 0.66              |
| 1:K:511:ARG:HD3  | 1:K:513:ARG:HH22 | 1.60                     | 0.66              |
| 1:E:434:THR:O    | 1:E:437:GLN:HB3  | 1.95                     | 0.66              |
| 1:F:113:ILE:HG13 | 1:F:148:PRO:HB2  | 1.77                     | 0.66              |
| 1:F:510:ILE:HG12 | 1:F:512:GLY:H    | 1.61                     | 0.66              |
| 1:G:87:ARG:HG2   | 1:G:89:ASP:H     | 1.61                     | 0.66              |
| 1:K:160:SER:OG   | 1:K:172:HIS:ND1  | 2.21                     | 0.66              |
| 1:E:164:LEU:HD12 | 1:E:166:ASP:HB3  | 1.76                     | 0.66              |
| 1:E:37:ARG:NH1   | 1:E:48:TYR:OH    | 2.29                     | 0.66              |
| 1:I:58:ASP:HB3   | 1:I:60:VAL:HG23  | 1.77                     | 0.65              |
| 1:F:457:MET:O    | 1:F:458:ARG:HG2  | 1.97                     | 0.65              |
| 1:I:134:ASP:OD1  | 1:I:141:ASN:ND2  | 2.25                     | 0.65              |
| 1:C:25:ALA:O     | 1:C:29:ALA:CB    | 2.44                     | 0.65              |
| 1:F:25:ALA:O     | 1:F:29:ALA:CB    | 2.44                     | 0.65              |
| 1:G:325:ASP:OD2  | 1:H:56:GLN:N     | 2.27                     | 0.65              |
| 1:K:164:LEU:HD12 | 1:K:166:ASP:HB3  | 1.77                     | 0.65              |
| 1:L:586:THR:HG22 | 1:L:590:GLN:HE22 | 1.61                     | 0.65              |
| 1:E:160:SER:OG   | 1:E:172:HIS:ND1  | 2.22                     | 0.65              |
| 1:E:650:ILE:HA   | 1:E:653:ILE:HD12 | 1.77                     | 0.65              |
| 1:D:457:MET:O    | 1:D:458:ARG:HG2  | 1.96                     | 0.65              |
| 1:H:22:SER:O     | 1:H:26:ARG:HG2   | 1.97                     | 0.65              |
| 1:I:87:ARG:HG2   | 1:I:89:ASP:H     | 1.60                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:457:MET:O    | 1:L:458:ARG:HG2  | 1.96                     | 0.65              |
| 1:F:221:GLU:HG2  | 1:F:280:ILE:HG12 | 1.79                     | 0.65              |
| 1:J:96:GLY:O     | 1:J:100:THR:OG1  | 2.10                     | 0.65              |
| 1:K:22:SER:O     | 1:K:26:ARG:HG2   | 1.96                     | 0.65              |
| 1:K:58:ASP:HA    | 1:K:327:GLN:OE1  | 1.95                     | 0.65              |
| 1:A:22:SER:O     | 1:A:26:ARG:HG2   | 1.96                     | 0.65              |
| 1:A:93:VAL:O     | 1:A:96:GLY:N     | 2.30                     | 0.65              |
| 1:E:83:LYS:HB2   | 1:E:515:GLU:HB3  | 1.78                     | 0.65              |
| 1:J:58:ASP:HB3   | 1:J:60:VAL:HG23  | 1.79                     | 0.65              |
| 1:A:510:ILE:HG12 | 1:A:512:GLY:H    | 1.62                     | 0.65              |
| 1:H:93:VAL:O     | 1:H:96:GLY:N     | 2.30                     | 0.65              |
| 1:C:160:SER:OG   | 1:C:172:HIS:ND1  | 2.23                     | 0.65              |
| 1:D:96:GLY:O     | 1:D:100:THR:OG1  | 2.08                     | 0.65              |
| 1:E:577:ILE:HD12 | 1:E:584:PRO:HB3  | 1.79                     | 0.65              |
| 1:H:221:GLU:HG2  | 1:H:280:ILE:HG12 | 1.78                     | 0.65              |
| 1:H:613:GLY:CA   | 1:H:616:LEU:HD13 | 2.26                     | 0.65              |
| 1:C:362:MET:HA   | 1:C:366:ASN:HB2  | 1.79                     | 0.64              |
| 1:I:22:SER:O     | 1:I:26:ARG:HG2   | 1.96                     | 0.64              |
| 1:I:38:VAL:HG21  | 1:I:324:LYS:HD2  | 1.79                     | 0.64              |
| 1:J:25:ALA:O     | 1:J:29:ALA:CB    | 2.45                     | 0.64              |
| 1:A:83:LYS:HB2   | 1:A:515:GLU:HB3  | 1.78                     | 0.64              |
| 1:C:96:GLY:O     | 1:C:100:THR:OG1  | 2.11                     | 0.64              |
| 1:C:457:MET:O    | 1:C:458:ARG:HG2  | 1.97                     | 0.64              |
| 1:E:22:SER:O     | 1:E:26:ARG:HG2   | 1.97                     | 0.64              |
| 1:K:270:GLN:NE2  | 1:K:271:ILE:O    | 2.30                     | 0.64              |
| 1:A:457:MET:O    | 1:A:458:ARG:HG2  | 1.98                     | 0.64              |
| 1:C:586:THR:HG22 | 1:C:590:GLN:HE22 | 1.61                     | 0.64              |
| 1:F:87:ARG:HG2   | 1:F:89:ASP:H     | 1.62                     | 0.64              |
| 1:G:58:ASP:HB3   | 1:G:60:VAL:HG23  | 1.78                     | 0.64              |
| 1:L:650:ILE:HA   | 1:L:653:ILE:HD12 | 1.78                     | 0.64              |
| 1:A:183:GLY:HA3  | 1:L:161:ASN:HD21 | 1.63                     | 0.64              |
| 1:C:510:ILE:HG12 | 1:C:512:GLY:H    | 1.62                     | 0.64              |
| 1:D:22:SER:O     | 1:D:26:ARG:HG2   | 1.96                     | 0.64              |
| 1:F:577:ILE:HG12 | 1:F:597:GLN:NE2  | 2.13                     | 0.64              |
| 1:K:650:ILE:HA   | 1:K:653:ILE:HD12 | 1.77                     | 0.64              |
| 1:L:25:ALA:O     | 1:L:29:ALA:CB    | 2.44                     | 0.64              |
| 1:A:58:ASP:HB3   | 1:A:60:VAL:HG23  | 1.79                     | 0.64              |
| 1:C:93:VAL:O     | 1:C:96:GLY:N     | 2.31                     | 0.64              |
| 1:E:79:LEU:H     | 1:E:520:VAL:HA   | 1.62                     | 0.64              |
| 1:G:310:VAL:HG22 | 1:H:40:GLN:HG3   | 1.79                     | 0.64              |
| 1:G:556:TYR:HB3  | 1:G:572:ALA:HB2  | 1.78                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:452:ASN:OD1  | 1:H:453:LEU:N    | 2.31                     | 0.64              |
| 1:C:87:ARG:HG2   | 1:C:89:ASP:H     | 1.63                     | 0.64              |
| 1:E:612:GLN:HA   | 1:E:615:LEU:HD13 | 1.78                     | 0.64              |
| 1:F:134:ASP:OD1  | 1:F:141:ASN:ND2  | 2.26                     | 0.64              |
| 1:F:270:GLN:NE2  | 1:F:271:ILE:O    | 2.31                     | 0.64              |
| 1:L:433:ASP:O    | 1:L:437:GLN:N    | 2.30                     | 0.64              |
| 1:B:164:LEU:HD12 | 1:B:166:ASP:HB3  | 1.79                     | 0.64              |
| 1:C:452:ASN:OD1  | 1:C:453:LEU:N    | 2.31                     | 0.64              |
| 1:D:510:ILE:HG12 | 1:D:512:GLY:H    | 1.63                     | 0.64              |
| 1:G:433:ASP:O    | 1:G:437:GLN:N    | 2.29                     | 0.64              |
| 1:B:87:ARG:HG2   | 1:B:89:ASP:H     | 1.62                     | 0.64              |
| 1:B:457:MET:O    | 1:B:458:ARG:HG2  | 1.98                     | 0.64              |
| 1:B:510:ILE:HG12 | 1:B:512:GLY:H    | 1.63                     | 0.64              |
| 1:D:113:ILE:HG13 | 1:D:148:PRO:HB2  | 1.80                     | 0.64              |
| 1:J:58:ASP:HA    | 1:J:327:GLN:OE1  | 1.97                     | 0.64              |
| 1:K:25:ALA:O     | 1:K:29:ALA:CB    | 2.45                     | 0.64              |
| 1:K:457:MET:O    | 1:K:458:ARG:HG2  | 1.98                     | 0.64              |
| 1:L:510:ILE:HG12 | 1:L:512:GLY:H    | 1.61                     | 0.64              |
| 1:A:96:GLY:O     | 1:A:100:THR:OG1  | 2.09                     | 0.64              |
| 1:F:353:PRO:HA   | 1:G:373:LEU:HD23 | 1.80                     | 0.64              |
| 1:A:38:VAL:HG21  | 1:A:324:LYS:HD2  | 1.79                     | 0.64              |
| 1:D:134:ASP:OD1  | 1:D:141:ASN:ND2  | 2.26                     | 0.64              |
| 1:E:457:MET:O    | 1:E:458:ARG:HG2  | 1.97                     | 0.64              |
| 1:H:577:ILE:HG12 | 1:H:597:GLN:NE2  | 2.11                     | 0.64              |
| 1:K:87:ARG:HG2   | 1:K:89:ASP:H     | 1.63                     | 0.64              |
| 1:D:650:ILE:HA   | 1:D:653:ILE:HD12 | 1.80                     | 0.63              |
| 1:I:270:GLN:NE2  | 1:I:271:ILE:O    | 2.31                     | 0.63              |
| 1:B:93:VAL:O     | 1:B:96:GLY:N     | 2.31                     | 0.63              |
| 1:D:79:LEU:H     | 1:D:520:VAL:HA   | 1.62                     | 0.63              |
| 1:D:93:VAL:O     | 1:D:96:GLY:N     | 2.30                     | 0.63              |
| 1:E:58:ASP:HB3   | 1:E:60:VAL:HG23  | 1.79                     | 0.63              |
| 1:F:93:VAL:O     | 1:F:96:GLY:N     | 2.31                     | 0.63              |
| 1:G:586:THR:HG22 | 1:G:590:GLN:HE22 | 1.61                     | 0.63              |
| 1:H:58:ASP:HB3   | 1:H:60:VAL:HG23  | 1.80                     | 0.63              |
| 1:I:339:ASP:HA   | 1:I:342:ALA:HB3  | 1.81                     | 0.63              |
| 1:I:510:ILE:HG12 | 1:I:512:GLY:H    | 1.63                     | 0.63              |
| 1:K:38:VAL:HG21  | 1:K:324:LYS:HD2  | 1.80                     | 0.63              |
| 1:A:79:LEU:H     | 1:A:520:VAL:HA   | 1.62                     | 0.63              |
| 1:C:353:PRO:HA   | 1:D:373:LEU:HD23 | 1.80                     | 0.63              |
| 1:E:117:GLU:HB3  | 1:E:123:VAL:HG23 | 1.81                     | 0.63              |
| 1:G:437:GLN:HG2  | 1:G:520:VAL:HG21 | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:457:MET:O    | 1:I:458:ARG:HG2  | 1.97                     | 0.63              |
| 1:J:93:VAL:O     | 1:J:96:GLY:N     | 2.31                     | 0.63              |
| 1:L:511:ARG:HD3  | 1:L:513:ARG:HH22 | 1.63                     | 0.63              |
| 1:G:457:MET:O    | 1:G:458:ARG:HG2  | 1.98                     | 0.63              |
| 1:L:80:TYR:HD1   | 1:L:518:THR:HA   | 1.64                     | 0.63              |
| 1:L:134:ASP:OD1  | 1:L:141:ASN:ND2  | 2.24                     | 0.63              |
| 1:B:309:PHE:HB3  | 1:B:312:ASP:HA   | 1.81                     | 0.63              |
| 1:H:339:ASP:HA   | 1:H:342:ALA:HB3  | 1.80                     | 0.63              |
| 1:L:58:ASP:HB3   | 1:L:60:VAL:HG23  | 1.79                     | 0.63              |
| 1:L:79:LEU:H     | 1:L:520:VAL:HA   | 1.62                     | 0.63              |
| 1:L:164:LEU:HD12 | 1:L:166:ASP:HB3  | 1.79                     | 0.63              |
| 1:J:164:LEU:HD12 | 1:J:166:ASP:HB3  | 1.81                     | 0.63              |
| 1:J:511:ARG:HD3  | 1:J:513:ARG:HH22 | 1.62                     | 0.63              |
| 1:L:87:ARG:HG2   | 1:L:89:ASP:H     | 1.62                     | 0.63              |
| 1:D:38:VAL:HG21  | 1:D:324:LYS:HD2  | 1.80                     | 0.63              |
| 1:G:339:ASP:HA   | 1:G:342:ALA:HB3  | 1.80                     | 0.63              |
| 1:J:362:MET:HA   | 1:J:366:ASN:HB2  | 1.80                     | 0.63              |
| 1:A:339:ASP:HA   | 1:A:342:ALA:HB3  | 1.79                     | 0.63              |
| 1:C:577:ILE:HD12 | 1:C:584:PRO:HB3  | 1.81                     | 0.63              |
| 1:F:297:HIS:CD2  | 1:F:298:ILE:HG13 | 2.33                     | 0.63              |
| 1:G:22:SER:O     | 1:G:26:ARG:HG2   | 1.98                     | 0.63              |
| 1:L:250:ASP:OD1  | 1:L:251:ILE:N    | 2.32                     | 0.63              |
| 1:L:613:GLY:O    | 1:L:616:LEU:HD12 | 1.99                     | 0.63              |
| 1:C:80:TYR:HD1   | 1:C:518:THR:HA   | 1.64                     | 0.63              |
| 1:D:250:ASP:OD1  | 1:D:251:ILE:N    | 2.32                     | 0.63              |
| 1:D:452:ASN:OD1  | 1:D:453:LEU:N    | 2.32                     | 0.63              |
| 1:E:452:ASN:OD1  | 1:E:453:LEU:N    | 2.32                     | 0.63              |
| 1:G:650:ILE:HA   | 1:G:653:ILE:HD12 | 1.81                     | 0.63              |
| 1:H:418:LEU:HD23 | 1:H:429:GLN:HB3  | 1.81                     | 0.63              |
| 1:A:577:ILE:HG12 | 1:A:597:GLN:NE2  | 2.13                     | 0.62              |
| 1:B:250:ASP:OD1  | 1:B:251:ILE:N    | 2.32                     | 0.62              |
| 1:F:339:ASP:HA   | 1:F:342:ALA:HB3  | 1.81                     | 0.62              |
| 1:K:577:ILE:HD12 | 1:K:584:PRO:HB3  | 1.81                     | 0.62              |
| 1:A:83:LYS:HE2   | 1:A:85:GLY:HA3   | 1.81                     | 0.62              |
| 1:A:666:ARG:NH1  | 1:L:667:GLU:HG2  | 2.14                     | 0.62              |
| 1:B:160:SER:OG   | 1:B:172:HIS:ND1  | 2.23                     | 0.62              |
| 1:B:276:VAL:HG22 | 1:B:296:GLU:HA   | 1.81                     | 0.62              |
| 1:E:38:VAL:HG21  | 1:E:324:LYS:HD2  | 1.79                     | 0.62              |
| 1:H:310:VAL:HG22 | 1:I:40:GLN:HG3   | 1.80                     | 0.62              |
| 1:J:577:ILE:HG12 | 1:J:597:GLN:NE2  | 2.15                     | 0.62              |
| 1:L:612:GLN:HA   | 1:L:615:LEU:HD13 | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:41:TRP:CH2   | 1:A:44:TRP:HB2   | 2.34                     | 0.62              |
| 1:B:437:GLN:HG2  | 1:B:520:VAL:HG21 | 1.82                     | 0.62              |
| 1:B:452:ASN:OD1  | 1:B:453:LEU:N    | 2.32                     | 0.62              |
| 1:C:250:ASP:OD1  | 1:C:251:ILE:N    | 2.32                     | 0.62              |
| 1:K:37:ARG:NH1   | 1:K:48:TYR:OH    | 2.29                     | 0.62              |
| 1:L:22:SER:O     | 1:L:26:ARG:HG2   | 2.00                     | 0.62              |
| 1:L:83:LYS:HE2   | 1:L:85:GLY:HA3   | 1.82                     | 0.62              |
| 1:A:297:HIS:CD2  | 1:A:298:ILE:HG13 | 2.35                     | 0.62              |
| 1:C:355:GLN:HG2  | 1:D:376:ARG:HH12 | 1.63                     | 0.62              |
| 1:G:113:ILE:HG13 | 1:G:148:PRO:HB2  | 1.81                     | 0.62              |
| 1:L:37:ARG:NH1   | 1:L:48:TYR:OH    | 2.29                     | 0.62              |
| 1:E:577:ILE:HG12 | 1:E:597:GLN:NE2  | 2.12                     | 0.62              |
| 1:F:79:LEU:H     | 1:F:520:VAL:HA   | 1.64                     | 0.62              |
| 1:G:434:THR:HG22 | 1:H:108:LYS:HE3  | 1.81                     | 0.62              |
| 1:I:83:LYS:HE2   | 1:I:85:GLY:HA3   | 1.80                     | 0.62              |
| 1:I:164:LEU:HD12 | 1:I:166:ASP:HB3  | 1.80                     | 0.62              |
| 1:K:362:MET:HA   | 1:K:366:ASN:HB2  | 1.80                     | 0.62              |
| 1:B:221:GLU:HG2  | 1:B:280:ILE:HG12 | 1.82                     | 0.62              |
| 1:H:510:ILE:HG12 | 1:H:512:GLY:H    | 1.63                     | 0.62              |
| 1:A:452:ASN:OD1  | 1:A:453:LEU:N    | 2.33                     | 0.62              |
| 1:A:556:TYR:HB3  | 1:A:572:ALA:HB2  | 1.80                     | 0.62              |
| 1:C:22:SER:O     | 1:C:26:ARG:HG2   | 2.00                     | 0.62              |
| 1:C:83:LYS:HE2   | 1:C:85:GLY:HA3   | 1.80                     | 0.62              |
| 1:E:297:HIS:CD2  | 1:E:298:ILE:HG13 | 2.35                     | 0.62              |
| 1:E:437:GLN:HG2  | 1:E:520:VAL:HG21 | 1.82                     | 0.62              |
| 1:G:250:ASP:OD1  | 1:G:251:ILE:N    | 2.33                     | 0.62              |
| 1:G:321:ARG:HA   | 1:G:324:LYS:HE2  | 1.81                     | 0.62              |
| 1:H:58:ASP:HA    | 1:H:327:GLN:OE1  | 1.98                     | 0.62              |
| 1:H:528:LYS:HZ3  | 1:H:560:LEU:HD23 | 1.65                     | 0.62              |
| 1:I:452:ASN:OD1  | 1:I:453:LEU:N    | 2.33                     | 0.62              |
| 1:I:511:ARG:HD3  | 1:I:513:ARG:HH22 | 1.62                     | 0.62              |
| 1:J:577:ILE:HD12 | 1:J:584:PRO:HB3  | 1.82                     | 0.62              |
| 1:J:250:ASP:OD1  | 1:J:251:ILE:N    | 2.33                     | 0.62              |
| 1:J:297:HIS:CD2  | 1:J:298:ILE:HG13 | 2.35                     | 0.62              |
| 1:K:664:GLU:HG3  | 1:L:659:LEU:HD22 | 1.80                     | 0.62              |
| 1:L:113:ILE:HG13 | 1:L:148:PRO:HB2  | 1.81                     | 0.62              |
| 1:L:362:MET:HA   | 1:L:366:ASN:HB2  | 1.80                     | 0.62              |
| 1:L:653:ILE:O    | 1:L:657:MET:HG2  | 2.00                     | 0.62              |
| 1:B:577:ILE:HG12 | 1:B:597:GLN:NE2  | 2.13                     | 0.62              |
| 1:G:79:LEU:H     | 1:G:520:VAL:HA   | 1.65                     | 0.62              |
| 1:I:83:LYS:HB2   | 1:I:515:GLU:HB3  | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:339:ASP:HA   | 1:J:342:ALA:HB3  | 1.82                     | 0.62              |
| 1:K:117:GLU:HB3  | 1:K:123:VAL:HG23 | 1.81                     | 0.62              |
| 1:K:236:GLN:HB2  | 1:K:265:LYS:HD2  | 1.81                     | 0.62              |
| 1:A:372:TYR:HB3  | 1:L:350:PHE:CD1  | 2.35                     | 0.61              |
| 1:H:653:ILE:O    | 1:H:657:MET:HG2  | 2.00                     | 0.61              |
| 1:C:41:TRP:CH2   | 1:C:44:TRP:HB2   | 2.34                     | 0.61              |
| 1:E:250:ASP:OD1  | 1:E:251:ILE:N    | 2.33                     | 0.61              |
| 1:H:113:ILE:HG13 | 1:H:148:PRO:HB2  | 1.81                     | 0.61              |
| 1:I:93:VAL:O     | 1:I:96:GLY:N     | 2.33                     | 0.61              |
| 1:L:577:ILE:HD12 | 1:L:584:PRO:HB3  | 1.81                     | 0.61              |
| 1:A:250:ASP:OD1  | 1:A:251:ILE:N    | 2.33                     | 0.61              |
| 1:B:134:ASP:OD1  | 1:B:141:ASN:ND2  | 2.30                     | 0.61              |
| 1:C:83:LYS:HB2   | 1:C:515:GLU:HB3  | 1.82                     | 0.61              |
| 1:J:113:ILE:HG13 | 1:J:148:PRO:HB2  | 1.81                     | 0.61              |
| 1:L:83:LYS:HB2   | 1:L:515:GLU:HB3  | 1.80                     | 0.61              |
| 1:A:113:ILE:HG13 | 1:A:148:PRO:HB2  | 1.82                     | 0.61              |
| 1:A:664:GLU:OE2  | 1:B:666:ARG:NH2  | 2.34                     | 0.61              |
| 1:A:667:GLU:HG2  | 1:B:666:ARG:NH1  | 2.15                     | 0.61              |
| 1:C:310:VAL:HG22 | 1:D:40:GLN:HG3   | 1.83                     | 0.61              |
| 1:C:339:ASP:HA   | 1:C:342:ALA:HB3  | 1.81                     | 0.61              |
| 1:E:667:GLU:HG2  | 1:F:666:ARG:NH1  | 2.14                     | 0.61              |
| 1:H:270:GLN:NE2  | 1:H:271:ILE:O    | 2.33                     | 0.61              |
| 1:H:362:MET:HA   | 1:H:366:ASN:HB2  | 1.81                     | 0.61              |
| 1:I:297:HIS:CD2  | 1:I:298:ILE:HG13 | 2.35                     | 0.61              |
| 1:I:577:ILE:HD12 | 1:I:584:PRO:HB3  | 1.82                     | 0.61              |
| 1:K:221:GLU:HG2  | 1:K:280:ILE:HG12 | 1.81                     | 0.61              |
| 1:L:270:GLN:NE2  | 1:L:271:ILE:O    | 2.33                     | 0.61              |
| 1:B:79:LEU:H     | 1:B:520:VAL:HA   | 1.64                     | 0.61              |
| 1:B:363:TYR:OH   | 1:B:373:LEU:O    | 2.14                     | 0.61              |
| 1:F:250:ASP:OD1  | 1:F:251:ILE:N    | 2.33                     | 0.61              |
| 1:H:236:GLN:HB2  | 1:H:265:LYS:HD2  | 1.83                     | 0.61              |
| 1:K:250:ASP:OD1  | 1:K:251:ILE:N    | 2.33                     | 0.61              |
| 1:H:83:LYS:HB2   | 1:H:515:GLU:HB3  | 1.81                     | 0.61              |
| 1:A:434:THR:HG22 | 1:B:108:LYS:HE3  | 1.83                     | 0.61              |
| 1:A:511:ARG:HD3  | 1:A:513:ARG:HH22 | 1.65                     | 0.61              |
| 1:E:434:THR:HG22 | 1:F:108:LYS:HE3  | 1.82                     | 0.61              |
| 1:G:362:MET:HA   | 1:G:366:ASN:HB2  | 1.82                     | 0.61              |
| 1:H:612:GLN:HA   | 1:H:615:LEU:CD1  | 2.31                     | 0.61              |
| 1:J:87:ARG:HG2   | 1:J:89:ASP:H     | 1.64                     | 0.61              |
| 1:J:452:ASN:OD1  | 1:J:453:LEU:N    | 2.33                     | 0.61              |
| 1:B:297:HIS:CD2  | 1:B:298:ILE:HG13 | 2.36                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:113:ILE:HG13 | 1:E:148:PRO:HB2  | 1.83                     | 0.61              |
| 1:G:134:ASP:OD1  | 1:G:141:ASN:ND2  | 2.27                     | 0.61              |
| 1:G:297:HIS:CD2  | 1:G:298:ILE:HG13 | 2.36                     | 0.61              |
| 1:A:134:ASP:OD1  | 1:A:141:ASN:ND2  | 2.25                     | 0.61              |
| 1:B:434:THR:HG22 | 1:C:108:LYS:HE3  | 1.83                     | 0.61              |
| 1:C:37:ARG:NH1   | 1:C:48:TYR:OH    | 2.33                     | 0.61              |
| 1:D:232:ALA:HB1  | 1:D:268:GLU:HA   | 1.82                     | 0.61              |
| 1:D:362:MET:HA   | 1:D:366:ASN:HB2  | 1.83                     | 0.61              |
| 1:D:399:GLN:HA   | 1:D:402:ALA:HB3  | 1.83                     | 0.61              |
| 1:E:350:PHE:N    | 1:E:390:ALA:O    | 2.29                     | 0.61              |
| 1:G:96:GLY:O     | 1:G:100:THR:OG1  | 2.10                     | 0.61              |
| 1:G:639:VAL:O    | 1:G:643:ASN:ND2  | 2.31                     | 0.61              |
| 1:J:510:ILE:HG12 | 1:J:512:GLY:H    | 1.64                     | 0.61              |
| 1:K:79:LEU:H     | 1:K:520:VAL:HA   | 1.65                     | 0.61              |
| 1:K:101:ASP:OD2  | 1:K:144:ILE:HG12 | 2.00                     | 0.61              |
| 1:D:87:ARG:HG2   | 1:D:89:ASP:H     | 1.66                     | 0.61              |
| 1:D:161:ASN:HD21 | 1:E:183:GLY:HA3  | 1.64                     | 0.61              |
| 1:K:96:GLY:O     | 1:K:100:THR:OG1  | 2.13                     | 0.61              |
| 1:K:161:ASN:HD21 | 1:L:183:GLY:HA3  | 1.66                     | 0.61              |
| 1:L:452:ASN:OD1  | 1:L:453:LEU:N    | 2.33                     | 0.61              |
| 1:A:58:ASP:HA    | 1:A:327:GLN:OE1  | 2.01                     | 0.60              |
| 1:I:434:THR:HG21 | 1:J:72:ARG:HG3   | 1.82                     | 0.60              |
| 1:B:38:VAL:HG21  | 1:B:324:LYS:HD2  | 1.83                     | 0.60              |
| 1:C:653:ILE:O    | 1:C:657:MET:HG2  | 2.01                     | 0.60              |
| 1:D:438:LEU:HD11 | 1:E:108:LYS:HD3  | 1.83                     | 0.60              |
| 1:F:556:TYR:HB3  | 1:F:572:ALA:HB2  | 1.83                     | 0.60              |
| 1:H:297:HIS:CD2  | 1:H:298:ILE:HG13 | 2.35                     | 0.60              |
| 1:D:37:ARG:NH1   | 1:D:48:TYR:OH    | 2.33                     | 0.60              |
| 1:E:603:GLN:O    | 1:E:606:PRO:HD3  | 2.01                     | 0.60              |
| 1:A:221:GLU:HG2  | 1:A:280:ILE:HG12 | 1.81                     | 0.60              |
| 1:F:452:ASN:OD1  | 1:F:453:LEU:N    | 2.33                     | 0.60              |
| 1:K:83:LYS:HB2   | 1:K:515:GLU:HB3  | 1.83                     | 0.60              |
| 1:C:297:HIS:CD2  | 1:C:298:ILE:HG13 | 2.35                     | 0.60              |
| 1:I:309:PHE:HB3  | 1:I:312:ASP:HA   | 1.83                     | 0.60              |
| 1:I:310:VAL:HG22 | 1:J:40:GLN:HG3   | 1.83                     | 0.60              |
| 1:J:236:GLN:HB2  | 1:J:265:LYS:HD2  | 1.84                     | 0.60              |
| 1:J:310:VAL:HG22 | 1:K:40:GLN:HG3   | 1.84                     | 0.60              |
| 1:B:603:GLN:O    | 1:B:606:PRO:HD3  | 2.01                     | 0.60              |
| 1:E:653:ILE:O    | 1:E:657:MET:HG2  | 2.02                     | 0.60              |
| 1:G:164:LEU:HD12 | 1:G:166:ASP:HB3  | 1.84                     | 0.60              |
| 1:H:250:ASP:OD1  | 1:H:251:ILE:N    | 2.34                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:250:ASP:OD1  | 1:I:251:ILE:N    | 2.34                     | 0.60              |
| 1:J:83:LYS:HB2   | 1:J:515:GLU:HB3  | 1.83                     | 0.60              |
| 1:K:434:THR:HG22 | 1:L:108:LYS:HE3  | 1.83                     | 0.60              |
| 1:K:452:ASN:OD1  | 1:K:453:LEU:N    | 2.34                     | 0.60              |
| 1:K:577:ILE:HG12 | 1:K:597:GLN:NE2  | 2.13                     | 0.60              |
| 1:A:362:MET:HA   | 1:A:366:ASN:HB2  | 1.83                     | 0.60              |
| 1:A:577:ILE:HD12 | 1:A:584:PRO:HB3  | 1.82                     | 0.60              |
| 1:B:426:ASN:O    | 1:B:429:GLN:NE2  | 2.34                     | 0.60              |
| 1:F:653:ILE:O    | 1:F:657:MET:HG2  | 2.02                     | 0.60              |
| 1:I:221:GLU:HG2  | 1:I:280:ILE:HG12 | 1.83                     | 0.60              |
| 1:J:433:ASP:O    | 1:J:437:GLN:N    | 2.30                     | 0.60              |
| 1:A:526:SER:O    | 1:A:530:GLN:HG3  | 2.01                     | 0.60              |
| 1:B:362:MET:HA   | 1:B:366:ASN:HB2  | 1.84                     | 0.60              |
| 1:E:134:ASP:OD1  | 1:E:141:ASN:ND2  | 2.24                     | 0.60              |
| 1:F:434:THR:HG22 | 1:G:108:LYS:HE3  | 1.83                     | 0.60              |
| 1:B:37:ARG:NH1   | 1:B:48:TYR:OH    | 2.35                     | 0.60              |
| 1:C:101:ASP:OD2  | 1:C:144:ILE:HG12 | 2.02                     | 0.60              |
| 1:C:263:PHE:O    | 1:C:265:LYS:HG3  | 2.02                     | 0.60              |
| 1:G:452:ASN:OD1  | 1:G:453:LEU:N    | 2.35                     | 0.60              |
| 1:I:362:MET:HA   | 1:I:366:ASN:HB2  | 1.82                     | 0.60              |
| 1:B:41:TRP:CH2   | 1:B:44:TRP:HB2   | 2.37                     | 0.60              |
| 1:D:310:VAL:HG22 | 1:E:40:GLN:HG3   | 1.83                     | 0.60              |
| 1:F:577:ILE:HD12 | 1:F:584:PRO:HB3  | 1.82                     | 0.60              |
| 1:H:79:LEU:H     | 1:H:520:VAL:HA   | 1.67                     | 0.60              |
| 1:L:117:GLU:HB3  | 1:L:123:VAL:HG23 | 1.82                     | 0.60              |
| 1:B:577:ILE:HD12 | 1:B:584:PRO:HB3  | 1.83                     | 0.59              |
| 1:B:653:ILE:O    | 1:B:657:MET:HG2  | 2.01                     | 0.59              |
| 1:E:362:MET:HA   | 1:E:366:ASN:HB2  | 1.84                     | 0.59              |
| 1:G:577:ILE:HD12 | 1:G:584:PRO:HB3  | 1.82                     | 0.59              |
| 1:H:321:ARG:HA   | 1:H:324:LYS:HE2  | 1.84                     | 0.59              |
| 1:I:363:TYR:OH   | 1:I:373:LEU:O    | 2.16                     | 0.59              |
| 1:J:433:ASP:HA   | 1:J:436:ASN:HB3  | 1.84                     | 0.59              |
| 1:A:108:LYS:HE3  | 1:L:434:THR:HG22 | 1.84                     | 0.59              |
| 1:C:528:LYS:HZ3  | 1:C:560:LEU:HD23 | 1.67                     | 0.59              |
| 1:E:526:SER:O    | 1:E:530:GLN:HG3  | 2.03                     | 0.59              |
| 1:F:310:VAL:HG22 | 1:G:40:GLN:HG3   | 1.84                     | 0.59              |
| 1:F:350:PHE:HB2  | 1:F:390:ALA:HB3  | 1.84                     | 0.59              |
| 1:F:433:ASP:O    | 1:F:437:GLN:N    | 2.34                     | 0.59              |
| 1:J:79:LEU:H     | 1:J:520:VAL:HA   | 1.67                     | 0.59              |
| 1:J:434:THR:HG22 | 1:K:108:LYS:HE3  | 1.83                     | 0.59              |
| 1:K:443:ASP:OD1  | 1:K:444:LEU:N    | 2.35                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:236:GLN:HB2  | 1:A:265:LYS:HD2  | 1.84                     | 0.59              |
| 1:D:410:SER:O    | 1:D:414:GLU:HG2  | 2.02                     | 0.59              |
| 1:D:526:SER:O    | 1:D:530:GLN:HG3  | 2.01                     | 0.59              |
| 1:D:603:GLN:O    | 1:D:606:PRO:HD3  | 2.02                     | 0.59              |
| 1:D:667:GLU:HG2  | 1:E:666:ARG:NH1  | 2.18                     | 0.59              |
| 1:E:236:GLN:HB2  | 1:E:265:LYS:HD2  | 1.84                     | 0.59              |
| 1:H:434:THR:HG22 | 1:I:108:LYS:HE3  | 1.83                     | 0.59              |
| 1:I:161:ASN:HD21 | 1:J:183:GLY:HA3  | 1.66                     | 0.59              |
| 1:A:399:GLN:HA   | 1:A:402:ALA:HB3  | 1.83                     | 0.59              |
| 1:C:221:GLU:HG2  | 1:C:280:ILE:HG12 | 1.82                     | 0.59              |
| 1:D:353:PRO:HA   | 1:E:373:LEU:HD23 | 1.85                     | 0.59              |
| 1:D:577:ILE:HD12 | 1:D:584:PRO:HB3  | 1.84                     | 0.59              |
| 1:E:556:TYR:HB3  | 1:E:572:ALA:HB2  | 1.84                     | 0.59              |
| 1:I:526:SER:O    | 1:I:530:GLN:HG3  | 2.02                     | 0.59              |
| 1:A:662:GLN:HA   | 1:A:665:PHE:CD2  | 2.38                     | 0.59              |
| 1:B:78:VAL:HG22  | 1:B:520:VAL:HG12 | 1.82                     | 0.59              |
| 1:B:80:TYR:HD1   | 1:B:518:THR:HA   | 1.67                     | 0.59              |
| 1:D:83:LYS:HE2   | 1:D:85:GLY:HA3   | 1.83                     | 0.59              |
| 1:G:443:ASP:OD1  | 1:G:444:LEU:N    | 2.36                     | 0.59              |
| 1:H:577:ILE:HD12 | 1:H:584:PRO:HB3  | 1.83                     | 0.59              |
| 1:I:79:LEU:H     | 1:I:520:VAL:HA   | 1.68                     | 0.59              |
| 1:J:221:GLU:HG2  | 1:J:280:ILE:HG12 | 1.84                     | 0.59              |
| 1:L:437:GLN:HG2  | 1:L:520:VAL:HG21 | 1.84                     | 0.59              |
| 1:L:603:GLN:O    | 1:L:606:PRO:HD3  | 2.01                     | 0.59              |
| 1:B:232:ALA:HB1  | 1:B:268:GLU:HA   | 1.84                     | 0.59              |
| 1:B:526:SER:O    | 1:B:530:GLN:HG3  | 2.03                     | 0.59              |
| 1:C:156:VAL:HA   | 1:C:174:THR:O    | 2.02                     | 0.59              |
| 1:E:433:ASP:O    | 1:E:437:GLN:N    | 2.34                     | 0.59              |
| 1:F:443:ASP:OD1  | 1:F:444:LEU:N    | 2.36                     | 0.59              |
| 1:G:526:SER:O    | 1:G:530:GLN:HG3  | 2.03                     | 0.59              |
| 1:H:603:GLN:O    | 1:H:606:PRO:HD3  | 2.02                     | 0.59              |
| 1:J:556:TYR:HB3  | 1:J:572:ALA:HB2  | 1.85                     | 0.59              |
| 1:K:418:LEU:HD23 | 1:K:429:GLN:HB3  | 1.84                     | 0.59              |
| 1:L:526:SER:O    | 1:L:530:GLN:HG3  | 2.03                     | 0.59              |
| 1:A:156:VAL:HA   | 1:A:174:THR:O    | 2.03                     | 0.59              |
| 1:C:443:ASP:OD1  | 1:C:444:LEU:N    | 2.35                     | 0.59              |
| 1:H:161:ASN:HD21 | 1:I:183:GLY:HA3  | 1.68                     | 0.59              |
| 1:K:83:LYS:HE2   | 1:K:85:GLY:HA3   | 1.85                     | 0.59              |
| 1:K:526:SER:O    | 1:K:530:GLN:HG3  | 2.03                     | 0.59              |
| 1:A:373:LEU:HD23 | 1:L:353:PRO:HA   | 1.85                     | 0.59              |
| 1:A:443:ASP:OD1  | 1:A:444:LEU:N    | 2.36                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:556:TYR:HB3  | 1:H:572:ALA:HB2  | 1.85                     | 0.59              |
| 1:I:434:THR:HG22 | 1:J:108:LYS:HE3  | 1.85                     | 0.59              |
| 1:B:350:PHE:CD1  | 1:C:372:TYR:HB3  | 2.38                     | 0.59              |
| 1:F:117:GLU:HB3  | 1:F:123:VAL:HG23 | 1.83                     | 0.59              |
| 1:J:526:SER:O    | 1:J:530:GLN:HG3  | 2.03                     | 0.59              |
| 1:K:410:SER:O    | 1:K:414:GLU:HG2  | 2.03                     | 0.59              |
| 1:A:433:ASP:O    | 1:A:437:GLN:N    | 2.35                     | 0.59              |
| 1:B:156:VAL:HA   | 1:B:174:THR:O    | 2.02                     | 0.59              |
| 1:B:443:ASP:OD1  | 1:B:444:LEU:N    | 2.35                     | 0.59              |
| 1:C:526:SER:O    | 1:C:530:GLN:HG3  | 2.02                     | 0.59              |
| 1:D:309:PHE:HB3  | 1:D:312:ASP:HA   | 1.85                     | 0.59              |
| 1:F:350:PHE:CD1  | 1:G:372:TYR:HB3  | 2.37                     | 0.59              |
| 1:G:156:VAL:HA   | 1:G:174:THR:O    | 2.03                     | 0.59              |
| 1:I:113:ILE:HG13 | 1:I:148:PRO:HB2  | 1.83                     | 0.59              |
| 1:A:375:ASN:OD1  | 1:A:376:ARG:N    | 2.36                     | 0.58              |
| 1:B:201:PHE:CD1  | 1:B:283:CYS:HB2  | 2.38                     | 0.58              |
| 1:C:603:GLN:O    | 1:C:606:PRO:HD3  | 2.03                     | 0.58              |
| 1:D:443:ASP:OD1  | 1:D:444:LEU:N    | 2.36                     | 0.58              |
| 1:D:653:ILE:O    | 1:D:657:MET:HG2  | 2.02                     | 0.58              |
| 1:E:41:TRP:CH2   | 1:E:44:TRP:HB2   | 2.37                     | 0.58              |
| 1:G:83:LYS:HB2   | 1:G:515:GLU:HB3  | 1.84                     | 0.58              |
| 1:A:363:TYR:OH   | 1:A:373:LEU:O    | 2.18                     | 0.58              |
| 1:C:613:GLY:HA2  | 1:C:616:LEU:HD13 | 1.83                     | 0.58              |
| 1:G:618:GLY:O    | 1:G:621:GLU:HB2  | 2.03                     | 0.58              |
| 1:H:433:ASP:O    | 1:H:437:GLN:N    | 2.33                     | 0.58              |
| 1:I:356:ILE:HG21 | 1:J:373:LEU:HD21 | 1.85                     | 0.58              |
| 1:J:83:LYS:HE2   | 1:J:85:GLY:HA3   | 1.85                     | 0.58              |
| 1:J:375:ASN:OD1  | 1:J:376:ARG:N    | 2.36                     | 0.58              |
| 1:G:612:GLN:HA   | 1:G:615:LEU:CD1  | 2.32                     | 0.58              |
| 1:I:653:ILE:O    | 1:I:657:MET:HG2  | 2.04                     | 0.58              |
| 1:A:310:VAL:HG22 | 1:B:40:GLN:HG3   | 1.85                     | 0.58              |
| 1:J:603:GLN:O    | 1:J:606:PRO:HD3  | 2.03                     | 0.58              |
| 1:B:83:LYS:HB2   | 1:B:515:GLU:HB3  | 1.85                     | 0.58              |
| 1:B:612:GLN:HA   | 1:B:615:LEU:CD1  | 2.33                     | 0.58              |
| 1:C:589:GLU:O    | 1:C:593:LEU:HB2  | 2.04                     | 0.58              |
| 1:D:434:THR:HG22 | 1:E:108:LYS:HE3  | 1.84                     | 0.58              |
| 1:G:83:LYS:HE2   | 1:G:85:GLY:HA3   | 1.86                     | 0.58              |
| 1:H:589:GLU:O    | 1:H:593:LEU:HB2  | 2.04                     | 0.58              |
| 1:I:418:LEU:HD23 | 1:I:429:GLN:HB3  | 1.85                     | 0.58              |
| 1:K:350:PHE:CD1  | 1:L:372:TYR:HB3  | 2.37                     | 0.58              |
| 1:L:443:ASP:OD1  | 1:L:444:LEU:N    | 2.36                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:82:PRO:HB3   | 1:B:90:ALA:HB3   | 1.86                     | 0.58              |
| 1:B:117:GLU:HB3  | 1:B:123:VAL:HG23 | 1.83                     | 0.58              |
| 1:B:618:GLY:O    | 1:B:621:GLU:HB2  | 2.03                     | 0.58              |
| 1:C:650:ILE:HA   | 1:C:653:ILE:HD12 | 1.86                     | 0.58              |
| 1:D:613:GLY:O    | 1:D:616:LEU:HD12 | 2.04                     | 0.58              |
| 1:E:87:ARG:HG2   | 1:E:89:ASP:H     | 1.67                     | 0.58              |
| 1:G:653:ILE:O    | 1:G:657:MET:HG2  | 2.03                     | 0.58              |
| 1:H:526:SER:O    | 1:H:530:GLN:HG3  | 2.03                     | 0.58              |
| 1:I:556:TYR:HB3  | 1:I:572:ALA:HB2  | 1.85                     | 0.58              |
| 1:J:29:ALA:O     | 1:J:33:LEU:HB2   | 2.04                     | 0.58              |
| 1:K:337:ASN:HA   | 1:K:340:ILE:HD12 | 1.86                     | 0.58              |
| 1:K:618:GLY:O    | 1:K:621:GLU:HB2  | 2.03                     | 0.58              |
| 1:C:236:GLN:HB2  | 1:C:265:LYS:HD2  | 1.85                     | 0.58              |
| 1:C:321:ARG:HA   | 1:C:324:LYS:HE2  | 1.84                     | 0.58              |
| 1:D:350:PHE:CD1  | 1:E:372:TYR:HB3  | 2.38                     | 0.58              |
| 1:E:339:ASP:HA   | 1:E:342:ALA:HB3  | 1.84                     | 0.58              |
| 1:F:362:MET:HA   | 1:F:366:ASN:HB2  | 1.85                     | 0.58              |
| 1:F:526:SER:O    | 1:F:530:GLN:HG3  | 2.03                     | 0.58              |
| 1:F:667:GLU:HG2  | 1:G:666:ARG:NH1  | 2.18                     | 0.58              |
| 1:H:399:GLN:HA   | 1:H:402:ALA:HB3  | 1.85                     | 0.58              |
| 1:A:603:GLN:O    | 1:A:606:PRO:HD3  | 2.02                     | 0.58              |
| 1:D:639:VAL:O    | 1:D:643:ASN:ND2  | 2.37                     | 0.58              |
| 1:E:263:PHE:O    | 1:E:265:LYS:HG3  | 2.04                     | 0.58              |
| 1:H:410:SER:O    | 1:H:414:GLU:HG2  | 2.03                     | 0.58              |
| 1:I:41:TRP:CH2   | 1:I:44:TRP:HB2   | 2.39                     | 0.58              |
| 1:J:117:GLU:HB3  | 1:J:123:VAL:HG23 | 1.86                     | 0.58              |
| 1:L:263:PHE:O    | 1:L:265:LYS:HG3  | 2.03                     | 0.58              |
| 1:D:263:PHE:O    | 1:D:265:LYS:HG3  | 2.03                     | 0.58              |
| 1:D:297:HIS:CD2  | 1:D:298:ILE:HG13 | 2.39                     | 0.58              |
| 1:G:80:TYR:HD1   | 1:G:518:THR:HA   | 1.69                     | 0.58              |
| 1:G:375:ASN:OD1  | 1:G:376:ARG:N    | 2.36                     | 0.58              |
| 1:H:350:PHE:CD1  | 1:I:372:TYR:HB3  | 2.39                     | 0.58              |
| 1:K:297:HIS:CD2  | 1:K:298:ILE:HG13 | 2.39                     | 0.58              |
| 1:K:375:ASN:OD1  | 1:K:376:ARG:N    | 2.35                     | 0.58              |
| 1:L:162:SER:HB2  | 1:L:170:ALA:HB2  | 1.84                     | 0.58              |
| 1:L:639:VAL:O    | 1:L:643:ASN:ND2  | 2.36                     | 0.58              |
| 1:C:434:THR:HG22 | 1:D:108:LYS:HE3  | 1.86                     | 0.58              |
| 1:C:577:ILE:HG12 | 1:C:597:GLN:NE2  | 2.13                     | 0.58              |
| 1:D:41:TRP:CH2   | 1:D:44:TRP:HB2   | 2.39                     | 0.58              |
| 1:D:221:GLU:HG2  | 1:D:280:ILE:HG12 | 1.86                     | 0.58              |
| 1:I:443:ASP:OD1  | 1:I:444:LEU:N    | 2.36                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:350:PHE:CD1  | 1:K:372:TYR:HB3  | 2.39                     | 0.58              |
| 1:L:236:GLN:HB2  | 1:L:265:LYS:HD2  | 1.84                     | 0.58              |
| 1:A:653:ILE:O    | 1:A:657:MET:HG2  | 2.04                     | 0.57              |
| 1:B:83:LYS:HE2   | 1:B:85:GLY:HA3   | 1.85                     | 0.57              |
| 1:B:375:ASN:OD1  | 1:B:376:ARG:N    | 2.37                     | 0.57              |
| 1:E:443:ASP:OD1  | 1:E:444:LEU:N    | 2.37                     | 0.57              |
| 1:G:603:GLN:O    | 1:G:606:PRO:HD3  | 2.04                     | 0.57              |
| 1:H:160:SER:OG   | 1:H:172:HIS:ND1  | 2.22                     | 0.57              |
| 1:I:399:GLN:HA   | 1:I:402:ALA:HB3  | 1.86                     | 0.57              |
| 1:K:612:GLN:HA   | 1:K:615:LEU:CD1  | 2.34                     | 0.57              |
| 1:L:193:LEU:HD21 | 1:L:288:LYS:HZ3  | 1.69                     | 0.57              |
| 1:A:117:GLU:HB3  | 1:A:123:VAL:HG23 | 1.86                     | 0.57              |
| 1:A:659:LEU:HD22 | 1:L:664:GLU:HG3  | 1.87                     | 0.57              |
| 1:C:511:ARG:HD3  | 1:C:513:ARG:HH22 | 1.68                     | 0.57              |
| 1:C:639:VAL:O    | 1:C:643:ASN:ND2  | 2.36                     | 0.57              |
| 1:D:80:TYR:HD1   | 1:D:518:THR:HA   | 1.69                     | 0.57              |
| 1:D:275:ARG:NH2  | 1:D:293:ILE:O    | 2.30                     | 0.57              |
| 1:E:96:GLY:O     | 1:E:100:THR:OG1  | 2.10                     | 0.57              |
| 1:G:263:PHE:O    | 1:G:265:LYS:HG3  | 2.04                     | 0.57              |
| 1:J:443:ASP:OD1  | 1:J:444:LEU:N    | 2.37                     | 0.57              |
| 1:L:399:GLN:HA   | 1:L:402:ALA:HB3  | 1.87                     | 0.57              |
| 1:A:127:ARG:HB3  | 1:A:147:GLU:HB2  | 1.87                     | 0.57              |
| 1:B:433:ASP:O    | 1:B:437:GLN:N    | 2.31                     | 0.57              |
| 1:D:433:ASP:O    | 1:D:437:GLN:N    | 2.32                     | 0.57              |
| 1:E:511:ARG:HD3  | 1:E:513:ARG:HH22 | 1.69                     | 0.57              |
| 1:F:603:GLN:O    | 1:F:606:PRO:HD3  | 2.05                     | 0.57              |
| 1:J:276:VAL:HG22 | 1:J:296:GLU:HA   | 1.85                     | 0.57              |
| 1:K:162:SER:HB2  | 1:K:170:ALA:HB2  | 1.86                     | 0.57              |
| 1:L:297:HIS:CD2  | 1:L:298:ILE:HG13 | 2.40                     | 0.57              |
| 1:C:438:LEU:HD11 | 1:D:108:LYS:HD3  | 1.85                     | 0.57              |
| 1:D:363:TYR:OH   | 1:D:373:LEU:O    | 2.14                     | 0.57              |
| 1:F:350:PHE:N    | 1:F:390:ALA:O    | 2.31                     | 0.57              |
| 1:I:96:GLY:O     | 1:I:100:THR:OG1  | 2.11                     | 0.57              |
| 1:J:410:SER:O    | 1:J:414:GLU:HG2  | 2.04                     | 0.57              |
| 1:K:232:ALA:HB1  | 1:K:268:GLU:HA   | 1.86                     | 0.57              |
| 1:L:232:ALA:HB1  | 1:L:268:GLU:HA   | 1.86                     | 0.57              |
| 1:F:83:LYS:HE2   | 1:F:85:GLY:HA3   | 1.86                     | 0.57              |
| 1:F:201:PHE:CD1  | 1:F:283:CYS:HB2  | 2.40                     | 0.57              |
| 1:K:113:ILE:HG13 | 1:K:148:PRO:HB2  | 1.85                     | 0.57              |
| 1:D:83:LYS:HB2   | 1:D:515:GLU:HB3  | 1.85                     | 0.57              |
| 1:E:321:ARG:HA   | 1:E:324:LYS:HE2  | 1.85                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:399:GLN:HA   | 1:E:402:ALA:HB3  | 1.86                     | 0.57              |
| 1:G:236:GLN:HB2  | 1:G:265:LYS:HD2  | 1.87                     | 0.57              |
| 1:H:83:LYS:HE2   | 1:H:85:GLY:HA3   | 1.86                     | 0.57              |
| 1:J:406:GLU:O    | 1:J:410:SER:OG   | 2.17                     | 0.57              |
| 1:J:434:THR:HG21 | 1:K:72:ARG:HG3   | 1.86                     | 0.57              |
| 1:K:556:TYR:HB3  | 1:K:572:ALA:HB2  | 1.86                     | 0.57              |
| 1:L:375:ASN:OD1  | 1:L:376:ARG:N    | 2.36                     | 0.57              |
| 1:A:276:VAL:HG22 | 1:A:296:GLU:HA   | 1.86                     | 0.57              |
| 1:B:667:GLU:HG2  | 1:C:666:ARG:NH1  | 2.20                     | 0.57              |
| 1:C:410:SER:O    | 1:C:414:GLU:HG2  | 2.04                     | 0.57              |
| 1:E:159:ASP:C    | 1:E:161:ASN:H    | 2.13                     | 0.57              |
| 1:E:221:GLU:HG2  | 1:E:280:ILE:HG12 | 1.86                     | 0.57              |
| 1:E:664:GLU:OE2  | 1:F:666:ARG:NH2  | 2.38                     | 0.57              |
| 1:F:80:TYR:HD1   | 1:F:518:THR:HA   | 1.69                     | 0.57              |
| 1:F:193:LEU:HD21 | 1:F:288:LYS:NZ   | 2.19                     | 0.57              |
| 1:G:47:GLN:HB2   | 1:G:50:THR:HG21  | 1.87                     | 0.57              |
| 1:G:232:ALA:HB1  | 1:G:268:GLU:HA   | 1.86                     | 0.57              |
| 1:G:613:GLY:HA2  | 1:G:616:LEU:CD1  | 2.33                     | 0.57              |
| 1:H:232:ALA:HB1  | 1:H:268:GLU:HA   | 1.87                     | 0.57              |
| 1:H:443:ASP:OD1  | 1:H:444:LEU:N    | 2.37                     | 0.57              |
| 1:K:263:PHE:O    | 1:K:265:LYS:HG3  | 2.05                     | 0.57              |
| 1:A:80:TYR:HD1   | 1:A:518:THR:HA   | 1.70                     | 0.57              |
| 1:B:223:TYR:HE1  | 1:B:278:LYS:HG3  | 1.70                     | 0.57              |
| 1:B:615:LEU:O    | 1:B:619:GLN:HG2  | 2.05                     | 0.57              |
| 1:B:639:VAL:O    | 1:B:643:ASN:ND2  | 2.38                     | 0.57              |
| 1:A:666:ARG:NH2  | 1:L:664:GLU:OE2  | 2.38                     | 0.57              |
| 1:C:615:LEU:O    | 1:C:619:GLN:HG2  | 2.04                     | 0.57              |
| 1:F:263:PHE:O    | 1:F:265:LYS:HG3  | 2.05                     | 0.57              |
| 1:F:589:GLU:O    | 1:F:593:LEU:HB2  | 2.05                     | 0.57              |
| 1:H:643:ASN:HA   | 1:H:646:ASN:ND2  | 2.20                     | 0.57              |
| 1:I:117:GLU:HB3  | 1:I:123:VAL:HG23 | 1.87                     | 0.57              |
| 1:J:270:GLN:NE2  | 1:J:271:ILE:O    | 2.38                     | 0.57              |
| 1:J:653:ILE:O    | 1:J:657:MET:HG2  | 2.05                     | 0.57              |
| 1:K:29:ALA:O     | 1:K:33:LEU:HB2   | 2.05                     | 0.57              |
| 1:B:159:ASP:C    | 1:B:161:ASN:H    | 2.13                     | 0.56              |
| 1:H:353:PRO:HA   | 1:I:373:LEU:HD23 | 1.87                     | 0.56              |
| 1:H:667:GLU:HG2  | 1:I:666:ARG:NH1  | 2.19                     | 0.56              |
| 1:J:263:PHE:O    | 1:J:265:LYS:HG3  | 2.05                     | 0.56              |
| 1:A:613:GLY:O    | 1:A:616:LEU:HD13 | 2.05                     | 0.56              |
| 1:C:612:GLN:HA   | 1:C:615:LEU:CD1  | 2.36                     | 0.56              |
| 1:D:236:GLN:HB2  | 1:D:265:LYS:HD2  | 1.85                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:615:LEU:O    | 1:E:619:GLN:HG2  | 2.05                     | 0.56              |
| 1:G:353:PRO:O    | 1:G:356:ILE:HG22 | 2.05                     | 0.56              |
| 1:I:37:ARG:NH1   | 1:I:48:TYR:OH    | 2.38                     | 0.56              |
| 1:I:162:SER:HA   | 1:I:169:ASP:OD1  | 2.06                     | 0.56              |
| 1:I:615:LEU:O    | 1:I:619:GLN:HG2  | 2.05                     | 0.56              |
| 1:I:650:ILE:HA   | 1:I:653:ILE:HD12 | 1.87                     | 0.56              |
| 1:K:353:PRO:HA   | 1:L:373:LEU:HD23 | 1.87                     | 0.56              |
| 1:B:577:ILE:HG21 | 1:B:593:LEU:HD13 | 1.87                     | 0.56              |
| 1:C:34:PHE:O     | 1:C:38:VAL:HG23  | 2.05                     | 0.56              |
| 1:C:350:PHE:CD1  | 1:D:372:TYR:HB3  | 2.39                     | 0.56              |
| 1:C:433:ASP:O    | 1:C:437:GLN:N    | 2.35                     | 0.56              |
| 1:C:667:GLU:HG2  | 1:D:666:ARG:NH1  | 2.20                     | 0.56              |
| 1:D:353:PRO:O    | 1:D:356:ILE:HG22 | 2.05                     | 0.56              |
| 1:D:426:ASN:O    | 1:D:429:GLN:NE2  | 2.39                     | 0.56              |
| 1:F:236:GLN:HB2  | 1:F:265:LYS:HD2  | 1.87                     | 0.56              |
| 1:G:577:ILE:HG12 | 1:G:597:GLN:NE2  | 2.14                     | 0.56              |
| 1:H:375:ASN:OD1  | 1:H:376:ARG:N    | 2.36                     | 0.56              |
| 1:I:433:ASP:O    | 1:I:437:GLN:N    | 2.37                     | 0.56              |
| 1:J:162:SER:HB2  | 1:J:170:ALA:HB2  | 1.86                     | 0.56              |
| 1:J:232:ALA:HB1  | 1:J:268:GLU:HA   | 1.86                     | 0.56              |
| 1:J:711:GLN:OE1  | 1:K:712:ARG:NH1  | 2.38                     | 0.56              |
| 1:K:433:ASP:O    | 1:K:437:GLN:N    | 2.37                     | 0.56              |
| 1:L:82:PRO:HB3   | 1:L:90:ALA:HB3   | 1.86                     | 0.56              |
| 1:A:589:GLU:O    | 1:A:593:LEU:HB2  | 2.05                     | 0.56              |
| 1:C:375:ASN:OD1  | 1:C:376:ARG:N    | 2.37                     | 0.56              |
| 1:C:386:THR:HG22 | 1:C:387:GLN:H    | 1.70                     | 0.56              |
| 1:I:232:ALA:HB1  | 1:I:268:GLU:HA   | 1.87                     | 0.56              |
| 1:B:113:ILE:HG13 | 1:B:148:PRO:HB2  | 1.88                     | 0.56              |
| 1:E:82:PRO:HB3   | 1:E:90:ALA:HB3   | 1.87                     | 0.56              |
| 1:G:276:VAL:HG22 | 1:G:296:GLU:HA   | 1.88                     | 0.56              |
| 1:J:34:PHE:O     | 1:J:38:VAL:HG23  | 2.05                     | 0.56              |
| 1:K:41:TRP:CH2   | 1:K:44:TRP:HB2   | 2.41                     | 0.56              |
| 1:K:603:GLN:O    | 1:K:606:PRO:HD3  | 2.04                     | 0.56              |
| 1:B:263:PHE:O    | 1:B:265:LYS:HG3  | 2.05                     | 0.56              |
| 1:B:386:THR:HG22 | 1:B:387:GLN:H    | 1.70                     | 0.56              |
| 1:B:511:ARG:HD3  | 1:B:513:ARG:HH22 | 1.71                     | 0.56              |
| 1:E:618:GLY:O    | 1:E:621:GLU:HB2  | 2.06                     | 0.56              |
| 1:F:41:TRP:CH2   | 1:F:44:TRP:HB2   | 2.41                     | 0.56              |
| 1:H:201:PHE:CD1  | 1:H:283:CYS:HB2  | 2.40                     | 0.56              |
| 1:I:276:VAL:HG22 | 1:I:296:GLU:HA   | 1.87                     | 0.56              |
| 1:I:639:VAL:O    | 1:I:643:ASN:ND2  | 2.37                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:667:GLU:HG2  | 1:J:666:ARG:NH1  | 2.20                     | 0.56              |
| 1:F:386:THR:HG22 | 1:F:387:GLN:H    | 1.71                     | 0.56              |
| 1:J:577:ILE:HG21 | 1:J:593:LEU:HD13 | 1.87                     | 0.56              |
| 1:A:193:LEU:HD21 | 1:A:288:LYS:NZ   | 2.21                     | 0.56              |
| 1:D:386:THR:HG22 | 1:D:387:GLN:H    | 1.71                     | 0.56              |
| 1:E:270:GLN:NE2  | 1:E:271:ILE:O    | 2.38                     | 0.56              |
| 1:E:375:ASN:OD1  | 1:E:376:ARG:N    | 2.35                     | 0.56              |
| 1:E:386:THR:HG22 | 1:E:387:GLN:H    | 1.70                     | 0.56              |
| 1:E:639:VAL:O    | 1:E:643:ASN:ND2  | 2.38                     | 0.56              |
| 1:G:309:PHE:HB3  | 1:G:312:ASP:HA   | 1.87                     | 0.56              |
| 1:I:193:LEU:HD21 | 1:I:288:LYS:HZ3  | 1.71                     | 0.56              |
| 1:B:410:SER:O    | 1:B:414:GLU:HG2  | 2.06                     | 0.56              |
| 1:D:577:ILE:HG12 | 1:D:597:GLN:NE2  | 2.16                     | 0.56              |
| 1:E:356:ILE:HG21 | 1:F:373:LEU:HD21 | 1.87                     | 0.56              |
| 1:G:272:LYS:O    | 1:H:134:ASP:HB2  | 2.06                     | 0.56              |
| 1:H:236:GLN:HB2  | 1:H:265:LYS:CD   | 2.36                     | 0.56              |
| 1:I:528:LYS:HZ3  | 1:I:560:LEU:HD23 | 1.71                     | 0.56              |
| 1:K:363:TYR:OH   | 1:K:373:LEU:O    | 2.18                     | 0.56              |
| 1:L:410:SER:O    | 1:L:414:GLU:HG2  | 2.05                     | 0.56              |
| 1:H:438:LEU:HD11 | 1:I:108:LYS:HD3  | 1.88                     | 0.56              |
| 1:J:159:ASP:C    | 1:J:161:ASN:H    | 2.14                     | 0.56              |
| 1:J:321:ARG:HA   | 1:J:324:LYS:HE2  | 1.87                     | 0.56              |
| 1:J:426:ASN:O    | 1:J:429:GLN:NE2  | 2.39                     | 0.56              |
| 1:J:639:VAL:O    | 1:J:643:ASN:ND2  | 2.37                     | 0.56              |
| 1:K:201:PHE:CD1  | 1:K:283:CYS:HB2  | 2.41                     | 0.56              |
| 1:B:220:ALA:CB   | 1:B:281:ILE:O    | 2.46                     | 0.55              |
| 1:D:55:GLY:H     | 1:D:335:SER:HG   | 1.54                     | 0.55              |
| 1:E:337:ASN:HA   | 1:E:340:ILE:HD12 | 1.88                     | 0.55              |
| 1:F:321:ARG:HA   | 1:F:324:LYS:HE2  | 1.87                     | 0.55              |
| 1:I:353:PRO:O    | 1:I:356:ILE:HG22 | 2.06                     | 0.55              |
| 1:I:589:GLU:O    | 1:I:593:LEU:HB2  | 2.06                     | 0.55              |
| 1:J:353:PRO:O    | 1:J:356:ILE:HG22 | 2.06                     | 0.55              |
| 1:J:386:THR:HG22 | 1:J:387:GLN:H    | 1.70                     | 0.55              |
| 1:K:386:THR:HG22 | 1:K:387:GLN:H    | 1.72                     | 0.55              |
| 1:A:433:ASP:HA   | 1:A:436:ASN:HB3  | 1.87                     | 0.55              |
| 1:B:335:SER:O    | 1:B:338:ALA:HB3  | 2.06                     | 0.55              |
| 1:B:337:ASN:HA   | 1:B:340:ILE:HD12 | 1.88                     | 0.55              |
| 1:C:577:ILE:HG21 | 1:C:593:LEU:HD13 | 1.86                     | 0.55              |
| 1:D:433:ASP:HA   | 1:D:436:ASN:HB3  | 1.88                     | 0.55              |
| 1:E:299:PRO:HG2  | 1:E:300:ILE:HD12 | 1.88                     | 0.55              |
| 1:E:438:LEU:HD11 | 1:F:108:LYS:HD3  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:299:PRO:HG2  | 1:F:300:ILE:HD12 | 1.87                     | 0.55              |
| 1:F:429:GLN:HA   | 1:F:432:PHE:HD2  | 1.71                     | 0.55              |
| 1:F:438:LEU:HD11 | 1:G:108:LYS:HD3  | 1.87                     | 0.55              |
| 1:F:618:GLY:O    | 1:F:621:GLU:HB2  | 2.05                     | 0.55              |
| 1:G:643:ASN:HA   | 1:G:646:ASN:ND2  | 2.21                     | 0.55              |
| 1:H:426:ASN:O    | 1:H:429:GLN:NE2  | 2.40                     | 0.55              |
| 1:I:429:GLN:HA   | 1:I:432:PHE:HD2  | 1.72                     | 0.55              |
| 1:K:193:LEU:HD21 | 1:K:288:LYS:HZ3  | 1.71                     | 0.55              |
| 1:L:386:THR:HG22 | 1:L:387:GLN:H    | 1.71                     | 0.55              |
| 1:A:263:PHE:O    | 1:A:265:LYS:HG3  | 2.06                     | 0.55              |
| 1:A:386:THR:HG22 | 1:A:387:GLN:H    | 1.71                     | 0.55              |
| 1:A:426:ASN:O    | 1:A:429:GLN:NE2  | 2.39                     | 0.55              |
| 1:C:664:GLU:HG3  | 1:D:659:LEU:HD22 | 1.88                     | 0.55              |
| 1:D:350:PHE:N    | 1:D:390:ALA:O    | 2.32                     | 0.55              |
| 1:D:612:GLN:HA   | 1:D:615:LEU:HG   | 1.88                     | 0.55              |
| 1:E:276:VAL:HG22 | 1:E:296:GLU:HA   | 1.88                     | 0.55              |
| 1:F:375:ASN:OD1  | 1:F:376:ARG:N    | 2.37                     | 0.55              |
| 1:F:612:GLN:HA   | 1:F:615:LEU:CD1  | 2.35                     | 0.55              |
| 1:G:386:THR:HG22 | 1:G:387:GLN:H    | 1.71                     | 0.55              |
| 1:G:426:ASN:O    | 1:G:429:GLN:NE2  | 2.40                     | 0.55              |
| 1:I:603:GLN:O    | 1:I:606:PRO:HD3  | 2.05                     | 0.55              |
| 1:J:353:PRO:HA   | 1:K:373:LEU:HD23 | 1.89                     | 0.55              |
| 1:B:236:GLN:HB2  | 1:B:265:LYS:HD2  | 1.89                     | 0.55              |
| 1:B:643:ASN:HA   | 1:B:646:ASN:ND2  | 2.21                     | 0.55              |
| 1:C:350:PHE:N    | 1:C:390:ALA:O    | 2.32                     | 0.55              |
| 1:D:159:ASP:C    | 1:D:161:ASN:H    | 2.13                     | 0.55              |
| 1:E:161:ASN:HD21 | 1:F:183:GLY:HA3  | 1.71                     | 0.55              |
| 1:E:350:PHE:CD1  | 1:F:372:TYR:HB3  | 2.42                     | 0.55              |
| 1:E:410:SER:O    | 1:E:414:GLU:HG2  | 2.06                     | 0.55              |
| 1:F:232:ALA:HB1  | 1:F:268:GLU:HA   | 1.87                     | 0.55              |
| 1:G:34:PHE:O     | 1:G:38:VAL:HG23  | 2.05                     | 0.55              |
| 1:I:34:PHE:O     | 1:I:38:VAL:HG23  | 2.06                     | 0.55              |
| 1:J:643:ASN:HA   | 1:J:646:ASN:ND2  | 2.21                     | 0.55              |
| 1:D:375:ASN:OD1  | 1:D:376:ARG:N    | 2.36                     | 0.55              |
| 1:E:193:LEU:HD21 | 1:E:288:LYS:NZ   | 2.22                     | 0.55              |
| 1:J:309:PHE:HB3  | 1:J:312:ASP:HA   | 1.88                     | 0.55              |
| 1:L:433:ASP:HA   | 1:L:436:ASN:HB3  | 1.88                     | 0.55              |
| 1:A:232:ALA:HB1  | 1:A:268:GLU:HA   | 1.87                     | 0.55              |
| 1:B:433:ASP:HA   | 1:B:436:ASN:HB3  | 1.88                     | 0.55              |
| 1:D:27:ARG:HD3   | 1:D:313:LYS:HE3  | 1.88                     | 0.55              |
| 1:D:556:TYR:HB3  | 1:D:572:ALA:HB2  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:643:ASN:HA   | 1:D:646:ASN:ND2  | 2.22                     | 0.55              |
| 1:E:363:TYR:HE1  | 1:E:372:TYR:HA   | 1.70                     | 0.55              |
| 1:H:263:PHE:O    | 1:H:265:LYS:HG3  | 2.05                     | 0.55              |
| 1:K:159:ASP:C    | 1:K:161:ASN:H    | 2.15                     | 0.55              |
| 1:K:438:LEU:HD11 | 1:L:108:LYS:HD3  | 1.89                     | 0.55              |
| 1:L:276:VAL:HG22 | 1:L:296:GLU:HA   | 1.88                     | 0.55              |
| 1:B:353:PRO:O    | 1:B:356:ILE:HG22 | 2.06                     | 0.55              |
| 1:B:418:LEU:HD23 | 1:B:429:GLN:HB3  | 1.89                     | 0.55              |
| 1:C:201:PHE:CD1  | 1:C:283:CYS:HB2  | 2.41                     | 0.55              |
| 1:C:399:GLN:HA   | 1:C:402:ALA:HB3  | 1.88                     | 0.55              |
| 1:D:117:GLU:HB3  | 1:D:123:VAL:HG23 | 1.88                     | 0.55              |
| 1:G:325:ASP:O    | 1:G:328:ARG:HG2  | 2.07                     | 0.55              |
| 1:H:615:LEU:O    | 1:H:619:GLN:HG2  | 2.07                     | 0.55              |
| 1:H:639:VAL:O    | 1:H:642:GLN:HG2  | 2.07                     | 0.55              |
| 1:J:272:LYS:O    | 1:K:134:ASP:HB2  | 2.06                     | 0.55              |
| 1:L:528:LYS:NZ   | 1:L:559:LEU:O    | 2.40                     | 0.55              |
| 1:B:589:GLU:O    | 1:B:593:LEU:HB2  | 2.07                     | 0.55              |
| 1:D:511:ARG:HD3  | 1:D:513:ARG:HH22 | 1.71                     | 0.55              |
| 1:E:353:PRO:HA   | 1:F:373:LEU:HD23 | 1.89                     | 0.55              |
| 1:E:426:ASN:O    | 1:E:429:GLN:NE2  | 2.38                     | 0.55              |
| 1:F:643:ASN:HA   | 1:F:646:ASN:ND2  | 2.21                     | 0.55              |
| 1:G:350:PHE:CD1  | 1:H:372:TYR:HB3  | 2.41                     | 0.55              |
| 1:I:32:ASP:O     | 1:I:35:PHE:HB2   | 2.07                     | 0.55              |
| 1:J:418:LEU:HD23 | 1:J:429:GLN:HB3  | 1.89                     | 0.55              |
| 1:K:193:LEU:HD21 | 1:K:288:LYS:NZ   | 2.22                     | 0.55              |
| 1:A:612:GLN:HA   | 1:A:615:LEU:CD1  | 2.37                     | 0.55              |
| 1:C:236:GLN:HB2  | 1:C:265:LYS:CD   | 2.36                     | 0.55              |
| 1:D:589:GLU:O    | 1:D:593:LEU:HB2  | 2.06                     | 0.55              |
| 1:I:433:ASP:O    | 1:I:436:ASN:HB3  | 2.07                     | 0.55              |
| 1:I:612:GLN:HA   | 1:I:615:LEU:CD1  | 2.36                     | 0.55              |
| 1:J:363:TYR:HE1  | 1:J:372:TYR:HA   | 1.72                     | 0.55              |
| 1:K:93:VAL:O     | 1:K:96:GLY:N     | 2.40                     | 0.55              |
| 1:K:309:PHE:HB3  | 1:K:312:ASP:HA   | 1.88                     | 0.55              |
| 1:L:337:ASN:HA   | 1:L:340:ILE:HD12 | 1.89                     | 0.55              |
| 1:L:589:GLU:O    | 1:L:593:LEU:HB2  | 2.06                     | 0.55              |
| 1:A:309:PHE:HB3  | 1:A:312:ASP:HA   | 1.88                     | 0.54              |
| 1:E:612:GLN:HA   | 1:E:615:LEU:CD1  | 2.37                     | 0.54              |
| 1:F:536:LEU:HD23 | 1:F:539:LEU:HD12 | 1.88                     | 0.54              |
| 1:H:276:VAL:HG22 | 1:H:296:GLU:HA   | 1.89                     | 0.54              |
| 1:I:263:PHE:O    | 1:I:265:LYS:HG3  | 2.07                     | 0.54              |
| 1:J:127:ARG:HB3  | 1:J:147:GLU:HB2  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:350:PHE:N    | 1:L:390:ALA:O    | 2.32                     | 0.54              |
| 1:C:162:SER:OG   | 1:C:164:LEU:O    | 2.25                     | 0.54              |
| 1:D:664:GLU:OE2  | 1:E:666:ARG:NH2  | 2.40                     | 0.54              |
| 1:G:117:GLU:HB3  | 1:G:123:VAL:HG23 | 1.89                     | 0.54              |
| 1:G:335:SER:O    | 1:G:338:ALA:HB3  | 2.07                     | 0.54              |
| 1:G:356:ILE:HG21 | 1:H:373:LEU:HD21 | 1.89                     | 0.54              |
| 1:K:536:LEU:HD23 | 1:K:539:LEU:HD12 | 1.89                     | 0.54              |
| 1:K:643:ASN:HA   | 1:K:646:ASN:ND2  | 2.22                     | 0.54              |
| 1:L:159:ASP:C    | 1:L:161:ASN:H    | 2.14                     | 0.54              |
| 1:L:201:PHE:CD1  | 1:L:283:CYS:HB2  | 2.42                     | 0.54              |
| 1:D:34:PHE:O     | 1:D:38:VAL:HG23  | 2.07                     | 0.54              |
| 1:D:156:VAL:HA   | 1:D:174:THR:O    | 2.07                     | 0.54              |
| 1:G:193:LEU:HD21 | 1:G:288:LYS:NZ   | 2.22                     | 0.54              |
| 1:G:350:PHE:HB2  | 1:G:390:ALA:HB3  | 1.88                     | 0.54              |
| 1:G:615:LEU:O    | 1:G:619:GLN:HG2  | 2.07                     | 0.54              |
| 1:H:353:PRO:O    | 1:H:356:ILE:HG22 | 2.07                     | 0.54              |
| 1:I:386:THR:HG22 | 1:I:387:GLN:H    | 1.72                     | 0.54              |
| 1:J:612:GLN:HA   | 1:J:615:LEU:CD1  | 2.36                     | 0.54              |
| 1:L:577:ILE:HG12 | 1:L:597:GLN:NE2  | 2.17                     | 0.54              |
| 1:A:307:TRP:HE1  | 1:A:314:GLU:HG2  | 1.71                     | 0.54              |
| 1:B:236:GLN:HB2  | 1:B:265:LYS:CD   | 2.38                     | 0.54              |
| 1:C:433:ASP:HA   | 1:C:436:ASN:HB3  | 1.89                     | 0.54              |
| 1:C:618:GLY:O    | 1:C:621:GLU:HB2  | 2.07                     | 0.54              |
| 1:D:236:GLN:HB2  | 1:D:265:LYS:CD   | 2.37                     | 0.54              |
| 1:E:349:PRO:HG3  | 1:E:391:TYR:CZ   | 2.42                     | 0.54              |
| 1:I:176:ILE:HD11 | 1:I:204:PRO:HB3  | 1.90                     | 0.54              |
| 1:K:276:VAL:HG22 | 1:K:296:GLU:HA   | 1.90                     | 0.54              |
| 1:L:27:ARG:HD3   | 1:L:313:LYS:HE3  | 1.89                     | 0.54              |
| 1:L:309:PHE:HB3  | 1:L:312:ASP:HA   | 1.88                     | 0.54              |
| 1:B:96:GLY:O     | 1:B:100:THR:OG1  | 2.08                     | 0.54              |
| 1:D:193:LEU:HD21 | 1:D:288:LYS:NZ   | 2.23                     | 0.54              |
| 1:D:348:LYS:HB2  | 1:E:372:TYR:CD2  | 2.43                     | 0.54              |
| 1:E:78:VAL:HG22  | 1:E:520:VAL:HG12 | 1.90                     | 0.54              |
| 1:F:236:GLN:HB2  | 1:F:265:LYS:CD   | 2.38                     | 0.54              |
| 1:I:375:ASN:OD1  | 1:I:376:ARG:N    | 2.36                     | 0.54              |
| 1:J:220:ALA:CB   | 1:J:281:ILE:O    | 2.43                     | 0.54              |
| 1:J:399:GLN:HA   | 1:J:402:ALA:HB3  | 1.88                     | 0.54              |
| 1:L:156:VAL:HA   | 1:L:174:THR:O    | 2.07                     | 0.54              |
| 1:A:159:ASP:C    | 1:A:161:ASN:H    | 2.14                     | 0.54              |
| 1:A:162:SER:HA   | 1:A:169:ASP:OD1  | 2.08                     | 0.54              |
| 1:D:176:ILE:HD11 | 1:D:204:PRO:HB3  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:159:ASP:C    | 1:F:161:ASN:H    | 2.14                     | 0.54              |
| 1:F:353:PRO:O    | 1:F:356:ILE:HG22 | 2.08                     | 0.54              |
| 1:G:221:GLU:HG2  | 1:G:280:ILE:HG12 | 1.89                     | 0.54              |
| 1:G:528:LYS:HZ3  | 1:G:560:LEU:HD23 | 1.72                     | 0.54              |
| 1:I:410:SER:O    | 1:I:414:GLU:HG2  | 2.08                     | 0.54              |
| 1:I:618:GLY:O    | 1:I:621:GLU:HB2  | 2.08                     | 0.54              |
| 1:J:363:TYR:OH   | 1:J:373:LEU:O    | 2.16                     | 0.54              |
| 1:B:399:GLN:HA   | 1:B:402:ALA:HB3  | 1.89                     | 0.54              |
| 1:E:350:PHE:HB2  | 1:E:390:ALA:HB3  | 1.89                     | 0.54              |
| 1:F:309:PHE:HB3  | 1:F:312:ASP:HA   | 1.88                     | 0.54              |
| 1:I:159:ASP:C    | 1:I:161:ASN:H    | 2.16                     | 0.54              |
| 1:I:236:GLN:HB2  | 1:I:265:LYS:HD2  | 1.89                     | 0.54              |
| 1:I:354:GLU:HG2  | 1:J:376:ARG:HD3  | 1.90                     | 0.54              |
| 1:J:193:LEU:HD21 | 1:J:288:LYS:NZ   | 2.23                     | 0.54              |
| 1:J:201:PHE:CD1  | 1:J:283:CYS:HB2  | 2.42                     | 0.54              |
| 1:J:589:GLU:O    | 1:J:593:LEU:HB2  | 2.07                     | 0.54              |
| 1:A:410:SER:O    | 1:A:414:GLU:HG2  | 2.07                     | 0.54              |
| 1:A:643:ASN:HA   | 1:A:646:ASN:ND2  | 2.22                     | 0.54              |
| 1:C:643:ASN:HA   | 1:C:646:ASN:ND2  | 2.22                     | 0.54              |
| 1:G:337:ASN:HA   | 1:G:340:ILE:HD12 | 1.88                     | 0.54              |
| 1:H:386:THR:HG22 | 1:H:387:GLN:H    | 1.73                     | 0.54              |
| 1:I:335:SER:O    | 1:I:338:ALA:HB3  | 2.07                     | 0.54              |
| 1:J:162:SER:HA   | 1:J:169:ASP:OD1  | 2.08                     | 0.54              |
| 1:J:275:ARG:NH2  | 1:J:293:ILE:O    | 2.35                     | 0.54              |
| 1:A:201:PHE:CD1  | 1:A:283:CYS:HB2  | 2.43                     | 0.54              |
| 1:C:15:PHE:HA    | 1:C:18:ASP:HB3   | 1.90                     | 0.54              |
| 1:C:418:LEU:HD23 | 1:C:429:GLN:HB3  | 1.88                     | 0.54              |
| 1:C:426:ASN:O    | 1:C:429:GLN:NE2  | 2.41                     | 0.54              |
| 1:E:83:LYS:HE2   | 1:E:85:GLY:HA3   | 1.89                     | 0.54              |
| 1:E:201:PHE:CD1  | 1:E:283:CYS:HB2  | 2.43                     | 0.54              |
| 1:J:32:ASP:O     | 1:J:35:PHE:HB2   | 2.07                     | 0.54              |
| 1:K:589:GLU:O    | 1:K:593:LEU:HB2  | 2.08                     | 0.54              |
| 1:K:653:ILE:O    | 1:K:657:MET:HG2  | 2.06                     | 0.54              |
| 1:A:321:ARG:HA   | 1:A:324:LYS:HE2  | 1.89                     | 0.54              |
| 1:A:353:PRO:O    | 1:A:356:ILE:HG22 | 2.08                     | 0.54              |
| 1:B:34:PHE:O     | 1:B:38:VAL:HG23  | 2.08                     | 0.54              |
| 1:D:350:PHE:HB2  | 1:D:390:ALA:HB3  | 1.88                     | 0.54              |
| 1:F:337:ASN:HA   | 1:F:340:ILE:HD12 | 1.89                     | 0.54              |
| 1:F:433:ASP:HA   | 1:F:436:ASN:HB3  | 1.89                     | 0.54              |
| 1:H:337:ASN:HA   | 1:H:340:ILE:HD12 | 1.89                     | 0.54              |
| 1:H:350:PHE:HB2  | 1:H:390:ALA:HB3  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:363:TYR:HE1  | 1:I:372:TYR:HA   | 1.73                     | 0.54              |
| 1:K:426:ASN:O    | 1:K:429:GLN:NE2  | 2.41                     | 0.54              |
| 1:C:335:SER:O    | 1:C:338:ALA:HB3  | 2.08                     | 0.53              |
| 1:E:232:ALA:HB1  | 1:E:268:GLU:HA   | 1.89                     | 0.53              |
| 1:E:309:PHE:HB3  | 1:E:312:ASP:HA   | 1.90                     | 0.53              |
| 1:J:618:GLY:O    | 1:J:621:GLU:HB2  | 2.07                     | 0.53              |
| 1:K:615:LEU:O    | 1:K:619:GLN:HG2  | 2.06                     | 0.53              |
| 1:L:34:PHE:O     | 1:L:38:VAL:HG23  | 2.08                     | 0.53              |
| 1:L:193:LEU:HD21 | 1:L:288:LYS:NZ   | 2.23                     | 0.53              |
| 1:L:429:GLN:HA   | 1:L:432:PHE:HD2  | 1.73                     | 0.53              |
| 1:E:236:GLN:HB2  | 1:E:265:LYS:CD   | 2.37                     | 0.53              |
| 1:E:353:PRO:O    | 1:E:356:ILE:HG22 | 2.08                     | 0.53              |
| 1:H:272:LYS:O    | 1:I:134:ASP:HB2  | 2.08                     | 0.53              |
| 1:H:335:SER:O    | 1:H:338:ALA:HB3  | 2.08                     | 0.53              |
| 1:J:528:LYS:HZ3  | 1:J:560:LEU:HD23 | 1.73                     | 0.53              |
| 1:K:433:ASP:HA   | 1:K:436:ASN:HB3  | 1.90                     | 0.53              |
| 1:A:235:TYR:HE1  | 1:A:264:ILE:HA   | 1.74                     | 0.53              |
| 1:B:556:TYR:HB3  | 1:B:572:ALA:HB2  | 1.90                     | 0.53              |
| 1:E:363:TYR:OH   | 1:E:373:LEU:O    | 2.20                     | 0.53              |
| 1:E:643:ASN:HA   | 1:E:646:ASN:ND2  | 2.23                     | 0.53              |
| 1:J:337:ASN:HA   | 1:J:340:ILE:HD12 | 1.90                     | 0.53              |
| 1:L:350:PHE:HB2  | 1:L:390:ALA:HB3  | 1.90                     | 0.53              |
| 1:L:618:GLY:O    | 1:L:621:GLU:HB2  | 2.08                     | 0.53              |
| 1:A:433:ASP:O    | 1:A:436:ASN:HB3  | 2.08                     | 0.53              |
| 1:E:335:SER:O    | 1:E:338:ALA:HB3  | 2.09                     | 0.53              |
| 1:E:515:GLU:OE1  | 1:E:515:GLU:N    | 2.41                     | 0.53              |
| 1:E:589:GLU:O    | 1:E:593:LEU:HB2  | 2.08                     | 0.53              |
| 1:F:577:ILE:HG21 | 1:F:593:LEU:HD13 | 1.89                     | 0.53              |
| 1:H:159:ASP:C    | 1:H:161:ASN:H    | 2.17                     | 0.53              |
| 1:I:577:ILE:HG21 | 1:I:593:LEU:HD13 | 1.89                     | 0.53              |
| 1:L:162:SER:HA   | 1:L:169:ASP:OD1  | 2.09                     | 0.53              |
| 1:B:223:TYR:CE1  | 1:B:278:LYS:HG3  | 2.43                     | 0.53              |
| 1:C:382:GLY:N    | 1:C:383:ASP:HA   | 2.23                     | 0.53              |
| 1:E:528:LYS:NZ   | 1:E:559:LEU:O    | 2.39                     | 0.53              |
| 1:F:276:VAL:HG22 | 1:F:296:GLU:HA   | 1.90                     | 0.53              |
| 1:F:591:GLN:HA   | 1:F:595:GLU:CD   | 2.33                     | 0.53              |
| 1:G:433:ASP:HA   | 1:G:436:ASN:HB3  | 1.91                     | 0.53              |
| 1:I:643:ASN:HA   | 1:I:646:ASN:ND2  | 2.23                     | 0.53              |
| 1:A:87:ARG:HD3   | 1:A:89:ASP:HB2   | 1.90                     | 0.53              |
| 1:B:193:LEU:HD21 | 1:B:288:LYS:NZ   | 2.23                     | 0.53              |
| 1:C:101:ASP:OD1  | 1:C:101:ASP:N    | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:618:GLY:O    | 1:D:621:GLU:HB2  | 2.08                     | 0.53              |
| 1:F:31:ASN:O     | 1:F:35:PHE:HD2   | 1.91                     | 0.53              |
| 1:F:156:VAL:HA   | 1:F:174:THR:O    | 2.08                     | 0.53              |
| 1:I:87:ARG:HD3   | 1:I:89:ASP:HB2   | 1.89                     | 0.53              |
| 1:K:32:ASP:O     | 1:K:35:PHE:HB2   | 2.09                     | 0.53              |
| 1:K:399:GLN:HA   | 1:K:402:ALA:HB3  | 1.89                     | 0.53              |
| 1:A:335:SER:O    | 1:A:338:ALA:HB3  | 2.08                     | 0.53              |
| 1:C:131:ASP:OD1  | 1:C:132:TYR:N    | 2.42                     | 0.53              |
| 1:D:528:LYS:NZ   | 1:D:559:LEU:O    | 2.40                     | 0.53              |
| 1:F:193:LEU:HD21 | 1:F:288:LYS:HZ3  | 1.74                     | 0.53              |
| 1:F:410:SER:O    | 1:F:414:GLU:HG2  | 2.08                     | 0.53              |
| 1:G:201:PHE:CD1  | 1:G:283:CYS:HB2  | 2.44                     | 0.53              |
| 1:L:124:GLY:HA3  | 1:L:303:VAL:HG22 | 1.91                     | 0.53              |
| 1:L:131:ASP:OD1  | 1:L:132:TYR:N    | 2.42                     | 0.53              |
| 1:L:221:GLU:HG2  | 1:L:280:ILE:HG12 | 1.90                     | 0.53              |
| 1:C:162:SER:HA   | 1:C:169:ASP:OD1  | 2.09                     | 0.53              |
| 1:C:230:GLU:OE2  | 1:C:249:ARG:HG2  | 2.09                     | 0.53              |
| 1:C:536:LEU:HD23 | 1:C:539:LEU:HD12 | 1.91                     | 0.53              |
| 1:F:78:VAL:HG22  | 1:F:520:VAL:HG12 | 1.90                     | 0.53              |
| 1:F:273:ARG:NE   | 1:F:296:GLU:OE2  | 2.42                     | 0.53              |
| 1:H:363:TYR:HE1  | 1:H:372:TYR:HA   | 1.74                     | 0.53              |
| 1:H:433:ASP:HA   | 1:H:436:ASN:HB3  | 1.91                     | 0.53              |
| 1:J:27:ARG:HD3   | 1:J:313:LYS:HE3  | 1.89                     | 0.53              |
| 1:B:15:PHE:HA    | 1:B:18:ASP:HB3   | 1.91                     | 0.53              |
| 1:D:235:TYR:HE1  | 1:D:264:ILE:HA   | 1.74                     | 0.53              |
| 1:H:309:PHE:HB3  | 1:H:312:ASP:HA   | 1.90                     | 0.53              |
| 1:H:577:ILE:HG21 | 1:H:593:LEU:HD13 | 1.91                     | 0.53              |
| 1:J:78:VAL:HG22  | 1:J:520:VAL:HG12 | 1.89                     | 0.53              |
| 1:A:536:LEU:HD23 | 1:A:539:LEU:HD12 | 1.91                     | 0.53              |
| 1:B:515:GLU:OE1  | 1:B:515:GLU:N    | 2.42                     | 0.53              |
| 1:C:159:ASP:C    | 1:C:161:ASN:H    | 2.16                     | 0.53              |
| 1:D:230:GLU:OE2  | 1:D:249:ARG:HG2  | 2.09                     | 0.53              |
| 1:F:538:LEU:O    | 1:F:542:THR:OG1  | 2.27                     | 0.53              |
| 1:G:353:PRO:HA   | 1:H:373:LEU:HD23 | 1.91                     | 0.53              |
| 1:I:80:TYR:HD1   | 1:I:518:THR:HA   | 1.74                     | 0.53              |
| 1:I:272:LYS:O    | 1:J:134:ASP:HB2  | 2.09                     | 0.53              |
| 1:L:168:SER:HA   | 1:L:297:HIS:NE2  | 2.24                     | 0.53              |
| 1:C:350:PHE:HB2  | 1:C:390:ALA:HB3  | 1.91                     | 0.52              |
| 1:E:162:SER:HA   | 1:E:169:ASP:OD1  | 2.09                     | 0.52              |
| 1:F:83:LYS:HB2   | 1:F:515:GLU:HB3  | 1.91                     | 0.52              |
| 1:F:528:LYS:HZ3  | 1:F:560:LEU:HD23 | 1.74                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:536:LEU:HD23 | 1:G:539:LEU:HD12 | 1.91                     | 0.52              |
| 1:H:618:GLY:O    | 1:H:621:GLU:HB2  | 2.09                     | 0.52              |
| 1:I:201:PHE:CD1  | 1:I:283:CYS:HB2  | 2.44                     | 0.52              |
| 1:J:382:GLY:N    | 1:J:383:ASP:HA   | 2.24                     | 0.52              |
| 1:J:438:LEU:HD11 | 1:K:108:LYS:HD3  | 1.91                     | 0.52              |
| 1:L:382:GLY:N    | 1:L:383:ASP:HA   | 2.24                     | 0.52              |
| 1:C:299:PRO:HG2  | 1:C:300:ILE:HD12 | 1.90                     | 0.52              |
| 1:G:399:GLN:HA   | 1:G:402:ALA:HB3  | 1.91                     | 0.52              |
| 1:G:438:LEU:HD11 | 1:H:108:LYS:HD3  | 1.91                     | 0.52              |
| 1:G:695:GLU:HA   | 1:G:698:HIS:HD1  | 1.73                     | 0.52              |
| 1:A:108:LYS:HD3  | 1:L:438:LEU:HD11 | 1.91                     | 0.52              |
| 1:A:615:LEU:O    | 1:A:619:GLN:HG2  | 2.08                     | 0.52              |
| 1:B:299:PRO:HG2  | 1:B:300:ILE:HD12 | 1.92                     | 0.52              |
| 1:F:15:PHE:HA    | 1:F:18:ASP:HB3   | 1.91                     | 0.52              |
| 1:I:101:ASP:OD2  | 1:I:144:ILE:HG12 | 2.09                     | 0.52              |
| 1:J:335:SER:O    | 1:J:338:ALA:HB3  | 2.09                     | 0.52              |
| 1:L:335:SER:O    | 1:L:338:ALA:HB3  | 2.09                     | 0.52              |
| 1:A:363:TYR:HE1  | 1:A:372:TYR:HA   | 1.74                     | 0.52              |
| 1:F:252:LYS:HD2  | 1:F:256:ASP:HB3  | 1.91                     | 0.52              |
| 1:F:325:ASP:O    | 1:F:328:ARG:HG2  | 2.09                     | 0.52              |
| 1:J:591:GLN:HA   | 1:J:595:GLU:CD   | 2.35                     | 0.52              |
| 1:A:235:TYR:CE1  | 1:A:264:ILE:HA   | 2.44                     | 0.52              |
| 1:A:618:GLY:O    | 1:A:621:GLU:HB2  | 2.09                     | 0.52              |
| 1:D:201:PHE:CD1  | 1:D:283:CYS:HB2  | 2.45                     | 0.52              |
| 1:K:353:PRO:O    | 1:K:356:ILE:HG22 | 2.09                     | 0.52              |
| 1:A:628:GLN:O    | 1:A:632:LEU:HB2  | 2.10                     | 0.52              |
| 1:A:663:SER:HA   | 1:A:666:ARG:NE   | 2.24                     | 0.52              |
| 1:C:161:ASN:HD21 | 1:D:183:GLY:HA3  | 1.73                     | 0.52              |
| 1:C:232:ALA:HB1  | 1:C:268:GLU:HA   | 1.90                     | 0.52              |
| 1:D:276:VAL:HG22 | 1:D:296:GLU:HA   | 1.90                     | 0.52              |
| 1:D:515:GLU:OE1  | 1:D:515:GLU:N    | 2.42                     | 0.52              |
| 1:E:162:SER:HB2  | 1:E:170:ALA:HB2  | 1.90                     | 0.52              |
| 1:E:433:ASP:HA   | 1:E:436:ASN:HB3  | 1.92                     | 0.52              |
| 1:H:41:TRP:CH2   | 1:H:44:TRP:HB2   | 2.44                     | 0.52              |
| 1:I:156:VAL:HA   | 1:I:174:THR:O    | 2.08                     | 0.52              |
| 1:I:577:ILE:HG12 | 1:I:597:GLN:NE2  | 2.16                     | 0.52              |
| 1:K:53:TYR:O     | 1:K:54:ARG:NH1   | 2.41                     | 0.52              |
| 1:L:299:PRO:HG2  | 1:L:300:ILE:HD12 | 1.90                     | 0.52              |
| 1:L:321:ARG:HA   | 1:L:324:LYS:HE2  | 1.91                     | 0.52              |
| 1:L:615:LEU:O    | 1:L:619:GLN:HG2  | 2.10                     | 0.52              |
| 1:H:156:VAL:HA   | 1:H:174:THR:O    | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:433:ASP:O    | 1:K:436:ASN:HB3  | 2.10                     | 0.52              |
| 1:L:353:PRO:O    | 1:L:356:ILE:HG22 | 2.09                     | 0.52              |
| 1:L:363:TYR:HE1  | 1:L:372:TYR:HA   | 1.75                     | 0.52              |
| 1:L:515:GLU:OE1  | 1:L:515:GLU:N    | 2.43                     | 0.52              |
| 1:A:15:PHE:HA    | 1:A:18:ASP:HB3   | 1.92                     | 0.52              |
| 1:A:429:GLN:HA   | 1:A:432:PHE:HD2  | 1.75                     | 0.52              |
| 1:F:615:LEU:O    | 1:F:619:GLN:HG2  | 2.10                     | 0.52              |
| 1:H:273:ARG:NE   | 1:H:296:GLU:OE2  | 2.43                     | 0.52              |
| 1:H:536:LEU:HD23 | 1:H:539:LEU:HD12 | 1.92                     | 0.52              |
| 1:J:168:SER:HA   | 1:J:297:HIS:NE2  | 2.25                     | 0.52              |
| 1:J:377:THR:HA   | 1:J:383:ASP:OD2  | 2.10                     | 0.52              |
| 1:L:536:LEU:HD23 | 1:L:539:LEU:HD12 | 1.90                     | 0.52              |
| 1:A:78:VAL:HG22  | 1:A:520:VAL:HG12 | 1.92                     | 0.52              |
| 1:A:338:ALA:O    | 1:A:342:ALA:N    | 2.41                     | 0.52              |
| 1:B:127:ARG:HB3  | 1:B:147:GLU:HB2  | 1.91                     | 0.52              |
| 1:D:78:VAL:HG22  | 1:D:520:VAL:HG12 | 1.92                     | 0.52              |
| 1:D:124:GLY:HA3  | 1:D:303:VAL:HG22 | 1.92                     | 0.52              |
| 1:D:615:LEU:O    | 1:D:619:GLN:HG2  | 2.10                     | 0.52              |
| 1:E:429:GLN:HA   | 1:E:432:PHE:HD2  | 1.75                     | 0.52              |
| 1:F:162:SER:HB2  | 1:F:170:ALA:HB2  | 1.92                     | 0.52              |
| 1:H:78:VAL:HG22  | 1:H:520:VAL:HG12 | 1.91                     | 0.52              |
| 1:H:299:PRO:HG2  | 1:H:300:ILE:HD12 | 1.91                     | 0.52              |
| 1:I:193:LEU:HD21 | 1:I:288:LYS:NZ   | 2.25                     | 0.52              |
| 1:J:80:TYR:HD1   | 1:J:518:THR:HA   | 1.74                     | 0.52              |
| 1:L:127:ARG:HB3  | 1:L:147:GLU:HB2  | 1.90                     | 0.52              |
| 1:D:127:ARG:HB3  | 1:D:147:GLU:HB2  | 1.92                     | 0.52              |
| 1:D:577:ILE:HG21 | 1:D:593:LEU:HD13 | 1.91                     | 0.52              |
| 1:E:382:GLY:N    | 1:E:383:ASP:HA   | 2.25                     | 0.52              |
| 1:G:159:ASP:C    | 1:G:161:ASN:H    | 2.16                     | 0.52              |
| 1:I:299:PRO:HG2  | 1:I:300:ILE:HD12 | 1.92                     | 0.52              |
| 1:J:355:GLN:HG2  | 1:K:376:ARG:NH1  | 2.22                     | 0.52              |
| 1:K:82:PRO:HB3   | 1:K:90:ALA:HB3   | 1.92                     | 0.52              |
| 1:L:612:GLN:HA   | 1:L:615:LEU:CD1  | 2.39                     | 0.52              |
| 1:A:27:ARG:HH11  | 1:A:313:LYS:HE3  | 1.74                     | 0.51              |
| 1:B:101:ASP:OD2  | 1:B:144:ILE:HG12 | 2.10                     | 0.51              |
| 1:B:152:ALA:HA   | 1:B:155:HIS:HB2  | 1.92                     | 0.51              |
| 1:B:353:PRO:HA   | 1:C:373:LEU:HD23 | 1.91                     | 0.51              |
| 1:B:433:ASP:O    | 1:B:436:ASN:HB3  | 2.11                     | 0.51              |
| 1:D:303:VAL:HB   | 1:D:439:ASN:ND2  | 2.25                     | 0.51              |
| 1:F:363:TYR:HE1  | 1:F:372:TYR:HA   | 1.75                     | 0.51              |
| 1:F:382:GLY:N    | 1:F:383:ASP:HA   | 2.25                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:230:GLU:OE2  | 1:I:249:ARG:HG2  | 2.09                     | 0.51              |
| 1:A:418:LEU:HD23 | 1:A:429:GLN:HB3  | 1.92                     | 0.51              |
| 1:A:613:GLY:HA2  | 1:A:616:LEU:CD1  | 2.32                     | 0.51              |
| 1:C:276:VAL:HG22 | 1:C:296:GLU:HA   | 1.92                     | 0.51              |
| 1:C:303:VAL:HB   | 1:C:439:ASN:ND2  | 2.26                     | 0.51              |
| 1:C:528:LYS:NZ   | 1:C:559:LEU:O    | 2.38                     | 0.51              |
| 1:G:299:PRO:HG2  | 1:G:300:ILE:HD12 | 1.92                     | 0.51              |
| 1:J:299:PRO:HG2  | 1:J:300:ILE:HD12 | 1.92                     | 0.51              |
| 1:L:643:ASN:HA   | 1:L:646:ASN:ND2  | 2.24                     | 0.51              |
| 1:A:348:LYS:HB2  | 1:B:372:TYR:CD2  | 2.46                     | 0.51              |
| 1:C:646:ASN:HA   | 1:D:644:GLN:HG2  | 1.91                     | 0.51              |
| 1:D:32:ASP:O     | 1:D:35:PHE:HB2   | 2.10                     | 0.51              |
| 1:D:321:ARG:HA   | 1:D:324:LYS:HE2  | 1.92                     | 0.51              |
| 1:D:353:PRO:HD3  | 1:E:374:LEU:O    | 2.10                     | 0.51              |
| 1:H:324:LYS:O    | 1:H:327:GLN:HB2  | 2.10                     | 0.51              |
| 1:I:273:ARG:NE   | 1:I:296:GLU:OE2  | 2.43                     | 0.51              |
| 1:K:127:ARG:HB3  | 1:K:147:GLU:HB2  | 1.91                     | 0.51              |
| 1:L:32:ASP:O     | 1:L:35:PHE:HB2   | 2.11                     | 0.51              |
| 1:B:664:GLU:OE2  | 1:C:666:ARG:NH2  | 2.43                     | 0.51              |
| 1:C:151:SER:HB2  | 1:C:155:HIS:CE1  | 2.46                     | 0.51              |
| 1:E:586:THR:CG2  | 1:E:590:GLN:HE22 | 2.24                     | 0.51              |
| 1:B:131:ASP:OD1  | 1:B:132:TYR:N    | 2.44                     | 0.51              |
| 1:B:281:ILE:HG12 | 1:B:287:LEU:H    | 1.74                     | 0.51              |
| 1:C:106:THR:HG23 | 1:C:146:ARG:HE   | 1.75                     | 0.51              |
| 1:C:252:LYS:HD2  | 1:C:256:ASP:HB3  | 1.91                     | 0.51              |
| 1:E:613:GLY:HA2  | 1:E:616:LEU:CD1  | 2.39                     | 0.51              |
| 1:G:131:ASP:OD1  | 1:G:132:TYR:N    | 2.44                     | 0.51              |
| 1:G:591:GLN:HA   | 1:G:595:GLU:CD   | 2.36                     | 0.51              |
| 1:H:417:THR:O    | 1:H:418:LEU:HD12 | 2.11                     | 0.51              |
| 1:H:515:GLU:OE1  | 1:H:515:GLU:N    | 2.44                     | 0.51              |
| 1:I:348:LYS:HB2  | 1:J:372:TYR:CD2  | 2.46                     | 0.51              |
| 1:I:587:PRO:HD2  | 1:I:589:GLU:HG3  | 1.92                     | 0.51              |
| 1:K:34:PHE:O     | 1:K:38:VAL:HG23  | 2.10                     | 0.51              |
| 1:K:162:SER:HA   | 1:K:169:ASP:OD1  | 2.11                     | 0.51              |
| 1:K:299:PRO:HG2  | 1:K:300:ILE:HD12 | 1.91                     | 0.51              |
| 1:K:667:GLU:HG2  | 1:L:666:ARG:NH1  | 2.25                     | 0.51              |
| 1:L:325:ASP:O    | 1:L:328:ARG:HG2  | 2.11                     | 0.51              |
| 1:A:438:LEU:HD11 | 1:B:108:LYS:HD3  | 1.92                     | 0.51              |
| 1:B:613:GLY:CA   | 1:B:616:LEU:HD13 | 2.33                     | 0.51              |
| 1:F:27:ARG:HH11  | 1:F:313:LYS:HE3  | 1.76                     | 0.51              |
| 1:F:433:ASP:O    | 1:F:436:ASN:HB3  | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:363:TYR:HE1  | 1:G:372:TYR:HA   | 1.75                     | 0.51              |
| 1:G:410:SER:O    | 1:G:414:GLU:HG2  | 2.11                     | 0.51              |
| 1:H:32:ASP:O     | 1:H:35:PHE:HB2   | 2.11                     | 0.51              |
| 1:A:325:ASP:O    | 1:A:328:ARG:HG2  | 2.11                     | 0.51              |
| 1:D:131:ASP:OD1  | 1:D:132:TYR:N    | 2.43                     | 0.51              |
| 1:D:299:PRO:HG2  | 1:D:300:ILE:HD12 | 1.93                     | 0.51              |
| 1:E:433:ASP:O    | 1:E:436:ASN:HB3  | 2.10                     | 0.51              |
| 1:F:335:SER:O    | 1:F:338:ALA:HB3  | 2.10                     | 0.51              |
| 1:G:586:THR:CG2  | 1:G:590:GLN:HE22 | 2.24                     | 0.51              |
| 1:H:97:MET:HE2   | 1:H:450:GLN:HE22 | 1.75                     | 0.51              |
| 1:I:382:GLY:N    | 1:I:383:ASP:HA   | 2.25                     | 0.51              |
| 1:J:303:VAL:HB   | 1:J:439:ASN:ND2  | 2.26                     | 0.51              |
| 1:K:220:ALA:CB   | 1:K:281:ILE:O    | 2.46                     | 0.51              |
| 1:A:34:PHE:O     | 1:A:38:VAL:HG23  | 2.10                     | 0.51              |
| 1:B:642:GLN:HA   | 1:B:645:LEU:HD12 | 1.92                     | 0.51              |
| 1:D:161:ASN:ND2  | 1:E:183:GLY:HA3  | 2.25                     | 0.51              |
| 1:F:101:ASP:OD2  | 1:F:144:ILE:HG12 | 2.11                     | 0.51              |
| 1:F:653:ILE:HG12 | 1:G:648:ALA:HA   | 1.92                     | 0.51              |
| 1:G:162:SER:HA   | 1:G:169:ASP:OD1  | 2.10                     | 0.51              |
| 1:G:273:ARG:NE   | 1:G:296:GLU:OE2  | 2.44                     | 0.51              |
| 1:H:34:PHE:O     | 1:H:38:VAL:HG23  | 2.11                     | 0.51              |
| 1:H:101:ASP:OD2  | 1:H:144:ILE:HG12 | 2.11                     | 0.51              |
| 1:J:325:ASP:O    | 1:J:328:ARG:HG2  | 2.10                     | 0.51              |
| 1:J:429:GLN:HA   | 1:J:432:PHE:HD2  | 1.75                     | 0.51              |
| 1:K:27:ARG:HD3   | 1:K:313:LYS:HE3  | 1.93                     | 0.51              |
| 1:C:272:LYS:O    | 1:D:134:ASP:HB2  | 2.10                     | 0.51              |
| 1:D:273:ARG:NE   | 1:D:296:GLU:OE2  | 2.44                     | 0.51              |
| 1:D:335:SER:O    | 1:D:338:ALA:HB3  | 2.10                     | 0.51              |
| 1:D:355:GLN:HG2  | 1:E:376:ARG:NH1  | 2.20                     | 0.51              |
| 1:E:559:LEU:HB3  | 1:E:565:VAL:HB   | 1.92                     | 0.51              |
| 1:G:303:VAL:HB   | 1:G:439:ASN:ND2  | 2.26                     | 0.51              |
| 1:G:382:GLY:N    | 1:G:383:ASP:HA   | 2.25                     | 0.51              |
| 1:H:223:TYR:CE1  | 1:H:278:LYS:HG3  | 2.46                     | 0.51              |
| 1:H:591:GLN:HA   | 1:H:595:GLU:CD   | 2.36                     | 0.51              |
| 1:J:156:VAL:HA   | 1:J:174:THR:O    | 2.10                     | 0.51              |
| 1:L:577:ILE:HG21 | 1:L:593:LEU:HD13 | 1.92                     | 0.51              |
| 1:A:434:THR:HG21 | 1:B:72:ARG:HG3   | 1.92                     | 0.51              |
| 1:C:309:PHE:HB3  | 1:C:312:ASP:HA   | 1.93                     | 0.51              |
| 1:E:307:TRP:HE1  | 1:E:314:GLU:HG2  | 1.75                     | 0.51              |
| 1:G:577:ILE:HG21 | 1:G:593:LEU:HD13 | 1.91                     | 0.51              |
| 1:H:162:SER:HA   | 1:H:169:ASP:OD1  | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:354:GLU:HG2  | 1:K:376:ARG:HD3  | 1.92                     | 0.51              |
| 1:K:78:VAL:HG22  | 1:K:520:VAL:HG12 | 1.92                     | 0.51              |
| 1:K:156:VAL:HA   | 1:K:174:THR:O    | 2.11                     | 0.51              |
| 1:K:325:ASP:O    | 1:K:328:ARG:HG2  | 2.10                     | 0.51              |
| 1:L:628:GLN:O    | 1:L:632:LEU:HB2  | 2.10                     | 0.51              |
| 1:A:273:ARG:NE   | 1:A:296:GLU:OE2  | 2.44                     | 0.50              |
| 1:B:24:GLU:N     | 1:B:24:GLU:OE1   | 2.44                     | 0.50              |
| 1:B:273:ARG:NE   | 1:B:296:GLU:OE2  | 2.44                     | 0.50              |
| 1:E:27:ARG:HD3   | 1:E:313:LYS:HE3  | 1.92                     | 0.50              |
| 1:E:228:LYS:HB2  | 1:E:275:ARG:HB3  | 1.93                     | 0.50              |
| 1:E:355:GLN:HA   | 1:E:375:ASN:HB3  | 1.93                     | 0.50              |
| 1:I:161:ASN:ND2  | 1:J:183:GLY:HA3  | 2.26                     | 0.50              |
| 1:I:236:GLN:HB2  | 1:I:265:LYS:CD   | 2.41                     | 0.50              |
| 1:I:350:PHE:CD1  | 1:J:372:TYR:HB3  | 2.46                     | 0.50              |
| 1:I:417:THR:O    | 1:I:418:LEU:HD12 | 2.11                     | 0.50              |
| 1:J:353:PRO:HD3  | 1:K:374:LEU:O    | 2.11                     | 0.50              |
| 1:J:587:PRO:HD2  | 1:J:589:GLU:HG3  | 1.93                     | 0.50              |
| 1:J:664:GLU:HG3  | 1:K:659:LEU:HD22 | 1.93                     | 0.50              |
| 1:K:577:ILE:HG21 | 1:K:593:LEU:HD13 | 1.92                     | 0.50              |
| 1:K:591:GLN:HA   | 1:K:595:GLU:CD   | 2.36                     | 0.50              |
| 1:L:53:TYR:O     | 1:L:54:ARG:NH1   | 2.43                     | 0.50              |
| 1:B:536:LEU:HD23 | 1:B:539:LEU:HD12 | 1.94                     | 0.50              |
| 1:B:591:GLN:HA   | 1:B:595:GLU:CD   | 2.36                     | 0.50              |
| 1:E:156:VAL:HA   | 1:E:174:THR:O    | 2.11                     | 0.50              |
| 1:H:348:LYS:HB2  | 1:I:372:TYR:CD2  | 2.46                     | 0.50              |
| 1:K:223:TYR:CE1  | 1:K:278:LYS:HG3  | 2.45                     | 0.50              |
| 1:L:236:GLN:HB2  | 1:L:265:LYS:CD   | 2.40                     | 0.50              |
| 1:A:655:ASN:ND2  | 1:L:657:MET:SD   | 2.85                     | 0.50              |
| 1:B:162:SER:OG   | 1:B:164:LEU:O    | 2.30                     | 0.50              |
| 1:B:349:PRO:HG3  | 1:B:391:TYR:CZ   | 2.47                     | 0.50              |
| 1:D:382:GLY:N    | 1:D:383:ASP:HA   | 2.25                     | 0.50              |
| 1:E:32:ASP:O     | 1:E:35:PHE:HB2   | 2.11                     | 0.50              |
| 1:G:168:SER:HA   | 1:G:297:HIS:NE2  | 2.26                     | 0.50              |
| 1:G:667:GLU:HG2  | 1:H:666:ARG:NH1  | 2.26                     | 0.50              |
| 1:J:615:LEU:O    | 1:J:619:GLN:HG2  | 2.10                     | 0.50              |
| 1:K:417:THR:O    | 1:K:418:LEU:HD12 | 2.12                     | 0.50              |
| 1:A:101:ASP:OD2  | 1:A:144:ILE:HG12 | 2.11                     | 0.50              |
| 1:B:382:GLY:N    | 1:B:383:ASP:HA   | 2.25                     | 0.50              |
| 1:B:434:THR:HG21 | 1:C:72:ARG:HG3   | 1.91                     | 0.50              |
| 1:B:663:SER:HA   | 1:B:666:ARG:NE   | 2.23                     | 0.50              |
| 1:D:349:PRO:HG3  | 1:D:391:TYR:CZ   | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:418:LEU:HD23 | 1:D:429:GLN:HB3  | 1.93                     | 0.50              |
| 1:E:325:ASP:O    | 1:E:328:ARG:HG2  | 2.10                     | 0.50              |
| 1:G:140:ASN:HB3  | 1:G:455:THR:OG1  | 2.11                     | 0.50              |
| 1:H:131:ASP:OD1  | 1:H:132:TYR:N    | 2.44                     | 0.50              |
| 1:J:559:LEU:HB3  | 1:J:565:VAL:HB   | 1.94                     | 0.50              |
| 1:J:667:GLU:HG2  | 1:K:666:ARG:NH1  | 2.26                     | 0.50              |
| 1:L:349:PRO:HG3  | 1:L:391:TYR:CZ   | 2.46                     | 0.50              |
| 1:C:444:LEU:O    | 1:C:447:TYR:HB3  | 2.12                     | 0.50              |
| 1:E:34:PHE:O     | 1:E:38:VAL:HG23  | 2.12                     | 0.50              |
| 1:F:168:SER:HA   | 1:F:297:HIS:NE2  | 2.27                     | 0.50              |
| 1:H:29:ALA:O     | 1:H:33:LEU:HB2   | 2.12                     | 0.50              |
| 1:I:343:ARG:HH22 | 1:K:368:ASP:HA   | 1.77                     | 0.50              |
| 1:J:581:VAL:HG22 | 1:K:567:MET:HB2  | 1.94                     | 0.50              |
| 1:C:436:ASN:HA   | 1:C:439:ASN:ND2  | 2.27                     | 0.50              |
| 1:C:586:THR:CG2  | 1:C:590:GLN:HE22 | 2.25                     | 0.50              |
| 1:D:278:LYS:HE2  | 1:D:280:ILE:HD11 | 1.93                     | 0.50              |
| 1:E:434:THR:HG21 | 1:F:72:ARG:HG3   | 1.94                     | 0.50              |
| 1:F:204:PRO:HD3  | 1:F:218:GLN:HG2  | 1.94                     | 0.50              |
| 1:H:230:GLU:OE2  | 1:H:249:ARG:HG2  | 2.11                     | 0.50              |
| 1:I:321:ARG:HA   | 1:I:324:LYS:HE2  | 1.94                     | 0.50              |
| 1:J:101:ASP:OD2  | 1:J:144:ILE:HG12 | 2.11                     | 0.50              |
| 1:K:62:PRO:HA    | 1:K:65:ARG:HH21  | 1.76                     | 0.50              |
| 1:K:228:LYS:HB2  | 1:K:275:ARG:HB3  | 1.93                     | 0.50              |
| 1:K:363:TYR:HE1  | 1:K:372:TYR:HA   | 1.76                     | 0.50              |
| 1:L:433:ASP:O    | 1:L:436:ASN:HB3  | 2.12                     | 0.50              |
| 1:A:124:GLY:HA3  | 1:A:303:VAL:HG22 | 1.93                     | 0.50              |
| 1:A:515:GLU:N    | 1:A:515:GLU:OE1  | 2.45                     | 0.50              |
| 1:B:272:LYS:O    | 1:C:134:ASP:HB2  | 2.12                     | 0.50              |
| 1:B:338:ALA:O    | 1:B:342:ALA:N    | 2.43                     | 0.50              |
| 1:C:29:ALA:O     | 1:C:33:LEU:HB2   | 2.11                     | 0.50              |
| 1:C:273:ARG:NE   | 1:C:296:GLU:OE2  | 2.44                     | 0.50              |
| 1:D:272:LYS:O    | 1:E:134:ASP:HB2  | 2.12                     | 0.50              |
| 1:E:101:ASP:OD2  | 1:E:144:ILE:HG12 | 2.12                     | 0.50              |
| 1:E:168:SER:HA   | 1:E:297:HIS:NE2  | 2.26                     | 0.50              |
| 1:E:230:GLU:OE2  | 1:E:249:ARG:HG2  | 2.12                     | 0.50              |
| 1:F:27:ARG:HD3   | 1:F:313:LYS:HE3  | 1.94                     | 0.50              |
| 1:F:140:ASN:HB3  | 1:F:455:THR:OG1  | 2.12                     | 0.50              |
| 1:I:131:ASP:OD1  | 1:I:132:TYR:N    | 2.44                     | 0.50              |
| 1:J:236:GLN:HB2  | 1:J:265:LYS:CD   | 2.41                     | 0.50              |
| 1:J:515:GLU:OE1  | 1:J:515:GLU:N    | 2.45                     | 0.50              |
| 1:A:24:GLU:OE1   | 1:A:24:GLU:N     | 2.44                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:193:LEU:HD21 | 1:C:288:LYS:NZ   | 2.26                     | 0.50              |
| 1:E:127:ARG:HB3  | 1:E:147:GLU:HB2  | 1.93                     | 0.50              |
| 1:E:273:ARG:NE   | 1:E:296:GLU:OE2  | 2.44                     | 0.50              |
| 1:G:24:GLU:OE1   | 1:G:24:GLU:N     | 2.45                     | 0.50              |
| 1:H:377:THR:HA   | 1:H:383:ASP:OD2  | 2.12                     | 0.50              |
| 1:I:127:ARG:HB3  | 1:I:147:GLU:HB2  | 1.94                     | 0.50              |
| 1:J:131:ASP:OD1  | 1:J:132:TYR:N    | 2.45                     | 0.50              |
| 1:K:24:GLU:OE1   | 1:K:24:GLU:N     | 2.45                     | 0.50              |
| 1:A:120:GLU:HA   | 1:A:320:VAL:HB   | 1.94                     | 0.50              |
| 1:B:162:SER:HA   | 1:B:169:ASP:OD1  | 2.12                     | 0.50              |
| 1:B:438:LEU:HD11 | 1:C:108:LYS:HD3  | 1.94                     | 0.50              |
| 1:B:528:LYS:HZ3  | 1:B:560:LEU:HD23 | 1.77                     | 0.50              |
| 1:D:680:SER:O    | 1:D:683:ALA:HB3  | 2.11                     | 0.50              |
| 1:I:235:TYR:HE1  | 1:I:264:ILE:HA   | 1.77                     | 0.50              |
| 1:K:515:GLU:OE1  | 1:K:515:GLU:N    | 2.45                     | 0.50              |
| 1:L:24:GLU:OE1   | 1:L:24:GLU:N     | 2.45                     | 0.50              |
| 1:B:303:VAL:HB   | 1:B:439:ASN:ND2  | 2.27                     | 0.49              |
| 1:C:417:THR:O    | 1:C:418:LEU:HD12 | 2.12                     | 0.49              |
| 1:D:101:ASP:OD2  | 1:D:144:ILE:HG12 | 2.12                     | 0.49              |
| 1:D:235:TYR:CE1  | 1:D:264:ILE:HA   | 2.47                     | 0.49              |
| 1:E:363:TYR:CE1  | 1:E:372:TYR:HA   | 2.47                     | 0.49              |
| 1:G:176:ILE:HD11 | 1:G:204:PRO:HB3  | 1.93                     | 0.49              |
| 1:J:230:GLU:OE2  | 1:J:249:ARG:HG2  | 2.11                     | 0.49              |
| 1:J:528:LYS:NZ   | 1:J:559:LEU:O    | 2.43                     | 0.49              |
| 1:L:78:VAL:HG22  | 1:L:520:VAL:HG12 | 1.93                     | 0.49              |
| 1:L:307:TRP:HE1  | 1:L:314:GLU:HG2  | 1.77                     | 0.49              |
| 1:A:161:ASN:HD21 | 1:B:183:GLY:HA3  | 1.77                     | 0.49              |
| 1:A:299:PRO:HG2  | 1:A:300:ILE:HD12 | 1.93                     | 0.49              |
| 1:B:201:PHE:HD1  | 1:B:283:CYS:HB2  | 1.77                     | 0.49              |
| 1:B:363:TYR:HE1  | 1:B:372:TYR:HA   | 1.77                     | 0.49              |
| 1:E:664:GLU:HG3  | 1:F:659:LEU:HD22 | 1.92                     | 0.49              |
| 1:F:45:LEU:HG    | 1:F:46:SER:H     | 1.76                     | 0.49              |
| 1:F:127:ARG:HB3  | 1:F:147:GLU:HB2  | 1.94                     | 0.49              |
| 1:F:161:ASN:HD21 | 1:G:183:GLY:HA3  | 1.78                     | 0.49              |
| 1:F:348:LYS:HB2  | 1:G:372:TYR:CD2  | 2.48                     | 0.49              |
| 1:G:248:LYS:HE3  | 1:G:252:LYS:HB2  | 1.93                     | 0.49              |
| 1:H:220:ALA:CB   | 1:H:281:ILE:O    | 2.48                     | 0.49              |
| 1:I:663:SER:O    | 1:I:666:ARG:HG3  | 2.12                     | 0.49              |
| 1:J:348:LYS:HB2  | 1:K:372:TYR:CD2  | 2.46                     | 0.49              |
| 1:A:168:SER:HA   | 1:A:297:HIS:NE2  | 2.26                     | 0.49              |
| 1:A:236:GLN:HG2  | 1:A:244:VAL:H    | 1.76                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:657:MET:SD   | 1:D:655:ASN:ND2  | 2.85                     | 0.49              |
| 1:D:53:TYR:O     | 1:D:54:ARG:NH1   | 2.43                     | 0.49              |
| 1:D:338:ALA:O    | 1:D:342:ALA:N    | 2.45                     | 0.49              |
| 1:D:536:LEU:HD23 | 1:D:539:LEU:HD12 | 1.94                     | 0.49              |
| 1:D:576:LEU:O    | 1:D:581:VAL:HG12 | 2.12                     | 0.49              |
| 1:F:34:PHE:O     | 1:F:38:VAL:HG23  | 2.13                     | 0.49              |
| 1:F:223:TYR:HE1  | 1:F:278:LYS:HG3  | 1.78                     | 0.49              |
| 1:G:162:SER:OG   | 1:G:164:LEU:O    | 2.31                     | 0.49              |
| 1:G:589:GLU:O    | 1:G:593:LEU:HB2  | 2.11                     | 0.49              |
| 1:I:80:TYR:CD1   | 1:I:444:LEU:HD21 | 2.47                     | 0.49              |
| 1:I:338:ALA:O    | 1:I:342:ALA:N    | 2.45                     | 0.49              |
| 1:J:350:PHE:HB2  | 1:J:390:ALA:HB3  | 1.94                     | 0.49              |
| 1:K:106:THR:HG23 | 1:K:146:ARG:HE   | 1.77                     | 0.49              |
| 1:K:622:LEU:O    | 1:K:626:GLN:HG3  | 2.11                     | 0.49              |
| 1:L:228:LYS:HB2  | 1:L:275:ARG:HB3  | 1.94                     | 0.49              |
| 1:B:78:VAL:HA    | 1:B:520:VAL:HA   | 1.92                     | 0.49              |
| 1:D:433:ASP:O    | 1:D:436:ASN:HB3  | 2.13                     | 0.49              |
| 1:E:348:LYS:HB2  | 1:F:372:TYR:CD2  | 2.47                     | 0.49              |
| 1:G:236:GLN:HB2  | 1:G:265:LYS:CD   | 2.43                     | 0.49              |
| 1:H:15:PHE:HA    | 1:H:18:ASP:HB3   | 1.94                     | 0.49              |
| 1:H:354:GLU:HG2  | 1:I:376:ARG:HD3  | 1.93                     | 0.49              |
| 1:I:433:ASP:HA   | 1:I:436:ASN:HB3  | 1.93                     | 0.49              |
| 1:J:176:ILE:HD11 | 1:J:204:PRO:HB3  | 1.94                     | 0.49              |
| 1:K:586:THR:CG2  | 1:K:590:GLN:HE22 | 2.24                     | 0.49              |
| 1:L:417:THR:O    | 1:L:418:LEU:HD12 | 2.12                     | 0.49              |
| 1:A:32:ASP:O     | 1:A:35:PHE:HB2   | 2.12                     | 0.49              |
| 1:B:348:LYS:HB2  | 1:C:372:TYR:CD2  | 2.48                     | 0.49              |
| 1:C:337:ASN:HA   | 1:C:340:ILE:HD12 | 1.95                     | 0.49              |
| 1:C:353:PRO:O    | 1:C:356:ILE:HG22 | 2.11                     | 0.49              |
| 1:D:591:GLN:HA   | 1:D:595:GLU:CD   | 2.37                     | 0.49              |
| 1:F:352:TRP:CB   | 1:G:376:ARG:HD2  | 2.39                     | 0.49              |
| 1:F:426:ASN:O    | 1:F:429:GLN:NE2  | 2.44                     | 0.49              |
| 1:G:528:LYS:NZ   | 1:G:559:LEU:O    | 2.42                     | 0.49              |
| 1:H:201:PHE:HD1  | 1:H:283:CYS:HB2  | 1.77                     | 0.49              |
| 1:K:348:LYS:HB2  | 1:L:372:TYR:CD2  | 2.48                     | 0.49              |
| 1:L:101:ASP:OD2  | 1:L:144:ILE:HG12 | 2.12                     | 0.49              |
| 1:L:363:TYR:OH   | 1:L:373:LEU:O    | 2.18                     | 0.49              |
| 1:A:223:TYR:CE1  | 1:A:278:LYS:HG3  | 2.48                     | 0.49              |
| 1:B:124:GLY:HA3  | 1:B:303:VAL:HG22 | 1.94                     | 0.49              |
| 1:C:124:GLY:HA3  | 1:C:303:VAL:HG22 | 1.94                     | 0.49              |
| 1:F:248:LYS:HE3  | 1:F:252:LYS:HB2  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:377:THR:HA   | 1:F:383:ASP:OD2  | 2.13                     | 0.49              |
| 1:G:101:ASP:OD2  | 1:G:144:ILE:HG12 | 2.13                     | 0.49              |
| 1:G:161:ASN:HD21 | 1:H:183:GLY:HA3  | 1.77                     | 0.49              |
| 1:H:525:GLN:HB2  | 1:H:529:GLN:OE1  | 2.13                     | 0.49              |
| 1:L:223:TYR:CE1  | 1:L:278:LYS:HG3  | 2.47                     | 0.49              |
| 1:A:80:TYR:CD1   | 1:A:444:LEU:HD21 | 2.47                     | 0.49              |
| 1:A:236:GLN:HB2  | 1:A:265:LYS:CD   | 2.43                     | 0.49              |
| 1:C:82:PRO:HB3   | 1:C:90:ALA:HB3   | 1.94                     | 0.49              |
| 1:C:613:GLY:CA   | 1:C:616:LEU:HD13 | 2.43                     | 0.49              |
| 1:E:24:GLU:N     | 1:E:24:GLU:OE1   | 2.45                     | 0.49              |
| 1:E:587:PRO:HD2  | 1:E:589:GLU:HG3  | 1.94                     | 0.49              |
| 1:E:663:SER:HA   | 1:E:666:ARG:NE   | 2.23                     | 0.49              |
| 1:F:613:GLY:O    | 1:F:616:LEU:HD13 | 2.13                     | 0.49              |
| 1:G:151:SER:HB2  | 1:G:155:HIS:CE1  | 2.48                     | 0.49              |
| 1:G:514:TYR:HB2  | 1:H:136:SER:OG   | 2.13                     | 0.49              |
| 1:I:78:VAL:HG22  | 1:I:520:VAL:HG12 | 1.95                     | 0.49              |
| 1:I:515:GLU:N    | 1:I:515:GLU:OE1  | 2.46                     | 0.49              |
| 1:A:350:PHE:HB2  | 1:A:390:ALA:HB3  | 1.94                     | 0.49              |
| 1:A:591:GLN:HA   | 1:A:595:GLU:CD   | 2.38                     | 0.49              |
| 1:A:639:VAL:O    | 1:A:642:GLN:HG2  | 2.12                     | 0.49              |
| 1:D:354:GLU:HG2  | 1:E:376:ARG:HD3  | 1.94                     | 0.49              |
| 1:E:639:VAL:O    | 1:E:642:GLN:HG2  | 2.13                     | 0.49              |
| 1:F:114:ALA:O    | 1:F:118:GLN:HB2  | 2.13                     | 0.49              |
| 1:G:377:THR:HA   | 1:G:383:ASP:OD2  | 2.11                     | 0.49              |
| 1:H:228:LYS:HB2  | 1:H:275:ARG:HB3  | 1.95                     | 0.49              |
| 1:H:382:GLY:N    | 1:H:383:ASP:HA   | 2.27                     | 0.49              |
| 1:H:590:GLN:HA   | 1:H:594:VAL:HB   | 1.94                     | 0.49              |
| 1:J:24:GLU:N     | 1:J:24:GLU:OE1   | 2.46                     | 0.49              |
| 1:L:96:GLY:O     | 1:L:100:THR:OG1  | 2.11                     | 0.49              |
| 1:L:124:GLY:CA   | 1:L:303:VAL:HG22 | 2.43                     | 0.49              |
| 1:B:325:ASP:O    | 1:B:328:ARG:HG2  | 2.12                     | 0.49              |
| 1:C:32:ASP:O     | 1:C:35:PHE:HB2   | 2.12                     | 0.49              |
| 1:C:55:GLY:N     | 1:C:335:SER:OG   | 2.43                     | 0.49              |
| 1:D:24:GLU:OE1   | 1:D:24:GLU:N     | 2.45                     | 0.49              |
| 1:E:642:GLN:HA   | 1:E:645:LEU:HD12 | 1.94                     | 0.49              |
| 1:E:646:ASN:HA   | 1:F:644:GLN:HG2  | 1.95                     | 0.49              |
| 1:J:417:THR:O    | 1:J:418:LEU:HD12 | 2.12                     | 0.49              |
| 1:J:628:GLN:O    | 1:J:632:LEU:HB2  | 2.13                     | 0.49              |
| 1:K:236:GLN:HB2  | 1:K:265:LYS:CD   | 2.43                     | 0.49              |
| 1:K:382:GLY:N    | 1:K:383:ASP:HA   | 2.25                     | 0.49              |
| 1:K:623:ALA:HA   | 1:K:626:GLN:CD   | 2.38                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:152:ALA:HA   | 1:C:155:HIS:HB2  | 1.94                     | 0.49              |
| 1:C:220:ALA:CB   | 1:C:281:ILE:O    | 2.48                     | 0.49              |
| 1:D:363:TYR:HE1  | 1:D:372:TYR:HA   | 1.77                     | 0.49              |
| 1:D:417:THR:O    | 1:D:418:LEU:HD12 | 2.13                     | 0.49              |
| 1:F:223:TYR:CE1  | 1:F:278:LYS:HG3  | 2.47                     | 0.49              |
| 1:F:230:GLU:OE2  | 1:F:249:ARG:HG2  | 2.12                     | 0.49              |
| 1:F:434:THR:HG21 | 1:G:72:ARG:HG3   | 1.95                     | 0.49              |
| 1:G:41:TRP:CH2   | 1:G:44:TRP:HB2   | 2.48                     | 0.49              |
| 1:G:193:LEU:HD21 | 1:G:288:LYS:HZ3  | 1.77                     | 0.49              |
| 1:I:168:SER:HA   | 1:I:297:HIS:NE2  | 2.27                     | 0.49              |
| 1:I:337:ASN:HA   | 1:I:340:ILE:HD12 | 1.95                     | 0.49              |
| 1:J:303:VAL:HG12 | 1:J:439:ASN:HB3  | 1.95                     | 0.49              |
| 1:K:176:ILE:HD11 | 1:K:204:PRO:HB3  | 1.95                     | 0.49              |
| 1:K:335:SER:O    | 1:K:338:ALA:HB3  | 2.13                     | 0.49              |
| 1:L:613:GLY:O    | 1:L:616:LEU:CD1  | 2.61                     | 0.49              |
| 1:B:32:ASP:O     | 1:B:35:PHE:HB2   | 2.12                     | 0.48              |
| 1:C:639:VAL:O    | 1:C:642:GLN:HG2  | 2.13                     | 0.48              |
| 1:D:249:ARG:HG3  | 1:D:250:ASP:N    | 2.28                     | 0.48              |
| 1:E:152:ALA:HA   | 1:E:155:HIS:HB2  | 1.94                     | 0.48              |
| 1:E:281:ILE:HG12 | 1:E:287:LEU:H    | 1.78                     | 0.48              |
| 1:F:639:VAL:O    | 1:F:642:GLN:HG2  | 2.13                     | 0.48              |
| 1:H:151:SER:HB2  | 1:H:155:HIS:CE1  | 2.48                     | 0.48              |
| 1:H:511:ARG:HD3  | 1:H:513:ARG:HH22 | 1.78                     | 0.48              |
| 1:I:162:SER:HB2  | 1:I:170:ALA:HB2  | 1.95                     | 0.48              |
| 1:I:613:GLY:CA   | 1:I:616:LEU:HD12 | 2.41                     | 0.48              |
| 1:J:433:ASP:O    | 1:J:436:ASN:HB3  | 2.13                     | 0.48              |
| 1:A:75:PRO:HD2   | 1:A:523:SER:HB3  | 1.94                     | 0.48              |
| 1:A:621:GLU:OE2  | 1:B:616:LEU:HB3  | 2.14                     | 0.48              |
| 1:B:576:LEU:O    | 1:B:581:VAL:HG12 | 2.13                     | 0.48              |
| 1:E:131:ASP:OD1  | 1:E:132:TYR:N    | 2.46                     | 0.48              |
| 1:G:32:ASP:O     | 1:G:35:PHE:HB2   | 2.13                     | 0.48              |
| 1:H:433:ASP:O    | 1:H:436:ASN:HB3  | 2.12                     | 0.48              |
| 1:J:324:LYS:O    | 1:J:327:GLN:HB2  | 2.13                     | 0.48              |
| 1:K:140:ASN:HB3  | 1:K:455:THR:OG1  | 2.13                     | 0.48              |
| 1:A:37:ARG:NH1   | 1:A:48:TYR:OH    | 2.42                     | 0.48              |
| 1:A:106:THR:HG23 | 1:A:146:ARG:HE   | 1.78                     | 0.48              |
| 1:A:230:GLU:OE2  | 1:A:249:ARG:HG2  | 2.12                     | 0.48              |
| 1:A:417:THR:O    | 1:A:418:LEU:HD12 | 2.12                     | 0.48              |
| 1:A:525:GLN:HB2  | 1:A:529:GLN:OE1  | 2.13                     | 0.48              |
| 1:A:528:LYS:NZ   | 1:A:559:LEU:O    | 2.44                     | 0.48              |
| 1:A:576:LEU:O    | 1:A:581:VAL:HG12 | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:168:SER:HA   | 1:B:297:HIS:NE2  | 2.29                     | 0.48              |
| 1:C:24:GLU:OE1   | 1:C:24:GLU:N     | 2.46                     | 0.48              |
| 1:E:235:TYR:HE1  | 1:E:264:ILE:HA   | 1.78                     | 0.48              |
| 1:E:303:VAL:HB   | 1:E:439:ASN:ND2  | 2.28                     | 0.48              |
| 1:F:399:GLN:HA   | 1:F:402:ALA:HB3  | 1.95                     | 0.48              |
| 1:H:99:ARG:NH2   | 1:H:525:GLN:HA   | 2.28                     | 0.48              |
| 1:H:356:ILE:HG21 | 1:I:373:LEU:HD21 | 1.95                     | 0.48              |
| 1:I:75:PRO:HD2   | 1:I:523:SER:HB3  | 1.95                     | 0.48              |
| 1:K:349:PRO:HG3  | 1:K:391:TYR:CZ   | 2.48                     | 0.48              |
| 1:K:377:THR:HA   | 1:K:383:ASP:OD2  | 2.14                     | 0.48              |
| 1:L:444:LEU:O    | 1:L:447:TYR:HB3  | 2.13                     | 0.48              |
| 1:L:576:LEU:O    | 1:L:581:VAL:HG12 | 2.12                     | 0.48              |
| 1:B:438:LEU:O    | 1:B:442:ALA:N    | 2.38                     | 0.48              |
| 1:C:201:PHE:HD1  | 1:C:283:CYS:HB2  | 1.77                     | 0.48              |
| 1:D:162:SER:OG   | 1:D:164:LEU:O    | 2.31                     | 0.48              |
| 1:D:281:ILE:HG12 | 1:D:287:LEU:H    | 1.78                     | 0.48              |
| 1:E:45:LEU:HG    | 1:E:46:SER:H     | 1.79                     | 0.48              |
| 1:E:235:TYR:CE1  | 1:E:264:ILE:HA   | 2.48                     | 0.48              |
| 1:E:248:LYS:HE3  | 1:E:252:LYS:HB2  | 1.95                     | 0.48              |
| 1:E:377:THR:HA   | 1:E:383:ASP:OD2  | 2.13                     | 0.48              |
| 1:F:24:GLU:OE1   | 1:F:24:GLU:N     | 2.47                     | 0.48              |
| 1:F:131:ASP:OD1  | 1:F:132:TYR:N    | 2.45                     | 0.48              |
| 1:I:320:VAL:O    | 1:I:323:THR:OG1  | 2.18                     | 0.48              |
| 1:J:536:LEU:HD23 | 1:J:539:LEU:HD12 | 1.93                     | 0.48              |
| 1:J:586:THR:CG2  | 1:J:590:GLN:HE22 | 2.26                     | 0.48              |
| 1:K:581:VAL:HG22 | 1:L:567:MET:HB2  | 1.94                     | 0.48              |
| 1:K:587:PRO:HD2  | 1:K:589:GLU:HG3  | 1.95                     | 0.48              |
| 1:B:354:GLU:HG2  | 1:C:376:ARG:HD3  | 1.95                     | 0.48              |
| 1:B:528:LYS:NZ   | 1:B:559:LEU:O    | 2.43                     | 0.48              |
| 1:B:581:VAL:HG22 | 1:C:567:MET:HB2  | 1.96                     | 0.48              |
| 1:C:664:GLU:OE2  | 1:D:666:ARG:NH2  | 2.46                     | 0.48              |
| 1:D:75:PRO:HD2   | 1:D:523:SER:HB3  | 1.95                     | 0.48              |
| 1:D:140:ASN:HB3  | 1:D:455:THR:OG1  | 2.14                     | 0.48              |
| 1:D:613:GLY:HA2  | 1:D:616:LEU:HD12 | 1.96                     | 0.48              |
| 1:E:220:ALA:CB   | 1:E:281:ILE:O    | 2.46                     | 0.48              |
| 1:E:438:LEU:O    | 1:E:442:ALA:N    | 2.40                     | 0.48              |
| 1:F:162:SER:HA   | 1:F:169:ASP:OD1  | 2.13                     | 0.48              |
| 1:F:444:LEU:O    | 1:F:447:TYR:HB3  | 2.13                     | 0.48              |
| 1:G:78:VAL:HG22  | 1:G:520:VAL:HG12 | 1.96                     | 0.48              |
| 1:G:80:TYR:CD1   | 1:G:444:LEU:HD21 | 2.49                     | 0.48              |
| 1:I:586:THR:CG2  | 1:I:590:GLN:HE22 | 2.25                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:82:PRO:HB3   | 1:J:90:ALA:HB3   | 1.96                     | 0.48              |
| 1:L:106:THR:HG23 | 1:L:146:ARG:HE   | 1.79                     | 0.48              |
| 1:L:586:THR:CG2  | 1:L:590:GLN:HE22 | 2.26                     | 0.48              |
| 1:L:593:LEU:O    | 1:L:597:GLN:HG3  | 2.12                     | 0.48              |
| 1:A:45:LEU:HG    | 1:A:46:SER:H     | 1.77                     | 0.48              |
| 1:A:306:GLU:OE2  | 1:B:61:ARG:NE    | 2.46                     | 0.48              |
| 1:A:350:PHE:CD1  | 1:B:372:TYR:HB3  | 2.48                     | 0.48              |
| 1:E:591:GLN:HA   | 1:E:595:GLU:CD   | 2.38                     | 0.48              |
| 1:F:272:LYS:O    | 1:G:134:ASP:HB2  | 2.13                     | 0.48              |
| 1:F:641:ALA:HA   | 1:F:644:GLN:OE1  | 2.14                     | 0.48              |
| 1:G:433:ASP:O    | 1:G:436:ASN:HB3  | 2.14                     | 0.48              |
| 1:I:353:PRO:HA   | 1:J:373:LEU:HD23 | 1.94                     | 0.48              |
| 1:L:591:GLN:HA   | 1:L:595:GLU:CD   | 2.38                     | 0.48              |
| 1:A:403:TYR:OH   | 1:B:397:VAL:HG11 | 2.14                     | 0.48              |
| 1:B:641:ALA:HA   | 1:B:644:GLN:OE1  | 2.14                     | 0.48              |
| 1:D:124:GLY:CA   | 1:D:303:VAL:HG22 | 2.43                     | 0.48              |
| 1:F:515:GLU:N    | 1:F:515:GLU:OE1  | 2.46                     | 0.48              |
| 1:G:230:GLU:OE2  | 1:G:249:ARG:HG2  | 2.14                     | 0.48              |
| 1:G:663:SER:O    | 1:G:666:ARG:HG3  | 2.14                     | 0.48              |
| 1:J:161:ASN:ND2  | 1:K:183:GLY:HA3  | 2.25                     | 0.48              |
| 1:K:528:LYS:HZ3  | 1:K:560:LEU:HD23 | 1.76                     | 0.48              |
| 1:A:641:ALA:HA   | 1:A:644:GLN:OE1  | 2.13                     | 0.48              |
| 1:C:223:TYR:CE1  | 1:C:278:LYS:HG3  | 2.49                     | 0.48              |
| 1:C:349:PRO:HG3  | 1:C:391:TYR:CZ   | 2.49                     | 0.48              |
| 1:E:80:TYR:CD1   | 1:E:444:LEU:HD21 | 2.49                     | 0.48              |
| 1:E:201:PHE:HD1  | 1:E:283:CYS:HB2  | 1.78                     | 0.48              |
| 1:E:417:THR:O    | 1:E:418:LEU:HD12 | 2.14                     | 0.48              |
| 1:F:32:ASP:O     | 1:F:35:PHE:HB2   | 2.14                     | 0.48              |
| 1:G:37:ARG:NH1   | 1:G:48:TYR:OH    | 2.38                     | 0.48              |
| 1:H:162:SER:OG   | 1:H:164:LEU:O    | 2.31                     | 0.48              |
| 1:I:24:GLU:OE1   | 1:I:24:GLU:N     | 2.47                     | 0.48              |
| 1:I:528:LYS:NZ   | 1:I:559:LEU:O    | 2.44                     | 0.48              |
| 1:K:21:ALA:HA    | 1:K:159:ASP:OD2  | 2.14                     | 0.48              |
| 1:L:99:ARG:NE    | 1:L:525:GLN:O    | 2.46                     | 0.48              |
| 1:L:528:LYS:HZ3  | 1:L:560:LEU:HD23 | 1.78                     | 0.48              |
| 1:A:220:ALA:CB   | 1:A:281:ILE:O    | 2.48                     | 0.48              |
| 1:C:21:ALA:HA    | 1:C:159:ASP:OD2  | 2.14                     | 0.48              |
| 1:C:363:TYR:HE1  | 1:C:372:TYR:HA   | 1.79                     | 0.48              |
| 1:D:223:TYR:CE1  | 1:D:278:LYS:HG3  | 2.48                     | 0.48              |
| 1:F:628:GLN:O    | 1:F:632:LEU:HB2  | 2.14                     | 0.48              |
| 1:G:664:GLU:HG3  | 1:H:659:LEU:HD22 | 1.94                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:228:LYS:HB2  | 1:J:275:ARG:HB3  | 1.95                     | 0.48              |
| 1:K:235:TYR:HE1  | 1:K:264:ILE:HA   | 1.78                     | 0.48              |
| 1:K:576:LEU:O    | 1:K:581:VAL:HG12 | 2.14                     | 0.48              |
| 1:L:587:PRO:HD2  | 1:L:589:GLU:HG3  | 1.95                     | 0.48              |
| 1:A:151:SER:HB2  | 1:A:155:HIS:CE1  | 2.48                     | 0.48              |
| 1:A:162:SER:HB2  | 1:A:170:ALA:HB2  | 1.96                     | 0.48              |
| 1:B:80:TYR:CZ    | 1:B:516:CYS:HB2  | 2.49                     | 0.48              |
| 1:B:444:LEU:O    | 1:B:448:VAL:HG23 | 2.14                     | 0.48              |
| 1:B:587:PRO:HD2  | 1:B:589:GLU:HG3  | 1.95                     | 0.48              |
| 1:C:363:TYR:OH   | 1:C:373:LEU:O    | 2.15                     | 0.48              |
| 1:C:433:ASP:O    | 1:C:436:ASN:HB3  | 2.13                     | 0.48              |
| 1:C:515:GLU:OE1  | 1:C:515:GLU:N    | 2.47                     | 0.48              |
| 1:E:35:PHE:CZ    | 1:E:321:ARG:HB2  | 2.49                     | 0.48              |
| 1:E:577:ILE:HG21 | 1:E:593:LEU:HD13 | 1.95                     | 0.48              |
| 1:E:641:ALA:HA   | 1:E:644:GLN:OE1  | 2.14                     | 0.48              |
| 1:F:82:PRO:HB3   | 1:F:90:ALA:HB3   | 1.96                     | 0.48              |
| 1:F:303:VAL:HB   | 1:F:439:ASN:ND2  | 2.29                     | 0.48              |
| 1:H:193:LEU:HD21 | 1:H:288:LYS:NZ   | 2.29                     | 0.48              |
| 1:I:325:ASP:O    | 1:I:328:ARG:HG2  | 2.14                     | 0.48              |
| 1:I:576:LEU:O    | 1:I:581:VAL:HG12 | 2.14                     | 0.48              |
| 1:J:124:GLY:HA3  | 1:J:303:VAL:HG22 | 1.96                     | 0.48              |
| 1:J:444:LEU:O    | 1:J:448:VAL:HG23 | 2.13                     | 0.48              |
| 1:K:303:VAL:HB   | 1:K:439:ASN:ND2  | 2.28                     | 0.48              |
| 1:A:131:ASP:OD1  | 1:A:132:TYR:N    | 2.46                     | 0.47              |
| 1:A:278:LYS:HE2  | 1:A:280:ILE:HD11 | 1.96                     | 0.47              |
| 1:A:577:ILE:HG21 | 1:A:593:LEU:HD13 | 1.94                     | 0.47              |
| 1:B:321:ARG:HA   | 1:B:324:LYS:HE2  | 1.95                     | 0.47              |
| 1:E:165:MET:HB3  | 1:E:304:PHE:CG   | 2.48                     | 0.47              |
| 1:G:82:PRO:HB3   | 1:G:90:ALA:HB3   | 1.94                     | 0.47              |
| 1:H:87:ARG:HD3   | 1:H:89:ASP:HB2   | 1.96                     | 0.47              |
| 1:H:441:ARG:NH2  | 1:H:519:ASP:OD1  | 2.47                     | 0.47              |
| 1:I:162:SER:OG   | 1:I:164:LEU:O    | 2.32                     | 0.47              |
| 1:I:350:PHE:HB2  | 1:I:390:ALA:HB3  | 1.95                     | 0.47              |
| 1:L:105:ASN:O    | 1:L:109:ILE:HG12 | 2.14                     | 0.47              |
| 1:L:152:ALA:HA   | 1:L:155:HIS:HB2  | 1.95                     | 0.47              |
| 1:L:662:GLN:HA   | 1:L:665:PHE:CD2  | 2.49                     | 0.47              |
| 1:A:382:GLY:N    | 1:A:383:ASP:HA   | 2.27                     | 0.47              |
| 1:C:27:ARG:HD3   | 1:C:313:LYS:HE3  | 1.97                     | 0.47              |
| 1:C:514:TYR:HB2  | 1:D:136:SER:OG   | 2.14                     | 0.47              |
| 1:C:532:ARG:HH22 | 1:C:560:LEU:HD11 | 1.78                     | 0.47              |
| 1:D:639:VAL:O    | 1:D:642:GLN:HG2  | 2.13                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:590:GLN:HA   | 1:E:594:VAL:HB   | 1.96                     | 0.47              |
| 1:F:587:PRO:HD2  | 1:F:589:GLU:HG3  | 1.96                     | 0.47              |
| 1:G:417:THR:O    | 1:G:418:LEU:HD12 | 2.14                     | 0.47              |
| 1:G:444:LEU:O    | 1:G:448:VAL:HG23 | 2.14                     | 0.47              |
| 1:G:444:LEU:O    | 1:G:447:TYR:HB3  | 2.15                     | 0.47              |
| 1:I:27:ARG:HD3   | 1:I:313:LYS:HE3  | 1.96                     | 0.47              |
| 1:K:15:PHE:HA    | 1:K:18:ASP:HB3   | 1.95                     | 0.47              |
| 1:A:136:SER:OG   | 1:L:514:TYR:HB2  | 2.14                     | 0.47              |
| 1:B:27:ARG:HA    | 1:B:30:LYS:HE2   | 1.97                     | 0.47              |
| 1:B:105:ASN:O    | 1:B:109:ILE:HG12 | 2.15                     | 0.47              |
| 1:B:228:LYS:HB2  | 1:B:275:ARG:HB3  | 1.96                     | 0.47              |
| 1:B:664:GLU:HG3  | 1:C:659:LEU:HD22 | 1.95                     | 0.47              |
| 1:E:140:ASN:HB3  | 1:E:455:THR:OG1  | 2.14                     | 0.47              |
| 1:F:249:ARG:HG3  | 1:F:250:ASP:N    | 2.29                     | 0.47              |
| 1:F:649:ARG:O    | 1:F:653:ILE:HG13 | 2.14                     | 0.47              |
| 1:G:303:VAL:HG12 | 1:G:439:ASN:HB3  | 1.96                     | 0.47              |
| 1:G:614:VAL:HG21 | 1:H:609:VAL:CG1  | 2.44                     | 0.47              |
| 1:I:664:GLU:OE2  | 1:J:666:ARG:NH2  | 2.47                     | 0.47              |
| 1:K:639:VAL:O    | 1:K:642:GLN:HG2  | 2.15                     | 0.47              |
| 1:L:164:LEU:HD11 | 1:L:168:SER:H    | 1.79                     | 0.47              |
| 1:L:203:ASN:OD1  | 1:L:205:ASN:N    | 2.34                     | 0.47              |
| 1:L:338:ALA:O    | 1:L:342:ALA:N    | 2.45                     | 0.47              |
| 1:A:324:LYS:O    | 1:A:327:GLN:HB2  | 2.14                     | 0.47              |
| 1:B:29:ALA:O     | 1:B:33:LEU:HB2   | 2.13                     | 0.47              |
| 1:B:80:TYR:CD1   | 1:B:444:LEU:HD21 | 2.49                     | 0.47              |
| 1:B:230:GLU:OE2  | 1:B:249:ARG:HG2  | 2.14                     | 0.47              |
| 1:C:193:LEU:HD21 | 1:C:288:LYS:HZ3  | 1.79                     | 0.47              |
| 1:D:105:ASN:O    | 1:D:109:ILE:HG12 | 2.14                     | 0.47              |
| 1:E:380:ASN:OD1  | 1:E:381:SER:N    | 2.47                     | 0.47              |
| 1:F:538:LEU:HB3  | 1:F:551:LEU:HD11 | 1.95                     | 0.47              |
| 1:G:47:GLN:HB2   | 1:G:50:THR:CG2   | 2.43                     | 0.47              |
| 1:G:363:TYR:OH   | 1:G:373:LEU:O    | 2.18                     | 0.47              |
| 1:H:53:TYR:CG    | 1:H:54:ARG:N     | 2.83                     | 0.47              |
| 1:H:303:VAL:HB   | 1:H:439:ASN:ND2  | 2.28                     | 0.47              |
| 1:I:223:TYR:CE1  | 1:I:278:LYS:HG3  | 2.50                     | 0.47              |
| 1:I:696:GLN:HE22 | 1:J:698:HIS:CE1  | 2.32                     | 0.47              |
| 1:J:380:ASN:OD1  | 1:J:381:SER:N    | 2.47                     | 0.47              |
| 1:K:80:TYR:CZ    | 1:K:516:CYS:HB2  | 2.50                     | 0.47              |
| 1:C:165:MET:HB3  | 1:C:304:PHE:CG   | 2.49                     | 0.47              |
| 1:E:663:SER:O    | 1:E:666:ARG:HG3  | 2.14                     | 0.47              |
| 1:F:80:TYR:CZ    | 1:F:516:CYS:HB2  | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:306:GLU:OE2  | 1:G:61:ARG:NE    | 2.48                     | 0.47              |
| 1:F:576:LEU:O    | 1:F:581:VAL:HG12 | 2.14                     | 0.47              |
| 1:G:124:GLY:HA3  | 1:G:303:VAL:HG22 | 1.96                     | 0.47              |
| 1:G:418:LEU:HD23 | 1:G:429:GLN:HB3  | 1.95                     | 0.47              |
| 1:G:587:PRO:HD2  | 1:G:589:GLU:HG3  | 1.97                     | 0.47              |
| 1:H:124:GLY:HA3  | 1:H:303:VAL:HG22 | 1.95                     | 0.47              |
| 1:H:176:ILE:HD11 | 1:H:204:PRO:HB3  | 1.96                     | 0.47              |
| 1:H:353:PRO:HD3  | 1:I:374:LEU:O    | 2.14                     | 0.47              |
| 1:J:641:ALA:HA   | 1:J:644:GLN:OE1  | 2.15                     | 0.47              |
| 1:J:657:MET:SD   | 1:K:655:ASN:ND2  | 2.88                     | 0.47              |
| 1:J:701:ARG:HA   | 1:J:704:ILE:HD12 | 1.97                     | 0.47              |
| 1:K:303:VAL:HG12 | 1:K:439:ASN:HB3  | 1.95                     | 0.47              |
| 1:L:223:TYR:HE1  | 1:L:278:LYS:HG3  | 1.79                     | 0.47              |
| 1:A:124:GLY:CA   | 1:A:303:VAL:HG22 | 2.45                     | 0.47              |
| 1:A:176:ILE:HD11 | 1:A:204:PRO:HB3  | 1.95                     | 0.47              |
| 1:B:161:ASN:HD21 | 1:C:183:GLY:HA3  | 1.79                     | 0.47              |
| 1:B:646:ASN:HA   | 1:C:644:GLN:HG2  | 1.97                     | 0.47              |
| 1:D:377:THR:HA   | 1:D:383:ASP:OD2  | 2.14                     | 0.47              |
| 1:F:417:THR:O    | 1:F:418:LEU:HD12 | 2.14                     | 0.47              |
| 1:F:661:LYS:HE3  | 1:F:665:PHE:CZ   | 2.50                     | 0.47              |
| 1:J:201:PHE:HD1  | 1:J:283:CYS:HB2  | 1.79                     | 0.47              |
| 1:J:350:PHE:N    | 1:J:390:ALA:O    | 2.36                     | 0.47              |
| 1:K:444:LEU:O    | 1:K:447:TYR:HB3  | 2.15                     | 0.47              |
| 1:L:235:TYR:CE1  | 1:L:264:ILE:HA   | 2.50                     | 0.47              |
| 1:A:53:TYR:CG    | 1:A:54:ARG:N     | 2.83                     | 0.47              |
| 1:A:193:LEU:HD21 | 1:A:288:LYS:HZ3  | 1.78                     | 0.47              |
| 1:A:528:LYS:HZ3  | 1:A:560:LEU:HD23 | 1.80                     | 0.47              |
| 1:A:586:THR:CG2  | 1:A:590:GLN:HE22 | 2.26                     | 0.47              |
| 1:A:661:LYS:HE3  | 1:A:665:PHE:CZ   | 2.49                     | 0.47              |
| 1:B:45:LEU:HG    | 1:B:46:SER:H     | 1.80                     | 0.47              |
| 1:B:248:LYS:HG2  | 1:B:511:ARG:HH21 | 1.80                     | 0.47              |
| 1:B:350:PHE:HB2  | 1:B:390:ALA:HB3  | 1.97                     | 0.47              |
| 1:B:417:THR:O    | 1:B:418:LEU:HD12 | 2.14                     | 0.47              |
| 1:B:649:ARG:O    | 1:B:653:ILE:HG13 | 2.14                     | 0.47              |
| 1:B:663:SER:O    | 1:B:666:ARG:HG3  | 2.15                     | 0.47              |
| 1:D:252:LYS:HD2  | 1:D:256:ASP:HB3  | 1.96                     | 0.47              |
| 1:D:303:VAL:HG12 | 1:D:439:ASN:HB3  | 1.96                     | 0.47              |
| 1:G:171:ARG:NH1  | 1:H:186:ASP:OD2  | 2.48                     | 0.47              |
| 1:H:576:LEU:O    | 1:H:581:VAL:HG12 | 2.15                     | 0.47              |
| 1:H:646:ASN:OD1  | 1:H:647:ALA:N    | 2.48                     | 0.47              |
| 1:I:201:PHE:HD1  | 1:I:283:CYS:HB2  | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:228:LYS:HB2  | 1:I:275:ARG:HB3  | 1.96                     | 0.47              |
| 1:I:426:ASN:O    | 1:I:429:GLN:NE2  | 2.48                     | 0.47              |
| 1:J:114:ALA:O    | 1:J:118:GLN:HB2  | 2.14                     | 0.47              |
| 1:J:621:GLU:OE2  | 1:K:616:LEU:HB3  | 2.15                     | 0.47              |
| 1:K:80:TYR:CD1   | 1:K:444:LEU:HD21 | 2.49                     | 0.47              |
| 1:K:80:TYR:HD1   | 1:K:518:THR:HA   | 1.78                     | 0.47              |
| 1:K:131:ASP:OD1  | 1:K:132:TYR:N    | 2.48                     | 0.47              |
| 1:K:646:ASN:HA   | 1:L:644:GLN:HG2  | 1.97                     | 0.47              |
| 1:L:21:ALA:HA    | 1:L:159:ASP:OD2  | 2.14                     | 0.47              |
| 1:L:201:PHE:HD1  | 1:L:283:CYS:HB2  | 1.80                     | 0.47              |
| 1:L:320:VAL:O    | 1:L:323:THR:OG1  | 2.18                     | 0.47              |
| 1:A:444:LEU:HD23 | 1:A:518:THR:HB   | 1.97                     | 0.47              |
| 1:B:657:MET:SD   | 1:C:655:ASN:ND2  | 2.88                     | 0.47              |
| 1:C:249:ARG:HG3  | 1:C:250:ASP:N    | 2.30                     | 0.47              |
| 1:C:641:ALA:HA   | 1:C:644:GLN:OE1  | 2.14                     | 0.47              |
| 1:D:613:GLY:O    | 1:D:616:LEU:CD1  | 2.63                     | 0.47              |
| 1:E:528:LYS:HZ3  | 1:E:560:LEU:HD23 | 1.79                     | 0.47              |
| 1:E:536:LEU:HD23 | 1:E:539:LEU:HD12 | 1.95                     | 0.47              |
| 1:E:538:LEU:HB3  | 1:E:551:LEU:HD11 | 1.97                     | 0.47              |
| 1:E:576:LEU:O    | 1:E:581:VAL:HG12 | 2.15                     | 0.47              |
| 1:F:151:SER:HB2  | 1:F:155:HIS:CE1  | 2.50                     | 0.47              |
| 1:F:162:SER:OG   | 1:F:164:LEU:O    | 2.33                     | 0.47              |
| 1:I:444:LEU:O    | 1:I:447:TYR:HB3  | 2.15                     | 0.47              |
| 1:I:641:ALA:HA   | 1:I:644:GLN:OE1  | 2.15                     | 0.47              |
| 1:K:663:SER:O    | 1:K:666:ARG:HG3  | 2.14                     | 0.47              |
| 1:A:134:ASP:HB2  | 1:L:272:LYS:O    | 2.14                     | 0.47              |
| 1:A:444:LEU:O    | 1:A:448:VAL:HG23 | 2.14                     | 0.47              |
| 1:C:117:GLU:HB3  | 1:C:123:VAL:HG23 | 1.97                     | 0.47              |
| 1:C:325:ASP:O    | 1:C:328:ARG:HG2  | 2.15                     | 0.47              |
| 1:D:80:TYR:CD1   | 1:D:444:LEU:HD21 | 2.49                     | 0.47              |
| 1:E:124:GLY:HA3  | 1:E:303:VAL:HG22 | 1.96                     | 0.47              |
| 1:E:695:GLU:HA   | 1:E:698:HIS:ND1  | 2.30                     | 0.47              |
| 1:F:238:PRO:HB3  | 1:F:263:PHE:CD1  | 2.50                     | 0.47              |
| 1:H:80:TYR:CD1   | 1:H:444:LEU:HD21 | 2.50                     | 0.47              |
| 1:H:238:PRO:HB3  | 1:H:263:PHE:CD1  | 2.49                     | 0.47              |
| 1:I:377:THR:HA   | 1:I:383:ASP:OD2  | 2.14                     | 0.47              |
| 1:J:363:TYR:CE1  | 1:J:372:TYR:HA   | 2.49                     | 0.47              |
| 1:L:387:GLN:HG3  | 1:L:387:GLN:O    | 2.15                     | 0.47              |
| 1:C:78:VAL:HG22  | 1:C:520:VAL:HG12 | 1.97                     | 0.47              |
| 1:C:333:ILE:HG22 | 1:C:337:ASN:OD1  | 2.15                     | 0.47              |
| 1:D:82:PRO:HB3   | 1:D:90:ALA:HB3   | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:590:GLN:HA   | 1:F:594:VAL:HB   | 1.96                     | 0.47              |
| 1:G:27:ARG:HH11  | 1:G:313:LYS:HE3  | 1.80                     | 0.47              |
| 1:G:380:ASN:OD1  | 1:G:381:SER:N    | 2.48                     | 0.47              |
| 1:G:434:THR:HG21 | 1:H:72:ARG:HG3   | 1.96                     | 0.47              |
| 1:H:27:ARG:HD3   | 1:H:313:LYS:HE3  | 1.96                     | 0.47              |
| 1:H:105:ASN:O    | 1:H:109:ILE:HG12 | 2.15                     | 0.47              |
| 1:H:223:TYR:HE1  | 1:H:278:LYS:HG3  | 1.80                     | 0.47              |
| 1:H:587:PRO:HD2  | 1:H:589:GLU:HG3  | 1.97                     | 0.47              |
| 1:I:403:TYR:OH   | 1:J:397:VAL:HG11 | 2.15                     | 0.47              |
| 1:A:444:LEU:O    | 1:A:447:TYR:HB3  | 2.15                     | 0.46              |
| 1:B:356:ILE:HG21 | 1:C:373:LEU:HD21 | 1.97                     | 0.46              |
| 1:C:21:ALA:HB2   | 1:C:172:HIS:CD2  | 2.50                     | 0.46              |
| 1:C:663:SER:HA   | 1:C:666:ARG:NE   | 2.25                     | 0.46              |
| 1:D:162:SER:HA   | 1:D:169:ASP:OD1  | 2.15                     | 0.46              |
| 1:E:15:PHE:HA    | 1:E:18:ASP:HB3   | 1.97                     | 0.46              |
| 1:E:164:LEU:HD11 | 1:E:168:SER:H    | 1.79                     | 0.46              |
| 1:F:105:ASN:O    | 1:F:109:ILE:HG12 | 2.15                     | 0.46              |
| 1:F:303:VAL:HG12 | 1:F:439:ASN:HB3  | 1.98                     | 0.46              |
| 1:F:353:PRO:HD3  | 1:G:374:LEU:O    | 2.14                     | 0.46              |
| 1:G:281:ILE:HG12 | 1:G:287:LEU:H    | 1.80                     | 0.46              |
| 1:H:117:GLU:HB3  | 1:H:123:VAL:HG23 | 1.96                     | 0.46              |
| 1:I:235:TYR:CE1  | 1:I:264:ILE:HA   | 2.49                     | 0.46              |
| 1:J:53:TYR:O     | 1:J:54:ARG:NH1   | 2.46                     | 0.46              |
| 1:J:306:GLU:HG3  | 1:K:116:ARG:NH2  | 2.30                     | 0.46              |
| 1:K:250:ASP:OD1  | 1:K:251:ILE:HG13 | 2.16                     | 0.46              |
| 1:K:350:PHE:N    | 1:K:390:ALA:O    | 2.37                     | 0.46              |
| 1:L:377:THR:HA   | 1:L:383:ASP:OD2  | 2.15                     | 0.46              |
| 1:L:527:MET:HA   | 1:L:530:GLN:CD   | 2.41                     | 0.46              |
| 1:A:328:ARG:HD2  | 1:B:53:TYR:OH    | 2.16                     | 0.46              |
| 1:A:642:GLN:HA   | 1:A:645:LEU:HD12 | 1.98                     | 0.46              |
| 1:B:387:GLN:HG3  | 1:B:387:GLN:O    | 2.15                     | 0.46              |
| 1:B:646:ASN:OD1  | 1:B:647:ALA:N    | 2.49                     | 0.46              |
| 1:D:646:ASN:OD1  | 1:D:647:ALA:N    | 2.49                     | 0.46              |
| 1:E:444:LEU:O    | 1:E:448:VAL:HG23 | 2.15                     | 0.46              |
| 1:F:387:GLN:HG3  | 1:F:387:GLN:O    | 2.15                     | 0.46              |
| 1:F:664:GLU:OE2  | 1:G:666:ARG:NH2  | 2.48                     | 0.46              |
| 1:G:21:ALA:HA    | 1:G:159:ASP:OD2  | 2.16                     | 0.46              |
| 1:G:350:PHE:N    | 1:G:390:ALA:O    | 2.35                     | 0.46              |
| 1:H:161:ASN:ND2  | 1:I:183:GLY:HA3  | 2.28                     | 0.46              |
| 1:I:303:VAL:HG12 | 1:I:439:ASN:HB3  | 1.97                     | 0.46              |
| 1:J:438:LEU:O    | 1:J:442:ALA:N    | 2.41                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:641:ALA:HA   | 1:K:644:GLN:OE1  | 2.15                     | 0.46              |
| 1:L:126:TRP:CD1  | 1:L:146:ARG:HG3  | 2.51                     | 0.46              |
| 1:B:458:ARG:HH21 | 1:B:500:ALA:HB1  | 1.81                     | 0.46              |
| 1:B:564:GLY:O    | 1:B:568:MET:HG2  | 2.15                     | 0.46              |
| 1:C:80:TYR:CZ    | 1:C:516:CYS:HB2  | 2.51                     | 0.46              |
| 1:C:398:PRO:HB3  | 1:D:394:ASN:HB3  | 1.96                     | 0.46              |
| 1:D:151:SER:HB2  | 1:D:155:HIS:CE1  | 2.50                     | 0.46              |
| 1:F:99:ARG:NH2   | 1:F:525:GLN:HA   | 2.31                     | 0.46              |
| 1:G:527:MET:HA   | 1:G:530:GLN:CD   | 2.40                     | 0.46              |
| 1:H:249:ARG:HG3  | 1:H:250:ASP:N    | 2.30                     | 0.46              |
| 1:H:420:VAL:HB   | 1:H:424:ALA:HA   | 1.97                     | 0.46              |
| 1:J:35:PHE:CZ    | 1:J:321:ARG:HB2  | 2.51                     | 0.46              |
| 1:J:41:TRP:CH2   | 1:J:44:TRP:HB2   | 2.49                     | 0.46              |
| 1:J:306:GLU:HG3  | 1:K:116:ARG:HH22 | 1.80                     | 0.46              |
| 1:K:321:ARG:HA   | 1:K:324:LYS:HE2  | 1.96                     | 0.46              |
| 1:K:354:GLU:HG2  | 1:L:376:ARG:HD3  | 1.96                     | 0.46              |
| 1:A:303:VAL:HB   | 1:A:439:ASN:ND2  | 2.30                     | 0.46              |
| 1:A:646:ASN:OD1  | 1:A:647:ALA:N    | 2.49                     | 0.46              |
| 1:B:151:SER:HB2  | 1:B:155:HIS:CE1  | 2.50                     | 0.46              |
| 1:B:350:PHE:N    | 1:B:390:ALA:O    | 2.33                     | 0.46              |
| 1:C:203:ASN:OD1  | 1:C:205:ASN:N    | 2.36                     | 0.46              |
| 1:D:444:LEU:O    | 1:D:448:VAL:HG23 | 2.15                     | 0.46              |
| 1:E:246:TYR:HB2  | 1:E:511:ARG:H    | 1.81                     | 0.46              |
| 1:E:272:LYS:O    | 1:F:134:ASP:HB2  | 2.15                     | 0.46              |
| 1:F:307:TRP:HE1  | 1:F:314:GLU:HG2  | 1.80                     | 0.46              |
| 1:G:436:ASN:HA   | 1:G:439:ASN:ND2  | 2.30                     | 0.46              |
| 1:G:515:GLU:OE1  | 1:G:515:GLU:N    | 2.48                     | 0.46              |
| 1:G:590:GLN:HA   | 1:G:594:VAL:HB   | 1.97                     | 0.46              |
| 1:G:646:ASN:OD1  | 1:G:647:ALA:N    | 2.49                     | 0.46              |
| 1:H:641:ALA:HA   | 1:H:644:GLN:OE1  | 2.16                     | 0.46              |
| 1:J:338:ALA:O    | 1:J:342:ALA:N    | 2.48                     | 0.46              |
| 1:J:349:PRO:HG3  | 1:J:391:TYR:CZ   | 2.50                     | 0.46              |
| 1:J:387:GLN:O    | 1:J:387:GLN:HG3  | 2.15                     | 0.46              |
| 1:J:590:GLN:HA   | 1:J:594:VAL:HB   | 1.97                     | 0.46              |
| 1:J:613:GLY:CA   | 1:J:616:LEU:HD12 | 2.43                     | 0.46              |
| 1:K:21:ALA:HB2   | 1:K:172:HIS:NE2  | 2.30                     | 0.46              |
| 1:K:701:ARG:HA   | 1:K:704:ILE:HD12 | 1.96                     | 0.46              |
| 1:A:249:ARG:HG3  | 1:A:250:ASP:N    | 2.30                     | 0.46              |
| 1:B:248:LYS:CD   | 1:B:251:ILE:HB   | 2.41                     | 0.46              |
| 1:B:699:LYS:O    | 1:B:702:MET:HB3  | 2.16                     | 0.46              |
| 1:C:576:LEU:O    | 1:C:581:VAL:HG12 | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:380:ASN:OD1  | 1:D:381:SER:N    | 2.48                     | 0.46              |
| 1:F:21:ALA:HA    | 1:F:159:ASP:OD2  | 2.16                     | 0.46              |
| 1:F:564:GLY:O    | 1:F:568:MET:HG2  | 2.15                     | 0.46              |
| 1:G:576:LEU:O    | 1:G:581:VAL:HG12 | 2.15                     | 0.46              |
| 1:I:53:TYR:CG    | 1:I:54:ARG:N     | 2.84                     | 0.46              |
| 1:I:82:PRO:HB3   | 1:I:90:ALA:HB3   | 1.96                     | 0.46              |
| 1:I:99:ARG:NE    | 1:I:525:GLN:O    | 2.48                     | 0.46              |
| 1:J:235:TYR:CE1  | 1:J:264:ILE:HA   | 2.51                     | 0.46              |
| 1:J:640:GLU:HA   | 1:J:643:ASN:HD22 | 1.81                     | 0.46              |
| 1:K:320:VAL:O    | 1:K:323:THR:OG1  | 2.19                     | 0.46              |
| 1:K:444:LEU:O    | 1:K:448:VAL:HG23 | 2.15                     | 0.46              |
| 1:K:609:VAL:O    | 1:K:612:GLN:HB2  | 2.16                     | 0.46              |
| 1:L:230:GLU:OE2  | 1:L:249:ARG:HG2  | 2.15                     | 0.46              |
| 1:B:444:LEU:O    | 1:B:447:TYR:HB3  | 2.16                     | 0.46              |
| 1:C:250:ASP:OD1  | 1:C:251:ILE:HG13 | 2.16                     | 0.46              |
| 1:C:387:GLN:HG3  | 1:C:387:GLN:O    | 2.14                     | 0.46              |
| 1:E:223:TYR:CE1  | 1:E:278:LYS:HG3  | 2.51                     | 0.46              |
| 1:E:235:TYR:HA   | 1:E:265:LYS:O    | 2.16                     | 0.46              |
| 1:E:387:GLN:HG3  | 1:E:387:GLN:O    | 2.16                     | 0.46              |
| 1:E:574:LYS:O    | 1:E:578:GLN:HG3  | 2.16                     | 0.46              |
| 1:G:348:LYS:HB2  | 1:H:372:TYR:CD2  | 2.51                     | 0.46              |
| 1:G:438:LEU:O    | 1:G:442:ALA:N    | 2.40                     | 0.46              |
| 1:H:45:LEU:HG    | 1:H:46:SER:H     | 1.81                     | 0.46              |
| 1:H:649:ARG:O    | 1:H:653:ILE:HG13 | 2.16                     | 0.46              |
| 1:I:591:GLN:HA   | 1:I:595:GLU:CD   | 2.40                     | 0.46              |
| 1:J:532:ARG:HH22 | 1:J:560:LEU:HD11 | 1.80                     | 0.46              |
| 1:K:564:GLY:O    | 1:K:568:MET:HG2  | 2.15                     | 0.46              |
| 1:L:235:TYR:HE1  | 1:L:264:ILE:HA   | 1.80                     | 0.46              |
| 1:A:72:ARG:HG3   | 1:L:434:THR:HG21 | 1.98                     | 0.46              |
| 1:A:133:GLU:O    | 1:A:137:PRO:HB3  | 2.16                     | 0.46              |
| 1:B:377:THR:HA   | 1:B:383:ASP:OD2  | 2.16                     | 0.46              |
| 1:D:444:LEU:O    | 1:D:447:TYR:HB3  | 2.16                     | 0.46              |
| 1:E:110:ALA:HB1  | 1:E:126:TRP:CE3  | 2.51                     | 0.46              |
| 1:F:201:PHE:HD1  | 1:F:283:CYS:HB2  | 1.81                     | 0.46              |
| 1:F:646:ASN:OD1  | 1:F:647:ALA:N    | 2.49                     | 0.46              |
| 1:J:120:GLU:HA   | 1:J:320:VAL:HB   | 1.98                     | 0.46              |
| 1:J:352:TRP:CB   | 1:K:376:ARG:HD2  | 2.39                     | 0.46              |
| 1:K:24:GLU:HB2   | 1:K:159:ASP:OD2  | 2.16                     | 0.46              |
| 1:L:151:SER:HB2  | 1:L:155:HIS:CE1  | 2.51                     | 0.46              |
| 1:L:623:ALA:HA   | 1:L:626:GLN:CD   | 2.40                     | 0.46              |
| 1:A:21:ALA:HA    | 1:A:159:ASP:OD2  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:238:PRO:HB3  | 1:A:263:PHE:CD1  | 2.51                     | 0.46              |
| 1:A:272:LYS:O    | 1:B:134:ASP:HB2  | 2.16                     | 0.46              |
| 1:A:372:TYR:CD2  | 1:L:348:LYS:HB2  | 2.50                     | 0.46              |
| 1:A:376:ARG:HD3  | 1:L:354:GLU:HG2  | 1.98                     | 0.46              |
| 1:B:124:GLY:CA   | 1:B:303:VAL:HG22 | 2.45                     | 0.46              |
| 1:B:225:VAL:HA   | 1:B:276:VAL:HG12 | 1.97                     | 0.46              |
| 1:C:228:LYS:HB2  | 1:C:275:ARG:HB3  | 1.97                     | 0.46              |
| 1:C:444:LEU:O    | 1:C:448:VAL:HG23 | 2.15                     | 0.46              |
| 1:D:649:ARG:O    | 1:D:653:ILE:HG13 | 2.16                     | 0.46              |
| 1:E:124:GLY:CA   | 1:E:303:VAL:HG22 | 2.46                     | 0.46              |
| 1:E:354:GLU:HG2  | 1:F:376:ARG:HD3  | 1.97                     | 0.46              |
| 1:E:646:ASN:OD1  | 1:E:647:ALA:N    | 2.48                     | 0.46              |
| 1:F:586:THR:CG2  | 1:F:590:GLN:HE22 | 2.27                     | 0.46              |
| 1:G:42:ASP:HB3   | 1:G:44:TRP:HD1   | 1.81                     | 0.46              |
| 1:G:114:ALA:O    | 1:G:118:GLN:HB2  | 2.16                     | 0.46              |
| 1:G:411:ALA:HA   | 1:H:57:PHE:HE1   | 1.81                     | 0.46              |
| 1:H:21:ALA:HA    | 1:H:159:ASP:OD2  | 2.16                     | 0.46              |
| 1:H:80:TYR:HD1   | 1:H:518:THR:HA   | 1.81                     | 0.46              |
| 1:H:193:LEU:HD21 | 1:H:288:LYS:HZ3  | 1.80                     | 0.46              |
| 1:H:325:ASP:O    | 1:H:328:ARG:HG2  | 2.15                     | 0.46              |
| 1:I:21:ALA:HA    | 1:I:159:ASP:OD2  | 2.15                     | 0.46              |
| 1:I:646:ASN:OD1  | 1:I:647:ALA:N    | 2.49                     | 0.46              |
| 1:K:223:TYR:HE1  | 1:K:278:LYS:HG3  | 1.80                     | 0.46              |
| 1:K:387:GLN:HG3  | 1:K:387:GLN:O    | 2.15                     | 0.46              |
| 1:K:528:LYS:NZ   | 1:K:559:LEU:O    | 2.44                     | 0.46              |
| 1:L:41:TRP:CH2   | 1:L:44:TRP:HB2   | 2.51                     | 0.46              |
| 1:A:82:PRO:HB3   | 1:A:90:ALA:HB3   | 1.98                     | 0.46              |
| 1:A:165:MET:HB3  | 1:A:304:PHE:CG   | 2.50                     | 0.46              |
| 1:A:350:PHE:N    | 1:A:390:ALA:O    | 2.38                     | 0.46              |
| 1:B:586:THR:CG2  | 1:B:590:GLN:HE22 | 2.26                     | 0.46              |
| 1:B:593:LEU:O    | 1:B:597:GLN:HG3  | 2.16                     | 0.46              |
| 1:C:306:GLU:OE2  | 1:D:61:ARG:NE    | 2.49                     | 0.46              |
| 1:D:642:GLN:HA   | 1:D:645:LEU:HD12 | 1.98                     | 0.46              |
| 1:E:249:ARG:HG3  | 1:E:250:ASP:N    | 2.30                     | 0.46              |
| 1:E:444:LEU:HD23 | 1:E:518:THR:HB   | 1.98                     | 0.46              |
| 1:G:87:ARG:HD3   | 1:G:89:ASP:HB2   | 1.98                     | 0.46              |
| 1:G:162:SER:HB2  | 1:G:170:ALA:HB2  | 1.97                     | 0.46              |
| 1:H:114:ALA:O    | 1:H:118:GLN:HB2  | 2.16                     | 0.46              |
| 1:H:350:PHE:N    | 1:H:390:ALA:O    | 2.35                     | 0.46              |
| 1:H:387:GLN:HG3  | 1:H:387:GLN:O    | 2.16                     | 0.46              |
| 1:I:124:GLY:HA3  | 1:I:303:VAL:HG22 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:249:ARG:HG3  | 1:I:250:ASP:N    | 2.31                     | 0.46              |
| 1:I:387:GLN:HG3  | 1:I:387:GLN:O    | 2.16                     | 0.46              |
| 1:I:590:GLN:HA   | 1:I:594:VAL:HB   | 1.98                     | 0.46              |
| 1:K:235:TYR:CE1  | 1:K:264:ILE:HA   | 2.49                     | 0.46              |
| 1:K:306:GLU:OE2  | 1:L:61:ARG:NE    | 2.49                     | 0.46              |
| 1:L:24:GLU:HB2   | 1:L:159:ASP:OD2  | 2.16                     | 0.46              |
| 1:A:248:LYS:HE3  | 1:A:252:LYS:HB2  | 1.98                     | 0.46              |
| 1:C:124:GLY:CA   | 1:C:303:VAL:HG22 | 2.46                     | 0.46              |
| 1:C:695:GLU:HA   | 1:C:698:HIS:ND1  | 2.31                     | 0.46              |
| 1:D:250:ASP:OD1  | 1:D:251:ILE:HG13 | 2.16                     | 0.46              |
| 1:F:87:ARG:HD3   | 1:F:89:ASP:HB2   | 1.98                     | 0.46              |
| 1:G:35:PHE:CZ    | 1:G:321:ARG:HB2  | 2.51                     | 0.46              |
| 1:G:45:LEU:HG    | 1:G:46:SER:H     | 1.81                     | 0.46              |
| 1:G:201:PHE:HD1  | 1:G:283:CYS:HB2  | 1.81                     | 0.46              |
| 1:G:663:SER:HA   | 1:G:666:ARG:NE   | 2.28                     | 0.46              |
| 1:H:140:ASN:HB3  | 1:H:455:THR:OG1  | 2.16                     | 0.46              |
| 1:H:429:GLN:HA   | 1:H:432:PHE:HD2  | 1.80                     | 0.46              |
| 1:I:117:GLU:OE1  | 1:I:124:GLY:HA2  | 2.16                     | 0.46              |
| 1:I:349:PRO:HG3  | 1:I:391:TYR:CZ   | 2.51                     | 0.46              |
| 1:I:527:MET:HA   | 1:I:530:GLN:CD   | 2.41                     | 0.46              |
| 1:J:80:TYR:CD1   | 1:J:444:LEU:HD21 | 2.51                     | 0.46              |
| 1:A:26:ARG:O     | 1:A:30:LYS:HG3   | 2.16                     | 0.45              |
| 1:A:587:PRO:HD2  | 1:A:589:GLU:HG3  | 1.97                     | 0.45              |
| 1:B:176:ILE:HD11 | 1:B:204:PRO:HB3  | 1.98                     | 0.45              |
| 1:B:303:VAL:HG12 | 1:B:439:ASN:HB3  | 1.97                     | 0.45              |
| 1:C:235:TYR:CE1  | 1:C:264:ILE:HA   | 2.51                     | 0.45              |
| 1:C:303:VAL:HG12 | 1:C:439:ASN:HB3  | 1.97                     | 0.45              |
| 1:D:641:ALA:HA   | 1:D:644:GLN:OE1  | 2.15                     | 0.45              |
| 1:E:21:ALA:HB2   | 1:E:172:HIS:CD2  | 2.51                     | 0.45              |
| 1:F:80:TYR:CD1   | 1:F:444:LEU:HD21 | 2.51                     | 0.45              |
| 1:G:10:SER:O     | 1:G:14:ARG:HG2   | 2.17                     | 0.45              |
| 1:G:15:PHE:HA    | 1:G:18:ASP:HB3   | 1.98                     | 0.45              |
| 1:G:53:TYR:CG    | 1:G:54:ARG:N     | 2.84                     | 0.45              |
| 1:G:338:ALA:O    | 1:G:342:ALA:N    | 2.46                     | 0.45              |
| 1:H:82:PRO:HB3   | 1:H:90:ALA:HB3   | 1.99                     | 0.45              |
| 1:J:574:LYS:O    | 1:J:578:GLN:HG3  | 2.16                     | 0.45              |
| 1:K:45:LEU:HG    | 1:K:46:SER:H     | 1.80                     | 0.45              |
| 1:K:142:GLN:NE2  | 1:K:455:THR:OG1  | 2.50                     | 0.45              |
| 1:K:230:GLU:OE2  | 1:K:249:ARG:HG2  | 2.15                     | 0.45              |
| 1:K:646:ASN:OD1  | 1:K:647:ALA:N    | 2.49                     | 0.45              |
| 1:B:250:ASP:OD1  | 1:B:251:ILE:HG13 | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:281:ILE:HG12 | 1:C:287:LEU:H    | 1.81                     | 0.45              |
| 1:C:429:GLN:HA   | 1:C:432:PHE:HD2  | 1.81                     | 0.45              |
| 1:D:223:TYR:HE1  | 1:D:278:LYS:HG3  | 1.81                     | 0.45              |
| 1:D:657:MET:SD   | 1:E:655:ASN:ND2  | 2.90                     | 0.45              |
| 1:E:203:ASN:OD1  | 1:E:205:ASN:N    | 2.37                     | 0.45              |
| 1:F:96:GLY:O     | 1:F:100:THR:OG1  | 2.11                     | 0.45              |
| 1:F:444:LEU:HD23 | 1:F:518:THR:HB   | 1.98                     | 0.45              |
| 1:H:42:ASP:HB3   | 1:H:44:TRP:HD1   | 1.81                     | 0.45              |
| 1:H:165:MET:HB3  | 1:H:304:PHE:CG   | 2.52                     | 0.45              |
| 1:H:528:LYS:NZ   | 1:H:559:LEU:O    | 2.45                     | 0.45              |
| 1:H:662:GLN:HA   | 1:H:665:PHE:CD2  | 2.51                     | 0.45              |
| 1:I:438:LEU:O    | 1:I:442:ALA:N    | 2.40                     | 0.45              |
| 1:J:151:SER:HB2  | 1:J:155:HIS:CE1  | 2.52                     | 0.45              |
| 1:J:236:GLN:HG2  | 1:J:244:VAL:H    | 1.81                     | 0.45              |
| 1:J:273:ARG:NE   | 1:J:296:GLU:OE2  | 2.49                     | 0.45              |
| 1:L:296:GLU:HB2  | 1:L:449:PHE:CD2  | 2.36                     | 0.45              |
| 1:L:564:GLY:O    | 1:L:568:MET:HG2  | 2.17                     | 0.45              |
| 1:A:355:GLN:HA   | 1:A:375:ASN:HB3  | 1.98                     | 0.45              |
| 1:A:377:THR:HA   | 1:A:383:ASP:OD2  | 2.16                     | 0.45              |
| 1:B:99:ARG:NE    | 1:B:525:GLN:O    | 2.49                     | 0.45              |
| 1:B:661:LYS:HE3  | 1:B:665:PHE:CZ   | 2.51                     | 0.45              |
| 1:C:623:ALA:HA   | 1:C:626:GLN:CD   | 2.41                     | 0.45              |
| 1:D:99:ARG:NH2   | 1:D:525:GLN:HA   | 2.31                     | 0.45              |
| 1:D:593:LEU:O    | 1:D:597:GLN:HG3  | 2.16                     | 0.45              |
| 1:E:444:LEU:O    | 1:E:447:TYR:HB3  | 2.16                     | 0.45              |
| 1:F:53:TYR:CG    | 1:F:54:ARG:N     | 2.83                     | 0.45              |
| 1:G:162:SER:OG   | 1:G:167:LYS:HA   | 2.16                     | 0.45              |
| 1:I:444:LEU:O    | 1:I:448:VAL:HG23 | 2.16                     | 0.45              |
| 1:J:193:LEU:HD21 | 1:J:288:LYS:HZ3  | 1.81                     | 0.45              |
| 1:L:133:GLU:O    | 1:L:137:PRO:HB3  | 2.16                     | 0.45              |
| 1:L:303:VAL:HG12 | 1:L:439:ASN:HB3  | 1.98                     | 0.45              |
| 1:L:363:TYR:CE1  | 1:L:372:TYR:HA   | 2.52                     | 0.45              |
| 1:A:21:ALA:HB2   | 1:A:172:HIS:NE2  | 2.31                     | 0.45              |
| 1:A:105:ASN:O    | 1:A:109:ILE:HG12 | 2.15                     | 0.45              |
| 1:A:303:VAL:HG12 | 1:A:439:ASN:HB3  | 1.98                     | 0.45              |
| 1:B:21:ALA:HB2   | 1:B:172:HIS:NE2  | 2.31                     | 0.45              |
| 1:C:99:ARG:NH2   | 1:C:525:GLN:HA   | 2.32                     | 0.45              |
| 1:C:377:THR:HA   | 1:C:383:ASP:OD2  | 2.15                     | 0.45              |
| 1:C:526:SER:O    | 1:C:530:GLN:N    | 2.45                     | 0.45              |
| 1:D:235:TYR:HA   | 1:D:265:LYS:O    | 2.16                     | 0.45              |
| 1:D:325:ASP:O    | 1:D:328:ARG:HG2  | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:80:TYR:CZ    | 1:G:516:CYS:HB2  | 2.52                     | 0.45              |
| 1:H:26:ARG:O     | 1:H:30:LYS:HG3   | 2.17                     | 0.45              |
| 1:H:250:ASP:OD1  | 1:H:251:ILE:HG13 | 2.17                     | 0.45              |
| 1:I:663:SER:HA   | 1:I:666:ARG:NE   | 2.29                     | 0.45              |
| 1:J:70:GLU:O     | 1:J:73:GLN:HG3   | 2.16                     | 0.45              |
| 1:J:576:LEU:O    | 1:J:581:VAL:HG12 | 2.15                     | 0.45              |
| 1:K:272:LYS:O    | 1:L:134:ASP:HB2  | 2.16                     | 0.45              |
| 1:K:355:GLN:HA   | 1:K:375:ASN:HB3  | 1.98                     | 0.45              |
| 1:L:250:ASP:OD1  | 1:L:251:ILE:HG13 | 2.16                     | 0.45              |
| 1:A:363:TYR:CE1  | 1:A:372:TYR:HA   | 2.52                     | 0.45              |
| 1:A:701:ARG:HA   | 1:A:704:ILE:HD12 | 1.99                     | 0.45              |
| 1:B:429:GLN:HA   | 1:B:432:PHE:HD2  | 1.82                     | 0.45              |
| 1:B:628:GLN:O    | 1:B:632:LEU:HB2  | 2.15                     | 0.45              |
| 1:C:438:LEU:O    | 1:C:442:ALA:N    | 2.40                     | 0.45              |
| 1:C:593:LEU:O    | 1:C:597:GLN:HG3  | 2.16                     | 0.45              |
| 1:D:53:TYR:CG    | 1:D:54:ARG:N     | 2.84                     | 0.45              |
| 1:D:203:ASN:OD1  | 1:D:205:ASN:N    | 2.38                     | 0.45              |
| 1:E:53:TYR:CG    | 1:E:54:ARG:N     | 2.85                     | 0.45              |
| 1:E:75:PRO:HD2   | 1:E:523:SER:HB3  | 1.98                     | 0.45              |
| 1:E:320:VAL:O    | 1:E:323:THR:OG1  | 2.18                     | 0.45              |
| 1:E:527:MET:HA   | 1:E:530:GLN:CD   | 2.41                     | 0.45              |
| 1:F:35:PHE:CZ    | 1:F:321:ARG:HB2  | 2.52                     | 0.45              |
| 1:H:406:GLU:O    | 1:H:410:SER:OG   | 2.20                     | 0.45              |
| 1:I:238:PRO:HB3  | 1:I:263:PHE:CD1  | 2.51                     | 0.45              |
| 1:I:380:ASN:OD1  | 1:I:381:SER:N    | 2.48                     | 0.45              |
| 1:I:623:ALA:HA   | 1:I:626:GLN:CD   | 2.41                     | 0.45              |
| 1:J:106:THR:HG23 | 1:J:146:ARG:HE   | 1.81                     | 0.45              |
| 1:J:642:GLN:HA   | 1:J:645:LEU:HD12 | 1.99                     | 0.45              |
| 1:K:248:LYS:HE3  | 1:K:252:LYS:HB2  | 1.99                     | 0.45              |
| 1:L:45:LEU:HG    | 1:L:46:SER:H     | 1.81                     | 0.45              |
| 1:A:387:GLN:HG3  | 1:A:387:GLN:O    | 2.15                     | 0.45              |
| 1:A:567:MET:HB2  | 1:L:581:VAL:HG22 | 1.98                     | 0.45              |
| 1:B:232:ALA:HA   | 1:B:269:ARG:H    | 1.81                     | 0.45              |
| 1:C:80:TYR:CD1   | 1:C:444:LEU:HD21 | 2.51                     | 0.45              |
| 1:C:105:ASN:O    | 1:C:109:ILE:HG12 | 2.17                     | 0.45              |
| 1:C:251:ILE:HD13 | 1:C:453:LEU:HD13 | 1.99                     | 0.45              |
| 1:C:356:ILE:HG21 | 1:D:373:LEU:HD21 | 1.99                     | 0.45              |
| 1:C:587:PRO:HD2  | 1:C:589:GLU:HG3  | 1.99                     | 0.45              |
| 1:C:590:GLN:HA   | 1:C:594:VAL:HB   | 1.99                     | 0.45              |
| 1:C:646:ASN:OD1  | 1:C:647:ALA:N    | 2.49                     | 0.45              |
| 1:D:21:ALA:HA    | 1:D:159:ASP:OD2  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:193:LEU:HD21 | 1:E:288:LYS:HZ3  | 1.81                     | 0.45              |
| 1:F:21:ALA:HB2   | 1:F:172:HIS:NE2  | 2.31                     | 0.45              |
| 1:F:355:GLN:HG2  | 1:G:376:ARG:NH1  | 2.25                     | 0.45              |
| 1:F:663:SER:HA   | 1:F:666:ARG:NE   | 2.25                     | 0.45              |
| 1:I:639:VAL:O    | 1:I:642:GLN:HG2  | 2.17                     | 0.45              |
| 1:J:444:LEU:HD23 | 1:J:518:THR:HB   | 1.98                     | 0.45              |
| 1:J:646:ASN:OD1  | 1:J:647:ALA:N    | 2.50                     | 0.45              |
| 1:L:15:PHE:HA    | 1:L:18:ASP:HB3   | 1.97                     | 0.45              |
| 1:L:380:ASN:OD1  | 1:L:381:SER:N    | 2.48                     | 0.45              |
| 1:L:663:SER:HA   | 1:L:666:ARG:NE   | 2.28                     | 0.45              |
| 1:D:24:GLU:HB2   | 1:D:159:ASP:OD2  | 2.17                     | 0.45              |
| 1:E:21:ALA:HB2   | 1:E:172:HIS:NE2  | 2.32                     | 0.45              |
| 1:E:418:LEU:HD23 | 1:E:429:GLN:HB3  | 1.99                     | 0.45              |
| 1:F:429:GLN:HA   | 1:F:432:PHE:CD2  | 2.49                     | 0.45              |
| 1:F:438:LEU:O    | 1:F:442:ALA:N    | 2.42                     | 0.45              |
| 1:G:593:LEU:O    | 1:G:597:GLN:HG3  | 2.17                     | 0.45              |
| 1:I:429:GLN:HA   | 1:I:432:PHE:CD2  | 2.51                     | 0.45              |
| 1:I:628:GLN:O    | 1:I:632:LEU:HB2  | 2.16                     | 0.45              |
| 1:J:403:TYR:OH   | 1:K:397:VAL:HG11 | 2.17                     | 0.45              |
| 1:J:639:VAL:O    | 1:J:642:GLN:HG2  | 2.17                     | 0.45              |
| 1:K:338:ALA:O    | 1:K:342:ALA:N    | 2.48                     | 0.45              |
| 1:L:297:HIS:CG   | 1:L:298:ILE:H    | 2.35                     | 0.45              |
| 1:A:99:ARG:NE    | 1:A:525:GLN:O    | 2.49                     | 0.45              |
| 1:A:380:ASN:OD1  | 1:A:381:SER:N    | 2.49                     | 0.45              |
| 1:A:527:MET:HA   | 1:A:530:GLN:CD   | 2.42                     | 0.45              |
| 1:D:80:TYR:CZ    | 1:D:516:CYS:HB2  | 2.52                     | 0.45              |
| 1:D:238:PRO:HB3  | 1:D:263:PHE:CD1  | 2.52                     | 0.45              |
| 1:D:436:ASN:HA   | 1:D:439:ASN:ND2  | 2.31                     | 0.45              |
| 1:D:528:LYS:HZ3  | 1:D:560:LEU:HD23 | 1.81                     | 0.45              |
| 1:D:538:LEU:HB3  | 1:D:551:LEU:HD11 | 1.99                     | 0.45              |
| 1:E:80:TYR:CZ    | 1:E:516:CYS:HB2  | 2.52                     | 0.45              |
| 1:E:640:GLU:HA   | 1:E:643:ASN:HD22 | 1.82                     | 0.45              |
| 1:F:124:GLY:HA3  | 1:F:303:VAL:HG22 | 1.99                     | 0.45              |
| 1:F:165:MET:HB3  | 1:F:304:PHE:CG   | 2.52                     | 0.45              |
| 1:F:398:PRO:HA   | 1:G:394:ASN:HB3  | 1.97                     | 0.45              |
| 1:F:406:GLU:O    | 1:F:410:SER:OG   | 2.26                     | 0.45              |
| 1:G:429:GLN:HA   | 1:G:432:PHE:HD2  | 1.82                     | 0.45              |
| 1:G:564:GLY:O    | 1:G:568:MET:HG2  | 2.17                     | 0.45              |
| 1:H:333:ILE:HG22 | 1:H:337:ASN:OD1  | 2.17                     | 0.45              |
| 1:I:29:ALA:O     | 1:I:33:LEU:HB2   | 2.17                     | 0.45              |
| 1:I:220:ALA:CB   | 1:I:281:ILE:O    | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:252:LYS:HD2  | 1:I:256:ASP:HB3  | 1.99                     | 0.45              |
| 1:J:29:ALA:O     | 1:J:33:LEU:CB    | 2.64                     | 0.45              |
| 1:J:45:LEU:HG    | 1:J:46:SER:H     | 1.82                     | 0.45              |
| 1:L:238:PRO:HB3  | 1:L:263:PHE:CD1  | 2.52                     | 0.45              |
| 1:L:426:ASN:O    | 1:L:429:GLN:NE2  | 2.50                     | 0.45              |
| 1:L:701:ARG:HA   | 1:L:704:ILE:HD12 | 1.99                     | 0.45              |
| 1:A:117:GLU:OE1  | 1:A:124:GLY:HA2  | 2.17                     | 0.45              |
| 1:A:354:GLU:HG2  | 1:B:376:ARG:HD3  | 1.99                     | 0.45              |
| 1:B:47:GLN:HB2   | 1:B:50:THR:CG2   | 2.47                     | 0.45              |
| 1:B:140:ASN:HB3  | 1:B:455:THR:OG1  | 2.16                     | 0.45              |
| 1:C:235:TYR:HA   | 1:C:265:LYS:O    | 2.16                     | 0.45              |
| 1:C:275:ARG:NH2  | 1:C:293:ILE:O    | 2.36                     | 0.45              |
| 1:D:387:GLN:HG3  | 1:D:387:GLN:O    | 2.16                     | 0.45              |
| 1:E:628:GLN:O    | 1:E:632:LEU:HB2  | 2.16                     | 0.45              |
| 1:F:176:ILE:HD11 | 1:F:204:PRO:HB3  | 1.97                     | 0.45              |
| 1:G:106:THR:HG23 | 1:G:146:ARG:HE   | 1.82                     | 0.45              |
| 1:G:320:VAL:O    | 1:G:324:LYS:HG3  | 2.17                     | 0.45              |
| 1:H:24:GLU:OE1   | 1:H:24:GLU:N     | 2.48                     | 0.45              |
| 1:H:80:TYR:CZ    | 1:H:516:CYS:HB2  | 2.52                     | 0.45              |
| 1:H:380:ASN:OD1  | 1:H:381:SER:N    | 2.49                     | 0.45              |
| 1:H:664:GLU:HG3  | 1:I:659:LEU:HD22 | 1.99                     | 0.45              |
| 1:I:232:ALA:HA   | 1:I:269:ARG:H    | 1.82                     | 0.45              |
| 1:I:420:VAL:HB   | 1:I:424:ALA:HA   | 1.99                     | 0.45              |
| 1:J:80:TYR:CZ    | 1:J:516:CYS:HB2  | 2.51                     | 0.45              |
| 1:K:297:HIS:CG   | 1:K:298:ILE:H    | 2.35                     | 0.45              |
| 1:A:201:PHE:HD1  | 1:A:283:CYS:HB2  | 1.81                     | 0.45              |
| 1:A:649:ARG:O    | 1:A:653:ILE:HG13 | 2.17                     | 0.45              |
| 1:A:663:SER:O    | 1:A:666:ARG:HG3  | 2.16                     | 0.45              |
| 1:B:21:ALA:HA    | 1:B:159:ASP:OD2  | 2.16                     | 0.45              |
| 1:B:259:ALA:HA   | 1:B:263:PHE:CD2  | 2.52                     | 0.45              |
| 1:C:642:GLN:HA   | 1:C:645:LEU:HD12 | 1.98                     | 0.45              |
| 1:D:640:GLU:HA   | 1:D:643:ASN:HD22 | 1.81                     | 0.45              |
| 1:F:246:TYR:C    | 1:F:247:PHE:HD1  | 2.25                     | 0.45              |
| 1:F:349:PRO:HG3  | 1:F:391:TYR:CZ   | 2.52                     | 0.45              |
| 1:G:75:PRO:HD2   | 1:G:523:SER:HB3  | 1.98                     | 0.45              |
| 1:H:35:PHE:CZ    | 1:H:321:ARG:HB2  | 2.52                     | 0.45              |
| 1:I:53:TYR:O     | 1:I:54:ARG:NH1   | 2.49                     | 0.45              |
| 1:J:203:ASN:OD1  | 1:J:205:ASN:N    | 2.35                     | 0.45              |
| 1:K:53:TYR:CG    | 1:K:54:ARG:N     | 2.85                     | 0.45              |
| 1:K:128:LEU:HD22 | 1:K:144:ILE:HD12 | 1.99                     | 0.45              |
| 1:K:628:GLN:O    | 1:K:632:LEU:HB2  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:695:GLU:HA   | 1:L:698:HIS:ND1  | 2.32                     | 0.45              |
| 1:A:35:PHE:CZ    | 1:A:321:ARG:HB2  | 2.52                     | 0.44              |
| 1:C:26:ARG:O     | 1:C:30:LYS:HG3   | 2.17                     | 0.44              |
| 1:C:53:TYR:CG    | 1:C:54:ARG:N     | 2.85                     | 0.44              |
| 1:D:168:SER:HA   | 1:D:297:HIS:NE2  | 2.32                     | 0.44              |
| 1:D:538:LEU:O    | 1:D:542:THR:OG1  | 2.34                     | 0.44              |
| 1:E:303:VAL:HG12 | 1:E:439:ASN:HB3  | 1.98                     | 0.44              |
| 1:E:593:LEU:O    | 1:E:597:GLN:HG3  | 2.17                     | 0.44              |
| 1:F:235:TYR:HE1  | 1:F:264:ILE:HA   | 1.82                     | 0.44              |
| 1:F:528:LYS:NZ   | 1:F:559:LEU:O    | 2.42                     | 0.44              |
| 1:F:642:GLN:HA   | 1:F:645:LEU:HD12 | 1.98                     | 0.44              |
| 1:G:184:TRP:CZ3  | 1:G:199:PRO:HG3  | 2.52                     | 0.44              |
| 1:G:228:LYS:HB2  | 1:G:275:ARG:HB3  | 1.98                     | 0.44              |
| 1:G:609:VAL:O    | 1:G:612:GLN:HB2  | 2.17                     | 0.44              |
| 1:I:15:PHE:HA    | 1:I:18:ASP:HB3   | 1.98                     | 0.44              |
| 1:K:75:PRO:HD2   | 1:K:523:SER:HB3  | 1.98                     | 0.44              |
| 1:K:526:SER:O    | 1:K:530:GLN:N    | 2.46                     | 0.44              |
| 1:D:356:ILE:HG21 | 1:E:373:LEU:HD21 | 1.99                     | 0.44              |
| 1:E:538:LEU:O    | 1:E:542:THR:OG1  | 2.34                     | 0.44              |
| 1:F:250:ASP:OD1  | 1:F:251:ILE:HG13 | 2.17                     | 0.44              |
| 1:H:663:SER:HA   | 1:H:666:ARG:HG2  | 1.98                     | 0.44              |
| 1:J:15:PHE:HA    | 1:J:18:ASP:HB3   | 1.98                     | 0.44              |
| 1:J:75:PRO:HD2   | 1:J:523:SER:HB3  | 1.99                     | 0.44              |
| 1:J:232:ALA:HA   | 1:J:269:ARG:H    | 1.83                     | 0.44              |
| 1:K:124:GLY:HA3  | 1:K:303:VAL:HG22 | 1.98                     | 0.44              |
| 1:K:273:ARG:NE   | 1:K:296:GLU:OE2  | 2.50                     | 0.44              |
| 1:K:363:TYR:CE1  | 1:K:372:TYR:HA   | 2.52                     | 0.44              |
| 1:K:695:GLU:HA   | 1:K:698:HIS:CE1  | 2.51                     | 0.44              |
| 1:L:140:ASN:HB3  | 1:L:455:THR:OG1  | 2.16                     | 0.44              |
| 1:L:249:ARG:HG3  | 1:L:250:ASP:N    | 2.32                     | 0.44              |
| 1:A:203:ASN:OD1  | 1:A:205:ASN:N    | 2.33                     | 0.44              |
| 1:A:657:MET:SD   | 1:B:655:ASN:ND2  | 2.90                     | 0.44              |
| 1:B:514:TYR:HB2  | 1:C:136:SER:OG   | 2.17                     | 0.44              |
| 1:B:653:ILE:HG12 | 1:C:648:ALA:HA   | 2.00                     | 0.44              |
| 1:C:21:ALA:HB2   | 1:C:172:HIS:NE2  | 2.32                     | 0.44              |
| 1:C:259:ALA:HA   | 1:C:263:PHE:CD2  | 2.53                     | 0.44              |
| 1:C:614:VAL:HG11 | 1:D:609:VAL:HG11 | 1.99                     | 0.44              |
| 1:D:646:ASN:HA   | 1:E:644:GLN:HG2  | 1.99                     | 0.44              |
| 1:E:21:ALA:HA    | 1:E:159:ASP:OD2  | 2.16                     | 0.44              |
| 1:E:246:TYR:HB2  | 1:E:510:ILE:HG13 | 1.99                     | 0.44              |
| 1:F:21:ALA:HB2   | 1:F:172:HIS:CD2  | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:363:TYR:CE1  | 1:F:372:TYR:HA   | 2.52                     | 0.44              |
| 1:G:398:PRO:O    | 1:G:399:GLN:HG2  | 2.18                     | 0.44              |
| 1:H:444:LEU:O    | 1:H:447:TYR:HB3  | 2.18                     | 0.44              |
| 1:H:444:LEU:HD23 | 1:H:518:THR:HB   | 1.99                     | 0.44              |
| 1:H:664:GLU:OE2  | 1:I:666:ARG:NH2  | 2.50                     | 0.44              |
| 1:J:78:VAL:HA    | 1:J:520:VAL:HA   | 1.99                     | 0.44              |
| 1:J:99:ARG:NH2   | 1:J:525:GLN:HA   | 2.31                     | 0.44              |
| 1:J:110:ALA:HB1  | 1:J:126:TRP:CE3  | 2.51                     | 0.44              |
| 1:K:168:SER:HA   | 1:K:297:HIS:NE2  | 2.32                     | 0.44              |
| 1:K:201:PHE:HD1  | 1:K:283:CYS:HB2  | 1.80                     | 0.44              |
| 1:K:324:LYS:O    | 1:K:327:GLN:HB2  | 2.18                     | 0.44              |
| 1:L:444:LEU:O    | 1:L:448:VAL:HG23 | 2.17                     | 0.44              |
| 1:L:526:SER:O    | 1:L:530:GLN:N    | 2.48                     | 0.44              |
| 1:A:223:TYR:HE1  | 1:A:278:LYS:HG3  | 1.81                     | 0.44              |
| 1:A:246:TYR:C    | 1:A:247:PHE:HD1  | 2.26                     | 0.44              |
| 1:A:578:GLN:HA   | 1:A:597:GLN:HE21 | 1.82                     | 0.44              |
| 1:B:26:ARG:O     | 1:B:30:LYS:HG3   | 2.16                     | 0.44              |
| 1:C:248:LYS:HG2  | 1:C:511:ARG:HH21 | 1.81                     | 0.44              |
| 1:D:458:ARG:NH2  | 1:D:500:ALA:HB1  | 2.32                     | 0.44              |
| 1:E:120:GLU:HA   | 1:E:320:VAL:HB   | 1.99                     | 0.44              |
| 1:E:231:THR:HG22 | 1:E:249:ARG:HE   | 1.82                     | 0.44              |
| 1:E:250:ASP:OD1  | 1:E:251:ILE:HG13 | 2.17                     | 0.44              |
| 1:G:223:TYR:HE1  | 1:G:278:LYS:HG3  | 1.83                     | 0.44              |
| 1:G:363:TYR:CE1  | 1:G:372:TYR:HA   | 2.51                     | 0.44              |
| 1:G:387:GLN:O    | 1:G:387:GLN:HG3  | 2.17                     | 0.44              |
| 1:H:124:GLY:CA   | 1:H:303:VAL:HG22 | 2.48                     | 0.44              |
| 1:H:203:ASN:OD1  | 1:H:205:ASN:N    | 2.33                     | 0.44              |
| 1:H:355:GLN:HA   | 1:H:375:ASN:HB3  | 1.98                     | 0.44              |
| 1:H:628:GLN:O    | 1:H:632:LEU:HB2  | 2.18                     | 0.44              |
| 1:J:47:GLN:HB2   | 1:J:50:THR:HG21  | 2.00                     | 0.44              |
| 1:J:124:GLY:CA   | 1:J:303:VAL:HG22 | 2.47                     | 0.44              |
| 1:K:80:TYR:HB3   | 1:K:95:MET:HE2   | 1.98                     | 0.44              |
| 1:K:203:ASN:HD21 | 1:K:209:PHE:HZ   | 1.65                     | 0.44              |
| 1:L:444:LEU:HD23 | 1:L:518:THR:HB   | 1.99                     | 0.44              |
| 1:A:250:ASP:OD1  | 1:A:251:ILE:HG13 | 2.17                     | 0.44              |
| 1:B:47:GLN:HB2   | 1:B:50:THR:HG21  | 2.00                     | 0.44              |
| 1:B:380:ASN:OD1  | 1:B:381:SER:N    | 2.49                     | 0.44              |
| 1:B:398:PRO:HA   | 1:C:394:ASN:HB3  | 1.99                     | 0.44              |
| 1:B:590:GLN:HA   | 1:B:594:VAL:HB   | 1.99                     | 0.44              |
| 1:C:663:SER:O    | 1:C:666:ARG:HG3  | 2.18                     | 0.44              |
| 1:E:649:ARG:O    | 1:E:653:ILE:HG13 | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:250:ASP:OD1  | 1:G:251:ILE:HG13 | 2.17                     | 0.44              |
| 1:G:613:GLY:CA   | 1:G:616:LEU:HD13 | 2.38                     | 0.44              |
| 1:H:27:ARG:HH11  | 1:H:313:LYS:HE3  | 1.83                     | 0.44              |
| 1:H:657:MET:SD   | 1:I:655:ASN:ND2  | 2.91                     | 0.44              |
| 1:I:21:ALA:HB2   | 1:I:172:HIS:NE2  | 2.32                     | 0.44              |
| 1:I:233:PHE:HB2  | 1:I:249:ARG:HB3  | 2.00                     | 0.44              |
| 1:J:233:PHE:HB2  | 1:J:249:ARG:HB3  | 1.98                     | 0.44              |
| 1:J:526:SER:O    | 1:J:530:GLN:N    | 2.45                     | 0.44              |
| 1:J:649:ARG:O    | 1:J:653:ILE:HG13 | 2.16                     | 0.44              |
| 1:K:47:GLN:HB2   | 1:K:50:THR:HG21  | 2.00                     | 0.44              |
| 1:K:614:VAL:HG11 | 1:L:609:VAL:HG11 | 2.00                     | 0.44              |
| 1:L:176:ILE:HD11 | 1:L:204:PRO:HB3  | 1.99                     | 0.44              |
| 1:L:418:LEU:HD23 | 1:L:429:GLN:HB3  | 2.00                     | 0.44              |
| 1:L:613:GLY:CA   | 1:L:616:LEU:HD12 | 2.47                     | 0.44              |
| 1:A:420:VAL:HB   | 1:A:424:ALA:HA   | 2.00                     | 0.44              |
| 1:A:613:GLY:CA   | 1:A:616:LEU:HD12 | 2.34                     | 0.44              |
| 1:B:27:ARG:HH11  | 1:B:313:LYS:HE3  | 1.83                     | 0.44              |
| 1:B:235:TYR:CE1  | 1:B:264:ILE:HA   | 2.52                     | 0.44              |
| 1:B:444:LEU:HD23 | 1:B:518:THR:HB   | 2.00                     | 0.44              |
| 1:C:444:LEU:HD23 | 1:C:518:THR:HB   | 2.00                     | 0.44              |
| 1:C:448:VAL:HA   | 1:C:451:ASP:OD2  | 2.18                     | 0.44              |
| 1:C:527:MET:HA   | 1:C:530:GLN:CD   | 2.43                     | 0.44              |
| 1:C:591:GLN:HA   | 1:C:595:GLU:CD   | 2.41                     | 0.44              |
| 1:D:228:LYS:HB2  | 1:D:275:ARG:HB3  | 1.99                     | 0.44              |
| 1:D:329:LEU:O    | 1:D:333:ILE:HG13 | 2.17                     | 0.44              |
| 1:E:162:SER:OG   | 1:E:164:LEU:O    | 2.35                     | 0.44              |
| 1:F:106:THR:HG23 | 1:F:146:ARG:HE   | 1.82                     | 0.44              |
| 1:F:418:LEU:HD23 | 1:F:429:GLN:HB3  | 1.99                     | 0.44              |
| 1:G:99:ARG:NE    | 1:G:525:GLN:O    | 2.50                     | 0.44              |
| 1:G:124:GLY:CA   | 1:G:303:VAL:HG22 | 2.48                     | 0.44              |
| 1:G:223:TYR:CE1  | 1:G:278:LYS:HG3  | 2.52                     | 0.44              |
| 1:J:527:MET:HA   | 1:J:530:GLN:CD   | 2.43                     | 0.44              |
| 1:L:97:MET:HE2   | 1:L:450:GLN:HE22 | 1.83                     | 0.44              |
| 1:A:162:SER:OG   | 1:A:164:LEU:O    | 2.35                     | 0.44              |
| 1:B:525:GLN:HB2  | 1:B:529:GLN:OE1  | 2.17                     | 0.44              |
| 1:B:527:MET:HA   | 1:B:530:GLN:CD   | 2.42                     | 0.44              |
| 1:C:75:PRO:HD2   | 1:C:523:SER:HB3  | 1.99                     | 0.44              |
| 1:C:348:LYS:HB2  | 1:D:372:TYR:CD2  | 2.53                     | 0.44              |
| 1:C:640:GLU:HA   | 1:C:643:ASN:HD22 | 1.83                     | 0.44              |
| 1:D:29:ALA:O     | 1:D:33:LEU:HB2   | 2.18                     | 0.44              |
| 1:E:99:ARG:NE    | 1:E:525:GLN:O    | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:126:TRP:CD1  | 1:F:146:ARG:HG3  | 2.53                     | 0.44              |
| 1:F:581:VAL:HG22 | 1:G:567:MET:HB2  | 2.00                     | 0.44              |
| 1:H:278:LYS:HE2  | 1:H:280:ILE:HD11 | 1.99                     | 0.44              |
| 1:I:45:LEU:HG    | 1:I:46:SER:H     | 1.82                     | 0.44              |
| 1:I:99:ARG:NH2   | 1:I:525:GLN:HA   | 2.32                     | 0.44              |
| 1:I:581:VAL:HG22 | 1:J:567:MET:HB2  | 1.99                     | 0.44              |
| 1:J:21:ALA:HB2   | 1:J:172:HIS:NE2  | 2.32                     | 0.44              |
| 1:J:320:VAL:O    | 1:J:323:THR:OG1  | 2.19                     | 0.44              |
| 1:J:436:ASN:HA   | 1:J:439:ASN:ND2  | 2.33                     | 0.44              |
| 1:J:525:GLN:HB2  | 1:J:529:GLN:OE1  | 2.18                     | 0.44              |
| 1:K:29:ALA:O     | 1:K:33:LEU:CB    | 2.66                     | 0.44              |
| 1:A:29:ALA:O     | 1:A:33:LEU:HB2   | 2.17                     | 0.44              |
| 1:A:664:GLU:HG3  | 1:B:659:LEU:HD22 | 1.99                     | 0.44              |
| 1:B:306:GLU:OE2  | 1:C:61:ARG:NE    | 2.50                     | 0.44              |
| 1:B:639:VAL:O    | 1:B:642:GLN:HG2  | 2.17                     | 0.44              |
| 1:C:140:ASN:HB3  | 1:C:455:THR:OG1  | 2.17                     | 0.44              |
| 1:C:559:LEU:HB3  | 1:C:565:VAL:HB   | 2.00                     | 0.44              |
| 1:E:573:ASN:HA   | 1:E:576:LEU:HD12 | 2.00                     | 0.44              |
| 1:F:235:TYR:CE1  | 1:F:264:ILE:HA   | 2.53                     | 0.44              |
| 1:F:525:GLN:HB2  | 1:F:529:GLN:OE1  | 2.17                     | 0.44              |
| 1:G:133:GLU:O    | 1:G:137:PRO:HB3  | 2.18                     | 0.44              |
| 1:G:646:ASN:HA   | 1:H:644:GLN:HG2  | 1.99                     | 0.44              |
| 1:I:250:ASP:OD1  | 1:I:251:ILE:HG13 | 2.17                     | 0.44              |
| 1:I:309:PHE:HB2  | 1:J:150:HIS:HB2  | 2.00                     | 0.44              |
| 1:I:363:TYR:CE1  | 1:I:372:TYR:HA   | 2.50                     | 0.44              |
| 1:J:140:ASN:HB3  | 1:J:455:THR:OG1  | 2.18                     | 0.44              |
| 1:J:250:ASP:OD1  | 1:J:251:ILE:HG13 | 2.17                     | 0.44              |
| 1:K:21:ALA:HB2   | 1:K:172:HIS:CD2  | 2.53                     | 0.44              |
| 1:K:124:GLY:CA   | 1:K:303:VAL:HG22 | 2.48                     | 0.44              |
| 1:K:204:PRO:HD3  | 1:K:218:GLN:HG2  | 2.00                     | 0.44              |
| 1:A:349:PRO:HG3  | 1:A:391:TYR:CZ   | 2.53                     | 0.44              |
| 1:B:458:ARG:NH2  | 1:B:500:ALA:HB1  | 2.33                     | 0.44              |
| 1:C:45:LEU:HG    | 1:C:46:SER:H     | 1.81                     | 0.44              |
| 1:C:320:VAL:O    | 1:C:324:LYS:HG3  | 2.18                     | 0.44              |
| 1:C:354:GLU:HG2  | 1:D:376:ARG:HD3  | 2.00                     | 0.44              |
| 1:C:701:ARG:HA   | 1:C:704:ILE:HD12 | 1.99                     | 0.44              |
| 1:E:29:ALA:O     | 1:E:33:LEU:HB2   | 2.17                     | 0.44              |
| 1:G:235:TYR:HE1  | 1:G:264:ILE:HA   | 1.83                     | 0.44              |
| 1:H:526:SER:O    | 1:H:530:GLN:N    | 2.47                     | 0.44              |
| 1:I:593:LEU:O    | 1:I:597:GLN:HG3  | 2.17                     | 0.44              |
| 1:K:10:SER:O     | 1:K:14:ARG:HG2   | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:151:SER:HB2  | 1:K:155:HIS:CE1  | 2.52                     | 0.44              |
| 1:K:252:LYS:HD2  | 1:K:256:ASP:HB3  | 1.99                     | 0.44              |
| 1:K:350:PHE:HB2  | 1:K:390:ALA:HB3  | 2.00                     | 0.44              |
| 1:K:590:GLN:HA   | 1:K:594:VAL:HB   | 2.00                     | 0.44              |
| 1:L:35:PHE:CZ    | 1:L:321:ARG:HB2  | 2.53                     | 0.44              |
| 1:L:53:TYR:CG    | 1:L:54:ARG:N     | 2.86                     | 0.44              |
| 1:L:80:TYR:CD1   | 1:L:444:LEU:HD21 | 2.52                     | 0.44              |
| 1:L:235:TYR:HA   | 1:L:265:LYS:O    | 2.18                     | 0.44              |
| 1:L:383:ASP:O    | 1:L:384:LEU:HD12 | 2.18                     | 0.44              |
| 1:L:646:ASN:OD1  | 1:L:647:ALA:N    | 2.50                     | 0.44              |
| 1:B:162:SER:OG   | 1:B:167:LYS:HA   | 2.17                     | 0.43              |
| 1:D:21:ALA:HB2   | 1:D:172:HIS:CD2  | 2.53                     | 0.43              |
| 1:D:514:TYR:HB2  | 1:E:136:SER:OG   | 2.17                     | 0.43              |
| 1:F:57:PHE:HB2   | 1:F:334:MET:SD   | 2.58                     | 0.43              |
| 1:F:203:ASN:HD21 | 1:F:209:PHE:HZ   | 1.65                     | 0.43              |
| 1:F:320:VAL:O    | 1:F:323:THR:OG1  | 2.19                     | 0.43              |
| 1:F:663:SER:O    | 1:F:666:ARG:HG3  | 2.18                     | 0.43              |
| 1:H:117:GLU:OE1  | 1:H:124:GLY:HA2  | 2.18                     | 0.43              |
| 1:J:333:ILE:HG22 | 1:J:337:ASN:OD1  | 2.19                     | 0.43              |
| 1:K:527:MET:HA   | 1:K:530:GLN:CD   | 2.42                     | 0.43              |
| 1:L:281:ILE:HG12 | 1:L:287:LEU:H    | 1.83                     | 0.43              |
| 1:L:663:SER:O    | 1:L:666:ARG:HG3  | 2.17                     | 0.43              |
| 1:A:228:LYS:HB2  | 1:A:275:ARG:HB3  | 1.99                     | 0.43              |
| 1:A:526:SER:O    | 1:A:530:GLN:N    | 2.45                     | 0.43              |
| 1:B:701:ARG:HA   | 1:B:704:ILE:HD12 | 2.00                     | 0.43              |
| 1:C:10:SER:O     | 1:C:14:ARG:HG2   | 2.18                     | 0.43              |
| 1:C:168:SER:HA   | 1:C:297:HIS:NE2  | 2.34                     | 0.43              |
| 1:C:278:LYS:HE2  | 1:C:280:ILE:HD11 | 2.00                     | 0.43              |
| 1:E:248:LYS:CD   | 1:E:251:ILE:HB   | 2.43                     | 0.43              |
| 1:F:26:ARG:O     | 1:F:30:LYS:HG3   | 2.18                     | 0.43              |
| 1:F:527:MET:HA   | 1:F:530:GLN:CD   | 2.43                     | 0.43              |
| 1:H:9:GLU:HB3    | 1:H:12:LEU:HG    | 2.00                     | 0.43              |
| 1:H:235:TYR:CE1  | 1:H:264:ILE:HA   | 2.53                     | 0.43              |
| 1:I:124:GLY:CA   | 1:I:303:VAL:HG22 | 2.49                     | 0.43              |
| 1:I:140:ASN:HB3  | 1:I:455:THR:OG1  | 2.18                     | 0.43              |
| 1:I:514:TYR:HB2  | 1:J:136:SER:OG   | 2.18                     | 0.43              |
| 1:J:695:GLU:HA   | 1:J:698:HIS:ND1  | 2.34                     | 0.43              |
| 1:K:162:SER:OG   | 1:K:164:LEU:O    | 2.36                     | 0.43              |
| 1:L:333:ILE:HG22 | 1:L:337:ASN:OD1  | 2.18                     | 0.43              |
| 1:L:590:GLN:HA   | 1:L:594:VAL:HB   | 1.99                     | 0.43              |
| 1:A:140:ASN:HB3  | 1:A:455:THR:OG1  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:564:GLY:O    | 1:A:568:MET:HG2  | 2.18                     | 0.43              |
| 1:B:609:VAL:O    | 1:B:612:GLN:HB2  | 2.18                     | 0.43              |
| 1:C:65:ARG:O     | 1:C:69:SER:HB2   | 2.17                     | 0.43              |
| 1:C:338:ALA:O    | 1:C:342:ALA:N    | 2.46                     | 0.43              |
| 1:D:204:PRO:HD3  | 1:D:218:GLN:HG2  | 2.00                     | 0.43              |
| 1:D:587:PRO:HD2  | 1:D:589:GLU:HG3  | 1.99                     | 0.43              |
| 1:E:383:ASP:O    | 1:E:384:LEU:HD12 | 2.19                     | 0.43              |
| 1:F:444:LEU:O    | 1:F:448:VAL:HG23 | 2.17                     | 0.43              |
| 1:G:444:LEU:HD23 | 1:G:518:THR:HB   | 2.00                     | 0.43              |
| 1:G:525:GLN:HB2  | 1:G:529:GLN:OE1  | 2.18                     | 0.43              |
| 1:H:21:ALA:HB2   | 1:H:172:HIS:CD2  | 2.52                     | 0.43              |
| 1:I:151:SER:HB2  | 1:I:155:HIS:CE1  | 2.52                     | 0.43              |
| 1:I:223:TYR:HE1  | 1:I:278:LYS:HG3  | 1.84                     | 0.43              |
| 1:I:350:PHE:N    | 1:I:390:ALA:O    | 2.36                     | 0.43              |
| 1:J:444:LEU:O    | 1:J:447:TYR:HB3  | 2.18                     | 0.43              |
| 1:K:99:ARG:NH2   | 1:K:525:GLN:HA   | 2.32                     | 0.43              |
| 1:K:162:SER:OG   | 1:K:167:LYS:HA   | 2.18                     | 0.43              |
| 1:K:649:ARG:O    | 1:K:653:ILE:HG13 | 2.18                     | 0.43              |
| 1:L:29:ALA:O     | 1:L:33:LEU:HB2   | 2.18                     | 0.43              |
| 1:L:33:LEU:HD12  | 1:L:33:LEU:HA    | 1.89                     | 0.43              |
| 1:L:87:ARG:HD3   | 1:L:89:ASP:HB2   | 2.00                     | 0.43              |
| 1:A:376:ARG:NH1  | 1:L:355:GLN:HG2  | 2.27                     | 0.43              |
| 1:A:383:ASP:O    | 1:A:384:LEU:HD12 | 2.19                     | 0.43              |
| 1:A:528:LYS:HE3  | 1:A:558:THR:HB   | 2.01                     | 0.43              |
| 1:B:35:PHE:CZ    | 1:B:321:ARG:HB2  | 2.53                     | 0.43              |
| 1:B:99:ARG:NH2   | 1:B:525:GLN:HA   | 2.33                     | 0.43              |
| 1:B:538:LEU:O    | 1:B:542:THR:OG1  | 2.37                     | 0.43              |
| 1:C:35:PHE:CZ    | 1:C:321:ARG:HB2  | 2.54                     | 0.43              |
| 1:D:31:ASN:O     | 1:D:35:PHE:HD2   | 2.02                     | 0.43              |
| 1:E:398:PRO:O    | 1:E:399:GLN:HG2  | 2.19                     | 0.43              |
| 1:E:526:SER:O    | 1:E:530:GLN:N    | 2.49                     | 0.43              |
| 1:E:657:MET:SD   | 1:F:655:ASN:ND2  | 2.91                     | 0.43              |
| 1:G:238:PRO:HB3  | 1:G:263:PHE:CD1  | 2.53                     | 0.43              |
| 1:G:649:ARG:O    | 1:G:653:ILE:HG13 | 2.19                     | 0.43              |
| 1:H:436:ASN:HA   | 1:H:439:ASN:ND2  | 2.33                     | 0.43              |
| 1:H:438:LEU:O    | 1:H:442:ALA:N    | 2.40                     | 0.43              |
| 1:H:527:MET:HA   | 1:H:530:GLN:CD   | 2.44                     | 0.43              |
| 1:H:653:ILE:HG12 | 1:I:648:ALA:HA   | 1.99                     | 0.43              |
| 1:I:532:ARG:HH22 | 1:I:560:LEU:HD11 | 1.83                     | 0.43              |
| 1:I:564:GLY:O    | 1:I:568:MET:HG2  | 2.18                     | 0.43              |
| 1:J:97:MET:HE2   | 1:J:450:GLN:HE22 | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:383:ASP:O    | 1:J:384:LEU:HD12 | 2.18                     | 0.43              |
| 1:J:663:SER:O    | 1:J:666:ARG:HG3  | 2.18                     | 0.43              |
| 1:K:126:TRP:CD1  | 1:K:146:ARG:HG3  | 2.53                     | 0.43              |
| 1:K:383:ASP:O    | 1:K:384:LEU:HD12 | 2.18                     | 0.43              |
| 1:K:398:PRO:O    | 1:K:399:GLN:HG2  | 2.18                     | 0.43              |
| 1:K:578:GLN:HA   | 1:K:597:GLN:HE21 | 1.82                     | 0.43              |
| 1:L:114:ALA:O    | 1:L:118:GLN:HB2  | 2.19                     | 0.43              |
| 1:L:525:GLN:HB2  | 1:L:529:GLN:OE1  | 2.19                     | 0.43              |
| 1:A:672:VAL:HA   | 1:A:675:PHE:CD2  | 2.54                     | 0.43              |
| 1:B:114:ALA:O    | 1:B:118:GLN:HB2  | 2.18                     | 0.43              |
| 1:B:436:ASN:HA   | 1:B:439:ASN:ND2  | 2.32                     | 0.43              |
| 1:D:297:HIS:CG   | 1:D:298:ILE:H    | 2.36                     | 0.43              |
| 1:D:590:GLN:HA   | 1:D:594:VAL:HB   | 1.99                     | 0.43              |
| 1:E:99:ARG:NH2   | 1:E:525:GLN:HA   | 2.34                     | 0.43              |
| 1:E:546:THR:OG1  | 1:E:547:PRO:HD3  | 2.19                     | 0.43              |
| 1:F:55:GLY:N     | 1:F:335:SER:OG   | 2.49                     | 0.43              |
| 1:F:77:ASP:HB2   | 1:F:522:PRO:O    | 2.19                     | 0.43              |
| 1:F:220:ALA:CB   | 1:F:281:ILE:O    | 2.50                     | 0.43              |
| 1:F:225:VAL:HG22 | 1:F:276:VAL:HG12 | 2.01                     | 0.43              |
| 1:F:664:GLU:HG3  | 1:G:659:LEU:HD22 | 1.99                     | 0.43              |
| 1:G:695:GLU:HA   | 1:G:698:HIS:ND1  | 2.34                     | 0.43              |
| 1:H:83:LYS:HD2   | 1:H:515:GLU:CG   | 2.49                     | 0.43              |
| 1:H:248:LYS:HG2  | 1:H:511:ARG:HH21 | 1.83                     | 0.43              |
| 1:I:21:ALA:HB1   | 1:I:157:ILE:HB   | 2.01                     | 0.43              |
| 1:I:114:ALA:O    | 1:I:118:GLN:HB2  | 2.18                     | 0.43              |
| 1:K:514:TYR:HB2  | 1:L:136:SER:OG   | 2.18                     | 0.43              |
| 1:K:695:GLU:HA   | 1:K:698:HIS:ND1  | 2.33                     | 0.43              |
| 1:L:546:THR:OG1  | 1:L:547:PRO:HD3  | 2.19                     | 0.43              |
| 1:B:133:GLU:O    | 1:B:137:PRO:HB3  | 2.19                     | 0.43              |
| 1:C:434:THR:HG21 | 1:D:72:ARG:HG3   | 2.01                     | 0.43              |
| 1:D:201:PHE:HD1  | 1:D:283:CYS:HB2  | 1.84                     | 0.43              |
| 1:D:527:MET:HA   | 1:D:530:GLN:CD   | 2.43                     | 0.43              |
| 1:E:117:GLU:OE1  | 1:E:124:GLY:HA2  | 2.19                     | 0.43              |
| 1:E:223:TYR:HE1  | 1:E:278:LYS:HG3  | 1.83                     | 0.43              |
| 1:E:436:ASN:HA   | 1:E:439:ASN:ND2  | 2.34                     | 0.43              |
| 1:F:363:TYR:OH   | 1:F:373:LEU:O    | 2.16                     | 0.43              |
| 1:H:89:ASP:O     | 1:H:92:ASP:HB2   | 2.18                     | 0.43              |
| 1:H:252:LYS:HD2  | 1:H:256:ASP:HB3  | 2.00                     | 0.43              |
| 1:I:248:LYS:HE3  | 1:I:252:LYS:HB2  | 2.00                     | 0.43              |
| 1:I:640:GLU:HA   | 1:I:643:ASN:HD22 | 1.83                     | 0.43              |
| 1:I:642:GLN:HA   | 1:I:645:LEU:HD12 | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:695:GLU:HA   | 1:I:698:HIS:ND1  | 2.33                     | 0.43              |
| 1:J:53:TYR:CG    | 1:J:54:ARG:N     | 2.86                     | 0.43              |
| 1:J:609:VAL:O    | 1:J:612:GLN:HB2  | 2.19                     | 0.43              |
| 1:J:663:SER:HA   | 1:J:666:ARG:NE   | 2.29                     | 0.43              |
| 1:K:193:LEU:HD23 | 1:K:193:LEU:HA   | 1.90                     | 0.43              |
| 1:K:403:TYR:OH   | 1:L:397:VAL:HG11 | 2.19                     | 0.43              |
| 1:L:72:ARG:HH22  | 1:L:112:ASN:HA   | 1.83                     | 0.43              |
| 1:A:373:LEU:HD21 | 1:L:356:ILE:HG21 | 2.01                     | 0.43              |
| 1:A:609:VAL:O    | 1:A:612:GLN:HB2  | 2.19                     | 0.43              |
| 1:B:353:PRO:HD3  | 1:C:374:LEU:O    | 2.19                     | 0.43              |
| 1:B:383:ASP:O    | 1:B:384:LEU:HD12 | 2.19                     | 0.43              |
| 1:C:47:GLN:HB2   | 1:C:50:THR:CG2   | 2.48                     | 0.43              |
| 1:C:695:GLU:HA   | 1:C:698:HIS:CE1  | 2.54                     | 0.43              |
| 1:D:383:ASP:O    | 1:D:384:LEU:HD12 | 2.18                     | 0.43              |
| 1:D:662:GLN:HA   | 1:D:665:PHE:CD2  | 2.54                     | 0.43              |
| 1:F:383:ASP:O    | 1:F:384:LEU:HD12 | 2.18                     | 0.43              |
| 1:G:235:TYR:CE1  | 1:G:264:ILE:HA   | 2.53                     | 0.43              |
| 1:H:303:VAL:HG12 | 1:H:439:ASN:HB3  | 1.99                     | 0.43              |
| 1:H:642:GLN:HA   | 1:H:645:LEU:HD12 | 2.01                     | 0.43              |
| 1:I:35:PHE:CZ    | 1:I:321:ARG:HB2  | 2.53                     | 0.43              |
| 1:I:70:GLU:O     | 1:I:73:GLN:HG3   | 2.18                     | 0.43              |
| 1:I:78:VAL:HA    | 1:I:520:VAL:HA   | 2.00                     | 0.43              |
| 1:I:333:ILE:HG22 | 1:I:337:ASN:OD1  | 2.18                     | 0.43              |
| 1:J:21:ALA:HA    | 1:J:159:ASP:OD2  | 2.19                     | 0.43              |
| 1:J:249:ARG:HG3  | 1:J:250:ASP:N    | 2.33                     | 0.43              |
| 1:K:249:ARG:HG3  | 1:K:250:ASP:N    | 2.34                     | 0.43              |
| 1:L:640:GLU:HA   | 1:L:643:ASN:HD22 | 1.84                     | 0.43              |
| 1:A:146:ARG:HG2  | 1:A:148:PRO:HD3  | 2.01                     | 0.43              |
| 1:A:376:ARG:HD2  | 1:L:352:TRP:CB   | 2.40                     | 0.43              |
| 1:B:53:TYR:CG    | 1:B:54:ARG:N     | 2.87                     | 0.43              |
| 1:C:662:GLN:HA   | 1:C:665:PHE:CD2  | 2.53                     | 0.43              |
| 1:D:126:TRP:CD1  | 1:D:146:ARG:HG3  | 2.54                     | 0.43              |
| 1:D:165:MET:HB3  | 1:D:304:PHE:CG   | 2.53                     | 0.43              |
| 1:E:10:SER:O     | 1:E:14:ARG:HG2   | 2.18                     | 0.43              |
| 1:E:246:TYR:C    | 1:E:247:PHE:HD1  | 2.27                     | 0.43              |
| 1:G:120:GLU:HA   | 1:G:320:VAL:HB   | 1.99                     | 0.43              |
| 1:G:272:LYS:N    | 1:H:134:ASP:OD2  | 2.52                     | 0.43              |
| 1:G:383:ASP:O    | 1:G:384:LEU:HD12 | 2.18                     | 0.43              |
| 1:H:162:SER:HB2  | 1:H:170:ALA:HB2  | 1.99                     | 0.43              |
| 1:H:168:SER:HA   | 1:H:297:HIS:NE2  | 2.34                     | 0.43              |
| 1:H:246:TYR:C    | 1:H:247:PHE:HD1  | 2.27                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:47:GLN:HB2   | 1:I:50:THR:HG21  | 2.01                     | 0.43              |
| 1:I:662:GLN:HA   | 1:I:665:PHE:CD2  | 2.53                     | 0.43              |
| 1:K:350:PHE:CE1  | 1:L:372:TYR:HB3  | 2.53                     | 0.43              |
| 1:K:429:GLN:HA   | 1:K:432:PHE:HD2  | 1.84                     | 0.43              |
| 1:K:525:GLN:HB2  | 1:K:529:GLN:OE1  | 2.19                     | 0.43              |
| 1:K:593:LEU:O    | 1:K:597:GLN:HG3  | 2.19                     | 0.43              |
| 1:L:21:ALA:HB2   | 1:L:172:HIS:CD2  | 2.54                     | 0.43              |
| 1:A:623:ALA:HA   | 1:A:626:GLN:CD   | 2.43                     | 0.43              |
| 1:B:355:GLN:HA   | 1:B:375:ASN:HB3  | 2.01                     | 0.43              |
| 1:C:162:SER:OG   | 1:C:167:LYS:HA   | 2.19                     | 0.43              |
| 1:C:233:PHE:HB2  | 1:C:249:ARG:HB3  | 1.99                     | 0.43              |
| 1:E:133:GLU:O    | 1:E:137:PRO:HB3  | 2.19                     | 0.43              |
| 1:F:354:GLU:HG2  | 1:G:376:ARG:HD3  | 2.00                     | 0.43              |
| 1:H:24:GLU:HB2   | 1:H:159:ASP:OD2  | 2.19                     | 0.43              |
| 1:H:444:LEU:O    | 1:H:448:VAL:HG23 | 2.18                     | 0.43              |
| 1:I:438:LEU:HD11 | 1:J:108:LYS:HD3  | 1.99                     | 0.43              |
| 1:I:612:GLN:O    | 1:I:615:LEU:HD22 | 2.19                     | 0.43              |
| 1:J:38:VAL:HG22  | 1:J:43:ASP:OD1   | 2.19                     | 0.43              |
| 1:K:42:ASP:HB3   | 1:K:44:TRP:HD1   | 1.82                     | 0.43              |
| 1:K:225:VAL:HG22 | 1:K:276:VAL:HG12 | 2.01                     | 0.43              |
| 1:K:233:PHE:HB2  | 1:K:249:ARG:HB3  | 2.00                     | 0.43              |
| 1:K:410:SER:O    | 1:K:413:LYS:HG2  | 2.18                     | 0.43              |
| 1:K:434:THR:HG21 | 1:L:72:ARG:HG3   | 2.01                     | 0.43              |
| 1:A:80:TYR:HB3   | 1:A:95:MET:HE2   | 2.01                     | 0.43              |
| 1:B:538:LEU:HB3  | 1:B:551:LEU:HD11 | 2.01                     | 0.43              |
| 1:C:161:ASN:ND2  | 1:D:183:GLY:HA3  | 2.34                     | 0.43              |
| 1:C:538:LEU:HB3  | 1:C:551:LEU:HD11 | 2.01                     | 0.43              |
| 1:D:99:ARG:NE    | 1:D:525:GLN:O    | 2.52                     | 0.43              |
| 1:E:47:GLN:HB2   | 1:E:50:THR:HG21  | 1.99                     | 0.43              |
| 1:E:73:GLN:C     | 1:E:75:PRO:HD3   | 2.44                     | 0.43              |
| 1:E:333:ILE:HG22 | 1:E:337:ASN:OD1  | 2.18                     | 0.43              |
| 1:F:228:LYS:HB2  | 1:F:275:ARG:HB3  | 2.01                     | 0.43              |
| 1:G:99:ARG:NH2   | 1:G:525:GLN:HA   | 2.34                     | 0.43              |
| 1:H:621:GLU:OE2  | 1:I:616:LEU:HA   | 2.19                     | 0.43              |
| 1:I:663:SER:HA   | 1:I:666:ARG:HG2  | 2.01                     | 0.43              |
| 1:L:613:GLY:O    | 1:L:616:LEU:N    | 2.51                     | 0.43              |
| 1:L:613:GLY:C    | 1:L:616:LEU:HD12 | 2.44                     | 0.43              |
| 1:A:559:LEU:HB3  | 1:A:565:VAL:HB   | 2.01                     | 0.42              |
| 1:B:75:PRO:HD2   | 1:B:523:SER:HB3  | 2.01                     | 0.42              |
| 1:C:117:GLU:OE1  | 1:C:124:GLY:HA2  | 2.19                     | 0.42              |
| 1:C:323:THR:HG22 | 1:C:415:VAL:CG2  | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:411:ALA:O    | 1:C:415:VAL:HG22 | 2.19                     | 0.42              |
| 1:D:57:PHE:HB2   | 1:D:334:MET:SD   | 2.59                     | 0.42              |
| 1:E:525:GLN:HB2  | 1:E:529:GLN:OE1  | 2.19                     | 0.42              |
| 1:F:32:ASP:HA    | 1:F:35:PHE:CD2   | 2.54                     | 0.42              |
| 1:F:133:GLU:O    | 1:F:137:PRO:HB3  | 2.19                     | 0.42              |
| 1:F:146:ARG:HG2  | 1:F:148:PRO:HD3  | 2.01                     | 0.42              |
| 1:F:380:ASN:OD1  | 1:F:381:SER:N    | 2.50                     | 0.42              |
| 1:F:398:PRO:O    | 1:F:399:GLN:HG2  | 2.19                     | 0.42              |
| 1:G:275:ARG:NH2  | 1:G:293:ILE:O    | 2.38                     | 0.42              |
| 1:H:57:PHE:CG    | 1:H:334:MET:HE1  | 2.54                     | 0.42              |
| 1:H:338:ALA:O    | 1:H:342:ALA:N    | 2.52                     | 0.42              |
| 1:H:514:TYR:HB2  | 1:I:136:SER:OG   | 2.19                     | 0.42              |
| 1:I:353:PRO:HD3  | 1:J:374:LEU:O    | 2.19                     | 0.42              |
| 1:I:538:LEU:O    | 1:I:542:THR:OG1  | 2.37                     | 0.42              |
| 1:I:559:LEU:HB3  | 1:I:565:VAL:HB   | 2.01                     | 0.42              |
| 1:K:35:PHE:CZ    | 1:K:321:ARG:HB2  | 2.54                     | 0.42              |
| 1:K:559:LEU:HB3  | 1:K:565:VAL:HB   | 2.01                     | 0.42              |
| 1:L:110:ALA:HB1  | 1:L:126:TRP:CE3  | 2.53                     | 0.42              |
| 1:L:429:GLN:HA   | 1:L:432:PHE:CD2  | 2.53                     | 0.42              |
| 1:A:99:ARG:NH2   | 1:A:525:GLN:HA   | 2.34                     | 0.42              |
| 1:A:126:TRP:CD1  | 1:A:146:ARG:HG3  | 2.54                     | 0.42              |
| 1:B:252:LYS:HD2  | 1:B:256:ASP:HB3  | 2.01                     | 0.42              |
| 1:C:42:ASP:HB3   | 1:C:44:TRP:HD1   | 1.84                     | 0.42              |
| 1:C:114:ALA:O    | 1:C:118:GLN:HB2  | 2.19                     | 0.42              |
| 1:C:564:GLY:O    | 1:C:568:MET:HG2  | 2.19                     | 0.42              |
| 1:D:664:GLU:HG3  | 1:E:659:LEU:HD22 | 2.01                     | 0.42              |
| 1:E:403:TYR:OH   | 1:F:397:VAL:HG11 | 2.19                     | 0.42              |
| 1:F:436:ASN:HA   | 1:F:439:ASN:ND2  | 2.34                     | 0.42              |
| 1:F:695:GLU:HA   | 1:F:698:HIS:ND1  | 2.34                     | 0.42              |
| 1:G:246:TYR:C    | 1:G:247:PHE:HD1  | 2.26                     | 0.42              |
| 1:G:311:GLU:O    | 1:G:312:ASP:CG   | 2.62                     | 0.42              |
| 1:I:248:LYS:CD   | 1:I:251:ILE:HB   | 2.42                     | 0.42              |
| 1:I:538:LEU:HB3  | 1:I:551:LEU:HD11 | 2.01                     | 0.42              |
| 1:J:133:GLU:O    | 1:J:137:PRO:HB3  | 2.19                     | 0.42              |
| 1:J:578:GLN:HA   | 1:J:597:GLN:HE21 | 1.83                     | 0.42              |
| 1:L:231:THR:HG22 | 1:L:249:ARG:HE   | 1.84                     | 0.42              |
| 1:B:10:SER:O     | 1:B:14:ARG:HG2   | 2.19                     | 0.42              |
| 1:C:31:ASN:O     | 1:C:35:PHE:HD2   | 2.02                     | 0.42              |
| 1:C:246:TYR:C    | 1:C:247:PHE:HD1  | 2.27                     | 0.42              |
| 1:C:383:ASP:O    | 1:C:384:LEU:HD12 | 2.19                     | 0.42              |
| 1:D:430:VAL:O    | 1:D:433:ASP:HB2  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:546:THR:OG1  | 1:D:547:PRO:HD3  | 2.19                     | 0.42              |
| 1:E:70:GLU:O     | 1:E:73:GLN:HG3   | 2.18                     | 0.42              |
| 1:E:297:HIS:CG   | 1:E:298:ILE:H    | 2.38                     | 0.42              |
| 1:H:21:ALA:HB2   | 1:H:172:HIS:NE2  | 2.34                     | 0.42              |
| 1:H:42:ASP:OD2   | 1:H:44:TRP:NE1   | 2.53                     | 0.42              |
| 1:H:311:GLU:O    | 1:H:312:ASP:CG   | 2.62                     | 0.42              |
| 1:I:383:ASP:O    | 1:I:384:LEU:HD12 | 2.19                     | 0.42              |
| 1:K:444:LEU:HD23 | 1:K:518:THR:HB   | 2.01                     | 0.42              |
| 1:L:649:ARG:O    | 1:L:653:ILE:HG13 | 2.19                     | 0.42              |
| 1:A:83:LYS:HG2   | 1:A:84:ASP:C     | 2.45                     | 0.42              |
| 1:A:204:PRO:HD3  | 1:A:218:GLN:HG2  | 2.01                     | 0.42              |
| 1:B:309:PHE:HB2  | 1:C:150:HIS:HB2  | 2.01                     | 0.42              |
| 1:C:400:ALA:O    | 1:C:404:MET:HB2  | 2.19                     | 0.42              |
| 1:C:613:GLY:C    | 1:C:616:LEU:HD13 | 2.45                     | 0.42              |
| 1:D:220:ALA:CB   | 1:D:281:ILE:O    | 2.52                     | 0.42              |
| 1:E:514:TYR:HB2  | 1:F:136:SER:OG   | 2.18                     | 0.42              |
| 1:E:661:LYS:HE3  | 1:E:665:PHE:CZ   | 2.54                     | 0.42              |
| 1:F:152:ALA:HA   | 1:F:155:HIS:HB2  | 2.01                     | 0.42              |
| 1:G:21:ALA:HB1   | 1:G:157:ILE:HB   | 2.01                     | 0.42              |
| 1:H:126:TRP:CD1  | 1:H:146:ARG:HG3  | 2.54                     | 0.42              |
| 1:H:204:PRO:HD3  | 1:H:218:GLN:HG2  | 2.02                     | 0.42              |
| 1:H:320:VAL:O    | 1:H:324:LYS:HG3  | 2.20                     | 0.42              |
| 1:I:325:ASP:O    | 1:I:326:GLY:C    | 2.63                     | 0.42              |
| 1:J:27:ARG:HH11  | 1:J:313:LYS:HE3  | 1.84                     | 0.42              |
| 1:J:73:GLN:C     | 1:J:75:PRO:HD3   | 2.43                     | 0.42              |
| 1:J:223:TYR:CE1  | 1:J:278:LYS:HG3  | 2.55                     | 0.42              |
| 1:L:613:GLY:HA2  | 1:L:616:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:337:ASN:HA   | 1:A:340:ILE:HD12 | 2.01                     | 0.42              |
| 1:A:374:LEU:O    | 1:L:353:PRO:HD3  | 2.18                     | 0.42              |
| 1:A:590:GLN:HA   | 1:A:594:VAL:HB   | 2.01                     | 0.42              |
| 1:A:695:GLU:HA   | 1:A:698:HIS:ND1  | 2.35                     | 0.42              |
| 1:B:281:ILE:HG23 | 1:B:286:VAL:HA   | 2.02                     | 0.42              |
| 1:C:133:GLU:O    | 1:C:137:PRO:HB3  | 2.19                     | 0.42              |
| 1:D:72:ARG:HH22  | 1:D:112:ASN:HA   | 1.84                     | 0.42              |
| 1:D:233:PHE:HB2  | 1:D:249:ARG:HB3  | 2.01                     | 0.42              |
| 1:D:246:TYR:C    | 1:D:247:PHE:HD1  | 2.27                     | 0.42              |
| 1:D:363:TYR:CE1  | 1:D:372:TYR:HA   | 2.54                     | 0.42              |
| 1:D:614:VAL:HG11 | 1:E:609:VAL:HG11 | 2.00                     | 0.42              |
| 1:E:24:GLU:HB2   | 1:E:159:ASP:OD2  | 2.20                     | 0.42              |
| 1:E:53:TYR:O     | 1:E:54:ARG:NH1   | 2.48                     | 0.42              |
| 1:E:78:VAL:HA    | 1:E:520:VAL:HA   | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:31:ASN:O     | 1:G:35:PHE:HD2   | 2.02                     | 0.42              |
| 1:G:248:LYS:CD   | 1:G:251:ILE:HB   | 2.44                     | 0.42              |
| 1:H:586:THR:CG2  | 1:H:590:GLN:HE22 | 2.27                     | 0.42              |
| 1:I:26:ARG:O     | 1:I:30:LYS:HG3   | 2.19                     | 0.42              |
| 1:I:57:PHE:HB2   | 1:I:334:MET:SD   | 2.60                     | 0.42              |
| 1:I:80:TYR:CZ    | 1:I:516:CYS:HB2  | 2.54                     | 0.42              |
| 1:J:65:ARG:O     | 1:J:69:SER:HB2   | 2.20                     | 0.42              |
| 1:J:311:GLU:O    | 1:J:312:ASP:CG   | 2.63                     | 0.42              |
| 1:K:99:ARG:NE    | 1:K:525:GLN:O    | 2.51                     | 0.42              |
| 1:K:133:GLU:O    | 1:K:137:PRO:HB3  | 2.19                     | 0.42              |
| 1:K:246:TYR:C    | 1:K:247:PHE:HD1  | 2.28                     | 0.42              |
| 1:L:447:TYR:O    | 1:L:450:GLN:HB3  | 2.19                     | 0.42              |
| 1:L:671:THR:HG22 | 1:L:675:PHE:CZ   | 2.54                     | 0.42              |
| 1:A:281:ILE:HG12 | 1:A:287:LEU:H    | 1.84                     | 0.42              |
| 1:A:652:GLU:O    | 1:A:656:ASN:HB2  | 2.19                     | 0.42              |
| 1:B:77:ASP:HB2   | 1:B:522:PRO:O    | 2.18                     | 0.42              |
| 1:C:325:ASP:O    | 1:C:326:GLY:C    | 2.63                     | 0.42              |
| 1:D:411:ALA:O    | 1:D:415:VAL:HG22 | 2.19                     | 0.42              |
| 1:D:429:GLN:HA   | 1:D:432:PHE:HD2  | 1.84                     | 0.42              |
| 1:D:663:SER:HA   | 1:D:666:ARG:HG2  | 2.01                     | 0.42              |
| 1:E:26:ARG:O     | 1:E:30:LYS:HG3   | 2.20                     | 0.42              |
| 1:E:233:PHE:HB2  | 1:E:249:ARG:HB3  | 2.01                     | 0.42              |
| 1:E:320:VAL:O    | 1:E:324:LYS:HG3  | 2.20                     | 0.42              |
| 1:E:701:ARG:HA   | 1:E:704:ILE:HD12 | 2.02                     | 0.42              |
| 1:G:232:ALA:HA   | 1:G:269:ARG:H    | 1.84                     | 0.42              |
| 1:H:248:LYS:CD   | 1:H:251:ILE:HB   | 2.41                     | 0.42              |
| 1:I:444:LEU:HD23 | 1:I:518:THR:HB   | 2.00                     | 0.42              |
| 1:J:248:LYS:CD   | 1:J:251:ILE:HB   | 2.43                     | 0.42              |
| 1:J:663:SER:HA   | 1:J:666:ARG:HG2  | 2.02                     | 0.42              |
| 1:K:447:TYR:O    | 1:K:450:GLN:HB3  | 2.19                     | 0.42              |
| 1:L:21:ALA:HB2   | 1:L:172:HIS:NE2  | 2.35                     | 0.42              |
| 1:L:73:GLN:C     | 1:L:75:PRO:HD3   | 2.45                     | 0.42              |
| 1:L:252:LYS:HD2  | 1:L:256:ASP:HB3  | 2.01                     | 0.42              |
| 1:A:21:ALA:HB1   | 1:A:157:ILE:HB   | 2.00                     | 0.42              |
| 1:A:31:ASN:O     | 1:A:35:PHE:HD2   | 2.01                     | 0.42              |
| 1:B:165:MET:HB3  | 1:B:304:PHE:CG   | 2.55                     | 0.42              |
| 1:B:236:GLN:HG2  | 1:B:244:VAL:H    | 1.84                     | 0.42              |
| 1:C:53:TYR:O     | 1:C:54:ARG:NH1   | 2.50                     | 0.42              |
| 1:D:695:GLU:HA   | 1:D:698:HIS:ND1  | 2.35                     | 0.42              |
| 1:E:31:ASN:O     | 1:E:35:PHE:HD2   | 2.02                     | 0.42              |
| 1:F:338:ALA:O    | 1:F:342:ALA:N    | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:142:GLN:NE2  | 1:G:455:THR:OG1  | 2.53                     | 0.42              |
| 1:G:546:THR:OG1  | 1:G:547:PRO:HD3  | 2.19                     | 0.42              |
| 1:J:10:SER:O     | 1:J:14:ARG:HG2   | 2.20                     | 0.42              |
| 1:L:420:VAL:HB   | 1:L:424:ALA:HA   | 2.00                     | 0.42              |
| 1:A:193:LEU:HD23 | 1:A:193:LEU:HA   | 1.92                     | 0.42              |
| 1:A:252:LYS:HD2  | 1:A:256:ASP:HB3  | 2.00                     | 0.42              |
| 1:A:297:HIS:CG   | 1:A:298:ILE:H    | 2.37                     | 0.42              |
| 1:A:653:ILE:HG12 | 1:B:648:ALA:HA   | 2.01                     | 0.42              |
| 1:B:307:TRP:HE1  | 1:B:314:GLU:HG2  | 1.85                     | 0.42              |
| 1:B:311:GLU:O    | 1:B:312:ASP:CG   | 2.63                     | 0.42              |
| 1:B:539:LEU:HG   | 1:B:551:LEU:HD22 | 2.02                     | 0.42              |
| 1:D:97:MET:HE2   | 1:D:450:GLN:HE22 | 1.84                     | 0.42              |
| 1:D:117:GLU:OE1  | 1:D:124:GLY:HA2  | 2.19                     | 0.42              |
| 1:D:248:LYS:CD   | 1:D:251:ILE:HB   | 2.44                     | 0.42              |
| 1:E:162:SER:OG   | 1:E:167:LYS:HA   | 2.20                     | 0.42              |
| 1:E:275:ARG:NH2  | 1:E:293:ILE:O    | 2.40                     | 0.42              |
| 1:E:564:GLY:O    | 1:E:568:MET:HG2  | 2.19                     | 0.42              |
| 1:G:249:ARG:HG3  | 1:G:250:ASP:N    | 2.34                     | 0.42              |
| 1:G:354:GLU:HG2  | 1:H:376:ARG:HD3  | 2.01                     | 0.42              |
| 1:H:383:ASP:O    | 1:H:384:LEU:HD12 | 2.19                     | 0.42              |
| 1:I:24:GLU:HB2   | 1:I:159:ASP:OD2  | 2.20                     | 0.42              |
| 1:I:404:MET:HA   | 1:I:407:ALA:HB3  | 2.02                     | 0.42              |
| 1:I:411:ALA:HA   | 1:J:57:PHE:HE1   | 1.83                     | 0.42              |
| 1:J:411:ALA:O    | 1:J:415:VAL:HG22 | 2.19                     | 0.42              |
| 1:K:546:THR:OG1  | 1:K:547:PRO:HD3  | 2.19                     | 0.42              |
| 1:K:613:GLY:HA2  | 1:K:616:LEU:CD1  | 2.46                     | 0.42              |
| 1:A:311:GLU:O    | 1:A:312:ASP:CG   | 2.63                     | 0.42              |
| 1:B:21:ALA:HB2   | 1:B:172:HIS:CD2  | 2.55                     | 0.42              |
| 1:B:81:ARG:HB2   | 1:B:517:TYR:CZ   | 2.55                     | 0.42              |
| 1:C:38:VAL:HG22  | 1:C:43:ASP:OD1   | 2.20                     | 0.42              |
| 1:C:609:VAL:O    | 1:C:612:GLN:HB2  | 2.20                     | 0.42              |
| 1:D:120:GLU:HA   | 1:D:320:VAL:HB   | 2.01                     | 0.42              |
| 1:D:203:ASN:HD21 | 1:D:209:PHE:HZ   | 1.68                     | 0.42              |
| 1:E:89:ASP:O     | 1:E:92:ASP:HB2   | 2.20                     | 0.42              |
| 1:E:99:ARG:O     | 1:E:103:ARG:N    | 2.53                     | 0.42              |
| 1:F:78:VAL:HA    | 1:F:520:VAL:HA   | 2.01                     | 0.42              |
| 1:F:193:LEU:HD23 | 1:F:193:LEU:HA   | 1.88                     | 0.42              |
| 1:F:246:TYR:HB2  | 1:F:511:ARG:H    | 1.85                     | 0.42              |
| 1:H:75:PRO:HD2   | 1:H:523:SER:HB3  | 2.01                     | 0.42              |
| 1:H:235:TYR:HE1  | 1:H:264:ILE:HA   | 1.85                     | 0.42              |
| 1:H:434:THR:HG21 | 1:I:72:ARG:HG3   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:622:LEU:O    | 1:I:626:GLN:HG3  | 2.20                     | 0.42              |
| 1:J:246:TYR:C    | 1:J:247:PHE:HD1  | 2.27                     | 0.42              |
| 1:K:311:GLU:O    | 1:K:312:ASP:CG   | 2.63                     | 0.42              |
| 1:L:297:HIS:CG   | 1:L:298:ILE:N    | 2.87                     | 0.42              |
| 1:L:538:LEU:O    | 1:L:542:THR:OG1  | 2.38                     | 0.42              |
| 1:A:21:ALA:HB2   | 1:A:172:HIS:CD2  | 2.54                     | 0.42              |
| 1:A:660:SER:O    | 1:A:663:SER:OG   | 2.24                     | 0.42              |
| 1:C:307:TRP:HE1  | 1:C:314:GLU:HG2  | 1.85                     | 0.42              |
| 1:C:649:ARG:O    | 1:C:653:ILE:HG13 | 2.20                     | 0.42              |
| 1:D:623:ALA:O    | 1:D:626:GLN:HB2  | 2.20                     | 0.42              |
| 1:D:628:GLN:O    | 1:D:632:LEU:HB2  | 2.19                     | 0.42              |
| 1:E:176:ILE:HD11 | 1:E:204:PRO:HB3  | 2.01                     | 0.42              |
| 1:E:623:ALA:O    | 1:E:626:GLN:HB2  | 2.19                     | 0.42              |
| 1:G:73:GLN:C     | 1:G:75:PRO:HD3   | 2.45                     | 0.42              |
| 1:G:642:GLN:HA   | 1:G:645:LEU:HD12 | 2.01                     | 0.42              |
| 1:H:235:TYR:HA   | 1:H:265:LYS:O    | 2.20                     | 0.42              |
| 1:H:447:TYR:O    | 1:H:450:GLN:HB3  | 2.20                     | 0.42              |
| 1:I:21:ALA:HB2   | 1:I:172:HIS:CD2  | 2.54                     | 0.42              |
| 1:J:162:SER:OG   | 1:J:164:LEU:O    | 2.38                     | 0.42              |
| 1:K:297:HIS:CG   | 1:K:298:ILE:N    | 2.88                     | 0.42              |
| 1:B:55:GLY:N     | 1:B:335:SER:OG   | 2.52                     | 0.41              |
| 1:C:236:GLN:HA   | 1:C:245:SER:H    | 1.85                     | 0.41              |
| 1:C:311:GLU:O    | 1:C:312:ASP:CG   | 2.63                     | 0.41              |
| 1:C:448:VAL:HG12 | 1:C:514:TYR:CE1  | 2.55                     | 0.41              |
| 1:C:622:LEU:O    | 1:C:626:GLN:HG3  | 2.20                     | 0.41              |
| 1:D:35:PHE:CZ    | 1:D:321:ARG:HB2  | 2.55                     | 0.41              |
| 1:D:581:VAL:HG22 | 1:E:567:MET:HB2  | 2.01                     | 0.41              |
| 1:D:623:ALA:HA   | 1:D:626:GLN:CD   | 2.44                     | 0.41              |
| 1:E:532:ARG:HH22 | 1:E:560:LEU:HD11 | 1.85                     | 0.41              |
| 1:E:660:SER:O    | 1:E:663:SER:OG   | 2.24                     | 0.41              |
| 1:F:47:GLN:HB2   | 1:F:50:THR:HG21  | 2.02                     | 0.41              |
| 1:F:57:PHE:CG    | 1:F:334:MET:HE1  | 2.55                     | 0.41              |
| 1:F:124:GLY:CA   | 1:F:303:VAL:HG22 | 2.49                     | 0.41              |
| 1:G:117:GLU:OE1  | 1:G:124:GLY:HA2  | 2.20                     | 0.41              |
| 1:G:628:GLN:O    | 1:G:632:LEU:HB2  | 2.19                     | 0.41              |
| 1:G:641:ALA:HA   | 1:G:644:GLN:OE1  | 2.20                     | 0.41              |
| 1:H:231:THR:HG22 | 1:H:249:ARG:HE   | 1.85                     | 0.41              |
| 1:H:410:SER:O    | 1:H:413:LYS:HG2  | 2.20                     | 0.41              |
| 1:J:162:SER:OG   | 1:J:167:LYS:HA   | 2.20                     | 0.41              |
| 1:J:297:HIS:CG   | 1:J:298:ILE:H    | 2.37                     | 0.41              |
| 1:K:532:ARG:HH22 | 1:K:560:LEU:HD11 | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:31:ASN:O     | 1:L:35:PHE:HD2   | 2.02                     | 0.41              |
| 1:A:83:LYS:HD2   | 1:A:515:GLU:CG   | 2.50                     | 0.41              |
| 1:B:238:PRO:HB3  | 1:B:263:PHE:CD1  | 2.55                     | 0.41              |
| 1:B:325:ASP:HA   | 1:B:328:ARG:NH1  | 2.36                     | 0.41              |
| 1:B:695:GLU:HA   | 1:B:698:HIS:ND1  | 2.35                     | 0.41              |
| 1:C:47:GLN:HB2   | 1:C:50:THR:HG21  | 2.01                     | 0.41              |
| 1:C:151:SER:O    | 1:C:155:HIS:ND1  | 2.44                     | 0.41              |
| 1:C:162:SER:HB2  | 1:C:170:ALA:HB2  | 2.02                     | 0.41              |
| 1:C:248:LYS:CD   | 1:C:251:ILE:HB   | 2.43                     | 0.41              |
| 1:C:357:ALA:HA   | 1:C:360:GLU:OE2  | 2.20                     | 0.41              |
| 1:C:710:SER:O    | 1:C:714:ASN:HB2  | 2.20                     | 0.41              |
| 1:D:73:GLN:C     | 1:D:75:PRO:HD3   | 2.45                     | 0.41              |
| 1:D:193:LEU:HD21 | 1:D:288:LYS:HZ3  | 1.85                     | 0.41              |
| 1:D:248:LYS:HE3  | 1:D:252:LYS:HB2  | 2.02                     | 0.41              |
| 1:D:323:THR:HG22 | 1:D:415:VAL:CG2  | 2.50                     | 0.41              |
| 1:D:564:GLY:O    | 1:D:568:MET:HG2  | 2.19                     | 0.41              |
| 1:D:663:SER:O    | 1:D:666:ARG:HG3  | 2.19                     | 0.41              |
| 1:E:171:ARG:NH1  | 1:F:186:ASP:OD2  | 2.52                     | 0.41              |
| 1:F:233:PHE:HB2  | 1:F:249:ARG:HB3  | 2.02                     | 0.41              |
| 1:G:21:ALA:HB2   | 1:G:172:HIS:CD2  | 2.54                     | 0.41              |
| 1:G:403:TYR:OH   | 1:H:397:VAL:HG11 | 2.21                     | 0.41              |
| 1:H:695:GLU:HA   | 1:H:698:HIS:ND1  | 2.34                     | 0.41              |
| 1:I:133:GLU:O    | 1:I:137:PRO:HB3  | 2.20                     | 0.41              |
| 1:I:307:TRP:HE1  | 1:I:314:GLU:HG2  | 1.85                     | 0.41              |
| 1:J:57:PHE:HB2   | 1:J:334:MET:SD   | 2.60                     | 0.41              |
| 1:J:146:ARG:HG2  | 1:J:148:PRO:HD3  | 2.02                     | 0.41              |
| 1:J:275:ARG:HD2  | 1:J:296:GLU:HG2  | 2.02                     | 0.41              |
| 1:J:546:THR:OG1  | 1:J:547:PRO:HD3  | 2.19                     | 0.41              |
| 1:J:564:GLY:O    | 1:J:568:MET:HG2  | 2.20                     | 0.41              |
| 1:K:652:GLU:O    | 1:K:656:ASN:HB2  | 2.21                     | 0.41              |
| 1:L:386:THR:HG22 | 1:L:387:GLN:N    | 2.35                     | 0.41              |
| 1:A:325:ASP:O    | 1:A:326:GLY:C    | 2.63                     | 0.41              |
| 1:C:120:GLU:HA   | 1:C:320:VAL:HB   | 2.02                     | 0.41              |
| 1:C:231:THR:HG22 | 1:C:249:ARG:HE   | 1.85                     | 0.41              |
| 1:D:444:LEU:HD23 | 1:D:518:THR:HB   | 2.01                     | 0.41              |
| 1:E:35:PHE:HD2   | 1:E:35:PHE:H     | 1.68                     | 0.41              |
| 1:F:623:ALA:O    | 1:F:626:GLN:HB2  | 2.21                     | 0.41              |
| 1:G:29:ALA:O     | 1:G:33:LEU:HB2   | 2.20                     | 0.41              |
| 1:G:231:THR:HG22 | 1:G:249:ARG:HE   | 1.84                     | 0.41              |
| 1:H:83:LYS:HG2   | 1:H:84:ASP:C     | 2.45                     | 0.41              |
| 1:H:120:GLU:HA   | 1:H:320:VAL:HB   | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:411:ALA:O    | 1:H:415:VAL:HG22 | 2.21                     | 0.41              |
| 1:I:276:VAL:HG11 | 1:I:297:HIS:O    | 2.20                     | 0.41              |
| 1:I:311:GLU:O    | 1:I:312:ASP:CG   | 2.63                     | 0.41              |
| 1:I:546:THR:OG1  | 1:I:547:PRO:HD3  | 2.21                     | 0.41              |
| 1:J:235:TYR:HE1  | 1:J:264:ILE:HA   | 1.84                     | 0.41              |
| 1:J:355:GLN:HA   | 1:J:375:ASN:HB3  | 2.02                     | 0.41              |
| 1:L:441:ARG:O    | 1:L:444:LEU:HB3  | 2.20                     | 0.41              |
| 1:B:57:PHE:HB2   | 1:B:334:MET:SD   | 2.60                     | 0.41              |
| 1:C:72:ARG:NH2   | 1:C:111:VAL:HG12 | 2.34                     | 0.41              |
| 1:D:45:LEU:HG    | 1:D:46:SER:H     | 1.84                     | 0.41              |
| 1:F:83:LYS:HD2   | 1:F:515:GLU:CG   | 2.51                     | 0.41              |
| 1:G:110:ALA:HB1  | 1:G:126:TRP:CE3  | 2.56                     | 0.41              |
| 1:H:246:TYR:HB2  | 1:H:511:ARG:H    | 1.85                     | 0.41              |
| 1:H:389:LEU:HD23 | 1:H:389:LEU:HA   | 1.89                     | 0.41              |
| 1:I:297:HIS:CG   | 1:I:298:ILE:H    | 2.38                     | 0.41              |
| 1:J:57:PHE:CG    | 1:J:334:MET:HE1  | 2.55                     | 0.41              |
| 1:J:83:LYS:HD2   | 1:J:515:GLU:CG   | 2.50                     | 0.41              |
| 1:J:398:PRO:O    | 1:J:399:GLN:HG2  | 2.20                     | 0.41              |
| 1:J:593:LEU:O    | 1:J:597:GLN:HG3  | 2.21                     | 0.41              |
| 1:K:509:ASP:OD2  | 1:K:513:ARG:NH2  | 2.53                     | 0.41              |
| 1:L:641:ALA:HA   | 1:L:644:GLN:OE1  | 2.21                     | 0.41              |
| 1:A:411:ALA:HA   | 1:B:57:PHE:HE1   | 1.84                     | 0.41              |
| 1:A:438:LEU:O    | 1:A:442:ALA:N    | 2.42                     | 0.41              |
| 1:A:646:ASN:HA   | 1:B:644:GLN:HG2  | 2.02                     | 0.41              |
| 1:B:231:THR:HG22 | 1:B:249:ARG:HE   | 1.85                     | 0.41              |
| 1:C:386:THR:HG22 | 1:C:387:GLN:N    | 2.35                     | 0.41              |
| 1:C:621:GLU:OE2  | 1:D:616:LEU:HA   | 2.20                     | 0.41              |
| 1:C:628:GLN:O    | 1:C:632:LEU:HB2  | 2.21                     | 0.41              |
| 1:D:386:THR:HG22 | 1:D:387:GLN:N    | 2.35                     | 0.41              |
| 1:D:441:ARG:O    | 1:D:444:LEU:HB3  | 2.21                     | 0.41              |
| 1:E:193:LEU:HD23 | 1:E:193:LEU:HA   | 1.91                     | 0.41              |
| 1:E:311:GLU:O    | 1:E:312:ASP:CG   | 2.63                     | 0.41              |
| 1:F:231:THR:HG22 | 1:F:249:ARG:HE   | 1.85                     | 0.41              |
| 1:F:386:THR:HG22 | 1:F:387:GLN:N    | 2.36                     | 0.41              |
| 1:F:509:ASP:OD2  | 1:F:513:ARG:NH2  | 2.53                     | 0.41              |
| 1:F:546:THR:OG1  | 1:F:547:PRO:HD3  | 2.21                     | 0.41              |
| 1:G:320:VAL:O    | 1:G:323:THR:OG1  | 2.21                     | 0.41              |
| 1:G:663:SER:HA   | 1:G:666:ARG:HG2  | 2.01                     | 0.41              |
| 1:H:564:GLY:O    | 1:H:568:MET:HG2  | 2.20                     | 0.41              |
| 1:I:105:ASN:O    | 1:I:109:ILE:HG12 | 2.21                     | 0.41              |
| 1:I:246:TYR:C    | 1:I:247:PHE:HD1  | 2.27                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:320:VAL:O    | 1:J:324:LYS:HG3  | 2.21                     | 0.41              |
| 1:K:120:GLU:HA   | 1:K:320:VAL:HB   | 2.03                     | 0.41              |
| 1:K:333:ILE:HG22 | 1:K:337:ASN:OD1  | 2.20                     | 0.41              |
| 1:L:47:GLN:HB2   | 1:L:50:THR:HG21  | 2.02                     | 0.41              |
| 1:L:162:SER:OG   | 1:L:167:LYS:HA   | 2.20                     | 0.41              |
| 1:L:246:TYR:C    | 1:L:247:PHE:HD1  | 2.27                     | 0.41              |
| 1:L:311:GLU:O    | 1:L:312:ASP:CG   | 2.63                     | 0.41              |
| 1:A:110:ALA:HB1  | 1:A:126:TRP:CE3  | 2.56                     | 0.41              |
| 1:A:436:ASN:HA   | 1:A:439:ASN:ND2  | 2.34                     | 0.41              |
| 1:B:447:TYR:O    | 1:B:450:GLN:HB3  | 2.20                     | 0.41              |
| 1:B:541:LYS:HE2  | 1:B:541:LYS:HB3  | 1.91                     | 0.41              |
| 1:C:281:ILE:HG23 | 1:C:286:VAL:HA   | 2.03                     | 0.41              |
| 1:C:546:THR:OG1  | 1:C:547:PRO:HD3  | 2.19                     | 0.41              |
| 1:E:106:THR:HG23 | 1:E:146:ARG:HE   | 1.86                     | 0.41              |
| 1:E:232:ALA:HA   | 1:E:269:ARG:H    | 1.86                     | 0.41              |
| 1:F:151:SER:HB3  | 1:F:154:SER:OG   | 2.20                     | 0.41              |
| 1:G:38:VAL:HG22  | 1:G:43:ASP:OD1   | 2.20                     | 0.41              |
| 1:G:325:ASP:O    | 1:G:326:GLY:C    | 2.63                     | 0.41              |
| 1:G:526:SER:O    | 1:G:530:GLN:N    | 2.49                     | 0.41              |
| 1:H:276:VAL:HG23 | 1:H:293:ILE:HD13 | 2.02                     | 0.41              |
| 1:H:325:ASP:O    | 1:H:326:GLY:C    | 2.63                     | 0.41              |
| 1:I:70:GLU:OE1   | 1:I:429:GLN:HG3  | 2.21                     | 0.41              |
| 1:I:126:TRP:CD1  | 1:I:146:ARG:HG3  | 2.56                     | 0.41              |
| 1:J:47:GLN:HB2   | 1:J:50:THR:CG2   | 2.50                     | 0.41              |
| 1:J:622:LEU:O    | 1:J:626:GLN:HG3  | 2.21                     | 0.41              |
| 1:K:73:GLN:C     | 1:K:75:PRO:HD3   | 2.45                     | 0.41              |
| 1:K:117:GLU:OE1  | 1:K:124:GLY:HA2  | 2.20                     | 0.41              |
| 1:K:231:THR:HG22 | 1:K:249:ARG:HE   | 1.86                     | 0.41              |
| 1:K:232:ALA:HA   | 1:K:269:ARG:H    | 1.85                     | 0.41              |
| 1:K:389:LEU:HD23 | 1:K:389:LEU:HA   | 1.90                     | 0.41              |
| 1:L:26:ARG:O     | 1:L:30:LYS:HG3   | 2.21                     | 0.41              |
| 1:L:77:ASP:HB2   | 1:L:523:SER:HA   | 2.03                     | 0.41              |
| 1:A:329:LEU:O    | 1:A:333:ILE:HG13 | 2.21                     | 0.41              |
| 1:A:350:PHE:CE1  | 1:B:372:TYR:HB3  | 2.56                     | 0.41              |
| 1:B:320:VAL:O    | 1:B:323:THR:OG1  | 2.18                     | 0.41              |
| 1:B:546:THR:OG1  | 1:B:547:PRO:HD3  | 2.21                     | 0.41              |
| 1:D:281:ILE:HG23 | 1:D:286:VAL:HA   | 2.02                     | 0.41              |
| 1:D:296:GLU:HB2  | 1:D:449:PHE:CD2  | 2.39                     | 0.41              |
| 1:D:311:GLU:O    | 1:D:312:ASP:CG   | 2.63                     | 0.41              |
| 1:F:514:TYR:HB2  | 1:G:136:SER:OG   | 2.20                     | 0.41              |
| 1:G:386:THR:HG22 | 1:G:387:GLN:N    | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:231:THR:HG22 | 1:I:249:ARG:HE   | 1.85                     | 0.41              |
| 1:I:238:PRO:HB3  | 1:I:263:PHE:CE1  | 2.56                     | 0.41              |
| 1:K:353:PRO:HD3  | 1:L:374:LEU:O    | 2.21                     | 0.41              |
| 1:L:83:LYS:HD2   | 1:L:515:GLU:CG   | 2.50                     | 0.41              |
| 1:L:83:LYS:HG2   | 1:L:84:ASP:C     | 2.46                     | 0.41              |
| 1:L:623:ALA:O    | 1:L:626:GLN:HB2  | 2.21                     | 0.41              |
| 1:L:652:GLU:O    | 1:L:656:ASN:HB2  | 2.20                     | 0.41              |
| 1:A:398:PRO:HB3  | 1:B:394:ASN:HB3  | 2.03                     | 0.41              |
| 1:B:31:ASN:O     | 1:B:35:PHE:HD2   | 2.03                     | 0.41              |
| 1:B:275:ARG:HD2  | 1:B:296:GLU:HG2  | 2.03                     | 0.41              |
| 1:B:359:PHE:HB3  | 1:B:363:TYR:HE2  | 1.85                     | 0.41              |
| 1:C:72:ARG:HH21  | 1:C:111:VAL:HG12 | 1.86                     | 0.41              |
| 1:D:325:ASP:O    | 1:D:326:GLY:C    | 2.63                     | 0.41              |
| 1:E:151:SER:HB2  | 1:E:155:HIS:CE1  | 2.55                     | 0.41              |
| 1:E:710:SER:O    | 1:E:714:ASN:HB2  | 2.21                     | 0.41              |
| 1:F:458:ARG:NH2  | 1:F:500:ALA:HB1  | 2.36                     | 0.41              |
| 1:F:663:SER:HA   | 1:F:666:ARG:HG2  | 2.03                     | 0.41              |
| 1:H:546:THR:OG1  | 1:H:547:PRO:HD3  | 2.20                     | 0.41              |
| 1:I:38:VAL:HG22  | 1:I:43:ASP:OD1   | 2.21                     | 0.41              |
| 1:I:110:ALA:HB1  | 1:I:126:TRP:CE3  | 2.55                     | 0.41              |
| 1:J:238:PRO:HB3  | 1:J:263:PHE:CE1  | 2.56                     | 0.41              |
| 1:J:646:ASN:HA   | 1:K:644:GLN:HG2  | 2.03                     | 0.41              |
| 1:J:667:GLU:HG2  | 1:K:666:ARG:CZ   | 2.51                     | 0.41              |
| 1:K:26:ARG:O     | 1:K:30:LYS:HG3   | 2.21                     | 0.41              |
| 1:K:436:ASN:HA   | 1:K:439:ASN:ND2  | 2.35                     | 0.41              |
| 1:L:509:ASP:N    | 1:L:509:ASP:OD1  | 2.54                     | 0.41              |
| 1:L:538:LEU:HB3  | 1:L:551:LEU:HD11 | 2.03                     | 0.41              |
| 1:A:276:VAL:HG11 | 1:A:297:HIS:O    | 2.20                     | 0.41              |
| 1:A:386:THR:HG22 | 1:A:387:GLN:N    | 2.35                     | 0.41              |
| 1:A:623:ALA:O    | 1:A:626:GLN:HB2  | 2.20                     | 0.41              |
| 1:B:117:GLU:OE1  | 1:B:124:GLY:HA2  | 2.21                     | 0.41              |
| 1:B:614:VAL:HG11 | 1:C:609:VAL:HG11 | 2.03                     | 0.41              |
| 1:B:623:ALA:HA   | 1:B:626:GLN:CD   | 2.46                     | 0.41              |
| 1:C:57:PHE:HB2   | 1:C:334:MET:SD   | 2.61                     | 0.41              |
| 1:C:297:HIS:CG   | 1:C:298:ILE:H    | 2.38                     | 0.41              |
| 1:C:538:LEU:O    | 1:C:542:THR:OG1  | 2.38                     | 0.41              |
| 1:E:42:ASP:HB3   | 1:E:44:TRP:HD1   | 1.86                     | 0.41              |
| 1:E:47:GLN:HB2   | 1:E:50:THR:CG2   | 2.51                     | 0.41              |
| 1:E:225:VAL:HA   | 1:E:276:VAL:HG12 | 2.02                     | 0.41              |
| 1:E:278:LYS:HB3  | 1:E:291:GLN:O    | 2.21                     | 0.41              |
| 1:E:623:ALA:HA   | 1:E:626:GLN:CD   | 2.44                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:89:ASP:O     | 1:F:92:ASP:HB2   | 2.21                     | 0.41              |
| 1:F:162:SER:OG   | 1:F:167:LYS:HA   | 2.20                     | 0.41              |
| 1:F:448:VAL:HA   | 1:F:451:ASP:OD2  | 2.21                     | 0.41              |
| 1:G:220:ALA:CB   | 1:G:281:ILE:O    | 2.48                     | 0.41              |
| 1:G:325:ASP:HA   | 1:G:328:ARG:NH1  | 2.35                     | 0.41              |
| 1:G:458:ARG:NH2  | 1:G:500:ALA:HB1  | 2.36                     | 0.41              |
| 1:G:623:ALA:HA   | 1:G:626:GLN:CD   | 2.46                     | 0.41              |
| 1:G:662:GLN:HA   | 1:G:665:PHE:CD2  | 2.55                     | 0.41              |
| 1:H:57:PHE:HB2   | 1:H:334:MET:SD   | 2.61                     | 0.41              |
| 1:H:127:ARG:HB3  | 1:H:147:GLU:HB2  | 2.02                     | 0.41              |
| 1:H:203:ASN:HD21 | 1:H:209:PHE:HZ   | 1.69                     | 0.41              |
| 1:H:306:GLU:OE2  | 1:I:61:ARG:NE    | 2.54                     | 0.41              |
| 1:H:363:TYR:CE1  | 1:H:372:TYR:HA   | 2.53                     | 0.41              |
| 1:H:593:LEU:O    | 1:H:597:GLN:HG3  | 2.21                     | 0.41              |
| 1:I:162:SER:OG   | 1:I:167:LYS:HA   | 2.20                     | 0.41              |
| 1:I:225:VAL:HG22 | 1:I:276:VAL:HG12 | 2.03                     | 0.41              |
| 1:I:236:GLN:HG2  | 1:I:244:VAL:H    | 1.86                     | 0.41              |
| 1:I:359:PHE:HB3  | 1:I:363:TYR:HE2  | 1.86                     | 0.41              |
| 1:I:410:SER:O    | 1:I:413:LYS:HG2  | 2.20                     | 0.41              |
| 1:I:458:ARG:NH2  | 1:I:500:ALA:HB1  | 2.35                     | 0.41              |
| 1:I:562:GLY:O    | 1:I:566:GLU:HG3  | 2.21                     | 0.41              |
| 1:I:615:LEU:O    | 1:I:618:GLY:N    | 2.54                     | 0.41              |
| 1:I:649:ARG:O    | 1:I:653:ILE:HG13 | 2.20                     | 0.41              |
| 1:J:42:ASP:HB3   | 1:J:44:TRP:HD1   | 1.85                     | 0.41              |
| 1:K:83:LYS:HG2   | 1:K:84:ASP:C     | 2.46                     | 0.41              |
| 1:K:235:TYR:HA   | 1:K:265:LYS:O    | 2.21                     | 0.41              |
| 1:K:238:PRO:HB3  | 1:K:263:PHE:CD1  | 2.56                     | 0.41              |
| 1:K:359:PHE:HB2  | 1:K:360:GLU:H    | 1.78                     | 0.41              |
| 1:K:407:ALA:HA   | 1:K:410:SER:HB2  | 2.03                     | 0.41              |
| 1:K:663:SER:HA   | 1:K:666:ARG:NE   | 2.28                     | 0.41              |
| 1:L:10:SER:O     | 1:L:14:ARG:HG2   | 2.21                     | 0.41              |
| 1:L:248:LYS:HG2  | 1:L:511:ARG:HH21 | 1.85                     | 0.41              |
| 1:L:282:THR:HG23 | 1:L:284:THR:H    | 1.85                     | 0.41              |
| 1:L:622:LEU:O    | 1:L:626:GLN:HG3  | 2.21                     | 0.41              |
| 1:A:47:GLN:HB2   | 1:A:50:THR:HG21  | 2.03                     | 0.41              |
| 1:A:184:TRP:CZ3  | 1:A:199:PRO:HG3  | 2.56                     | 0.41              |
| 1:A:458:ARG:NH2  | 1:A:500:ALA:HB1  | 2.36                     | 0.41              |
| 1:B:73:GLN:C     | 1:B:75:PRO:HD3   | 2.46                     | 0.41              |
| 1:B:87:ARG:HD3   | 1:B:89:ASP:HB2   | 2.02                     | 0.41              |
| 1:B:398:PRO:O    | 1:B:399:GLN:HG2  | 2.20                     | 0.41              |
| 1:C:83:LYS:HD2   | 1:C:515:GLU:CG   | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:282:THR:HG23 | 1:C:284:THR:H    | 1.86                     | 0.41              |
| 1:C:562:GLY:O    | 1:C:566:GLU:HG3  | 2.20                     | 0.41              |
| 1:D:282:THR:HG23 | 1:D:284:THR:H    | 1.86                     | 0.41              |
| 1:D:448:VAL:HA   | 1:D:451:ASP:OD2  | 2.21                     | 0.41              |
| 1:D:526:SER:O    | 1:D:530:GLN:N    | 2.47                     | 0.41              |
| 1:D:663:SER:HA   | 1:D:666:ARG:NE   | 2.27                     | 0.41              |
| 1:F:311:GLU:O    | 1:F:312:ASP:CG   | 2.64                     | 0.41              |
| 1:F:460:ASP:HA   | 1:F:499:LEU:O    | 2.21                     | 0.41              |
| 1:F:574:LYS:O    | 1:F:578:GLN:HG3  | 2.21                     | 0.41              |
| 1:G:165:MET:HB3  | 1:G:304:PHE:CG   | 2.56                     | 0.41              |
| 1:G:236:GLN:HG2  | 1:G:244:VAL:H    | 1.86                     | 0.41              |
| 1:H:72:ARG:HH21  | 1:H:111:VAL:HG12 | 1.86                     | 0.41              |
| 1:H:297:HIS:CG   | 1:H:298:ILE:H    | 2.38                     | 0.41              |
| 1:H:403:TYR:OH   | 1:I:397:VAL:HG11 | 2.20                     | 0.41              |
| 1:J:21:ALA:HB2   | 1:J:172:HIS:CD2  | 2.56                     | 0.41              |
| 1:J:386:THR:HG22 | 1:J:387:GLN:N    | 2.35                     | 0.41              |
| 1:L:438:LEU:O    | 1:L:442:ALA:N    | 2.42                     | 0.41              |
| 1:A:114:ALA:O    | 1:A:118:GLN:HB2  | 2.20                     | 0.40              |
| 1:A:233:PHE:HB2  | 1:A:249:ARG:HB3  | 2.03                     | 0.40              |
| 1:C:35:PHE:HD2   | 1:C:35:PHE:H     | 1.68                     | 0.40              |
| 1:C:176:ILE:HG21 | 1:C:201:PHE:CE2  | 2.56                     | 0.40              |
| 1:D:26:ARG:O     | 1:D:30:LYS:HG3   | 2.22                     | 0.40              |
| 1:D:398:PRO:O    | 1:D:399:GLN:HG2  | 2.20                     | 0.40              |
| 1:E:83:LYS:HD2   | 1:E:515:GLU:CG   | 2.52                     | 0.40              |
| 1:E:252:LYS:NZ   | 1:E:256:ASP:HB3  | 2.36                     | 0.40              |
| 1:F:556:TYR:HB3  | 1:F:572:ALA:CB   | 2.48                     | 0.40              |
| 1:F:593:LEU:O    | 1:F:597:GLN:HG3  | 2.20                     | 0.40              |
| 1:G:26:ARG:O     | 1:G:30:LYS:HG3   | 2.20                     | 0.40              |
| 1:G:89:ASP:O     | 1:G:92:ASP:HB2   | 2.21                     | 0.40              |
| 1:G:252:LYS:HD2  | 1:G:256:ASP:HB3  | 2.04                     | 0.40              |
| 1:H:236:GLN:HG2  | 1:H:244:VAL:H    | 1.85                     | 0.40              |
| 1:H:559:LEU:HB3  | 1:H:565:VAL:HB   | 2.04                     | 0.40              |
| 1:J:662:GLN:HA   | 1:J:665:PHE:CD2  | 2.56                     | 0.40              |
| 1:K:83:LYS:HD2   | 1:K:515:GLU:CG   | 2.52                     | 0.40              |
| 1:K:362:MET:HA   | 1:K:366:ASN:CB   | 2.50                     | 0.40              |
| 1:K:685:ALA:O    | 1:K:689:LEU:HG   | 2.21                     | 0.40              |
| 1:L:47:GLN:HB2   | 1:L:50:THR:CG2   | 2.51                     | 0.40              |
| 1:L:248:LYS:CD   | 1:L:251:ILE:HB   | 2.45                     | 0.40              |
| 1:L:259:ALA:HA   | 1:L:263:PHE:CD2  | 2.56                     | 0.40              |
| 1:L:325:ASP:O    | 1:L:326:GLY:C    | 2.63                     | 0.40              |
| 1:L:398:PRO:O    | 1:L:399:GLN:HG2  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:35:PHE:HD2   | 1:A:35:PHE:H     | 1.69                     | 0.40              |
| 1:A:116:ARG:NH2  | 1:L:306:GLU:HG3  | 2.36                     | 0.40              |
| 1:A:183:GLY:HA3  | 1:L:161:ASN:ND2  | 2.33                     | 0.40              |
| 1:A:644:GLN:HG2  | 1:L:646:ASN:HA   | 2.03                     | 0.40              |
| 1:B:297:HIS:CG   | 1:B:298:ILE:H    | 2.38                     | 0.40              |
| 1:B:363:TYR:CE1  | 1:B:372:TYR:HA   | 2.55                     | 0.40              |
| 1:B:562:GLY:O    | 1:B:566:GLU:HG3  | 2.21                     | 0.40              |
| 1:D:35:PHE:HD2   | 1:D:35:PHE:H     | 1.68                     | 0.40              |
| 1:D:297:HIS:CG   | 1:D:298:ILE:N    | 2.90                     | 0.40              |
| 1:D:323:THR:HG22 | 1:D:415:VAL:HG23 | 2.02                     | 0.40              |
| 1:E:31:ASN:O     | 1:E:35:PHE:CD2   | 2.75                     | 0.40              |
| 1:E:114:ALA:O    | 1:E:118:GLN:HB2  | 2.22                     | 0.40              |
| 1:E:353:PRO:HD3  | 1:F:374:LEU:O    | 2.20                     | 0.40              |
| 1:E:509:ASP:OD1  | 1:E:509:ASP:N    | 2.54                     | 0.40              |
| 1:F:10:SER:O     | 1:F:14:ARG:HG2   | 2.21                     | 0.40              |
| 1:F:117:GLU:OE1  | 1:F:124:GLY:HA2  | 2.21                     | 0.40              |
| 1:F:411:ALA:HA   | 1:G:57:PHE:HE1   | 1.86                     | 0.40              |
| 1:G:105:ASN:O    | 1:G:109:ILE:HG12 | 2.20                     | 0.40              |
| 1:G:276:VAL:HG11 | 1:G:297:HIS:O    | 2.21                     | 0.40              |
| 1:G:581:VAL:HG22 | 1:H:567:MET:HB2  | 2.02                     | 0.40              |
| 1:H:10:SER:O     | 1:H:14:ARG:HG2   | 2.21                     | 0.40              |
| 1:H:80:TYR:HB3   | 1:H:95:MET:HE2   | 2.04                     | 0.40              |
| 1:H:573:ASN:HA   | 1:H:576:LEU:HD12 | 2.03                     | 0.40              |
| 1:J:623:ALA:HA   | 1:J:626:GLN:CD   | 2.46                     | 0.40              |
| 1:J:623:ALA:O    | 1:J:626:GLN:HB2  | 2.21                     | 0.40              |
| 1:K:152:ALA:HA   | 1:K:155:HIS:HB2  | 2.04                     | 0.40              |
| 1:K:411:ALA:O    | 1:K:415:VAL:HG22 | 2.21                     | 0.40              |
| 1:L:117:GLU:OE1  | 1:L:124:GLY:HA2  | 2.22                     | 0.40              |
| 1:L:609:VAL:O    | 1:L:612:GLN:HB2  | 2.20                     | 0.40              |
| 1:A:398:PRO:CB   | 1:B:394:ASN:HB3  | 2.52                     | 0.40              |
| 1:A:404:MET:HA   | 1:A:407:ALA:HB3  | 2.03                     | 0.40              |
| 1:A:671:THR:O    | 1:A:674:SER:OG   | 2.31                     | 0.40              |
| 1:B:89:ASP:O     | 1:B:92:ASP:HB2   | 2.20                     | 0.40              |
| 1:B:101:ASP:OD1  | 1:B:101:ASP:N    | 2.55                     | 0.40              |
| 1:B:246:TYR:C    | 1:B:247:PHE:HD1  | 2.29                     | 0.40              |
| 1:C:73:GLN:C     | 1:C:75:PRO:HD3   | 2.47                     | 0.40              |
| 1:C:363:TYR:CE1  | 1:C:372:TYR:HA   | 2.56                     | 0.40              |
| 1:D:15:PHE:HA    | 1:D:18:ASP:HB3   | 2.03                     | 0.40              |
| 1:D:21:ALA:HB2   | 1:D:172:HIS:NE2  | 2.36                     | 0.40              |
| 1:D:133:GLU:O    | 1:D:137:PRO:HB3  | 2.21                     | 0.40              |
| 1:D:320:VAL:O    | 1:D:323:THR:OG1  | 2.19                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:83:LYS:HD2   | 1:E:515:GLU:HG3  | 2.03                     | 0.40              |
| 1:G:562:GLY:O    | 1:G:566:GLU:HG3  | 2.21                     | 0.40              |
| 1:H:176:ILE:HG21 | 1:H:201:PHE:CE2  | 2.56                     | 0.40              |
| 1:I:64:VAL:HG22  | 1:I:119:ILE:HG21 | 2.04                     | 0.40              |
| 1:L:278:LYS:HB3  | 1:L:291:GLN:O    | 2.21                     | 0.40              |
| 1:A:546:THR:OG1  | 1:A:547:PRO:HD3  | 2.20                     | 0.40              |
| 1:B:151:SER:O    | 1:B:155:HIS:ND1  | 2.43                     | 0.40              |
| 1:B:526:SER:O    | 1:B:530:GLN:N    | 2.52                     | 0.40              |
| 1:C:137:PRO:HG3  | 1:C:141:ASN:OD1  | 2.21                     | 0.40              |
| 1:D:400:ALA:O    | 1:D:404:MET:HB2  | 2.22                     | 0.40              |
| 1:E:325:ASP:O    | 1:E:326:GLY:C    | 2.63                     | 0.40              |
| 1:F:83:LYS:HG2   | 1:F:84:ASP:C     | 2.47                     | 0.40              |
| 1:F:609:VAL:O    | 1:F:612:GLN:HB2  | 2.22                     | 0.40              |
| 1:F:657:MET:SD   | 1:G:655:ASN:ND2  | 2.94                     | 0.40              |
| 1:G:65:ARG:O     | 1:G:69:SER:HB2   | 2.22                     | 0.40              |
| 1:G:161:ASN:ND2  | 1:H:183:GLY:HA3  | 2.37                     | 0.40              |
| 1:G:374:LEU:HD13 | 1:G:374:LEU:HA   | 1.97                     | 0.40              |
| 1:H:47:GLN:HB2   | 1:H:50:THR:HG21  | 2.03                     | 0.40              |
| 1:I:398:PRO:O    | 1:I:399:GLN:HG2  | 2.21                     | 0.40              |
| 1:I:623:ALA:O    | 1:I:626:GLN:HB2  | 2.22                     | 0.40              |
| 1:J:573:ASN:HA   | 1:J:576:LEU:HD12 | 2.03                     | 0.40              |
| 1:K:657:MET:SD   | 1:L:655:ASN:ND2  | 2.94                     | 0.40              |
| 1:L:248:LYS:CG   | 1:L:511:ARG:HH21 | 2.35                     | 0.40              |
| 1:L:448:VAL:HA   | 1:L:451:ASP:OD2  | 2.21                     | 0.40              |
| 1:B:57:PHE:CG    | 1:B:334:MET:HE1  | 2.57                     | 0.40              |
| 1:B:248:LYS:HE3  | 1:B:252:LYS:HB2  | 2.02                     | 0.40              |
| 1:B:325:ASP:O    | 1:B:326:GLY:C    | 2.63                     | 0.40              |
| 1:D:621:GLU:OE2  | 1:E:616:LEU:HB3  | 2.21                     | 0.40              |
| 1:D:685:ALA:O    | 1:D:689:LEU:HG   | 2.21                     | 0.40              |
| 1:F:42:ASP:HB3   | 1:F:44:TRP:HD1   | 1.87                     | 0.40              |
| 1:G:297:HIS:CG   | 1:G:298:ILE:H    | 2.40                     | 0.40              |
| 1:G:407:ALA:HA   | 1:G:410:SER:HB2  | 2.04                     | 0.40              |
| 1:G:538:LEU:HB3  | 1:G:551:LEU:HD11 | 2.03                     | 0.40              |
| 1:H:72:ARG:HH22  | 1:H:112:ASN:HA   | 1.85                     | 0.40              |
| 1:H:78:VAL:HA    | 1:H:520:VAL:HA   | 2.04                     | 0.40              |
| 1:H:238:PRO:HB3  | 1:H:263:PHE:CE1  | 2.57                     | 0.40              |
| 1:H:407:ALA:HA   | 1:H:410:SER:HB2  | 2.04                     | 0.40              |
| 1:K:87:ARG:HD3   | 1:K:89:ASP:HB2   | 2.02                     | 0.40              |
| 1:K:236:GLN:OE1  | 1:K:265:LYS:HD3  | 2.22                     | 0.40              |
| 1:K:441:ARG:O    | 1:K:444:LEU:HB3  | 2.22                     | 0.40              |
| 1:K:663:SER:HA   | 1:K:666:ARG:HG2  | 2.04                     | 0.40              |

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| Atom-1        | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------|--------------------------|-------------------|
| 1:L:626:GLN:O | 1:L:630:LEU:HB2 | 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     | 669/725 (92%)   | 562 (84%)  | 102 (15%)  | 5 (1%)   | 18          | 56 |
| 1   | B     | 669/725 (92%)   | 561 (84%)  | 103 (15%)  | 5 (1%)   | 18          | 56 |
| 1   | C     | 669/725 (92%)   | 560 (84%)  | 104 (16%)  | 5 (1%)   | 18          | 56 |
| 1   | D     | 669/725 (92%)   | 561 (84%)  | 103 (15%)  | 5 (1%)   | 18          | 56 |
| 1   | E     | 669/725 (92%)   | 562 (84%)  | 101 (15%)  | 6 (1%)   | 14          | 51 |
| 1   | F     | 669/725 (92%)   | 561 (84%)  | 103 (15%)  | 5 (1%)   | 18          | 56 |
| 1   | G     | 669/725 (92%)   | 563 (84%)  | 100 (15%)  | 6 (1%)   | 14          | 51 |
| 1   | H     | 669/725 (92%)   | 561 (84%)  | 103 (15%)  | 5 (1%)   | 18          | 56 |
| 1   | I     | 669/725 (92%)   | 560 (84%)  | 105 (16%)  | 4 (1%)   | 21          | 59 |
| 1   | J     | 669/725 (92%)   | 559 (84%)  | 106 (16%)  | 4 (1%)   | 21          | 59 |
| 1   | K     | 669/725 (92%)   | 560 (84%)  | 104 (16%)  | 5 (1%)   | 18          | 56 |
| 1   | L     | 669/725 (92%)   | 562 (84%)  | 101 (15%)  | 6 (1%)   | 14          | 51 |
| All | All   | 8028/8700 (92%) | 6732 (84%) | 1235 (15%) | 61 (1%)  | 16          | 54 |

All (61) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 58  | ASP  |
| 1   | B     | 58  | ASP  |
| 1   | C     | 58  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 58  | ASP  |
| 1   | E     | 58  | ASP  |
| 1   | F     | 58  | ASP  |
| 1   | G     | 58  | ASP  |
| 1   | H     | 58  | ASP  |
| 1   | I     | 58  | ASP  |
| 1   | J     | 58  | ASP  |
| 1   | K     | 58  | ASP  |
| 1   | L     | 58  | ASP  |
| 1   | A     | 587 | PRO  |
| 1   | C     | 587 | PRO  |
| 1   | D     | 587 | PRO  |
| 1   | H     | 587 | PRO  |
| 1   | I     | 587 | PRO  |
| 1   | B     | 587 | PRO  |
| 1   | E     | 587 | PRO  |
| 1   | F     | 587 | PRO  |
| 1   | G     | 587 | PRO  |
| 1   | J     | 587 | PRO  |
| 1   | K     | 587 | PRO  |
| 1   | L     | 587 | PRO  |
| 1   | A     | 203 | ASN  |
| 1   | B     | 203 | ASN  |
| 1   | C     | 203 | ASN  |
| 1   | D     | 203 | ASN  |
| 1   | E     | 31  | ASN  |
| 1   | E     | 203 | ASN  |
| 1   | F     | 203 | ASN  |
| 1   | G     | 120 | GLU  |
| 1   | G     | 203 | ASN  |
| 1   | H     | 203 | ASN  |
| 1   | I     | 203 | ASN  |
| 1   | J     | 203 | ASN  |
| 1   | K     | 31  | ASN  |
| 1   | K     | 203 | ASN  |
| 1   | L     | 31  | ASN  |
| 1   | L     | 203 | ASN  |
| 1   | A     | 76  | ILE  |
| 1   | B     | 76  | ILE  |
| 1   | C     | 76  | ILE  |
| 1   | D     | 76  | ILE  |
| 1   | E     | 76  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 76  | ILE  |
| 1   | G     | 76  | ILE  |
| 1   | H     | 76  | ILE  |
| 1   | I     | 76  | ILE  |
| 1   | J     | 76  | ILE  |
| 1   | K     | 76  | ILE  |
| 1   | L     | 76  | ILE  |
| 1   | B     | 653 | ILE  |
| 1   | C     | 653 | ILE  |
| 1   | E     | 653 | ILE  |
| 1   | F     | 653 | ILE  |
| 1   | H     | 653 | ILE  |
| 1   | L     | 653 | ILE  |
| 1   | A     | 653 | ILE  |
| 1   | D     | 653 | ILE  |
| 1   | G     | 653 | ILE  |

### 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     | 572/630 (91%) | 570 (100%) | 2 (0%)   | 86          | 86 |
| 1   | B     | 572/630 (91%) | 570 (100%) | 2 (0%)   | 86          | 86 |
| 1   | C     | 572/630 (91%) | 570 (100%) | 2 (0%)   | 86          | 86 |
| 1   | D     | 572/630 (91%) | 571 (100%) | 1 (0%)   | 87          | 87 |
| 1   | E     | 572/630 (91%) | 570 (100%) | 2 (0%)   | 86          | 86 |
| 1   | F     | 572/630 (91%) | 570 (100%) | 2 (0%)   | 86          | 86 |
| 1   | G     | 572/630 (91%) | 570 (100%) | 2 (0%)   | 86          | 86 |
| 1   | H     | 572/630 (91%) | 570 (100%) | 2 (0%)   | 86          | 86 |
| 1   | I     | 572/630 (91%) | 570 (100%) | 2 (0%)   | 86          | 86 |
| 1   | J     | 572/630 (91%) | 570 (100%) | 2 (0%)   | 86          | 86 |
| 1   | K     | 572/630 (91%) | 570 (100%) | 2 (0%)   | 86          | 86 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-----------------|-------------|----------|-------------|----|
| 1   | L     | 572/630 (91%)   | 570 (100%)  | 2 (0%)   | 86          | 86 |
| All | All   | 6864/7560 (91%) | 6841 (100%) | 23 (0%)  | 86          | 86 |

All (23) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 615 | LEU  |
| 1   | A     | 616 | LEU  |
| 1   | B     | 615 | LEU  |
| 1   | B     | 616 | LEU  |
| 1   | C     | 615 | LEU  |
| 1   | C     | 616 | LEU  |
| 1   | D     | 616 | LEU  |
| 1   | E     | 615 | LEU  |
| 1   | E     | 616 | LEU  |
| 1   | F     | 615 | LEU  |
| 1   | F     | 616 | LEU  |
| 1   | G     | 615 | LEU  |
| 1   | G     | 616 | LEU  |
| 1   | H     | 615 | LEU  |
| 1   | H     | 616 | LEU  |
| 1   | I     | 615 | LEU  |
| 1   | I     | 616 | LEU  |
| 1   | J     | 615 | LEU  |
| 1   | J     | 616 | LEU  |
| 1   | K     | 615 | LEU  |
| 1   | K     | 616 | LEU  |
| 1   | L     | 615 | LEU  |
| 1   | L     | 616 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 40  | GLN  |
| 1   | A     | 52  | GLN  |
| 1   | A     | 135 | GLN  |
| 1   | A     | 142 | GLN  |
| 1   | A     | 161 | ASN  |
| 1   | A     | 361 | HIS  |
| 1   | A     | 439 | ASN  |
| 1   | A     | 550 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 597 | GLN  |
| 1   | A     | 676 | GLN  |
| 1   | B     | 40  | GLN  |
| 1   | B     | 52  | GLN  |
| 1   | B     | 135 | GLN  |
| 1   | B     | 142 | GLN  |
| 1   | B     | 161 | ASN  |
| 1   | B     | 337 | ASN  |
| 1   | B     | 361 | HIS  |
| 1   | B     | 439 | ASN  |
| 1   | B     | 597 | GLN  |
| 1   | C     | 52  | GLN  |
| 1   | C     | 104 | HIS  |
| 1   | C     | 135 | GLN  |
| 1   | C     | 161 | ASN  |
| 1   | C     | 337 | ASN  |
| 1   | C     | 361 | HIS  |
| 1   | C     | 439 | ASN  |
| 1   | C     | 550 | GLN  |
| 1   | C     | 597 | GLN  |
| 1   | C     | 706 | ASN  |
| 1   | D     | 40  | GLN  |
| 1   | D     | 52  | GLN  |
| 1   | D     | 135 | GLN  |
| 1   | D     | 161 | ASN  |
| 1   | D     | 361 | HIS  |
| 1   | D     | 439 | ASN  |
| 1   | D     | 597 | GLN  |
| 1   | E     | 40  | GLN  |
| 1   | E     | 52  | GLN  |
| 1   | E     | 135 | GLN  |
| 1   | E     | 161 | ASN  |
| 1   | E     | 361 | HIS  |
| 1   | E     | 439 | ASN  |
| 1   | E     | 550 | GLN  |
| 1   | E     | 597 | GLN  |
| 1   | F     | 40  | GLN  |
| 1   | F     | 52  | GLN  |
| 1   | F     | 135 | GLN  |
| 1   | F     | 142 | GLN  |
| 1   | F     | 161 | ASN  |
| 1   | F     | 337 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 361 | HIS  |
| 1   | F     | 439 | ASN  |
| 1   | F     | 550 | GLN  |
| 1   | F     | 597 | GLN  |
| 1   | G     | 40  | GLN  |
| 1   | G     | 52  | GLN  |
| 1   | G     | 135 | GLN  |
| 1   | G     | 142 | GLN  |
| 1   | G     | 161 | ASN  |
| 1   | G     | 337 | ASN  |
| 1   | G     | 361 | HIS  |
| 1   | G     | 439 | ASN  |
| 1   | G     | 550 | GLN  |
| 1   | G     | 597 | GLN  |
| 1   | H     | 40  | GLN  |
| 1   | H     | 52  | GLN  |
| 1   | H     | 135 | GLN  |
| 1   | H     | 161 | ASN  |
| 1   | H     | 337 | ASN  |
| 1   | H     | 439 | ASN  |
| 1   | H     | 597 | GLN  |
| 1   | I     | 40  | GLN  |
| 1   | I     | 52  | GLN  |
| 1   | I     | 135 | GLN  |
| 1   | I     | 142 | GLN  |
| 1   | I     | 161 | ASN  |
| 1   | I     | 550 | GLN  |
| 1   | I     | 597 | GLN  |
| 1   | I     | 696 | GLN  |
| 1   | J     | 40  | GLN  |
| 1   | J     | 52  | GLN  |
| 1   | J     | 135 | GLN  |
| 1   | J     | 161 | ASN  |
| 1   | J     | 361 | HIS  |
| 1   | J     | 439 | ASN  |
| 1   | J     | 550 | GLN  |
| 1   | J     | 597 | GLN  |
| 1   | J     | 706 | ASN  |
| 1   | K     | 52  | GLN  |
| 1   | K     | 142 | GLN  |
| 1   | K     | 161 | ASN  |
| 1   | K     | 337 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 361 | HIS  |
| 1   | K     | 439 | ASN  |
| 1   | K     | 597 | GLN  |
| 1   | L     | 52  | GLN  |
| 1   | L     | 135 | GLN  |
| 1   | L     | 161 | ASN  |
| 1   | L     | 337 | ASN  |
| 1   | L     | 361 | HIS  |
| 1   | L     | 550 | GLN  |
| 1   | L     | 597 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |    |    | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|----|----|-----------------------|---------|
| 1   | A     | 673/725 (92%)   | 0.11   | 15 (2%)   | 62 | 53 | 46, 96, 204, 282      | 0       |
| 1   | B     | 673/725 (92%)   | 0.21   | 36 (5%)   | 32 | 34 | 31, 97, 169, 284      | 0       |
| 1   | C     | 673/725 (92%)   | 0.22   | 24 (3%)   | 46 | 43 | 47, 81, 181, 288      | 0       |
| 1   | D     | 673/725 (92%)   | 0.22   | 28 (4%)   | 40 | 40 | 51, 97, 160, 240      | 0       |
| 1   | E     | 673/725 (92%)   | 0.26   | 31 (4%)   | 37 | 37 | 54, 100, 176, 292     | 0       |
| 1   | F     | 673/725 (92%)   | 0.17   | 18 (2%)   | 56 | 48 | 73, 110, 184, 317     | 0       |
| 1   | G     | 673/725 (92%)   | 0.27   | 36 (5%)   | 32 | 34 | 71, 117, 190, 362     | 0       |
| 1   | H     | 673/725 (92%)   | 0.21   | 23 (3%)   | 48 | 44 | 77, 127, 205, 345     | 0       |
| 1   | I     | 673/725 (92%)   | 0.24   | 30 (4%)   | 38 | 38 | 90, 134, 222, 333     | 0       |
| 1   | J     | 673/725 (92%)   | 0.24   | 25 (3%)   | 45 | 43 | 70, 139, 211, 312     | 0       |
| 1   | K     | 673/725 (92%)   | 0.18   | 21 (3%)   | 51 | 46 | 65, 113, 182, 250     | 0       |
| 1   | L     | 673/725 (92%)   | 0.17   | 26 (3%)   | 43 | 42 | 63, 106, 203, 303     | 0       |
| All | All   | 8076/8700 (92%) | 0.21   | 313 (3%)  | 43 | 42 | 31, 112, 196, 362     | 0       |

All (313) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 43  | ASP  | 8.8  |
| 1   | G     | 50  | THR  | 8.4  |
| 1   | B     | 50  | THR  | 6.8  |
| 1   | G     | 48  | TYR  | 6.7  |
| 1   | D     | 43  | ASP  | 6.1  |
| 1   | I     | 354 | GLU  | 5.8  |
| 1   | B     | 51  | LEU  | 5.6  |
| 1   | A     | 362 | MET  | 5.2  |
| 1   | E     | 591 | GLN  | 5.2  |
| 1   | B     | 43  | ASP  | 4.9  |
| 1   | J     | 714 | ASN  | 4.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 48  | TYR  | 4.9  |
| 1   | J     | 710 | SER  | 4.8  |
| 1   | B     | 47  | GLN  | 4.8  |
| 1   | G     | 258 | LEU  | 4.6  |
| 1   | J     | 314 | GLU  | 4.5  |
| 1   | B     | 159 | ASP  | 4.5  |
| 1   | C     | 316 | TYR  | 4.5  |
| 1   | J     | 518 | THR  | 4.3  |
| 1   | C     | 236 | GLN  | 4.3  |
| 1   | C     | 362 | MET  | 4.2  |
| 1   | G     | 214 | GLN  | 4.2  |
| 1   | G     | 47  | GLN  | 4.2  |
| 1   | G     | 603 | GLN  | 4.2  |
| 1   | B     | 49  | THR  | 4.1  |
| 1   | G     | 213 | THR  | 4.1  |
| 1   | I     | 204 | PRO  | 4.1  |
| 1   | G     | 712 | ARG  | 4.0  |
| 1   | J     | 43  | ASP  | 4.0  |
| 1   | H     | 635 | ASP  | 4.0  |
| 1   | E     | 354 | GLU  | 4.0  |
| 1   | G     | 32  | ASP  | 3.9  |
| 1   | I     | 203 | ASN  | 3.9  |
| 1   | E     | 362 | MET  | 3.8  |
| 1   | L     | 681 | GLU  | 3.8  |
| 1   | I     | 709 | GLN  | 3.8  |
| 1   | J     | 621 | GLU  | 3.8  |
| 1   | G     | 635 | ASP  | 3.8  |
| 1   | D     | 578 | GLN  | 3.7  |
| 1   | F     | 163 | LYS  | 3.7  |
| 1   | C     | 43  | ASP  | 3.7  |
| 1   | H     | 210 | PRO  | 3.7  |
| 1   | B     | 195 | ALA  | 3.7  |
| 1   | D     | 314 | GLU  | 3.7  |
| 1   | J     | 362 | MET  | 3.6  |
| 1   | B     | 214 | GLN  | 3.6  |
| 1   | C     | 621 | GLU  | 3.6  |
| 1   | D     | 603 | GLN  | 3.6  |
| 1   | K     | 686 | ASN  | 3.5  |
| 1   | G     | 51  | LEU  | 3.5  |
| 1   | D     | 240 | THR  | 3.5  |
| 1   | E     | 635 | ASP  | 3.5  |
| 1   | C     | 591 | GLN  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 635 | ASP  | 3.5  |
| 1   | I     | 610 | GLN  | 3.5  |
| 1   | G     | 208 | VAL  | 3.4  |
| 1   | D     | 573 | ASN  | 3.4  |
| 1   | A     | 159 | ASP  | 3.4  |
| 1   | B     | 218 | GLN  | 3.4  |
| 1   | H     | 709 | GLN  | 3.4  |
| 1   | I     | 573 | ASN  | 3.4  |
| 1   | C     | 608 | MET  | 3.4  |
| 1   | D     | 236 | GLN  | 3.4  |
| 1   | K     | 386 | THR  | 3.4  |
| 1   | I     | 233 | PHE  | 3.4  |
| 1   | I     | 286 | VAL  | 3.4  |
| 1   | D     | 635 | ASP  | 3.4  |
| 1   | E     | 661 | LYS  | 3.4  |
| 1   | B     | 505 | GLN  | 3.4  |
| 1   | B     | 609 | VAL  | 3.4  |
| 1   | K     | 684 | ARG  | 3.4  |
| 1   | A     | 518 | THR  | 3.4  |
| 1   | G     | 591 | GLN  | 3.3  |
| 1   | L     | 354 | GLU  | 3.3  |
| 1   | H     | 316 | TYR  | 3.3  |
| 1   | K     | 236 | GLN  | 3.3  |
| 1   | C     | 214 | GLN  | 3.3  |
| 1   | G     | 159 | ASP  | 3.3  |
| 1   | E     | 316 | TYR  | 3.3  |
| 1   | G     | 25  | ALA  | 3.2  |
| 1   | A     | 588 | GLU  | 3.2  |
| 1   | L     | 573 | ASN  | 3.2  |
| 1   | A     | 272 | LYS  | 3.2  |
| 1   | G     | 207 | TRP  | 3.2  |
| 1   | C     | 578 | GLN  | 3.1  |
| 1   | C     | 28  | GLU  | 3.1  |
| 1   | E     | 662 | GLN  | 3.1  |
| 1   | E     | 159 | ASP  | 3.1  |
| 1   | F     | 354 | GLU  | 3.1  |
| 1   | B     | 678 | ASP  | 3.1  |
| 1   | K     | 373 | LEU  | 3.1  |
| 1   | K     | 43  | ASP  | 3.0  |
| 1   | K     | 635 | ASP  | 3.0  |
| 1   | C     | 609 | VAL  | 3.0  |
| 1   | A     | 517 | TYR  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 605 | ASP  | 3.0  |
| 1   | G     | 362 | MET  | 3.0  |
| 1   | F     | 50  | THR  | 3.0  |
| 1   | J     | 159 | ASP  | 3.0  |
| 1   | E     | 314 | GLU  | 3.0  |
| 1   | D     | 258 | LEU  | 3.0  |
| 1   | G     | 43  | ASP  | 3.0  |
| 1   | J     | 573 | ASN  | 2.9  |
| 1   | D     | 203 | ASN  | 2.9  |
| 1   | C     | 178 | SER  | 2.9  |
| 1   | I     | 316 | TYR  | 2.9  |
| 1   | F     | 154 | SER  | 2.9  |
| 1   | I     | 578 | GLN  | 2.9  |
| 1   | G     | 202 | GLN  | 2.9  |
| 1   | I     | 693 | GLY  | 2.9  |
| 1   | H     | 195 | ALA  | 2.9  |
| 1   | J     | 245 | SER  | 2.9  |
| 1   | H     | 612 | GLN  | 2.9  |
| 1   | B     | 367 | ASP  | 2.8  |
| 1   | G     | 621 | GLU  | 2.8  |
| 1   | B     | 578 | GLN  | 2.8  |
| 1   | G     | 332 | MET  | 2.8  |
| 1   | E     | 212 | LEU  | 2.8  |
| 1   | C     | 598 | GLN  | 2.8  |
| 1   | F     | 49  | THR  | 2.8  |
| 1   | D     | 159 | ASP  | 2.8  |
| 1   | F     | 43  | ASP  | 2.8  |
| 1   | E     | 273 | ARG  | 2.7  |
| 1   | E     | 43  | ASP  | 2.7  |
| 1   | J     | 711 | GLN  | 2.7  |
| 1   | F     | 178 | SER  | 2.7  |
| 1   | B     | 573 | ASN  | 2.7  |
| 1   | J     | 706 | ASN  | 2.7  |
| 1   | C     | 713 | GLN  | 2.7  |
| 1   | D     | 41  | TRP  | 2.7  |
| 1   | G     | 610 | GLN  | 2.7  |
| 1   | L     | 240 | THR  | 2.7  |
| 1   | L     | 578 | GLN  | 2.7  |
| 1   | F     | 364 | ASP  | 2.6  |
| 1   | B     | 272 | LYS  | 2.6  |
| 1   | L     | 590 | GLN  | 2.6  |
| 1   | E     | 573 | ASN  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 612 | GLN  | 2.6  |
| 1   | E     | 631 | SER  | 2.6  |
| 1   | J     | 699 | LYS  | 2.6  |
| 1   | D     | 664 | GLU  | 2.6  |
| 1   | F     | 646 | ASN  | 2.6  |
| 1   | G     | 664 | GLU  | 2.6  |
| 1   | H     | 56  | GLN  | 2.6  |
| 1   | K     | 706 | ASN  | 2.6  |
| 1   | E     | 163 | LYS  | 2.6  |
| 1   | E     | 518 | THR  | 2.6  |
| 1   | K     | 363 | TYR  | 2.6  |
| 1   | D     | 386 | THR  | 2.6  |
| 1   | I     | 49  | THR  | 2.6  |
| 1   | L     | 316 | TYR  | 2.6  |
| 1   | E     | 272 | LYS  | 2.5  |
| 1   | J     | 595 | GLU  | 2.5  |
| 1   | G     | 578 | GLN  | 2.5  |
| 1   | I     | 635 | ASP  | 2.5  |
| 1   | E     | 713 | GLN  | 2.5  |
| 1   | C     | 573 | ASN  | 2.5  |
| 1   | H     | 375 | ASN  | 2.5  |
| 1   | D     | 507 | LEU  | 2.5  |
| 1   | H     | 691 | LEU  | 2.5  |
| 1   | A     | 460 | ASP  | 2.5  |
| 1   | I     | 691 | LEU  | 2.5  |
| 1   | B     | 208 | VAL  | 2.5  |
| 1   | G     | 49  | THR  | 2.5  |
| 1   | H     | 228 | LYS  | 2.5  |
| 1   | I     | 52  | GLN  | 2.5  |
| 1   | E     | 258 | LEU  | 2.5  |
| 1   | I     | 614 | VAL  | 2.5  |
| 1   | E     | 233 | PHE  | 2.4  |
| 1   | E     | 681 | GLU  | 2.4  |
| 1   | I     | 695 | GLU  | 2.4  |
| 1   | L     | 236 | GLN  | 2.4  |
| 1   | J     | 204 | PRO  | 2.4  |
| 1   | A     | 43  | ASP  | 2.4  |
| 1   | I     | 706 | ASN  | 2.4  |
| 1   | C     | 677 | GLN  | 2.4  |
| 1   | B     | 614 | VAL  | 2.4  |
| 1   | F     | 273 | ARG  | 2.4  |
| 1   | G     | 44  | TRP  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 517 | TYR  | 2.4  |
| 1   | L     | 595 | GLU  | 2.4  |
| 1   | L     | 621 | GLU  | 2.4  |
| 1   | J     | 661 | LYS  | 2.4  |
| 1   | H     | 43  | ASP  | 2.4  |
| 1   | G     | 281 | ILE  | 2.4  |
| 1   | C     | 204 | PRO  | 2.4  |
| 1   | J     | 709 | GLN  | 2.4  |
| 1   | C     | 195 | ALA  | 2.4  |
| 1   | H     | 362 | MET  | 2.3  |
| 1   | L     | 258 | LEU  | 2.3  |
| 1   | D     | 591 | GLN  | 2.3  |
| 1   | H     | 218 | GLN  | 2.3  |
| 1   | D     | 213 | THR  | 2.3  |
| 1   | C     | 498 | ASP  | 2.3  |
| 1   | B     | 598 | GLN  | 2.3  |
| 1   | J     | 664 | GLU  | 2.3  |
| 1   | B     | 671 | THR  | 2.3  |
| 1   | J     | 697 | THR  | 2.3  |
| 1   | L     | 439 | ASN  | 2.3  |
| 1   | A     | 98  | TYR  | 2.3  |
| 1   | F     | 204 | PRO  | 2.3  |
| 1   | L     | 43  | ASP  | 2.3  |
| 1   | E     | 636 | ALA  | 2.3  |
| 1   | C     | 711 | GLN  | 2.3  |
| 1   | D     | 595 | GLU  | 2.3  |
| 1   | E     | 28  | GLU  | 2.3  |
| 1   | I     | 621 | GLU  | 2.3  |
| 1   | L     | 680 | SER  | 2.3  |
| 1   | B     | 332 | MET  | 2.3  |
| 1   | B     | 709 | GLN  | 2.3  |
| 1   | D     | 56  | GLN  | 2.3  |
| 1   | L     | 373 | LEU  | 2.3  |
| 1   | L     | 362 | MET  | 2.3  |
| 1   | B     | 52  | GLN  | 2.3  |
| 1   | B     | 118 | GLN  | 2.3  |
| 1   | I     | 644 | GLN  | 2.3  |
| 1   | B     | 44  | TRP  | 2.2  |
| 1   | E     | 25  | ALA  | 2.2  |
| 1   | A     | 99  | ARG  | 2.2  |
| 1   | F     | 179 | MET  | 2.2  |
| 1   | F     | 588 | GLU  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 52  | GLN  | 2.2  |
| 1   | H     | 713 | GLN  | 2.2  |
| 1   | I     | 591 | GLN  | 2.2  |
| 1   | J     | 591 | GLN  | 2.2  |
| 1   | D     | 316 | TYR  | 2.2  |
| 1   | B     | 216 | THR  | 2.2  |
| 1   | G     | 518 | THR  | 2.2  |
| 1   | I     | 310 | VAL  | 2.2  |
| 1   | A     | 591 | GLN  | 2.2  |
| 1   | L     | 224 | GLU  | 2.2  |
| 1   | H     | 130 | THR  | 2.2  |
| 1   | A     | 598 | GLN  | 2.2  |
| 1   | H     | 529 | GLN  | 2.2  |
| 1   | D     | 596 | ALA  | 2.2  |
| 1   | D     | 686 | ASN  | 2.2  |
| 1   | J     | 310 | VAL  | 2.2  |
| 1   | E     | 361 | HIS  | 2.2  |
| 1   | J     | 361 | HIS  | 2.2  |
| 1   | G     | 233 | PHE  | 2.2  |
| 1   | G     | 525 | GLN  | 2.2  |
| 1   | E     | 664 | GLU  | 2.2  |
| 1   | E     | 225 | VAL  | 2.2  |
| 1   | H     | 702 | MET  | 2.2  |
| 1   | E     | 656 | ASN  | 2.2  |
| 1   | C     | 514 | TYR  | 2.2  |
| 1   | L     | 591 | GLN  | 2.2  |
| 1   | D     | 354 | GLU  | 2.2  |
| 1   | K     | 688 | GLU  | 2.2  |
| 1   | H     | 712 | ARG  | 2.2  |
| 1   | E     | 665 | PHE  | 2.2  |
| 1   | B     | 364 | ASP  | 2.1  |
| 1   | D     | 204 | PRO  | 2.1  |
| 1   | K     | 353 | PRO  | 2.1  |
| 1   | L     | 170 | ALA  | 2.1  |
| 1   | L     | 678 | ASP  | 2.1  |
| 1   | B     | 675 | PHE  | 2.1  |
| 1   | I     | 622 | LEU  | 2.1  |
| 1   | K     | 33  | LEU  | 2.1  |
| 1   | I     | 698 | HIS  | 2.1  |
| 1   | B     | 712 | ARG  | 2.1  |
| 1   | G     | 649 | ARG  | 2.1  |
| 1   | A     | 224 | GLU  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 365 | GLY  | 2.1  |
| 1   | K     | 592 | TRP  | 2.1  |
| 1   | A     | 316 | TYR  | 2.1  |
| 1   | K     | 578 | GLN  | 2.1  |
| 1   | I     | 705 | ALA  | 2.1  |
| 1   | D     | 403 | TYR  | 2.1  |
| 1   | E     | 213 | THR  | 2.1  |
| 1   | G     | 386 | THR  | 2.1  |
| 1   | I     | 363 | TYR  | 2.1  |
| 1   | L     | 102 | MET  | 2.1  |
| 1   | H     | 347 | LYS  | 2.1  |
| 1   | K     | 695 | GLU  | 2.1  |
| 1   | F     | 531 | ASN  | 2.1  |
| 1   | C     | 381 | SER  | 2.1  |
| 1   | F     | 286 | VAL  | 2.1  |
| 1   | J     | 635 | ASP  | 2.1  |
| 1   | L     | 397 | VAL  | 2.1  |
| 1   | H     | 556 | TYR  | 2.1  |
| 1   | A     | 573 | ASN  | 2.1  |
| 1   | B     | 347 | LYS  | 2.1  |
| 1   | D     | 212 | LEU  | 2.1  |
| 1   | H     | 212 | LEU  | 2.1  |
| 1   | F     | 56  | GLN  | 2.1  |
| 1   | H     | 578 | GLN  | 2.1  |
| 1   | I     | 242 | GLU  | 2.1  |
| 1   | K     | 621 | GLU  | 2.1  |
| 1   | K     | 233 | PHE  | 2.1  |
| 1   | L     | 607 | ALA  | 2.1  |
| 1   | B     | 236 | GLN  | 2.1  |
| 1   | B     | 133 | GLU  | 2.1  |
| 1   | C     | 373 | LEU  | 2.0  |
| 1   | F     | 616 | LEU  | 2.0  |
| 1   | K     | 661 | LYS  | 2.0  |
| 1   | E     | 125 | ALA  | 2.0  |
| 1   | K     | 266 | ILE  | 2.0  |
| 1   | I     | 386 | THR  | 2.0  |
| 1   | H     | 54  | ARG  | 2.0  |
| 1   | J     | 657 | MET  | 2.0  |
| 1   | B     | 163 | LYS  | 2.0  |
| 1   | I     | 140 | ASN  | 2.0  |
| 1   | F     | 621 | GLU  | 2.0  |
| 1   | J     | 684 | ARG  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 710 | SER  | 2.0  |
| 1   | G     | 236 | GLN  | 2.0  |
| 1   | G     | 609 | VAL  | 2.0  |
| 1   | L     | 709 | GLN  | 2.0  |
| 1   | B     | 377 | THR  | 2.0  |
| 1   | G     | 203 | ASN  | 2.0  |
| 1   | K     | 212 | LEU  | 2.0  |
| 1   | K     | 691 | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.