



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:37 AM UTC

PDB ID : 6LT4 / pdb\_00006lt4  
EMDB ID : EMD-0967  
Title : AAA+ ATPase, ClpL from Streptococcus pneumoniae: ATP<sub>r</sub>S-bound  
Authors : Kim, G.; Lee, S.G.; Han, S.; Jung, J.; Jeong, H.S.; Hyun, J.K.; Rhee, D.K.;  
Kim, H.M.; Lee, S.  
Deposited on : 2020-01-21  
Resolution : 4.50 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>  
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:

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

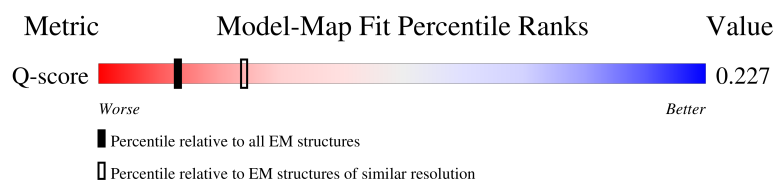
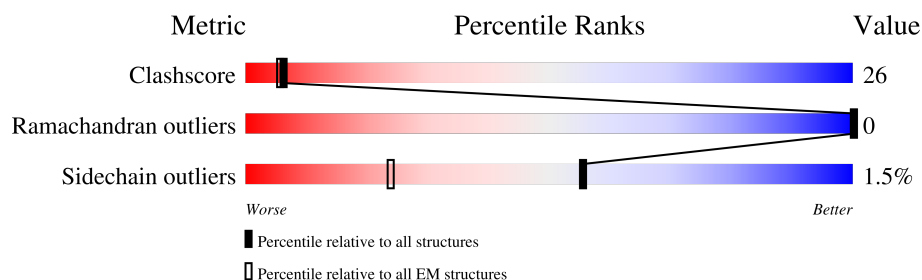
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 2937 ( 4.00 - 5.00 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 701    |                  |
| 1   | B     | 701    |                  |
| 1   | C     | 701    |                  |
| 1   | D     | 701    |                  |

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| Mol | Chain | Length | Quality of chain                                                           |
|-----|-------|--------|----------------------------------------------------------------------------|
| 1   | E     | 701    | <div> <div>39%</div> <div>50%</div> <div>38%</div> <div>• 11%</div> </div> |
| 1   | F     | 701    | <div> <div>39%</div> <div>52%</div> <div>36%</div> <div>• 11%</div> </div> |
| 1   | G     | 701    | <div> <div>39%</div> <div>51%</div> <div>37%</div> <div>• 11%</div> </div> |
| 1   | H     | 701    | <div> <div>42%</div> <div>51%</div> <div>37%</div> <div>• 11%</div> </div> |
| 1   | I     | 701    | <div> <div>44%</div> <div>51%</div> <div>37%</div> <div>• 11%</div> </div> |
| 1   | J     | 701    | <div> <div>43%</div> <div>51%</div> <div>37%</div> <div>• 11%</div> </div> |
| 1   | K     | 701    | <div> <div>40%</div> <div>51%</div> <div>37%</div> <div>• 11%</div> </div> |
| 1   | L     | 701    | <div> <div>40%</div> <div>51%</div> <div>37%</div> <div>• 11%</div> </div> |
| 1   | M     | 701    | <div> <div>42%</div> <div>51%</div> <div>36%</div> <div>• 11%</div> </div> |
| 1   | N     | 701    | <div> <div>42%</div> <div>50%</div> <div>38%</div> <div>• 11%</div> </div> |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 68432 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP-dependent Clp protease, ATP-binding subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |
| 1   | B     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |
| 1   | C     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |
| 1   | D     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |
| 1   | E     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |
| 1   | F     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |
| 1   | G     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |
| 1   | H     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |
| 1   | I     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |
| 1   | J     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |
| 1   | K     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |
| 1   | L     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |
| 1   | M     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |
| 1   | N     | 623      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4824  | 3005 | 850 | 958 | 11 |         |       |

There are 28 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference      |
|-------|---------|----------|--------|---------------------|----------------|
| A     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| A     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference      |
|-------|---------|----------|--------|---------------------|----------------|
| B     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| B     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| C     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| C     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| D     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| D     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| E     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| E     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| F     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| F     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| G     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| G     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| H     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| H     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| I     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| I     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| J     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| J     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| K     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| K     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| L     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| L     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| M     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| M     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| N     | 193     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |
| N     | 526     | ALA      | GLU    | engineered mutation | UNP A0A0H2ZMB9 |

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

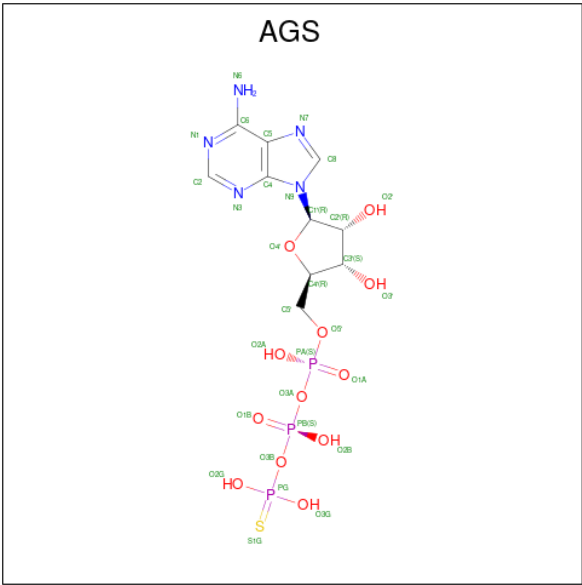
| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 2   | A     | 2        | Total Mg<br>2 2 | 0       |
| 2   | B     | 2        | Total Mg<br>2 2 | 0       |
| 2   | C     | 2        | Total Mg<br>2 2 | 0       |
| 2   | D     | 2        |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

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 2   | G     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 2   | H     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 2   | I     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 2   | J     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 2   | K     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 2   | L     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 2   | M     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 2   | N     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms       |         |        |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|--------|---------|
| 3   | A     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | A     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | B     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|--------|---------|
| 3   | B     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | C     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | C     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | D     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | D     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | E     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | E     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | F     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | F     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | G     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | G     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | H     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | H     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | I     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | I     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | J     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | J     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | K     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | K     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | L     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 3   | L     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |

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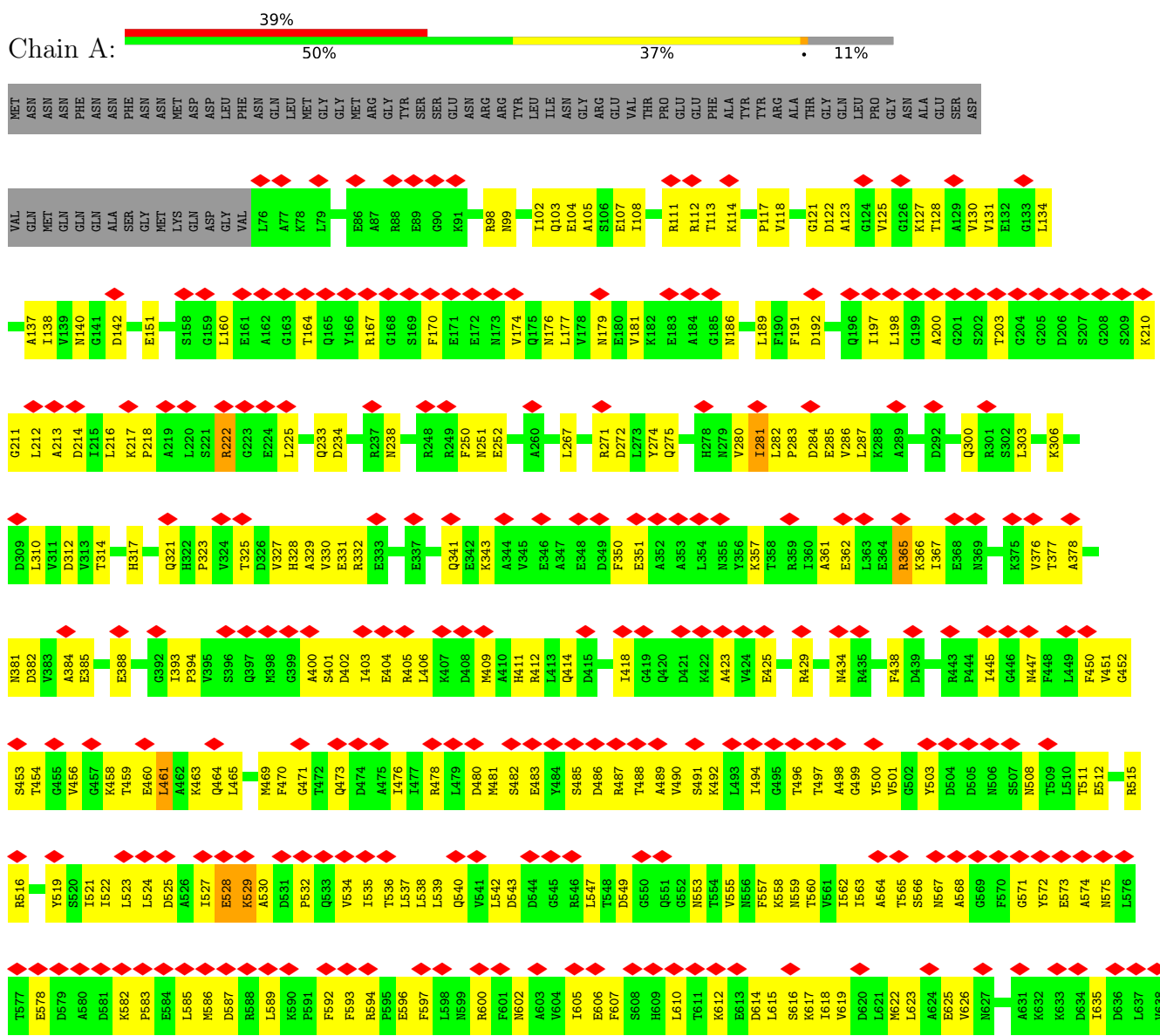
| Mol | Chain | Residues | Atoms |    |   |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---|---------|
| 3   | M     | 1        | Total | C  | N | O  | P | S | 0       |
|     |       |          | 31    | 10 | 5 | 12 | 3 | 1 |         |
| 3   | M     | 1        | Total | C  | N | O  | P | S | 0       |
|     |       |          | 31    | 10 | 5 | 12 | 3 | 1 |         |
| 3   | N     | 1        | Total | C  | N | O  | P | S | 0       |
|     |       |          | 31    | 10 | 5 | 12 | 3 | 1 |         |
| 3   | N     | 1        | Total | C  | N | O  | P | S | 0       |
|     |       |          | 31    | 10 | 5 | 12 | 3 | 1 |         |

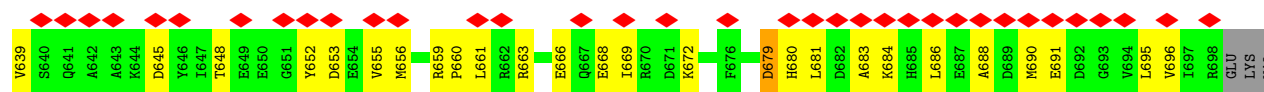


### 3 Residue-property plots

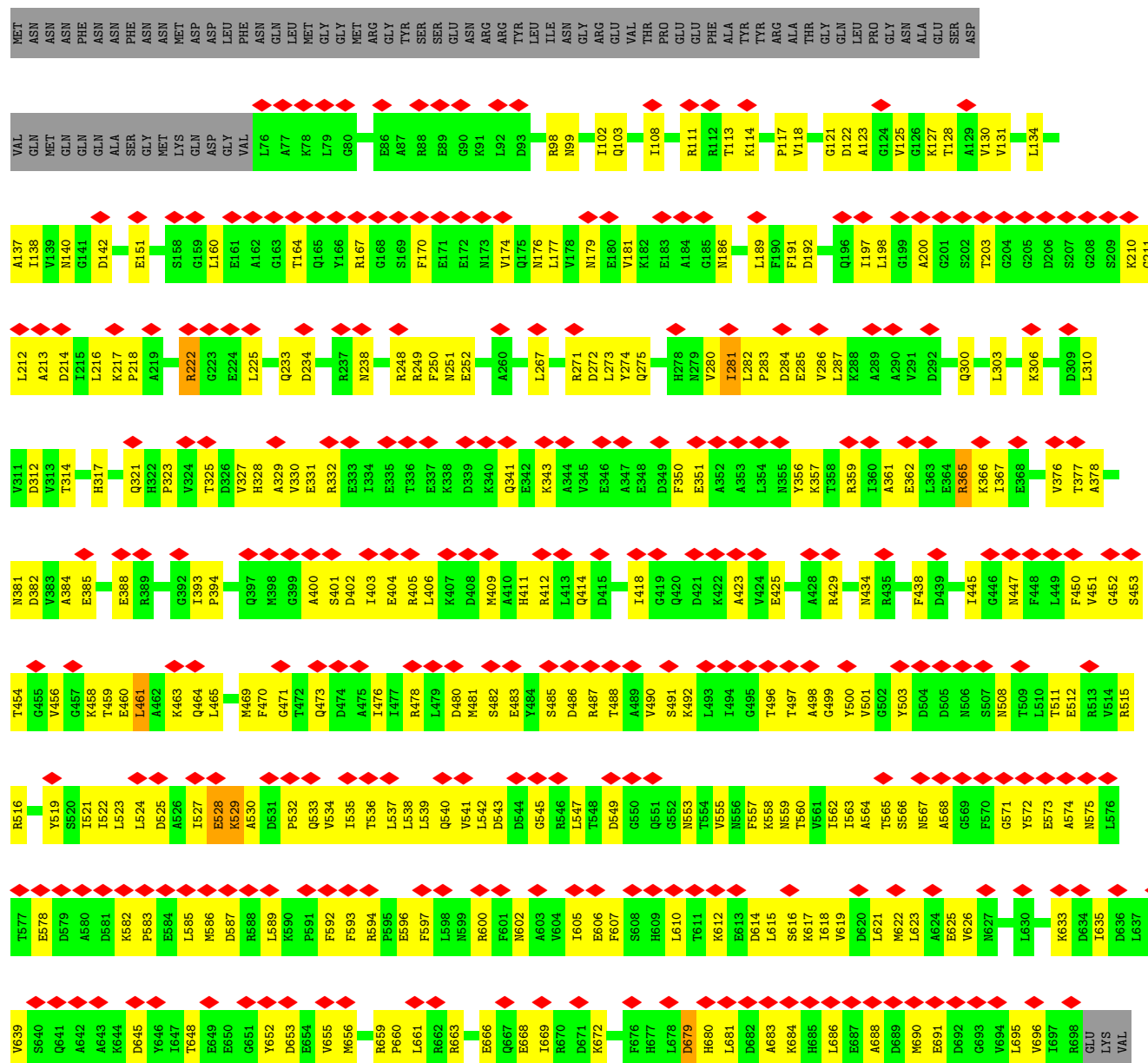
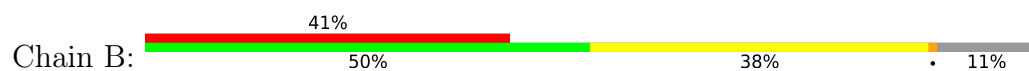
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: ATP-dependent Clp protease, ATP-binding subunit

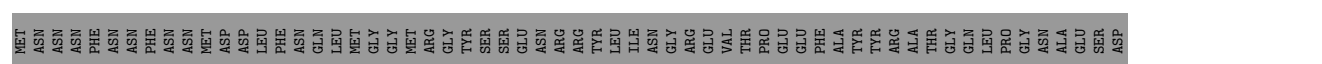
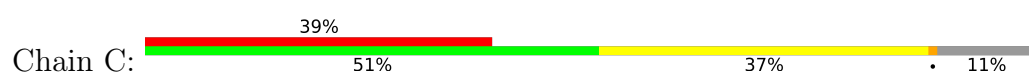


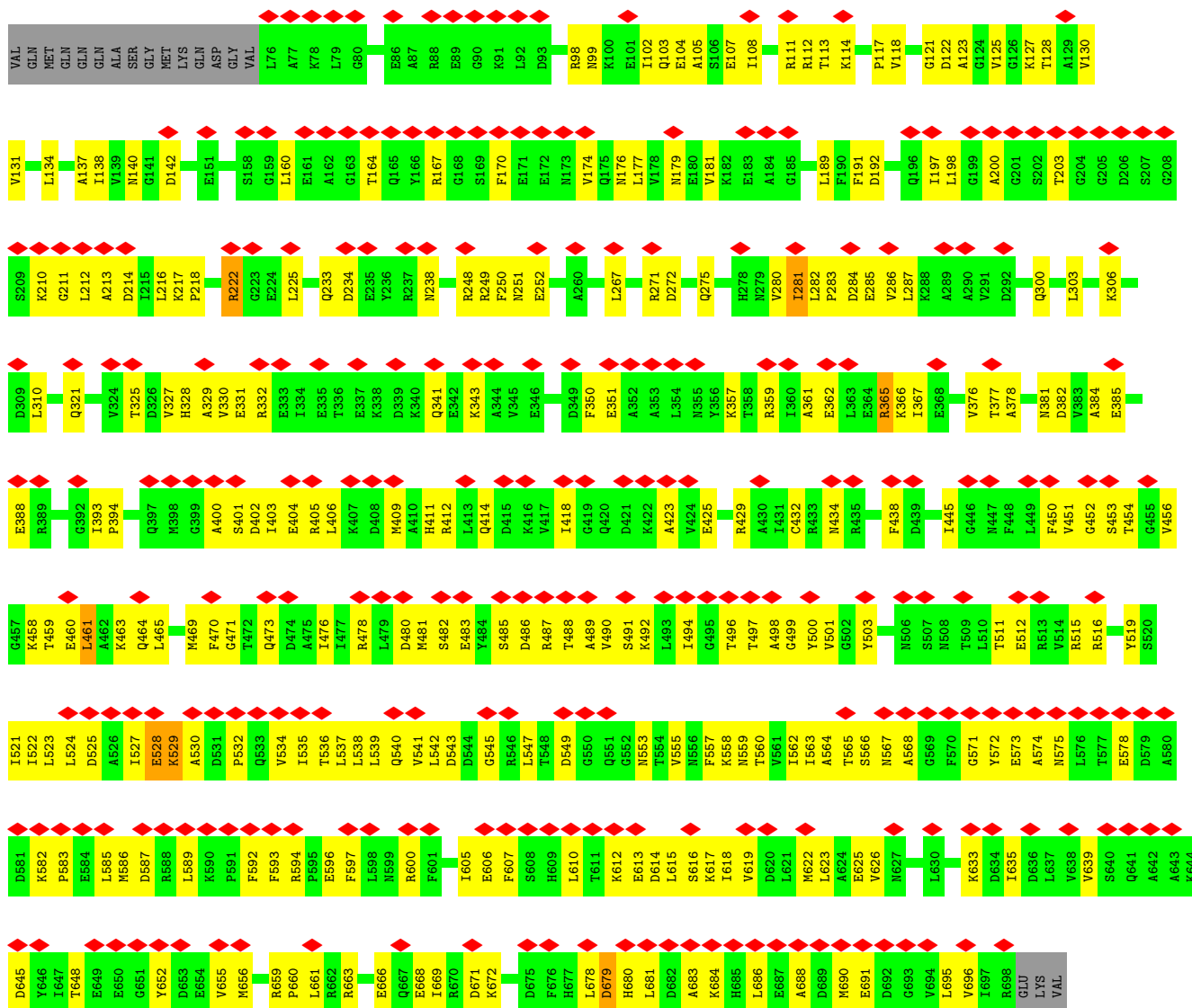


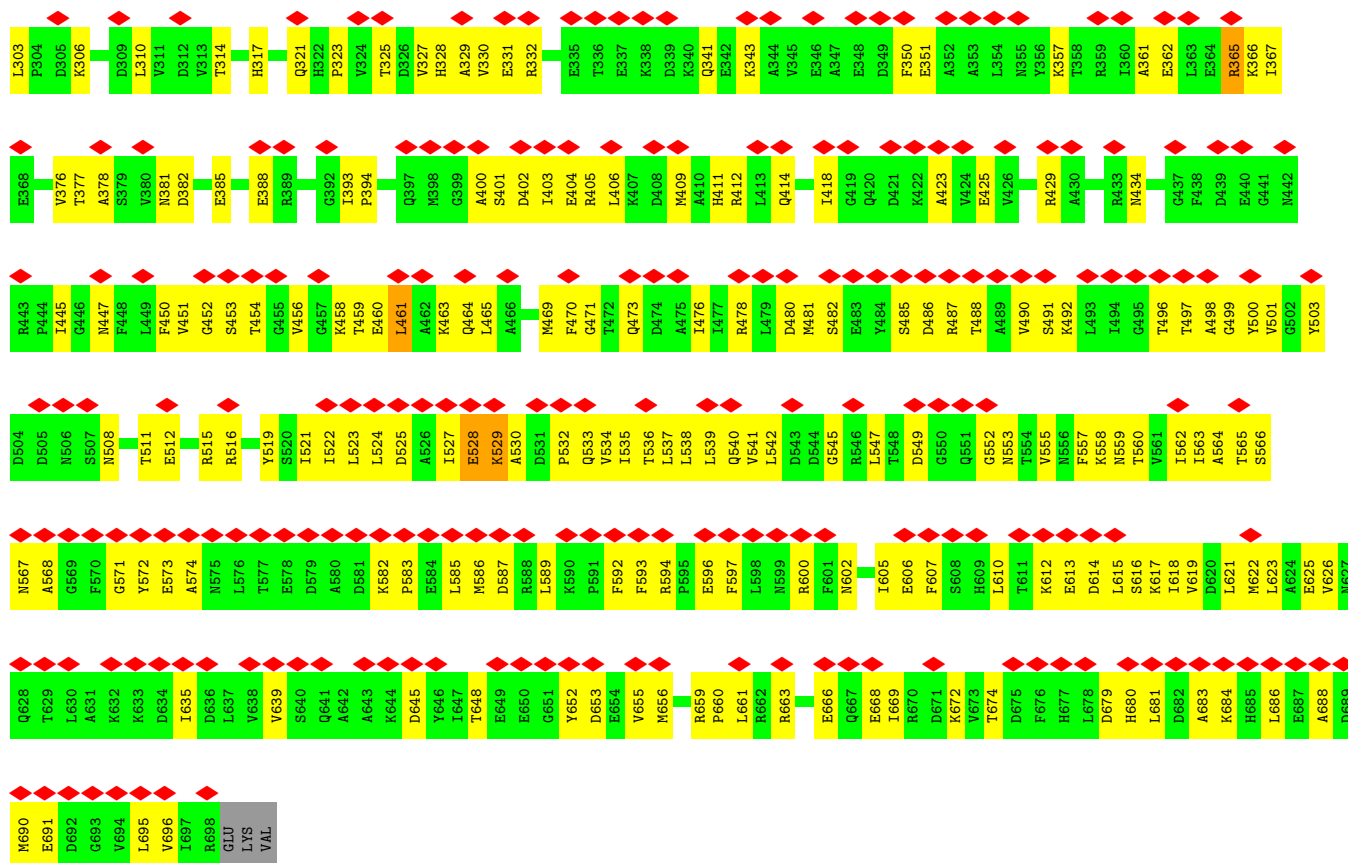
- Molecule 1: ATP-dependent Clp protease, ATP-binding subunit



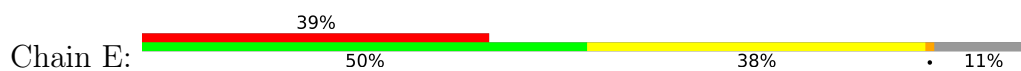
- Molecule 1: ATP-dependent Clp protease, ATP-binding subunit



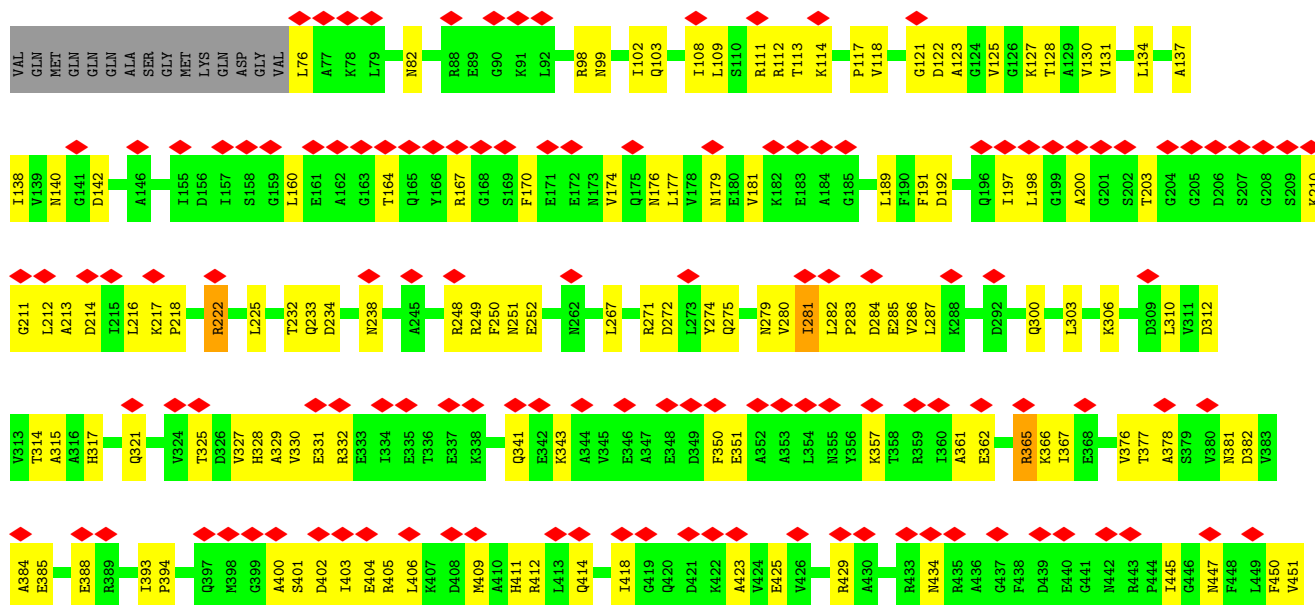


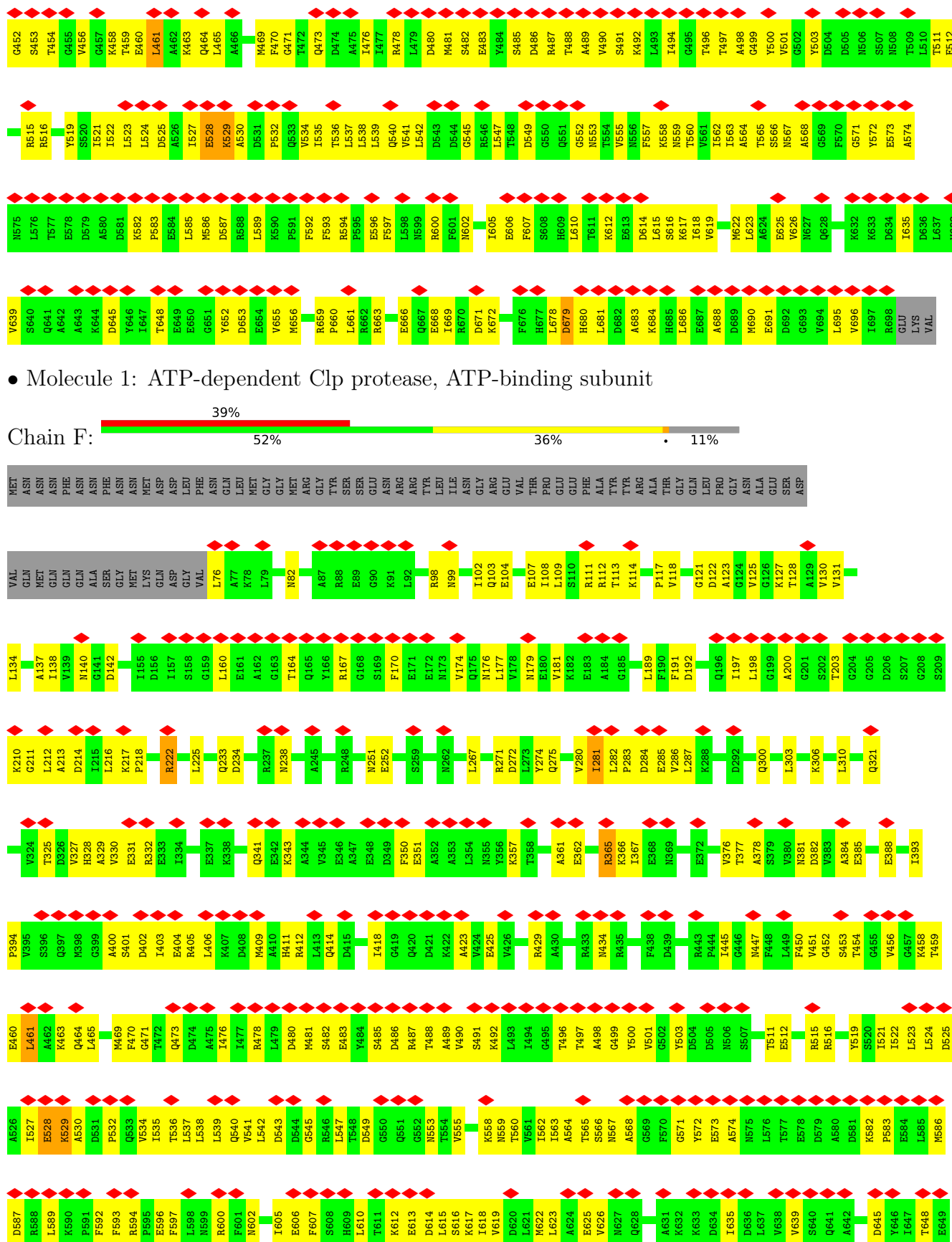


• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit



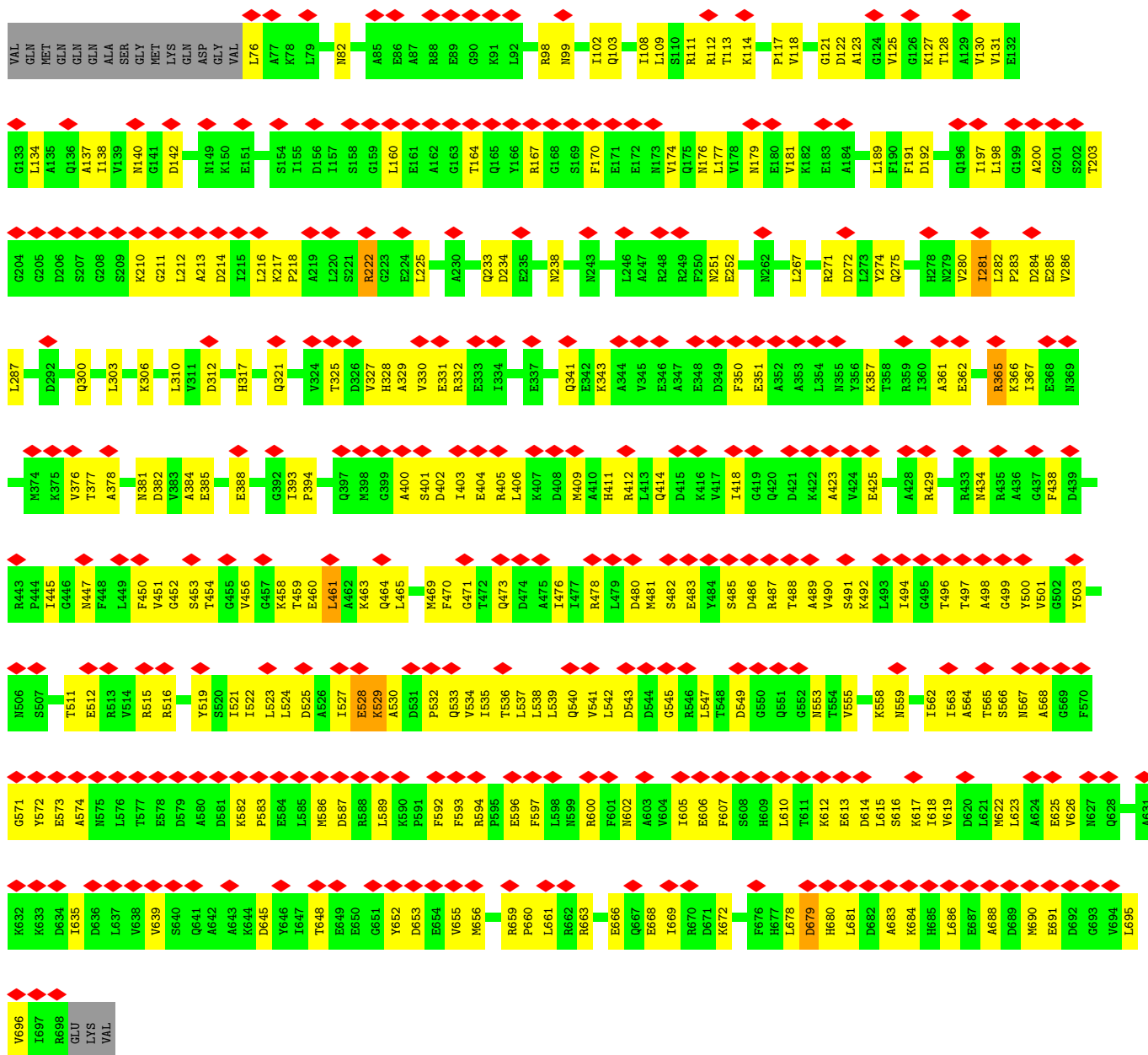
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ASN | ASN | ASN | PHE | ASN | ASN | PHE | ASN | ASN | ASN | ASP | ASP | LEU | PHE | ASN | GLN | LEU | MET | GLY | GLY | MET | ARG | GLY | TYR | SER | SER | GLU | ASN | ARG | ARG | TYR | LEU | ILE | ASN | GLY | ARG | GLU | VAL | THR | PRO | GLU | GLU | PHE | ALA | TYR | THR | ALA | GLY | GLN | LEU | PRO | GLY | ALA | SER | ASP |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

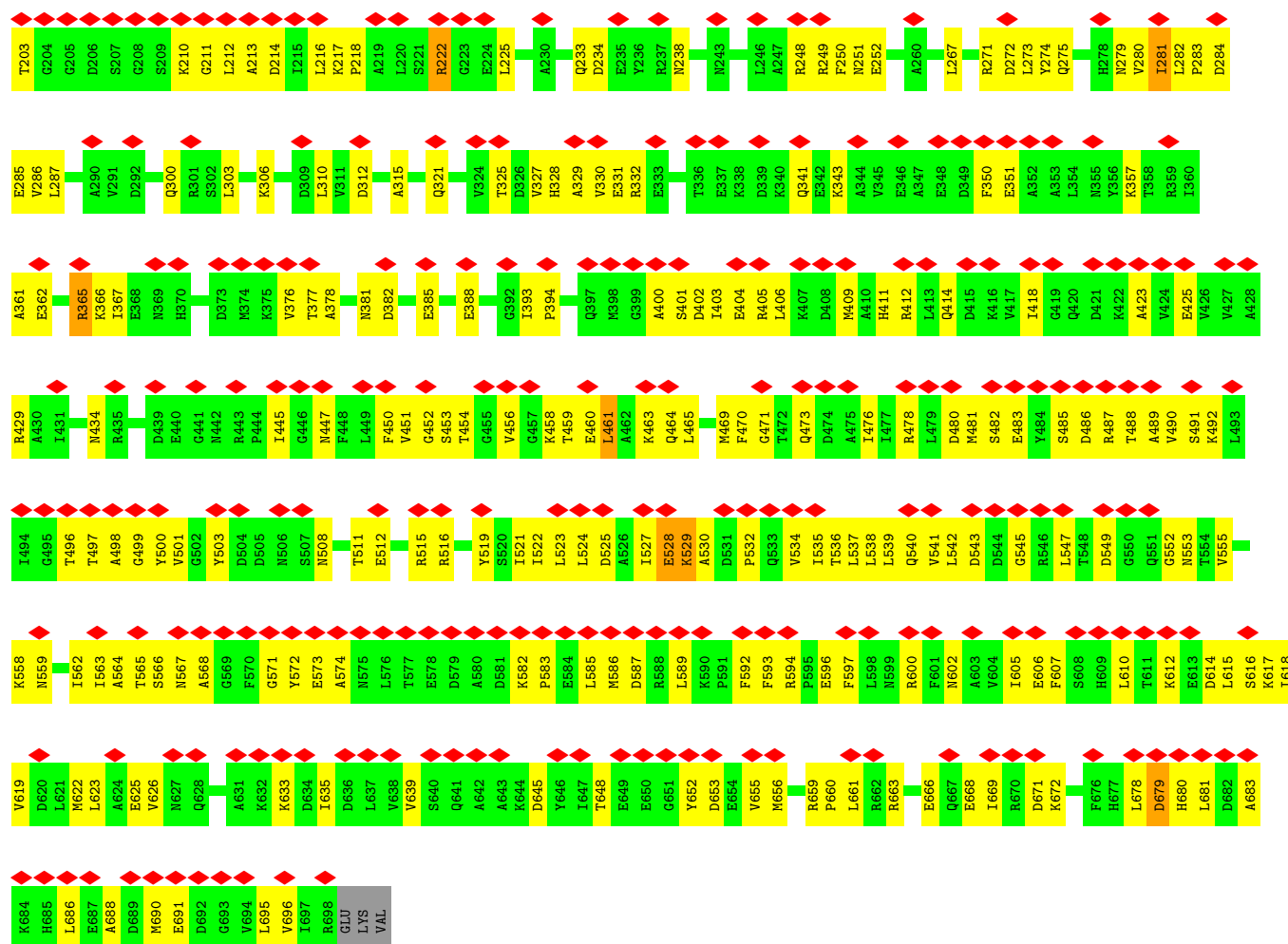




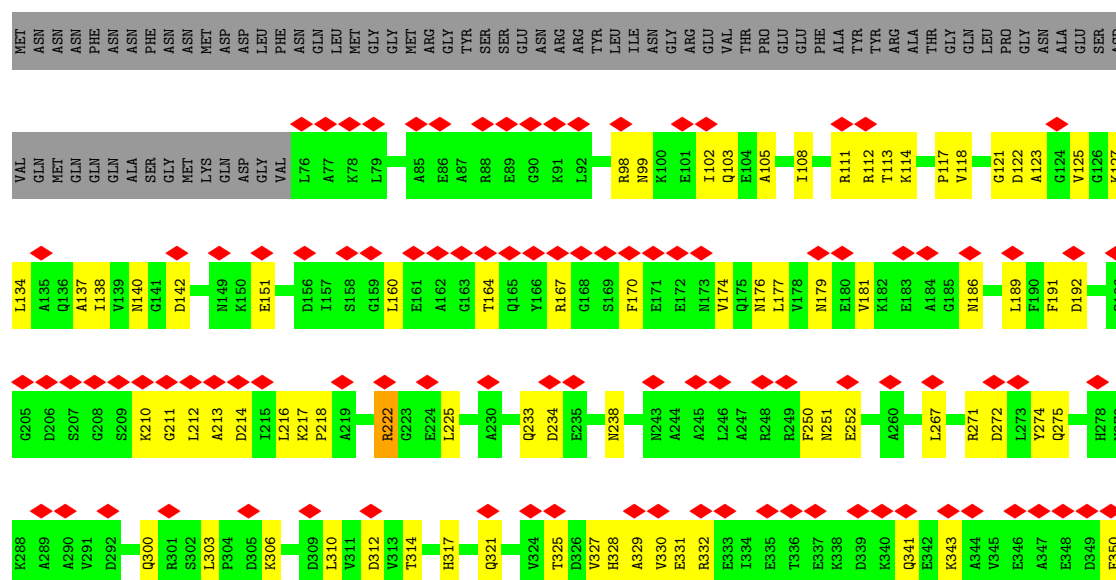
• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit



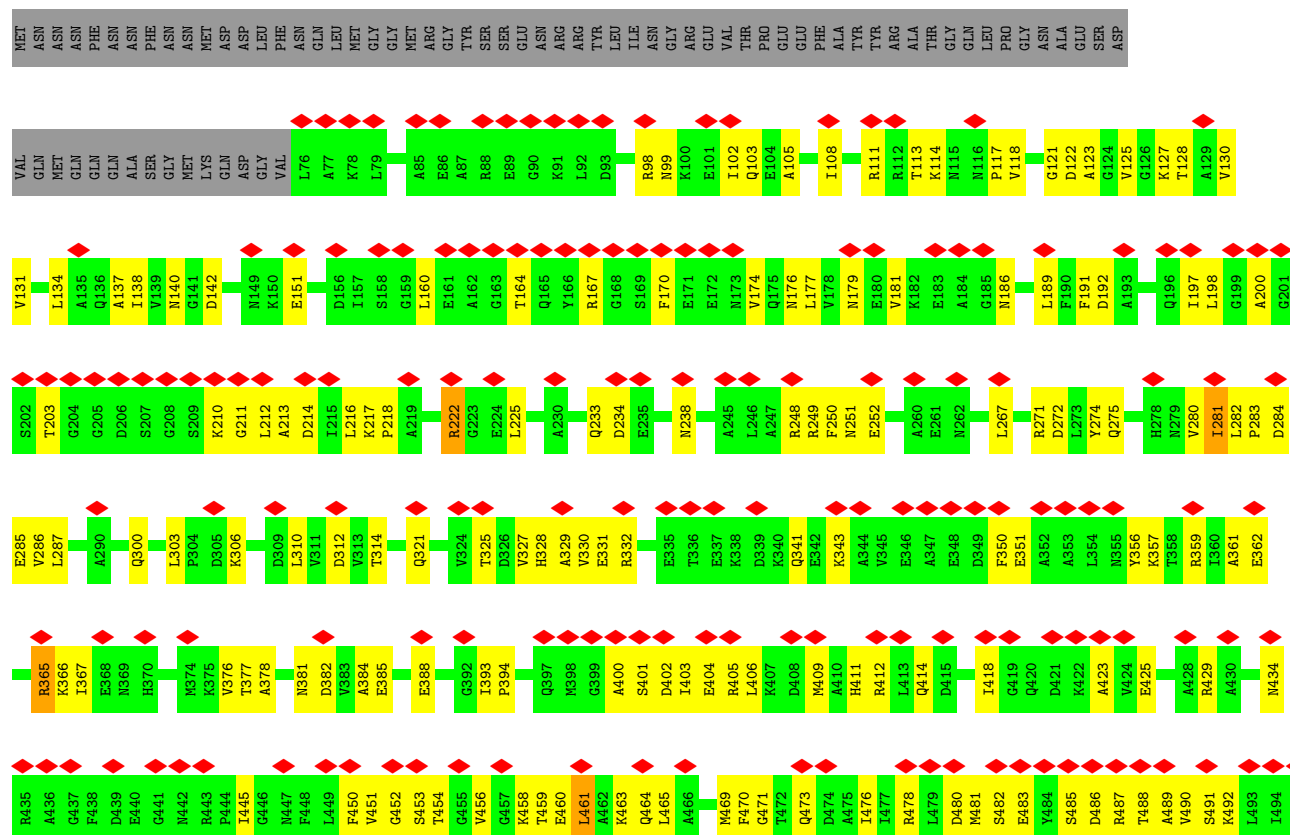


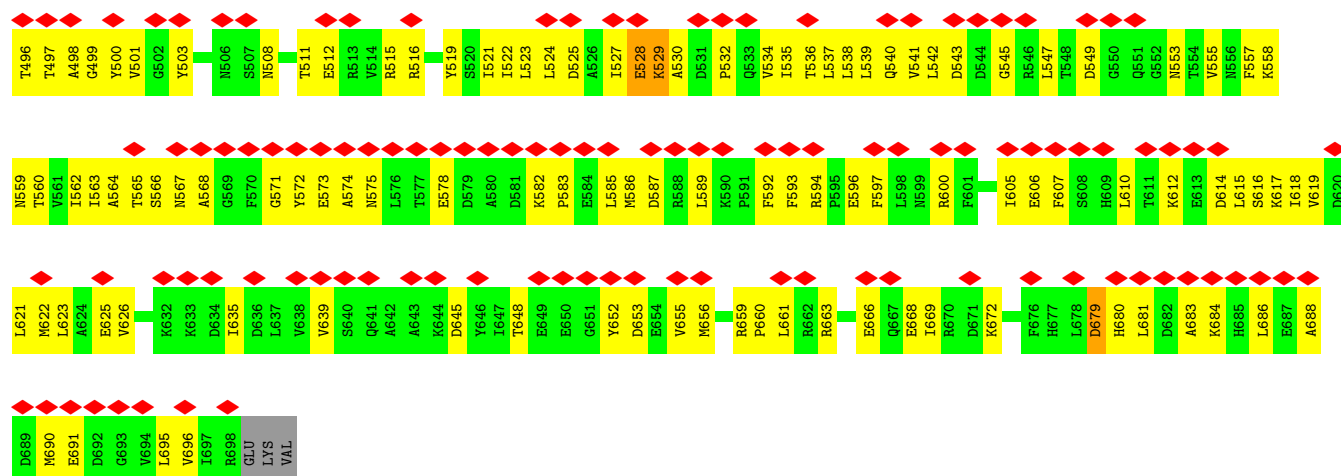


### • Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

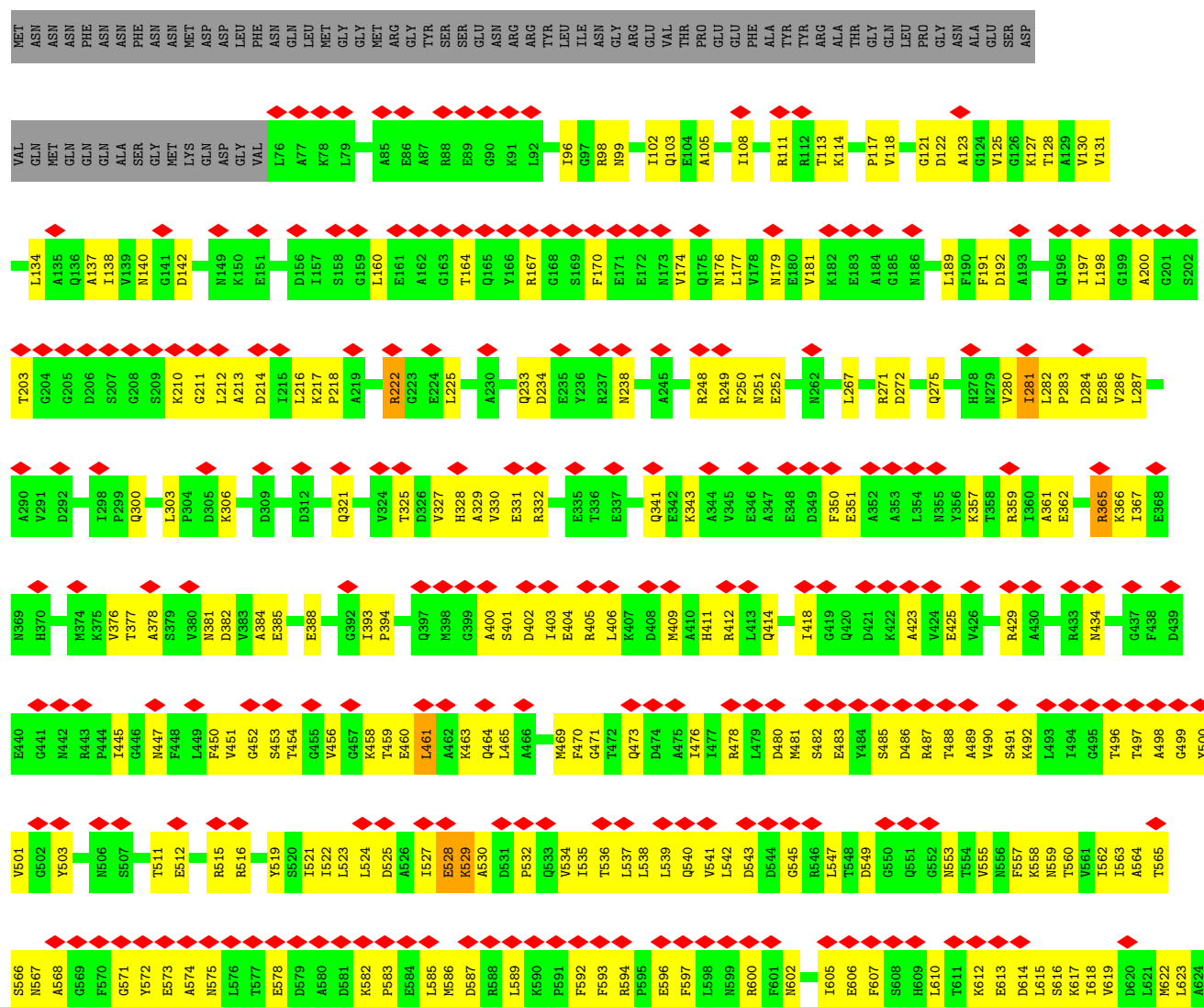
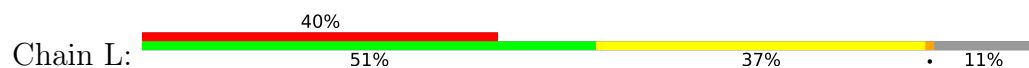


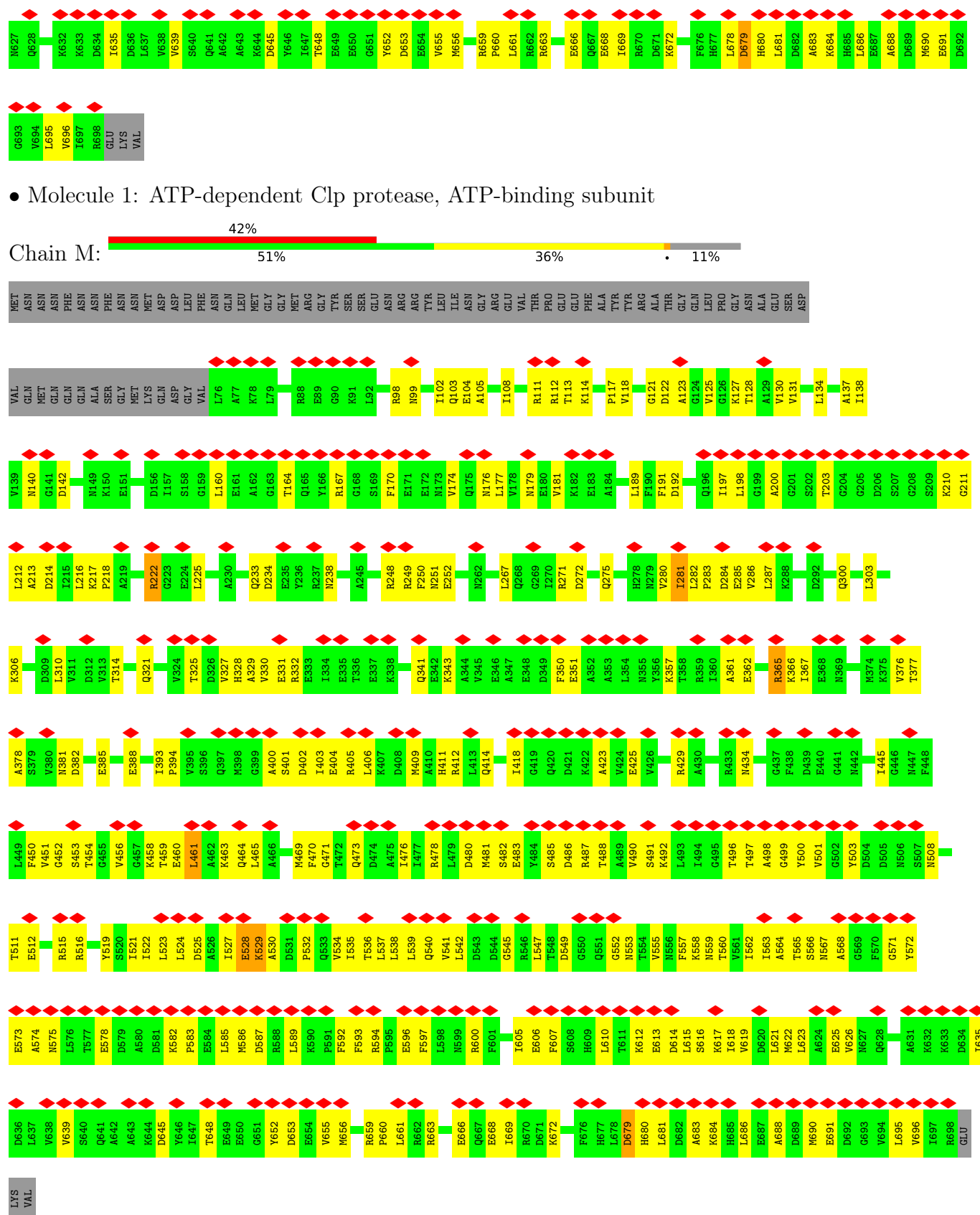






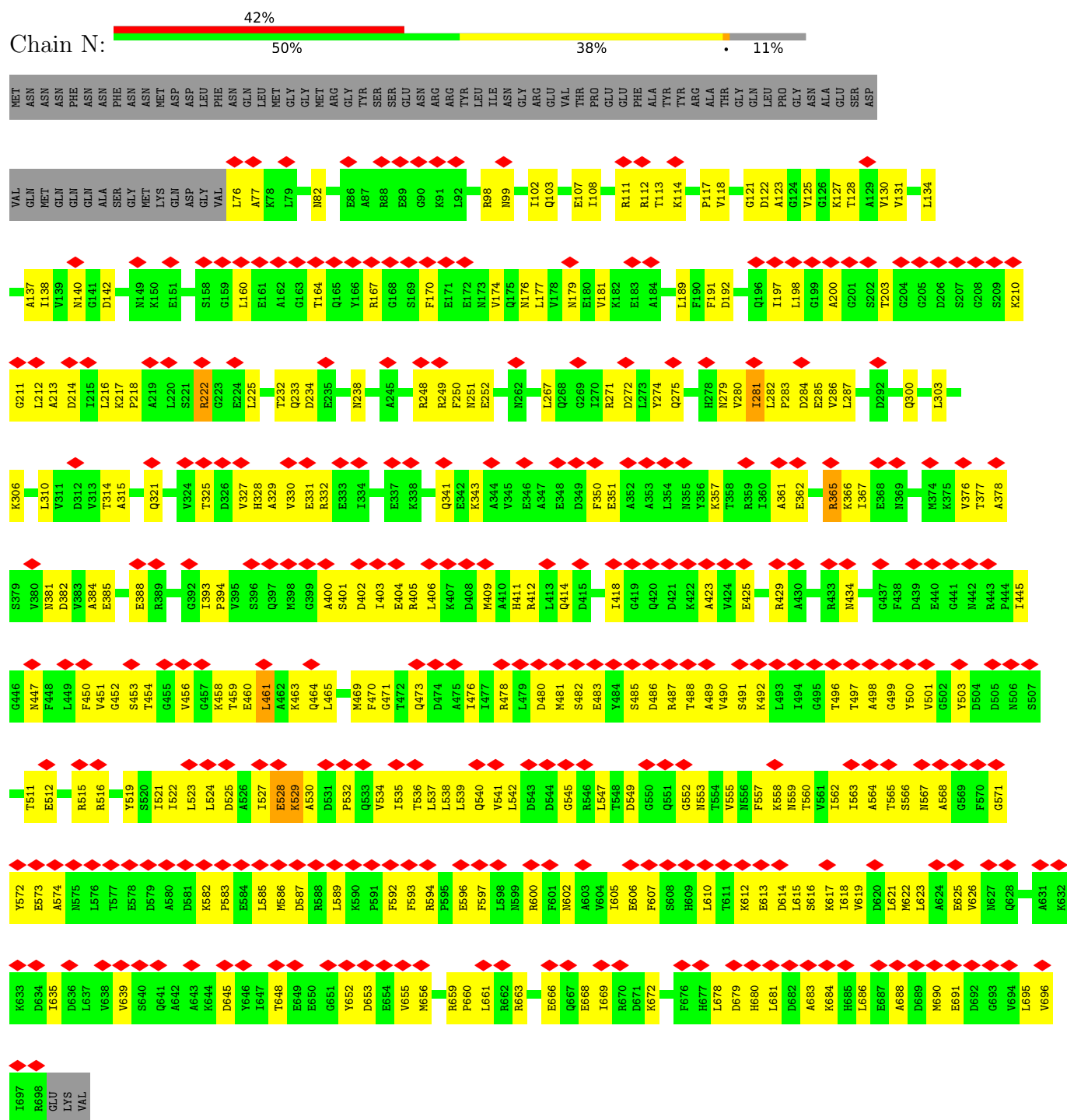
- Molecule 1: ATP-dependent Clp protease, ATP-binding subunit





• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit

• Molecule 1: ATP-dependent Clp protease, ATP-binding subunit



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 49797                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 0.717                                   | Depositor |
| Minimum map value                    | -0.436                                  | Depositor |
| Average map value                    | 0.009                                   | Depositor |
| Map value standard deviation         | 0.045                                   | Depositor |
| Recommended contour level            | 0.2                                     | Depositor |
| Map size (Å)                         | 280.0, 280.0, 280.0                     | wwPDB     |
| Map dimensions                       | 200, 200, 200                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.4, 1.4, 1.4                           | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.29         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| 1   | B     | 0.29         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| 1   | C     | 0.29         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| 1   | D     | 0.29         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| 1   | E     | 0.28         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| 1   | F     | 0.29         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| 1   | G     | 0.29         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| 1   | H     | 0.29         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| 1   | I     | 0.29         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| 1   | J     | 0.28         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| 1   | K     | 0.29         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| 1   | L     | 0.29         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| 1   | M     | 0.29         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| 1   | N     | 0.29         | 0/4883      | 0.57        | 1/6603 (0.0%)   |
| All | All   | 0.29         | 0/68362     | 0.57        | 14/92442 (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                   | 3                   |
| 1   | B     | 0                   | 3                   |
| 1   | C     | 0                   | 3                   |
| 1   | D     | 0                   | 2                   |
| 1   | E     | 0                   | 3                   |
| 1   | F     | 0                   | 3                   |
| 1   | G     | 0                   | 3                   |
| 1   | H     | 0                   | 3                   |
| 1   | I     | 0                   | 3                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | J     | 0                   | 3                   |
| 1   | K     | 0                   | 3                   |
| 1   | L     | 0                   | 3                   |
| 1   | M     | 0                   | 3                   |
| 1   | N     | 0                   | 2                   |
| All | All   | 0                   | 40                  |

There are no bond length outliers.

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 529 | LYS  | N-CA-C | -8.88 | 103.57      | 114.75   |
| 1   | N     | 529 | LYS  | N-CA-C | -8.87 | 103.57      | 114.75   |
| 1   | E     | 529 | LYS  | N-CA-C | -8.87 | 103.58      | 114.75   |
| 1   | M     | 529 | LYS  | N-CA-C | -8.87 | 103.58      | 114.75   |
| 1   | D     | 529 | LYS  | N-CA-C | -8.86 | 103.58      | 114.75   |
| 1   | H     | 529 | LYS  | N-CA-C | -8.85 | 103.60      | 114.75   |
| 1   | L     | 529 | LYS  | N-CA-C | -8.84 | 103.61      | 114.75   |
| 1   | F     | 529 | LYS  | N-CA-C | -8.84 | 103.61      | 114.75   |
| 1   | K     | 529 | LYS  | N-CA-C | -8.84 | 103.61      | 114.75   |
| 1   | I     | 529 | LYS  | N-CA-C | -8.84 | 103.62      | 114.75   |
| 1   | J     | 529 | LYS  | N-CA-C | -8.84 | 103.62      | 114.75   |
| 1   | A     | 529 | LYS  | N-CA-C | -8.83 | 103.62      | 114.75   |
| 1   | G     | 529 | LYS  | N-CA-C | -8.82 | 103.64      | 114.75   |
| 1   | C     | 529 | LYS  | N-CA-C | -8.81 | 103.65      | 114.75   |

There are no chirality outliers.

All (40) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 281 | ILE  | Peptide |
| 1   | A     | 528 | GLU  | Peptide |
| 1   | A     | 679 | ASP  | Peptide |
| 1   | B     | 281 | ILE  | Peptide |
| 1   | B     | 528 | GLU  | Peptide |
| 1   | B     | 679 | ASP  | Peptide |
| 1   | C     | 281 | ILE  | Peptide |
| 1   | C     | 528 | GLU  | Peptide |
| 1   | C     | 679 | ASP  | Peptide |
| 1   | D     | 281 | ILE  | Peptide |
| 1   | D     | 528 | GLU  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | E     | 281 | ILE  | Peptide |
| 1   | E     | 528 | GLU  | Peptide |
| 1   | E     | 679 | ASP  | Peptide |
| 1   | F     | 281 | ILE  | Peptide |
| 1   | F     | 528 | GLU  | Peptide |
| 1   | F     | 679 | ASP  | Peptide |
| 1   | G     | 281 | ILE  | Peptide |
| 1   | G     | 528 | GLU  | Peptide |
| 1   | G     | 679 | ASP  | Peptide |
| 1   | H     | 281 | ILE  | Peptide |
| 1   | H     | 528 | GLU  | Peptide |
| 1   | H     | 679 | ASP  | Peptide |
| 1   | I     | 281 | ILE  | Peptide |
| 1   | I     | 528 | GLU  | Peptide |
| 1   | I     | 679 | ASP  | Peptide |
| 1   | J     | 281 | ILE  | Peptide |
| 1   | J     | 528 | GLU  | Peptide |
| 1   | J     | 679 | ASP  | Peptide |
| 1   | K     | 281 | ILE  | Peptide |
| 1   | K     | 528 | GLU  | Peptide |
| 1   | K     | 679 | ASP  | Peptide |
| 1   | L     | 281 | ILE  | Peptide |
| 1   | L     | 528 | GLU  | Peptide |
| 1   | L     | 679 | ASP  | Peptide |
| 1   | M     | 281 | ILE  | Peptide |
| 1   | M     | 528 | GLU  | Peptide |
| 1   | M     | 679 | ASP  | Peptide |
| 1   | N     | 281 | ILE  | Peptide |
| 1   | N     | 528 | GLU  | 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     | 4824  | 0        | 4841     | 259     | 0            |
| 1   | B     | 4824  | 0        | 4841     | 269     | 0            |
| 1   | C     | 4824  | 0        | 4841     | 263     | 0            |
| 1   | D     | 4824  | 0        | 4841     | 274     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | E     | 4824  | 0        | 4841     | 272     | 0            |
| 1   | F     | 4824  | 0        | 4841     | 251     | 0            |
| 1   | G     | 4824  | 0        | 4841     | 263     | 0            |
| 1   | H     | 4824  | 0        | 4841     | 264     | 0            |
| 1   | I     | 4824  | 0        | 4841     | 267     | 0            |
| 1   | J     | 4824  | 0        | 4841     | 253     | 0            |
| 1   | K     | 4824  | 0        | 4841     | 258     | 0            |
| 1   | L     | 4824  | 0        | 4841     | 253     | 0            |
| 1   | M     | 4824  | 0        | 4841     | 258     | 0            |
| 1   | N     | 4824  | 0        | 4841     | 266     | 0            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| 2   | C     | 2     | 0        | 0        | 0       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 2   | E     | 2     | 0        | 0        | 0       | 0            |
| 2   | F     | 2     | 0        | 0        | 0       | 0            |
| 2   | G     | 2     | 0        | 0        | 0       | 0            |
| 2   | H     | 2     | 0        | 0        | 0       | 0            |
| 2   | I     | 2     | 0        | 0        | 0       | 0            |
| 2   | J     | 2     | 0        | 0        | 0       | 0            |
| 2   | K     | 2     | 0        | 0        | 0       | 0            |
| 2   | L     | 2     | 0        | 0        | 0       | 0            |
| 2   | M     | 2     | 0        | 0        | 0       | 0            |
| 2   | N     | 2     | 0        | 0        | 0       | 0            |
| 3   | A     | 62    | 0        | 24       | 6       | 0            |
| 3   | B     | 62    | 0        | 24       | 7       | 0            |
| 3   | C     | 62    | 0        | 24       | 6       | 0            |
| 3   | D     | 62    | 0        | 24       | 7       | 0            |
| 3   | E     | 62    | 0        | 24       | 6       | 0            |
| 3   | F     | 62    | 0        | 24       | 6       | 0            |
| 3   | G     | 62    | 0        | 24       | 6       | 0            |
| 3   | H     | 62    | 0        | 24       | 6       | 0            |
| 3   | I     | 62    | 0        | 24       | 6       | 0            |
| 3   | J     | 62    | 0        | 24       | 6       | 0            |
| 3   | K     | 62    | 0        | 24       | 7       | 0            |
| 3   | L     | 62    | 0        | 24       | 7       | 0            |
| 3   | M     | 62    | 0        | 24       | 6       | 0            |
| 3   | N     | 62    | 0        | 24       | 6       | 0            |
| All | All   | 68432 | 0        | 68110    | 3519    | 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 26.

All (3519) 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:H:103:GLN:NE2  | 1:I:321:GLN:OE1  | 1.97                     | 0.95              |
| 1:M:365:ARG:HH11 | 1:M:365:ARG:HG3  | 1.32                     | 0.95              |
| 1:D:365:ARG:HH11 | 1:D:365:ARG:HG3  | 1.31                     | 0.95              |
| 1:K:365:ARG:HG3  | 1:K:365:ARG:HH11 | 1.32                     | 0.95              |
| 1:B:365:ARG:HH11 | 1:B:365:ARG:HG3  | 1.32                     | 0.95              |
| 1:G:365:ARG:HH11 | 1:G:365:ARG:HG3  | 1.32                     | 0.95              |
| 1:I:365:ARG:HH11 | 1:I:365:ARG:HG3  | 1.32                     | 0.95              |
| 1:B:482:SER:HA   | 1:B:530:ALA:HB2  | 1.49                     | 0.95              |
| 1:K:482:SER:HA   | 1:K:530:ALA:HB2  | 1.48                     | 0.95              |
| 1:J:482:SER:HA   | 1:J:530:ALA:HB2  | 1.49                     | 0.94              |
| 1:A:482:SER:HA   | 1:A:530:ALA:HB2  | 1.49                     | 0.94              |
| 1:E:365:ARG:HH11 | 1:E:365:ARG:HG3  | 1.32                     | 0.94              |
| 1:H:365:ARG:HH11 | 1:H:365:ARG:HG3  | 1.31                     | 0.94              |
| 1:C:482:SER:HA   | 1:C:530:ALA:HB2  | 1.49                     | 0.94              |
| 1:D:534:VAL:HG22 | 1:E:492:LYS:HB3  | 1.46                     | 0.94              |
| 1:N:365:ARG:HG3  | 1:N:365:ARG:HH11 | 1.32                     | 0.94              |
| 1:F:365:ARG:HG3  | 1:F:365:ARG:HH11 | 1.31                     | 0.93              |
| 1:L:482:SER:HA   | 1:L:530:ALA:HB2  | 1.49                     | 0.93              |
| 1:E:482:SER:HA   | 1:E:530:ALA:HB2  | 1.48                     | 0.93              |
| 1:N:482:SER:HA   | 1:N:530:ALA:HB2  | 1.48                     | 0.93              |
| 1:C:365:ARG:HG3  | 1:C:365:ARG:HH11 | 1.31                     | 0.93              |
| 1:F:482:SER:HA   | 1:F:530:ALA:HB2  | 1.49                     | 0.93              |
| 1:H:482:SER:HA   | 1:H:530:ALA:HB2  | 1.49                     | 0.93              |
| 1:A:365:ARG:HH11 | 1:A:365:ARG:HG3  | 1.32                     | 0.92              |
| 1:L:365:ARG:HH11 | 1:L:365:ARG:HG3  | 1.32                     | 0.92              |
| 1:M:482:SER:HA   | 1:M:530:ALA:HB2  | 1.48                     | 0.92              |
| 1:D:482:SER:HA   | 1:D:530:ALA:HB2  | 1.48                     | 0.92              |
| 1:I:482:SER:HA   | 1:I:530:ALA:HB2  | 1.49                     | 0.92              |
| 1:J:365:ARG:HH11 | 1:J:365:ARG:HG3  | 1.32                     | 0.92              |
| 1:G:482:SER:HA   | 1:G:530:ALA:HB2  | 1.49                     | 0.92              |
| 1:H:532:PRO:HB3  | 1:I:491:SER:H    | 1.35                     | 0.90              |
| 1:B:534:VAL:HG22 | 1:C:492:LYS:HB3  | 1.53                     | 0.89              |
| 1:M:532:PRO:HB3  | 1:N:491:SER:H    | 1.38                     | 0.87              |
| 1:J:532:PRO:HB3  | 1:K:491:SER:H    | 1.40                     | 0.85              |
| 1:C:350:PHE:HB3  | 1:M:350:PHE:HB3  | 1.58                     | 0.84              |
| 1:D:532:PRO:HA   | 1:E:490:VAL:HB   | 1.57                     | 0.84              |
| 1:D:536:THR:HG21 | 1:E:483:GLU:HG3  | 1.58                     | 0.83              |
| 1:C:234:ASP:OD1  | 1:C:238:ASN:ND2  | 2.13                     | 0.81              |
| 1:L:234:ASP:OD1  | 1:L:238:ASN:ND2  | 2.13                     | 0.81              |
| 1:K:234:ASP:OD1  | 1:K:238:ASN:ND2  | 2.13                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:234:ASP:OD1  | 1:B:238:ASN:ND2  | 2.13                     | 0.81              |
| 1:D:234:ASP:OD1  | 1:D:238:ASN:ND2  | 2.14                     | 0.81              |
| 1:I:234:ASP:OD1  | 1:I:238:ASN:ND2  | 2.13                     | 0.81              |
| 1:M:234:ASP:OD1  | 1:M:238:ASN:ND2  | 2.13                     | 0.81              |
| 1:G:234:ASP:OD1  | 1:G:238:ASN:ND2  | 2.13                     | 0.81              |
| 1:D:532:PRO:HB3  | 1:E:491:SER:H    | 1.45                     | 0.81              |
| 1:F:234:ASP:OD1  | 1:F:238:ASN:ND2  | 2.13                     | 0.81              |
| 1:H:234:ASP:OD1  | 1:H:238:ASN:ND2  | 2.13                     | 0.81              |
| 1:N:234:ASP:OD1  | 1:N:238:ASN:ND2  | 2.13                     | 0.81              |
| 1:E:234:ASP:OD1  | 1:E:238:ASN:ND2  | 2.13                     | 0.81              |
| 1:J:234:ASP:OD1  | 1:J:238:ASN:ND2  | 2.13                     | 0.80              |
| 1:A:234:ASP:OD1  | 1:A:238:ASN:ND2  | 2.14                     | 0.80              |
| 1:H:321:GLN:OE1  | 1:N:103:GLN:NE2  | 2.12                     | 0.80              |
| 1:K:103:GLN:NE2  | 1:L:321:GLN:OE1  | 2.15                     | 0.80              |
| 1:H:532:PRO:HA   | 1:I:490:VAL:HB   | 1.63                     | 0.79              |
| 1:B:536:THR:HG21 | 1:C:483:GLU:HG3  | 1.63                     | 0.79              |
| 1:M:532:PRO:HA   | 1:N:490:VAL:HB   | 1.64                     | 0.79              |
| 1:H:536:THR:HG21 | 1:I:483:GLU:HG3  | 1.63                     | 0.78              |
| 1:A:492:LYS:HB3  | 1:G:534:VAL:HG22 | 1.64                     | 0.78              |
| 1:L:496:THR:HG23 | 1:L:499:GLY:H    | 1.49                     | 0.78              |
| 1:A:523:LEU:HD23 | 1:A:563:ILE:HB   | 1.66                     | 0.78              |
| 1:C:496:THR:HG23 | 1:C:499:GLY:H    | 1.49                     | 0.78              |
| 1:G:523:LEU:HD23 | 1:G:563:ILE:HB   | 1.66                     | 0.78              |
| 1:I:523:LEU:HD23 | 1:I:563:ILE:HB   | 1.66                     | 0.78              |
| 1:M:496:THR:HG23 | 1:M:499:GLY:H    | 1.49                     | 0.78              |
| 1:J:523:LEU:HD23 | 1:J:563:ILE:HB   | 1.66                     | 0.78              |
| 1:D:496:THR:HG23 | 1:D:499:GLY:H    | 1.49                     | 0.78              |
| 1:J:103:GLN:NE2  | 1:K:321:GLN:OE1  | 2.16                     | 0.78              |
| 1:F:523:LEU:HD23 | 1:F:563:ILE:HB   | 1.66                     | 0.78              |
| 1:K:496:THR:HG23 | 1:K:499:GLY:H    | 1.49                     | 0.78              |
| 1:N:496:THR:HG23 | 1:N:499:GLY:H    | 1.49                     | 0.78              |
| 1:D:532:PRO:HB2  | 1:D:534:VAL:HG23 | 1.66                     | 0.77              |
| 1:E:496:THR:HG23 | 1:E:499:GLY:H    | 1.49                     | 0.77              |
| 1:E:532:PRO:HB2  | 1:E:534:VAL:HG23 | 1.66                     | 0.77              |
| 1:H:523:LEU:HD23 | 1:H:563:ILE:HB   | 1.66                     | 0.77              |
| 1:L:451:VAL:HG22 | 1:L:566:SER:HB3  | 1.66                     | 0.77              |
| 1:B:496:THR:HG23 | 1:B:499:GLY:H    | 1.49                     | 0.77              |
| 1:B:523:LEU:HD23 | 1:B:563:ILE:HB   | 1.66                     | 0.77              |
| 1:D:451:VAL:HG22 | 1:D:566:SER:HB3  | 1.67                     | 0.77              |
| 1:H:451:VAL:HG22 | 1:H:566:SER:HB3  | 1.67                     | 0.77              |
| 1:K:523:LEU:HD23 | 1:K:563:ILE:HB   | 1.66                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:451:VAL:HG22 | 1:M:566:SER:HB3  | 1.67                     | 0.77              |
| 1:F:451:VAL:HG22 | 1:F:566:SER:HB3  | 1.67                     | 0.77              |
| 1:G:451:VAL:HG22 | 1:G:566:SER:HB3  | 1.67                     | 0.77              |
| 1:H:496:THR:HG23 | 1:H:499:GLY:H    | 1.49                     | 0.77              |
| 1:I:451:VAL:HG22 | 1:I:566:SER:HB3  | 1.67                     | 0.77              |
| 1:J:496:THR:HG23 | 1:J:499:GLY:H    | 1.49                     | 0.77              |
| 1:N:532:PRO:HB2  | 1:N:534:VAL:HG23 | 1.66                     | 0.77              |
| 1:A:496:THR:HG23 | 1:A:499:GLY:H    | 1.49                     | 0.77              |
| 1:C:451:VAL:HG22 | 1:C:566:SER:HB3  | 1.67                     | 0.77              |
| 1:E:451:VAL:HG22 | 1:E:566:SER:HB3  | 1.67                     | 0.77              |
| 1:I:103:GLN:NE2  | 1:J:321:GLN:OE1  | 2.16                     | 0.77              |
| 1:M:532:PRO:HB2  | 1:M:534:VAL:HG23 | 1.66                     | 0.77              |
| 1:M:672:LYS:HG3  | 1:M:695:LEU:HD23 | 1.66                     | 0.77              |
| 1:F:496:THR:HG23 | 1:F:499:GLY:H    | 1.49                     | 0.77              |
| 1:C:532:PRO:HB2  | 1:C:534:VAL:HG23 | 1.66                     | 0.77              |
| 1:I:496:THR:HG23 | 1:I:499:GLY:H    | 1.49                     | 0.77              |
| 1:N:451:VAL:HG22 | 1:N:566:SER:HB3  | 1.67                     | 0.77              |
| 1:A:451:VAL:HG22 | 1:A:566:SER:HB3  | 1.67                     | 0.77              |
| 1:D:497:THR:HB   | 1:E:489:ALA:O    | 1.84                     | 0.77              |
| 1:F:500:TYR:HA   | 1:F:503:TYR:HD1  | 1.50                     | 0.77              |
| 1:H:500:TYR:HA   | 1:H:503:TYR:HD1  | 1.50                     | 0.77              |
| 1:N:672:LYS:HG3  | 1:N:695:LEU:HD23 | 1.66                     | 0.77              |
| 1:F:532:PRO:HB2  | 1:F:534:VAL:HG23 | 1.66                     | 0.77              |
| 1:G:496:THR:HG23 | 1:G:499:GLY:H    | 1.49                     | 0.77              |
| 1:J:451:VAL:HG22 | 1:J:566:SER:HB3  | 1.67                     | 0.77              |
| 1:L:672:LYS:HG3  | 1:L:695:LEU:HD23 | 1.66                     | 0.77              |
| 1:A:500:TYR:HA   | 1:A:503:TYR:HD1  | 1.50                     | 0.77              |
| 1:B:451:VAL:HG22 | 1:B:566:SER:HB3  | 1.67                     | 0.77              |
| 1:D:672:LYS:HG3  | 1:D:695:LEU:HD23 | 1.66                     | 0.77              |
| 1:E:672:LYS:HG3  | 1:E:695:LEU:HD23 | 1.66                     | 0.77              |
| 1:H:532:PRO:HB2  | 1:H:534:VAL:HG23 | 1.66                     | 0.76              |
| 1:J:500:TYR:HA   | 1:J:503:TYR:HD1  | 1.50                     | 0.76              |
| 1:K:451:VAL:HG22 | 1:K:566:SER:HB3  | 1.67                     | 0.76              |
| 1:L:532:PRO:HB2  | 1:L:534:VAL:HG23 | 1.66                     | 0.76              |
| 1:E:523:LEU:HD23 | 1:E:563:ILE:HB   | 1.66                     | 0.76              |
| 1:A:103:GLN:NE2  | 1:B:321:GLN:OE1  | 2.17                     | 0.76              |
| 1:C:672:LYS:HG3  | 1:C:695:LEU:HD23 | 1.66                     | 0.76              |
| 1:N:523:LEU:HD23 | 1:N:563:ILE:HB   | 1.66                     | 0.76              |
| 1:A:350:PHE:HB3  | 1:H:350:PHE:HB3  | 1.67                     | 0.76              |
| 1:B:532:PRO:HB2  | 1:B:534:VAL:HG23 | 1.66                     | 0.76              |
| 1:C:523:LEU:HD23 | 1:C:563:ILE:HB   | 1.66                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:672:LYS:HG3  | 1:H:695:LEU:HD23 | 1.66                     | 0.76              |
| 1:K:672:LYS:HG3  | 1:K:695:LEU:HD23 | 1.66                     | 0.76              |
| 1:M:523:LEU:HD23 | 1:M:563:ILE:HB   | 1.66                     | 0.76              |
| 1:B:539:LEU:HD23 | 1:B:542:LEU:HD12 | 1.68                     | 0.76              |
| 1:D:523:LEU:HD23 | 1:D:563:ILE:HB   | 1.66                     | 0.76              |
| 1:L:523:LEU:HD23 | 1:L:563:ILE:HB   | 1.66                     | 0.76              |
| 1:M:534:VAL:HG22 | 1:N:492:LYS:HB3  | 1.67                     | 0.76              |
| 1:K:532:PRO:HB2  | 1:K:534:VAL:HG23 | 1.66                     | 0.76              |
| 1:K:539:LEU:HD23 | 1:K:542:LEU:HD12 | 1.68                     | 0.76              |
| 1:C:539:LEU:HD23 | 1:C:542:LEU:HD12 | 1.68                     | 0.76              |
| 1:F:672:LYS:HG3  | 1:F:695:LEU:HD23 | 1.66                     | 0.76              |
| 1:B:672:LYS:HG3  | 1:B:695:LEU:HD23 | 1.66                     | 0.75              |
| 1:D:533:GLN:O    | 1:E:492:LYS:NZ   | 2.13                     | 0.75              |
| 1:G:532:PRO:HB2  | 1:G:534:VAL:HG23 | 1.66                     | 0.75              |
| 1:K:500:TYR:HA   | 1:K:503:TYR:HD1  | 1.50                     | 0.75              |
| 1:M:539:LEU:HD23 | 1:M:542:LEU:HD12 | 1.68                     | 0.75              |
| 1:B:500:TYR:HA   | 1:B:503:TYR:HD1  | 1.50                     | 0.75              |
| 1:D:539:LEU:HD23 | 1:D:542:LEU:HD12 | 1.68                     | 0.75              |
| 1:I:532:PRO:HB2  | 1:I:534:VAL:HG23 | 1.66                     | 0.75              |
| 1:J:539:LEU:HD23 | 1:J:542:LEU:HD12 | 1.68                     | 0.75              |
| 1:L:539:LEU:HD23 | 1:L:542:LEU:HD12 | 1.68                     | 0.75              |
| 1:A:532:PRO:HB2  | 1:A:534:VAL:HG23 | 1.66                     | 0.75              |
| 1:A:539:LEU:HD23 | 1:A:542:LEU:HD12 | 1.68                     | 0.75              |
| 1:H:534:VAL:HG22 | 1:I:492:LYS:HB3  | 1.69                     | 0.75              |
| 1:I:672:LYS:HG3  | 1:I:695:LEU:HD23 | 1.66                     | 0.75              |
| 1:J:532:PRO:HB2  | 1:J:534:VAL:HG23 | 1.66                     | 0.75              |
| 1:M:536:THR:HG21 | 1:N:483:GLU:HG3  | 1.69                     | 0.75              |
| 1:E:500:TYR:HA   | 1:E:503:TYR:HD1  | 1.50                     | 0.75              |
| 1:G:672:LYS:HG3  | 1:G:695:LEU:HD23 | 1.66                     | 0.75              |
| 1:J:672:LYS:HG3  | 1:J:695:LEU:HD23 | 1.66                     | 0.75              |
| 1:E:539:LEU:HD23 | 1:E:542:LEU:HD12 | 1.68                     | 0.75              |
| 1:N:539:LEU:HD23 | 1:N:542:LEU:HD12 | 1.68                     | 0.75              |
| 1:A:672:LYS:HG3  | 1:A:695:LEU:HD23 | 1.66                     | 0.75              |
| 1:I:500:TYR:HA   | 1:I:503:TYR:HD1  | 1.50                     | 0.74              |
| 1:N:500:TYR:HA   | 1:N:503:TYR:HD1  | 1.50                     | 0.74              |
| 1:C:418:ILE:O    | 3:C:803:AGS:N6   | 2.21                     | 0.74              |
| 1:N:418:ILE:O    | 3:N:803:AGS:N6   | 2.21                     | 0.74              |
| 1:D:418:ILE:O    | 3:D:803:AGS:N6   | 2.21                     | 0.74              |
| 1:E:418:ILE:O    | 3:E:803:AGS:N6   | 2.21                     | 0.74              |
| 1:G:500:TYR:HA   | 1:G:503:TYR:HD1  | 1.50                     | 0.74              |
| 1:L:418:ILE:O    | 3:L:803:AGS:N6   | 2.21                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:539:LEU:HD23 | 1:G:542:LEU:HD12 | 1.68                     | 0.74              |
| 1:I:539:LEU:HD23 | 1:I:542:LEU:HD12 | 1.68                     | 0.74              |
| 1:J:532:PRO:HA   | 1:K:490:VAL:HB   | 1.70                     | 0.74              |
| 1:M:418:ILE:O    | 3:M:803:AGS:N6   | 2.21                     | 0.74              |
| 1:M:614:ASP:OD1  | 1:M:617:LYS:NZ   | 2.21                     | 0.74              |
| 1:D:614:ASP:OD1  | 1:D:617:LYS:NZ   | 2.21                     | 0.74              |
| 1:E:614:ASP:OD1  | 1:E:617:LYS:NZ   | 2.21                     | 0.74              |
| 1:K:418:ILE:O    | 3:K:803:AGS:N6   | 2.21                     | 0.74              |
| 1:M:500:TYR:HA   | 1:M:503:TYR:HD1  | 1.50                     | 0.74              |
| 1:H:539:LEU:HD23 | 1:H:542:LEU:HD12 | 1.68                     | 0.74              |
| 1:L:500:TYR:HA   | 1:L:503:TYR:HD1  | 1.50                     | 0.74              |
| 1:N:614:ASP:OD1  | 1:N:617:LYS:NZ   | 2.21                     | 0.74              |
| 1:B:418:ILE:O    | 3:B:803:AGS:N6   | 2.21                     | 0.74              |
| 1:B:497:THR:HB   | 1:C:489:ALA:O    | 1.87                     | 0.74              |
| 1:B:614:ASP:OD1  | 1:B:617:LYS:NZ   | 2.21                     | 0.74              |
| 1:F:539:LEU:HD23 | 1:F:542:LEU:HD12 | 1.68                     | 0.74              |
| 1:C:500:TYR:HA   | 1:C:503:TYR:HD1  | 1.50                     | 0.74              |
| 1:F:614:ASP:OD1  | 1:F:617:LYS:NZ   | 2.21                     | 0.74              |
| 1:K:614:ASP:OD1  | 1:K:617:LYS:NZ   | 2.21                     | 0.74              |
| 1:H:418:ILE:O    | 3:H:803:AGS:N6   | 2.21                     | 0.74              |
| 1:H:614:ASP:OD1  | 1:H:617:LYS:NZ   | 2.21                     | 0.74              |
| 1:D:500:TYR:HA   | 1:D:503:TYR:HD1  | 1.50                     | 0.73              |
| 1:F:418:ILE:O    | 3:F:803:AGS:N6   | 2.21                     | 0.73              |
| 1:J:614:ASP:OD1  | 1:J:617:LYS:NZ   | 2.21                     | 0.73              |
| 1:A:614:ASP:OD1  | 1:A:617:LYS:NZ   | 2.21                     | 0.73              |
| 1:A:418:ILE:O    | 3:A:803:AGS:N6   | 2.21                     | 0.73              |
| 1:G:614:ASP:OD1  | 1:G:617:LYS:NZ   | 2.21                     | 0.73              |
| 1:J:418:ILE:O    | 3:J:803:AGS:N6   | 2.21                     | 0.73              |
| 1:J:478:ARG:HG3  | 1:J:523:LEU:HB2  | 1.70                     | 0.73              |
| 1:A:478:ARG:HG3  | 1:A:523:LEU:HB2  | 1.71                     | 0.73              |
| 1:D:400:ALA:O    | 1:D:405:ARG:NH1  | 2.22                     | 0.73              |
| 1:I:418:ILE:O    | 3:I:803:AGS:N6   | 2.21                     | 0.73              |
| 1:I:614:ASP:OD1  | 1:I:617:LYS:NZ   | 2.21                     | 0.73              |
| 1:G:418:ILE:O    | 3:G:803:AGS:N6   | 2.21                     | 0.73              |
| 1:M:400:ALA:O    | 1:M:405:ARG:NH1  | 2.22                     | 0.73              |
| 1:C:400:ALA:O    | 1:C:405:ARG:NH1  | 2.22                     | 0.73              |
| 1:F:350:PHE:HB3  | 1:J:350:PHE:HB3  | 1.71                     | 0.73              |
| 1:I:478:ARG:HG3  | 1:I:523:LEU:HB2  | 1.70                     | 0.73              |
| 1:L:400:ALA:O    | 1:L:405:ARG:NH1  | 2.22                     | 0.73              |
| 1:L:614:ASP:OD1  | 1:L:617:LYS:NZ   | 2.21                     | 0.73              |
| 1:B:478:ARG:HG3  | 1:B:523:LEU:HB2  | 1.70                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:400:ALA:O    | 1:G:405:ARG:NH1  | 2.22                     | 0.73              |
| 1:G:478:ARG:HG3  | 1:G:523:LEU:HB2  | 1.70                     | 0.73              |
| 1:F:103:GLN:NE2  | 1:G:321:GLN:OE1  | 2.17                     | 0.73              |
| 1:I:400:ALA:O    | 1:I:405:ARG:NH1  | 2.22                     | 0.73              |
| 1:K:478:ARG:HG3  | 1:K:523:LEU:HB2  | 1.71                     | 0.73              |
| 1:A:400:ALA:O    | 1:A:405:ARG:NH1  | 2.22                     | 0.73              |
| 1:B:400:ALA:O    | 1:B:405:ARG:NH1  | 2.22                     | 0.73              |
| 1:C:614:ASP:OD1  | 1:C:617:LYS:NZ   | 2.21                     | 0.73              |
| 1:J:400:ALA:O    | 1:J:405:ARG:NH1  | 2.22                     | 0.72              |
| 1:K:400:ALA:O    | 1:K:405:ARG:NH1  | 2.22                     | 0.72              |
| 1:E:400:ALA:O    | 1:E:405:ARG:NH1  | 2.22                     | 0.72              |
| 1:F:478:ARG:HG3  | 1:F:523:LEU:HB2  | 1.70                     | 0.72              |
| 1:H:478:ARG:HG3  | 1:H:523:LEU:HB2  | 1.70                     | 0.72              |
| 1:N:400:ALA:O    | 1:N:405:ARG:NH1  | 2.22                     | 0.72              |
| 1:C:107:GLU:OE2  | 1:D:317:HIS:ND1  | 2.19                     | 0.72              |
| 1:H:400:ALA:O    | 1:H:405:ARG:NH1  | 2.22                     | 0.72              |
| 1:F:400:ALA:O    | 1:F:405:ARG:NH1  | 2.22                     | 0.72              |
| 1:H:492:LYS:HB3  | 1:N:534:VAL:HG22 | 1.71                     | 0.72              |
| 1:A:321:GLN:OE1  | 1:G:103:GLN:NE2  | 2.22                     | 0.72              |
| 1:B:635:ILE:HA   | 1:B:683:ALA:HB1  | 1.71                     | 0.72              |
| 1:C:478:ARG:HG3  | 1:C:523:LEU:HB2  | 1.70                     | 0.72              |
| 1:C:635:ILE:HA   | 1:C:683:ALA:HB1  | 1.71                     | 0.72              |
| 1:K:635:ILE:HA   | 1:K:683:ALA:HB1  | 1.71                     | 0.72              |
| 1:M:681:LEU:HD11 | 1:M:686:LEU:HD21 | 1.72                     | 0.72              |
| 1:B:532:PRO:HA   | 1:C:490:VAL:HB   | 1.70                     | 0.71              |
| 1:D:681:LEU:HD11 | 1:D:686:LEU:HD21 | 1.72                     | 0.71              |
| 1:L:635:ILE:HA   | 1:L:683:ALA:HB1  | 1.71                     | 0.71              |
| 1:M:478:ARG:HG3  | 1:M:523:LEU:HB2  | 1.70                     | 0.71              |
| 1:B:103:GLN:NE2  | 1:C:321:GLN:OE1  | 2.17                     | 0.71              |
| 1:D:478:ARG:HG3  | 1:D:523:LEU:HB2  | 1.70                     | 0.71              |
| 1:E:478:ARG:HG3  | 1:E:523:LEU:HB2  | 1.70                     | 0.71              |
| 1:F:635:ILE:HA   | 1:F:683:ALA:HB1  | 1.71                     | 0.71              |
| 1:M:103:GLN:NE2  | 1:N:321:GLN:OE1  | 2.21                     | 0.71              |
| 1:N:478:ARG:HG3  | 1:N:523:LEU:HB2  | 1.70                     | 0.71              |
| 1:E:681:LEU:HD11 | 1:E:686:LEU:HD21 | 1.72                     | 0.71              |
| 1:G:635:ILE:HA   | 1:G:683:ALA:HB1  | 1.71                     | 0.71              |
| 1:H:635:ILE:HA   | 1:H:683:ALA:HB1  | 1.71                     | 0.71              |
| 1:I:635:ILE:HA   | 1:I:683:ALA:HB1  | 1.71                     | 0.71              |
| 1:L:478:ARG:HG3  | 1:L:523:LEU:HB2  | 1.71                     | 0.71              |
| 1:M:635:ILE:HA   | 1:M:683:ALA:HB1  | 1.71                     | 0.71              |
| 1:D:635:ILE:HA   | 1:D:683:ALA:HB1  | 1.71                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:681:LEU:HD11 | 1:C:686:LEU:HD21 | 1.72                     | 0.71              |
| 1:L:681:LEU:HD11 | 1:L:686:LEU:HD21 | 1.72                     | 0.71              |
| 1:N:681:LEU:HD11 | 1:N:686:LEU:HD21 | 1.72                     | 0.71              |
| 1:E:635:ILE:HA   | 1:E:683:ALA:HB1  | 1.71                     | 0.71              |
| 1:N:635:ILE:HA   | 1:N:683:ALA:HB1  | 1.71                     | 0.71              |
| 1:E:480:ASP:HA   | 1:E:525:ASP:HB2  | 1.73                     | 0.71              |
| 1:J:635:ILE:HA   | 1:J:683:ALA:HB1  | 1.71                     | 0.71              |
| 1:N:480:ASP:HA   | 1:N:525:ASP:HB2  | 1.73                     | 0.71              |
| 1:A:681:LEU:HD11 | 1:A:686:LEU:HD21 | 1.72                     | 0.70              |
| 1:E:532:PRO:HB3  | 1:F:491:SER:H    | 1.54                     | 0.70              |
| 1:I:681:LEU:HD11 | 1:I:686:LEU:HD21 | 1.72                     | 0.70              |
| 1:J:681:LEU:HD11 | 1:J:686:LEU:HD21 | 1.72                     | 0.70              |
| 1:A:635:ILE:HA   | 1:A:683:ALA:HB1  | 1.71                     | 0.70              |
| 1:G:681:LEU:HD11 | 1:G:686:LEU:HD21 | 1.72                     | 0.70              |
| 1:M:480:ASP:HA   | 1:M:525:ASP:HB2  | 1.73                     | 0.70              |
| 1:D:480:ASP:HA   | 1:D:525:ASP:HB2  | 1.73                     | 0.70              |
| 1:F:480:ASP:HA   | 1:F:525:ASP:HB2  | 1.73                     | 0.70              |
| 1:K:476:ILE:HG22 | 1:K:521:ILE:HB   | 1.74                     | 0.70              |
| 1:B:486:ASP:O    | 1:B:497:THR:OG1  | 2.10                     | 0.70              |
| 1:B:681:LEU:HD11 | 1:B:686:LEU:HD21 | 1.72                     | 0.70              |
| 1:D:476:ILE:HG22 | 1:D:521:ILE:HB   | 1.74                     | 0.70              |
| 1:E:486:ASP:O    | 1:E:497:THR:OG1  | 2.10                     | 0.70              |
| 1:F:681:LEU:HD11 | 1:F:686:LEU:HD21 | 1.72                     | 0.70              |
| 1:G:198:LEU:O    | 1:G:203:THR:OG1  | 2.10                     | 0.70              |
| 1:H:480:ASP:HA   | 1:H:525:ASP:HB2  | 1.73                     | 0.70              |
| 1:I:198:LEU:O    | 1:I:203:THR:OG1  | 2.10                     | 0.70              |
| 1:K:486:ASP:O    | 1:K:497:THR:OG1  | 2.10                     | 0.70              |
| 1:K:681:LEU:HD11 | 1:K:686:LEU:HD21 | 1.72                     | 0.70              |
| 1:N:486:ASP:O    | 1:N:497:THR:OG1  | 2.10                     | 0.70              |
| 1:A:200:ALA:HB3  | 1:A:213:ALA:HB3  | 1.74                     | 0.70              |
| 1:B:476:ILE:HG22 | 1:B:521:ILE:HB   | 1.74                     | 0.70              |
| 1:C:476:ILE:HG22 | 1:C:521:ILE:HB   | 1.74                     | 0.70              |
| 1:D:486:ASP:O    | 1:D:497:THR:OG1  | 2.10                     | 0.70              |
| 1:H:476:ILE:HG22 | 1:H:521:ILE:HB   | 1.74                     | 0.70              |
| 1:H:534:VAL:HA   | 1:I:492:LYS:HD2  | 1.72                     | 0.70              |
| 1:H:681:LEU:HD11 | 1:H:686:LEU:HD21 | 1.72                     | 0.70              |
| 1:I:476:ILE:HG22 | 1:I:521:ILE:HB   | 1.74                     | 0.70              |
| 1:J:476:ILE:HG22 | 1:J:521:ILE:HB   | 1.74                     | 0.70              |
| 1:L:476:ILE:HG22 | 1:L:521:ILE:HB   | 1.74                     | 0.70              |
| 1:A:476:ILE:HG22 | 1:A:521:ILE:HB   | 1.74                     | 0.70              |
| 1:A:486:ASP:O    | 1:A:497:THR:OG1  | 2.10                     | 0.70              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:198:LEU:O    | 1:C:203:THR:OG1 | 2.10                     | 0.70              |
| 1:E:476:ILE:HG22 | 1:E:521:ILE:HB  | 1.74                     | 0.70              |
| 1:F:476:ILE:HG22 | 1:F:521:ILE:HB  | 1.74                     | 0.70              |
| 1:G:476:ILE:HG22 | 1:G:521:ILE:HB  | 1.74                     | 0.70              |
| 1:J:200:ALA:HB3  | 1:J:213:ALA:HB3 | 1.74                     | 0.70              |
| 1:J:534:VAL:HG22 | 1:K:492:LYS:HB3 | 1.74                     | 0.70              |
| 1:L:486:ASP:O    | 1:L:497:THR:OG1 | 2.10                     | 0.70              |
| 1:M:476:ILE:HG22 | 1:M:521:ILE:HB  | 1.74                     | 0.70              |
| 1:C:486:ASP:O    | 1:C:497:THR:OG1 | 2.10                     | 0.70              |
| 1:E:198:LEU:O    | 1:E:203:THR:OG1 | 2.10                     | 0.70              |
| 1:G:200:ALA:HB3  | 1:G:213:ALA:HB3 | 1.74                     | 0.70              |
| 1:I:200:ALA:HB3  | 1:I:213:ALA:HB3 | 1.74                     | 0.70              |
| 1:J:486:ASP:O    | 1:J:497:THR:OG1 | 2.10                     | 0.70              |
| 1:L:198:LEU:O    | 1:L:203:THR:OG1 | 2.10                     | 0.70              |
| 1:M:486:ASP:O    | 1:M:497:THR:OG1 | 2.10                     | 0.70              |
| 1:N:198:LEU:O    | 1:N:203:THR:OG1 | 2.10                     | 0.70              |
| 1:F:486:ASP:O    | 1:F:497:THR:OG1 | 2.10                     | 0.69              |
| 1:H:486:ASP:O    | 1:H:497:THR:OG1 | 2.10                     | 0.69              |
| 1:N:476:ILE:HG22 | 1:N:521:ILE:HB  | 1.74                     | 0.69              |
| 1:M:198:LEU:O    | 1:M:203:THR:OG1 | 2.10                     | 0.69              |
| 1:D:198:LEU:O    | 1:D:203:THR:OG1 | 2.10                     | 0.69              |
| 1:G:486:ASP:O    | 1:G:497:THR:OG1 | 2.10                     | 0.69              |
| 1:I:486:ASP:O    | 1:I:497:THR:OG1 | 2.10                     | 0.69              |
| 1:A:198:LEU:O    | 1:A:203:THR:OG1 | 2.10                     | 0.69              |
| 1:J:198:LEU:O    | 1:J:203:THR:OG1 | 2.10                     | 0.69              |
| 1:L:480:ASP:HA   | 1:L:525:ASP:HB2 | 1.73                     | 0.69              |
| 3:A:802:AGS:O5'  | 3:A:802:AGS:O2B | 2.11                     | 0.69              |
| 1:B:200:ALA:HB3  | 1:B:213:ALA:HB3 | 1.74                     | 0.69              |
| 1:B:480:ASP:HA   | 1:B:525:ASP:HB2 | 1.73                     | 0.69              |
| 1:G:480:ASP:HA   | 1:G:525:ASP:HB2 | 1.73                     | 0.69              |
| 1:I:480:ASP:HA   | 1:I:525:ASP:HB2 | 1.73                     | 0.69              |
| 3:J:802:AGS:O2B  | 3:J:802:AGS:O5' | 2.11                     | 0.69              |
| 1:M:200:ALA:HB3  | 1:M:213:ALA:HB3 | 1.74                     | 0.69              |
| 1:C:480:ASP:HA   | 1:C:525:ASP:HB2 | 1.73                     | 0.69              |
| 1:D:103:GLN:NE2  | 1:E:321:GLN:OE1 | 2.21                     | 0.69              |
| 3:G:802:AGS:O2B  | 3:G:802:AGS:O5' | 2.11                     | 0.69              |
| 3:I:802:AGS:O5'  | 3:I:802:AGS:O2B | 2.11                     | 0.69              |
| 1:K:200:ALA:HB3  | 1:K:213:ALA:HB3 | 1.74                     | 0.69              |
| 1:K:480:ASP:HA   | 1:K:525:ASP:HB2 | 1.73                     | 0.69              |
| 1:A:480:ASP:HA   | 1:A:525:ASP:HB2 | 1.73                     | 0.69              |
| 1:A:534:VAL:HG22 | 1:B:492:LYS:HB3 | 1.75                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:198:LEU:O    | 1:H:203:THR:OG1  | 2.10                     | 0.69              |
| 1:H:200:ALA:HB3  | 1:H:213:ALA:HB3  | 1.74                     | 0.69              |
| 1:F:198:LEU:O    | 1:F:203:THR:OG1  | 2.10                     | 0.69              |
| 1:F:200:ALA:HB3  | 1:F:213:ALA:HB3  | 1.74                     | 0.69              |
| 1:B:533:GLN:O    | 1:C:492:LYS:NZ   | 2.19                     | 0.68              |
| 1:C:618:ILE:HG12 | 1:C:622:MET:HE1  | 1.75                     | 0.68              |
| 1:D:112:ARG:HD2  | 1:E:274:TYR:CE1  | 2.28                     | 0.68              |
| 1:D:200:ALA:HB3  | 1:D:213:ALA:HB3  | 1.74                     | 0.68              |
| 1:E:200:ALA:HB3  | 1:E:213:ALA:HB3  | 1.74                     | 0.68              |
| 1:J:480:ASP:HA   | 1:J:525:ASP:HB2  | 1.73                     | 0.68              |
| 1:L:618:ILE:HG12 | 1:L:622:MET:HE1  | 1.75                     | 0.68              |
| 1:N:200:ALA:HB3  | 1:N:213:ALA:HB3  | 1.74                     | 0.68              |
| 1:B:532:PRO:HB3  | 1:C:491:SER:H    | 1.58                     | 0.68              |
| 1:I:534:VAL:HG22 | 1:J:492:LYS:HB3  | 1.75                     | 0.68              |
| 1:D:618:ILE:HG12 | 1:D:622:MET:HE1  | 1.75                     | 0.68              |
| 1:L:200:ALA:HB3  | 1:L:213:ALA:HB3  | 1.74                     | 0.68              |
| 1:C:200:ALA:HB3  | 1:C:213:ALA:HB3  | 1.74                     | 0.68              |
| 3:D:802:AGS:O5'  | 3:D:802:AGS:O2B  | 2.11                     | 0.68              |
| 1:K:198:LEU:O    | 1:K:203:THR:OG1  | 2.10                     | 0.68              |
| 1:L:351:GLU:OE1  | 1:L:351:GLU:N    | 2.27                     | 0.68              |
| 3:M:802:AGS:O5'  | 3:M:802:AGS:O2B  | 2.11                     | 0.68              |
| 1:C:351:GLU:OE1  | 1:C:351:GLU:N    | 2.27                     | 0.68              |
| 1:D:351:GLU:OE1  | 1:D:351:GLU:N    | 2.27                     | 0.68              |
| 1:M:351:GLU:OE1  | 1:M:351:GLU:N    | 2.27                     | 0.68              |
| 1:B:351:GLU:N    | 1:B:351:GLU:OE1  | 2.27                     | 0.68              |
| 1:K:351:GLU:OE1  | 1:K:351:GLU:N    | 2.27                     | 0.68              |
| 1:M:618:ILE:HG12 | 1:M:622:MET:HE1  | 1.75                     | 0.68              |
| 1:A:481:MET:HB2  | 1:A:524:LEU:HD12 | 1.76                     | 0.68              |
| 1:K:618:ILE:HG12 | 1:K:622:MET:HE1  | 1.75                     | 0.68              |
| 1:B:198:LEU:O    | 1:B:203:THR:OG1  | 2.10                     | 0.68              |
| 1:B:618:ILE:HG12 | 1:B:622:MET:HE1  | 1.75                     | 0.68              |
| 3:C:802:AGS:O5'  | 3:C:802:AGS:O2B  | 2.11                     | 0.68              |
| 1:E:351:GLU:OE1  | 1:E:351:GLU:N    | 2.27                     | 0.68              |
| 1:J:481:MET:HB2  | 1:J:524:LEU:HD12 | 1.76                     | 0.68              |
| 3:L:802:AGS:O5'  | 3:L:802:AGS:O2B  | 2.11                     | 0.68              |
| 3:N:802:AGS:O5'  | 3:N:802:AGS:O2B  | 2.11                     | 0.68              |
| 3:B:802:AGS:O2B  | 3:B:802:AGS:O5'  | 2.11                     | 0.67              |
| 3:E:802:AGS:O5'  | 3:E:802:AGS:O2B  | 2.11                     | 0.67              |
| 1:N:351:GLU:OE1  | 1:N:351:GLU:N    | 2.27                     | 0.67              |
| 3:F:802:AGS:O5'  | 3:F:802:AGS:O2B  | 2.11                     | 0.67              |
| 3:H:802:AGS:O5'  | 3:H:802:AGS:O2B  | 2.11                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:481:MET:HB2  | 1:I:524:LEU:HD12 | 1.76                     | 0.67              |
| 3:K:802:AGS:O5'  | 3:K:802:AGS:O2B  | 2.11                     | 0.67              |
| 1:N:618:ILE:HG12 | 1:N:622:MET:HE1  | 1.75                     | 0.67              |
| 1:G:481:MET:HB2  | 1:G:524:LEU:HD12 | 1.76                     | 0.67              |
| 1:E:618:ILE:HG12 | 1:E:622:MET:HE1  | 1.75                     | 0.67              |
| 1:A:351:GLU:OE1  | 1:A:351:GLU:N    | 2.27                     | 0.67              |
| 1:B:481:MET:HB2  | 1:B:524:LEU:HD12 | 1.76                     | 0.67              |
| 1:C:112:ARG:HD2  | 1:D:274:TYR:CE1  | 2.29                     | 0.67              |
| 1:D:498:ALA:HB1  | 1:E:494:ILE:HA   | 1.75                     | 0.67              |
| 1:J:351:GLU:N    | 1:J:351:GLU:OE1  | 2.27                     | 0.67              |
| 1:J:536:THR:HG21 | 1:K:483:GLU:HG3  | 1.77                     | 0.67              |
| 1:E:500:TYR:HA   | 1:E:503:TYR:CD1  | 2.29                     | 0.67              |
| 1:G:618:ILE:HG12 | 1:G:622:MET:HE1  | 1.75                     | 0.67              |
| 1:K:481:MET:HB2  | 1:K:524:LEU:HD12 | 1.76                     | 0.67              |
| 1:A:500:TYR:HA   | 1:A:503:TYR:CD1  | 2.29                     | 0.67              |
| 1:J:500:TYR:HA   | 1:J:503:TYR:CD1  | 2.30                     | 0.67              |
| 1:D:660:PRO:HA   | 1:D:663:ARG:HB3  | 1.77                     | 0.66              |
| 1:G:660:PRO:HA   | 1:G:663:ARG:HB3  | 1.77                     | 0.66              |
| 1:I:618:ILE:HG12 | 1:I:622:MET:HE1  | 1.75                     | 0.66              |
| 1:L:660:PRO:HA   | 1:L:663:ARG:HB3  | 1.77                     | 0.66              |
| 1:N:500:TYR:HA   | 1:N:503:TYR:CD1  | 2.29                     | 0.66              |
| 1:F:618:ILE:HG12 | 1:F:622:MET:HE1  | 1.75                     | 0.66              |
| 1:I:500:TYR:HA   | 1:I:503:TYR:CD1  | 2.29                     | 0.66              |
| 1:M:660:PRO:HA   | 1:M:663:ARG:HB3  | 1.77                     | 0.66              |
| 1:C:660:PRO:HA   | 1:C:663:ARG:HB3  | 1.77                     | 0.66              |
| 1:D:500:TYR:HA   | 1:D:503:TYR:CD1  | 2.29                     | 0.66              |
| 1:H:618:ILE:HG12 | 1:H:622:MET:HE1  | 1.75                     | 0.66              |
| 1:I:660:PRO:HA   | 1:I:663:ARG:HB3  | 1.77                     | 0.66              |
| 1:G:500:TYR:HA   | 1:G:503:TYR:CD1  | 2.30                     | 0.66              |
| 1:H:351:GLU:OE1  | 1:H:351:GLU:N    | 2.27                     | 0.66              |
| 1:H:500:TYR:HA   | 1:H:503:TYR:CD1  | 2.29                     | 0.66              |
| 1:F:351:GLU:OE1  | 1:F:351:GLU:N    | 2.27                     | 0.66              |
| 1:F:660:PRO:HA   | 1:F:663:ARG:HB3  | 1.77                     | 0.66              |
| 1:H:660:PRO:HA   | 1:H:663:ARG:HB3  | 1.77                     | 0.66              |
| 1:J:618:ILE:HG12 | 1:J:622:MET:HE1  | 1.75                     | 0.66              |
| 1:A:618:ILE:HG12 | 1:A:622:MET:HE1  | 1.75                     | 0.66              |
| 1:F:500:TYR:HA   | 1:F:503:TYR:CD1  | 2.30                     | 0.66              |
| 1:M:500:TYR:HA   | 1:M:503:TYR:CD1  | 2.29                     | 0.66              |
| 1:D:107:GLU:OE2  | 1:E:317:HIS:ND1  | 2.26                     | 0.66              |
| 1:A:660:PRO:HA   | 1:A:663:ARG:HB3  | 1.77                     | 0.66              |
| 1:K:537:LEU:HD13 | 1:L:492:LYS:HA   | 1.78                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:481:MET:HB2  | 1:H:524:LEU:HD12 | 1.76                     | 0.66              |
| 1:J:660:PRO:HA   | 1:J:663:ARG:HB3  | 1.77                     | 0.66              |
| 1:G:351:GLU:N    | 1:G:351:GLU:OE1  | 2.27                     | 0.66              |
| 1:M:481:MET:HB2  | 1:M:524:LEU:HD12 | 1.76                     | 0.66              |
| 1:A:330:VAL:HG21 | 1:A:366:LYS:HZ3  | 1.61                     | 0.65              |
| 1:B:500:TYR:HA   | 1:B:503:TYR:CD1  | 2.30                     | 0.65              |
| 1:D:534:VAL:HA   | 1:E:492:LYS:HD2  | 1.78                     | 0.65              |
| 1:F:481:MET:HB2  | 1:F:524:LEU:HD12 | 1.77                     | 0.65              |
| 1:I:351:GLU:OE1  | 1:I:351:GLU:N    | 2.27                     | 0.65              |
| 1:J:330:VAL:HG21 | 1:J:366:LYS:HZ3  | 1.62                     | 0.65              |
| 1:D:481:MET:HB2  | 1:D:524:LEU:HD12 | 1.77                     | 0.65              |
| 1:E:481:MET:HB2  | 1:E:524:LEU:HD12 | 1.76                     | 0.65              |
| 1:D:536:THR:HA   | 1:D:539:LEU:HG   | 1.79                     | 0.65              |
| 1:E:660:PRO:HA   | 1:E:663:ARG:HB3  | 1.77                     | 0.65              |
| 1:K:500:TYR:HA   | 1:K:503:TYR:CD1  | 2.29                     | 0.65              |
| 1:M:536:THR:HA   | 1:M:539:LEU:HG   | 1.79                     | 0.65              |
| 1:N:481:MET:HB2  | 1:N:524:LEU:HD12 | 1.76                     | 0.65              |
| 1:A:112:ARG:HD2  | 1:B:274:TYR:CE1  | 2.31                     | 0.65              |
| 1:C:500:TYR:HA   | 1:C:503:TYR:CD1  | 2.30                     | 0.65              |
| 1:E:536:THR:HA   | 1:E:539:LEU:HG   | 1.79                     | 0.65              |
| 1:F:536:THR:HA   | 1:F:539:LEU:HG   | 1.79                     | 0.65              |
| 1:C:481:MET:HB2  | 1:C:524:LEU:HD12 | 1.76                     | 0.65              |
| 1:H:536:THR:HA   | 1:H:539:LEU:HG   | 1.79                     | 0.65              |
| 1:L:500:TYR:HA   | 1:L:503:TYR:CD1  | 2.29                     | 0.65              |
| 1:N:536:THR:HA   | 1:N:539:LEU:HG   | 1.79                     | 0.65              |
| 1:N:660:PRO:HA   | 1:N:663:ARG:HB3  | 1.77                     | 0.65              |
| 1:L:532:PRO:HB3  | 1:M:491:SER:H    | 1.62                     | 0.65              |
| 1:L:536:THR:HA   | 1:L:539:LEU:HG   | 1.79                     | 0.65              |
| 1:C:536:THR:HA   | 1:C:539:LEU:HG   | 1.79                     | 0.65              |
| 1:F:325:THR:HA   | 1:F:328:HIS:HB3  | 1.79                     | 0.65              |
| 1:G:536:THR:HA   | 1:G:539:LEU:HG   | 1.79                     | 0.65              |
| 1:H:325:THR:HA   | 1:H:328:HIS:HB3  | 1.79                     | 0.65              |
| 1:I:536:THR:HA   | 1:I:539:LEU:HG   | 1.79                     | 0.65              |
| 1:L:481:MET:HB2  | 1:L:524:LEU:HD12 | 1.76                     | 0.65              |
| 1:G:325:THR:HA   | 1:G:328:HIS:HB3  | 1.79                     | 0.65              |
| 1:B:451:VAL:HG12 | 1:B:568:ALA:HB2  | 1.79                     | 0.64              |
| 1:I:325:THR:HA   | 1:I:328:HIS:HB3  | 1.79                     | 0.64              |
| 1:K:451:VAL:HG12 | 1:K:568:ALA:HB2  | 1.79                     | 0.64              |
| 1:K:660:PRO:HA   | 1:K:663:ARG:HB3  | 1.77                     | 0.64              |
| 1:E:325:THR:HA   | 1:E:328:HIS:HB3  | 1.79                     | 0.64              |
| 1:C:451:VAL:HG12 | 1:C:568:ALA:HB2  | 1.79                     | 0.64              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:E:434:ASN:ND2  | 1:E:445:ILE:O   | 2.31                     | 0.64              |
| 1:L:451:VAL:HG12 | 1:L:568:ALA:HB2 | 1.79                     | 0.64              |
| 1:N:325:THR:HA   | 1:N:328:HIS:HB3 | 1.79                     | 0.64              |
| 1:N:434:ASN:ND2  | 1:N:445:ILE:O   | 2.31                     | 0.64              |
| 1:B:660:PRO:HA   | 1:B:663:ARG:HB3 | 1.77                     | 0.64              |
| 1:E:534:VAL:HG22 | 1:F:492:LYS:HB3 | 1.78                     | 0.64              |
| 1:E:451:VAL:HG12 | 1:E:568:ALA:HB2 | 1.79                     | 0.64              |
| 1:J:536:THR:HA   | 1:J:539:LEU:HG  | 1.79                     | 0.64              |
| 1:A:536:THR:HA   | 1:A:539:LEU:HG  | 1.79                     | 0.64              |
| 1:K:536:THR:HG21 | 1:L:483:GLU:HG3 | 1.79                     | 0.64              |
| 1:M:434:ASN:ND2  | 1:M:445:ILE:O   | 2.31                     | 0.64              |
| 1:A:451:VAL:HG12 | 1:A:568:ALA:HB2 | 1.79                     | 0.64              |
| 1:F:330:VAL:HG21 | 1:F:366:LYS:HZ3 | 1.63                     | 0.64              |
| 1:J:451:VAL:HG12 | 1:J:568:ALA:HB2 | 1.79                     | 0.64              |
| 1:N:451:VAL:HG12 | 1:N:568:ALA:HB2 | 1.79                     | 0.64              |
| 1:D:434:ASN:ND2  | 1:D:445:ILE:O   | 2.31                     | 0.64              |
| 1:J:534:VAL:HA   | 1:K:492:LYS:HD2 | 1.79                     | 0.64              |
| 1:K:536:THR:HA   | 1:K:539:LEU:HG  | 1.79                     | 0.64              |
| 1:B:536:THR:HA   | 1:B:539:LEU:HG  | 1.79                     | 0.64              |
| 1:M:451:VAL:HG12 | 1:M:568:ALA:HB2 | 1.79                     | 0.64              |
| 1:D:451:VAL:HG12 | 1:D:568:ALA:HB2 | 1.79                     | 0.63              |
| 1:E:532:PRO:HA   | 1:F:490:VAL:HB  | 1.81                     | 0.63              |
| 1:F:532:PRO:HB3  | 1:G:491:SER:H   | 1.62                     | 0.63              |
| 1:B:330:VAL:HG21 | 1:B:366:LYS:HZ3 | 1.63                     | 0.63              |
| 1:C:434:ASN:ND2  | 1:C:445:ILE:O   | 2.31                     | 0.63              |
| 1:G:451:VAL:HG12 | 1:G:568:ALA:HB2 | 1.79                     | 0.63              |
| 1:I:451:VAL:HG12 | 1:I:568:ALA:HB2 | 1.79                     | 0.63              |
| 1:F:434:ASN:ND2  | 1:F:445:ILE:O   | 2.31                     | 0.63              |
| 1:G:434:ASN:ND2  | 1:G:445:ILE:O   | 2.31                     | 0.63              |
| 1:C:104:GLU:HA   | 1:D:321:GLN:NE2 | 2.13                     | 0.63              |
| 1:H:434:ASN:ND2  | 1:H:445:ILE:O   | 2.31                     | 0.63              |
| 1:I:434:ASN:ND2  | 1:I:445:ILE:O   | 2.31                     | 0.63              |
| 1:L:325:THR:HA   | 1:L:328:HIS:HB3 | 1.79                     | 0.63              |
| 1:L:434:ASN:ND2  | 1:L:445:ILE:O   | 2.31                     | 0.63              |
| 1:B:200:ALA:HB2  | 1:B:211:GLY:H   | 1.64                     | 0.63              |
| 1:H:330:VAL:HG21 | 1:H:366:LYS:HZ3 | 1.64                     | 0.63              |
| 1:K:200:ALA:HB2  | 1:K:211:GLY:H   | 1.64                     | 0.63              |
| 1:K:434:ASN:ND2  | 1:K:445:ILE:O   | 2.31                     | 0.63              |
| 1:A:200:ALA:HB2  | 1:A:211:GLY:H   | 1.64                     | 0.63              |
| 1:C:325:THR:HA   | 1:C:328:HIS:HB3 | 1.79                     | 0.63              |
| 1:H:451:VAL:HG12 | 1:H:568:ALA:HB2 | 1.79                     | 0.63              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:J:200:ALA:HB2  | 1:J:211:GLY:H   | 1.64                     | 0.63              |
| 1:J:325:THR:HA   | 1:J:328:HIS:HB3 | 1.79                     | 0.63              |
| 1:A:325:THR:HA   | 1:A:328:HIS:HB3 | 1.79                     | 0.63              |
| 1:B:434:ASN:ND2  | 1:B:445:ILE:O   | 2.31                     | 0.63              |
| 1:F:451:VAL:HG12 | 1:F:568:ALA:HB2 | 1.79                     | 0.63              |
| 1:B:325:THR:HA   | 1:B:328:HIS:HB3 | 1.79                     | 0.62              |
| 1:B:362:GLU:HA   | 1:B:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:D:362:GLU:HA   | 1:D:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:F:200:ALA:HB2  | 1:F:211:GLY:H   | 1.64                     | 0.62              |
| 1:H:200:ALA:HB2  | 1:H:211:GLY:H   | 1.64                     | 0.62              |
| 1:K:362:GLU:HA   | 1:K:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:L:200:ALA:HB2  | 1:L:211:GLY:H   | 1.64                     | 0.62              |
| 1:I:362:GLU:HA   | 1:I:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:M:362:GLU:HA   | 1:M:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:C:200:ALA:HB2  | 1:C:211:GLY:H   | 1.64                     | 0.62              |
| 1:D:325:THR:HA   | 1:D:328:HIS:HB3 | 1.79                     | 0.62              |
| 1:G:362:GLU:HA   | 1:G:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:K:325:THR:HA   | 1:K:328:HIS:HB3 | 1.79                     | 0.62              |
| 3:B:802:AGS:O2G  | 3:B:802:AGS:O3A | 2.18                     | 0.62              |
| 1:F:534:VAL:HG22 | 1:G:492:LYS:HB3 | 1.81                     | 0.62              |
| 1:C:362:GLU:HA   | 1:C:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:E:362:GLU:HA   | 1:E:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:F:362:GLU:HA   | 1:F:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:N:362:GLU:HA   | 1:N:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:E:200:ALA:HB2  | 1:E:211:GLY:H   | 1.64                     | 0.62              |
| 1:H:362:GLU:HA   | 1:H:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:M:325:THR:HA   | 1:M:328:HIS:HB3 | 1.79                     | 0.62              |
| 1:M:330:VAL:HG21 | 1:M:366:LYS:HZ3 | 1.64                     | 0.62              |
| 1:M:200:ALA:HB2  | 1:M:211:GLY:H   | 1.64                     | 0.62              |
| 1:A:434:ASN:ND2  | 1:A:445:ILE:O   | 2.31                     | 0.62              |
| 1:A:481:MET:HE1  | 1:A:529:LYS:H   | 1.65                     | 0.62              |
| 1:G:481:MET:HE1  | 1:G:529:LYS:H   | 1.65                     | 0.62              |
| 1:I:481:MET:HE1  | 1:I:529:LYS:H   | 1.65                     | 0.62              |
| 1:L:362:GLU:HA   | 1:L:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:N:200:ALA:HB2  | 1:N:211:GLY:H   | 1.64                     | 0.62              |
| 1:A:362:GLU:HA   | 1:A:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:J:362:GLU:HA   | 1:J:365:ARG:NH1 | 2.14                     | 0.62              |
| 1:J:434:ASN:ND2  | 1:J:445:ILE:O   | 2.31                     | 0.62              |
| 1:B:481:MET:HE1  | 1:B:529:LYS:H   | 1.65                     | 0.62              |
| 1:D:200:ALA:HB2  | 1:D:211:GLY:H   | 1.64                     | 0.62              |
| 1:J:481:MET:HE1  | 1:J:529:LYS:H   | 1.65                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:481:MET:HE1  | 1:K:529:LYS:H    | 1.65                     | 0.61              |
| 1:K:534:VAL:HG22 | 1:L:492:LYS:HB3  | 1.80                     | 0.61              |
| 1:K:688:ALA:HB1  | 1:K:695:LEU:HD11 | 1.82                     | 0.61              |
| 1:A:274:TYR:CE1  | 1:G:112:ARG:HD2  | 2.34                     | 0.61              |
| 1:B:688:ALA:HB1  | 1:B:695:LEU:HD11 | 1.82                     | 0.61              |
| 1:F:481:MET:HE1  | 1:F:529:LYS:H    | 1.65                     | 0.61              |
| 1:G:303:LEU:HA   | 1:G:306:LYS:HE2  | 1.82                     | 0.61              |
| 1:H:303:LEU:HA   | 1:H:306:LYS:HE2  | 1.82                     | 0.61              |
| 1:J:688:ALA:HB1  | 1:J:695:LEU:HD11 | 1.82                     | 0.61              |
| 1:A:688:ALA:HB1  | 1:A:695:LEU:HD11 | 1.82                     | 0.61              |
| 1:F:303:LEU:HA   | 1:F:306:LYS:HE2  | 1.82                     | 0.61              |
| 1:H:481:MET:HE1  | 1:H:529:LYS:H    | 1.65                     | 0.61              |
| 1:I:303:LEU:HA   | 1:I:306:LYS:HE2  | 1.82                     | 0.61              |
| 1:J:612:LYS:O    | 1:J:652:TYR:OH   | 2.17                     | 0.61              |
| 1:K:539:LEU:HA   | 1:K:542:LEU:HB2  | 1.83                     | 0.61              |
| 3:K:802:AGS:O2G  | 3:K:802:AGS:O3A  | 2.18                     | 0.61              |
| 1:A:612:LYS:O    | 1:A:652:TYR:OH   | 2.17                     | 0.61              |
| 1:K:330:VAL:HG21 | 1:K:366:LYS:HZ3  | 1.65                     | 0.61              |
| 1:K:532:PRO:HB3  | 1:L:491:SER:H    | 1.65                     | 0.61              |
| 1:B:539:LEU:HA   | 1:B:542:LEU:HB2  | 1.83                     | 0.61              |
| 1:G:102:ILE:HG22 | 1:G:130:VAL:HG13 | 1.83                     | 0.61              |
| 1:I:688:ALA:HB1  | 1:I:695:LEU:HD11 | 1.82                     | 0.61              |
| 1:A:102:ILE:HG22 | 1:A:130:VAL:HG13 | 1.83                     | 0.61              |
| 3:E:802:AGS:O2G  | 3:E:802:AGS:O3A  | 2.17                     | 0.61              |
| 1:G:688:ALA:HB1  | 1:G:695:LEU:HD11 | 1.82                     | 0.61              |
| 1:I:102:ILE:HG22 | 1:I:130:VAL:HG13 | 1.83                     | 0.61              |
| 1:J:102:ILE:HG22 | 1:J:130:VAL:HG13 | 1.83                     | 0.61              |
| 1:J:539:LEU:HA   | 1:J:542:LEU:HB2  | 1.83                     | 0.61              |
| 1:L:102:ILE:HG22 | 1:L:130:VAL:HG13 | 1.83                     | 0.61              |
| 1:L:303:LEU:HA   | 1:L:306:LYS:HE2  | 1.82                     | 0.61              |
| 3:N:802:AGS:O2G  | 3:N:802:AGS:O3A  | 2.18                     | 0.61              |
| 1:A:490:VAL:HB   | 1:G:532:PRO:HA   | 1.83                     | 0.61              |
| 1:A:539:LEU:HA   | 1:A:542:LEU:HB2  | 1.83                     | 0.61              |
| 1:C:112:ARG:HD2  | 1:D:274:TYR:HE1  | 1.63                     | 0.61              |
| 1:C:303:LEU:HA   | 1:C:306:LYS:HE2  | 1.82                     | 0.61              |
| 1:C:539:LEU:HA   | 1:C:542:LEU:HB2  | 1.83                     | 0.61              |
| 1:D:350:PHE:HB3  | 1:L:350:PHE:HB3  | 1.82                     | 0.61              |
| 1:F:102:ILE:HG22 | 1:F:130:VAL:HG13 | 1.83                     | 0.61              |
| 1:G:200:ALA:HB2  | 1:G:211:GLY:H    | 1.64                     | 0.61              |
| 1:H:102:ILE:HG22 | 1:H:130:VAL:HG13 | 1.83                     | 0.61              |
| 1:J:303:LEU:HA   | 1:J:306:LYS:HE2  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:688:ALA:HB1  | 1:L:695:LEU:HD11 | 1.82                     | 0.61              |
| 1:N:121:GLY:O    | 1:N:127:LYS:NZ   | 2.34                     | 0.61              |
| 1:A:303:LEU:HA   | 1:A:306:LYS:HE2  | 1.82                     | 0.61              |
| 1:C:102:ILE:HG22 | 1:C:130:VAL:HG13 | 1.83                     | 0.61              |
| 1:I:200:ALA:HB2  | 1:I:211:GLY:H    | 1.64                     | 0.61              |
| 1:K:102:ILE:HG22 | 1:K:130:VAL:HG13 | 1.83                     | 0.61              |
| 1:K:534:VAL:HA   | 1:L:492:LYS:HD2  | 1.83                     | 0.61              |
| 1:L:539:LEU:HA   | 1:L:542:LEU:HB2  | 1.83                     | 0.61              |
| 3:M:802:AGS:O2G  | 3:M:802:AGS:O3A  | 2.17                     | 0.61              |
| 1:N:303:LEU:HA   | 1:N:306:LYS:HE2  | 1.82                     | 0.61              |
| 1:B:102:ILE:HG22 | 1:B:130:VAL:HG13 | 1.83                     | 0.60              |
| 1:B:534:VAL:HA   | 1:C:492:LYS:HD2  | 1.83                     | 0.60              |
| 1:C:688:ALA:HB1  | 1:C:695:LEU:HD11 | 1.82                     | 0.60              |
| 1:D:481:MET:HE1  | 1:D:529:LYS:H    | 1.65                     | 0.60              |
| 3:D:802:AGS:O2G  | 3:D:802:AGS:O3A  | 2.18                     | 0.60              |
| 1:E:303:LEU:HA   | 1:E:306:LYS:HE2  | 1.82                     | 0.60              |
| 1:F:688:ALA:HB1  | 1:F:695:LEU:HD11 | 1.82                     | 0.60              |
| 1:H:688:ALA:HB1  | 1:H:695:LEU:HD11 | 1.82                     | 0.60              |
| 1:I:539:LEU:HA   | 1:I:542:LEU:HB2  | 1.83                     | 0.60              |
| 3:J:802:AGS:O2G  | 3:J:802:AGS:O3A  | 2.18                     | 0.60              |
| 1:K:303:LEU:HA   | 1:K:306:LYS:HE2  | 1.82                     | 0.60              |
| 1:C:121:GLY:O    | 1:C:127:LYS:NZ   | 2.34                     | 0.60              |
| 1:C:481:MET:HE1  | 1:C:529:LYS:H    | 1.65                     | 0.60              |
| 3:F:802:AGS:O2G  | 3:F:802:AGS:O3A  | 2.18                     | 0.60              |
| 1:G:539:LEU:HA   | 1:G:542:LEU:HB2  | 1.83                     | 0.60              |
| 3:H:802:AGS:O2G  | 3:H:802:AGS:O3A  | 2.18                     | 0.60              |
| 1:L:481:MET:HE1  | 1:L:529:LYS:H    | 1.65                     | 0.60              |
| 1:M:481:MET:HE1  | 1:M:529:LYS:H    | 1.65                     | 0.60              |
| 3:A:802:AGS:O2G  | 3:A:802:AGS:O3A  | 2.17                     | 0.60              |
| 1:B:303:LEU:HA   | 1:B:306:LYS:HE2  | 1.82                     | 0.60              |
| 1:L:121:GLY:O    | 1:L:127:LYS:NZ   | 2.34                     | 0.60              |
| 1:N:102:ILE:HG22 | 1:N:130:VAL:HG13 | 1.83                     | 0.60              |
| 1:D:121:GLY:O    | 1:D:127:LYS:NZ   | 2.34                     | 0.60              |
| 1:M:102:ILE:HG22 | 1:M:130:VAL:HG13 | 1.83                     | 0.60              |
| 1:M:303:LEU:HA   | 1:M:306:LYS:HE2  | 1.82                     | 0.60              |
| 1:D:102:ILE:HG22 | 1:D:130:VAL:HG13 | 1.83                     | 0.60              |
| 1:E:102:ILE:HG22 | 1:E:130:VAL:HG13 | 1.83                     | 0.60              |
| 1:H:483:GLU:HG3  | 1:N:536:THR:HG21 | 1.82                     | 0.60              |
| 1:D:303:LEU:HA   | 1:D:306:LYS:HE2  | 1.82                     | 0.60              |
| 1:M:121:GLY:O    | 1:M:127:LYS:NZ   | 2.34                     | 0.60              |
| 1:B:528:GLU:HB3  | 1:B:529:LYS:HA   | 1.84                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:622:MET:HG3  | 1:C:625:GLU:OE2  | 2.02                     | 0.60              |
| 1:K:511:THR:HG23 | 1:K:555:VAL:HG21 | 1.84                     | 0.60              |
| 1:K:612:LYS:O    | 1:K:652:TYR:OH   | 2.17                     | 0.60              |
| 1:M:688:ALA:HB1  | 1:M:695:LEU:HD11 | 1.82                     | 0.60              |
| 1:N:688:ALA:HB1  | 1:N:695:LEU:HD11 | 1.82                     | 0.60              |
| 1:C:423:ALA:HB2  | 1:C:605:ILE:HG21 | 1.83                     | 0.60              |
| 1:D:423:ALA:HB2  | 1:D:605:ILE:HG21 | 1.83                     | 0.60              |
| 1:L:582:LYS:HE2  | 1:L:586:MET:HE1  | 1.84                     | 0.60              |
| 1:L:622:MET:HG3  | 1:L:625:GLU:OE2  | 2.02                     | 0.60              |
| 1:M:534:VAL:HA   | 1:N:492:LYS:HD2  | 1.81                     | 0.60              |
| 1:A:511:THR:HG23 | 1:A:555:VAL:HG21 | 1.84                     | 0.60              |
| 1:B:511:THR:HG23 | 1:B:555:VAL:HG21 | 1.84                     | 0.60              |
| 1:C:218:PRO:O    | 1:C:222:ARG:HD3  | 2.02                     | 0.60              |
| 1:D:582:LYS:HE2  | 1:D:586:MET:HE1  | 1.84                     | 0.60              |
| 1:D:688:ALA:HB1  | 1:D:695:LEU:HD11 | 1.82                     | 0.60              |
| 1:F:528:GLU:HB3  | 1:F:529:LYS:HA   | 1.84                     | 0.60              |
| 1:G:528:GLU:HB3  | 1:G:529:LYS:HA   | 1.84                     | 0.60              |
| 1:G:582:LYS:HE2  | 1:G:586:MET:HE1  | 1.84                     | 0.60              |
| 3:G:802:AGS:O2G  | 3:G:802:AGS:O3A  | 2.18                     | 0.60              |
| 1:H:403:ILE:HG23 | 1:I:678:LEU:HD22 | 1.83                     | 0.60              |
| 1:I:528:GLU:HB3  | 1:I:529:LYS:HA   | 1.84                     | 0.60              |
| 1:I:582:LYS:HE2  | 1:I:586:MET:HE1  | 1.84                     | 0.60              |
| 1:J:511:THR:HG23 | 1:J:555:VAL:HG21 | 1.84                     | 0.60              |
| 1:K:528:GLU:HB3  | 1:K:529:LYS:HA   | 1.84                     | 0.60              |
| 1:N:511:THR:HG23 | 1:N:555:VAL:HG21 | 1.84                     | 0.60              |
| 1:A:528:GLU:HB3  | 1:A:529:LYS:HA   | 1.84                     | 0.60              |
| 1:A:532:PRO:HB3  | 1:B:491:SER:H    | 1.66                     | 0.60              |
| 1:B:423:ALA:HB2  | 1:B:605:ILE:HG21 | 1.83                     | 0.60              |
| 1:E:511:THR:HG23 | 1:E:555:VAL:HG21 | 1.84                     | 0.60              |
| 1:E:688:ALA:HB1  | 1:E:695:LEU:HD11 | 1.82                     | 0.60              |
| 1:F:511:THR:HG23 | 1:F:555:VAL:HG21 | 1.84                     | 0.60              |
| 3:I:802:AGS:O2G  | 3:I:802:AGS:O3A  | 2.18                     | 0.60              |
| 1:K:423:ALA:HB2  | 1:K:605:ILE:HG21 | 1.83                     | 0.60              |
| 1:L:218:PRO:O    | 1:L:222:ARG:HD3  | 2.02                     | 0.60              |
| 1:L:423:ALA:HB2  | 1:L:605:ILE:HG21 | 1.83                     | 0.60              |
| 1:M:582:LYS:HE2  | 1:M:586:MET:HE1  | 1.84                     | 0.60              |
| 1:A:483:GLU:HG3  | 1:G:536:THR:HG21 | 1.82                     | 0.59              |
| 1:A:622:MET:HG3  | 1:A:625:GLU:OE2  | 2.02                     | 0.59              |
| 1:B:612:LYS:O    | 1:B:652:TYR:OH   | 2.17                     | 0.59              |
| 1:C:582:LYS:HE2  | 1:C:586:MET:HE1  | 1.84                     | 0.59              |
| 1:E:481:MET:HE1  | 1:E:529:LYS:H    | 1.65                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:582:LYS:HE2  | 1:E:586:MET:HE1  | 1.84                     | 0.59              |
| 1:F:539:LEU:HA   | 1:F:542:LEU:HB2  | 1.83                     | 0.59              |
| 1:H:511:THR:HG23 | 1:H:555:VAL:HG21 | 1.84                     | 0.59              |
| 1:H:528:GLU:HB3  | 1:H:529:LYS:HA   | 1.84                     | 0.59              |
| 1:H:539:LEU:HA   | 1:H:542:LEU:HB2  | 1.83                     | 0.59              |
| 1:I:622:MET:HG3  | 1:I:625:GLU:OE2  | 2.02                     | 0.59              |
| 1:J:218:PRO:O    | 1:J:222:ARG:HD3  | 2.02                     | 0.59              |
| 1:J:528:GLU:HB3  | 1:J:529:LYS:HA   | 1.84                     | 0.59              |
| 1:J:622:MET:HG3  | 1:J:625:GLU:OE2  | 2.02                     | 0.59              |
| 1:L:528:GLU:HB3  | 1:L:529:LYS:HA   | 1.84                     | 0.59              |
| 1:A:218:PRO:O    | 1:A:222:ARG:HD3  | 2.02                     | 0.59              |
| 1:A:491:SER:H    | 1:G:532:PRO:HB3  | 1.67                     | 0.59              |
| 1:A:582:LYS:HE2  | 1:A:586:MET:HE1  | 1.84                     | 0.59              |
| 1:C:528:GLU:HB3  | 1:C:529:LYS:HA   | 1.84                     | 0.59              |
| 1:D:218:PRO:O    | 1:D:222:ARG:HD3  | 2.02                     | 0.59              |
| 1:D:539:LEU:HA   | 1:D:542:LEU:HB2  | 1.83                     | 0.59              |
| 1:E:423:ALA:HB2  | 1:E:605:ILE:HG21 | 1.83                     | 0.59              |
| 1:G:218:PRO:O    | 1:G:222:ARG:HD3  | 2.02                     | 0.59              |
| 1:G:330:VAL:HG21 | 1:G:366:LYS:HZ3  | 1.67                     | 0.59              |
| 1:G:622:MET:HG3  | 1:G:625:GLU:OE2  | 2.02                     | 0.59              |
| 1:H:582:LYS:HE2  | 1:H:586:MET:HE1  | 1.84                     | 0.59              |
| 1:I:218:PRO:O    | 1:I:222:ARG:HD3  | 2.02                     | 0.59              |
| 1:J:423:ALA:HB2  | 1:J:605:ILE:HG21 | 1.83                     | 0.59              |
| 1:M:218:PRO:O    | 1:M:222:ARG:HD3  | 2.02                     | 0.59              |
| 1:M:423:ALA:HB2  | 1:M:605:ILE:HG21 | 1.83                     | 0.59              |
| 1:M:511:THR:HG23 | 1:M:555:VAL:HG21 | 1.84                     | 0.59              |
| 1:N:481:MET:HE1  | 1:N:529:LYS:H    | 1.65                     | 0.59              |
| 1:N:582:LYS:HE2  | 1:N:586:MET:HE1  | 1.84                     | 0.59              |
| 1:A:423:ALA:HB2  | 1:A:605:ILE:HG21 | 1.83                     | 0.59              |
| 1:A:498:ALA:O    | 1:A:501:VAL:HG12 | 2.03                     | 0.59              |
| 1:F:582:LYS:HE2  | 1:F:586:MET:HE1  | 1.84                     | 0.59              |
| 1:J:498:ALA:O    | 1:J:501:VAL:HG12 | 2.03                     | 0.59              |
| 1:J:582:LYS:HE2  | 1:J:586:MET:HE1  | 1.84                     | 0.59              |
| 1:K:498:ALA:O    | 1:K:501:VAL:HG12 | 2.03                     | 0.59              |
| 1:M:539:LEU:HA   | 1:M:542:LEU:HB2  | 1.83                     | 0.59              |
| 1:M:622:MET:HG3  | 1:M:625:GLU:OE2  | 2.02                     | 0.59              |
| 1:N:539:LEU:HA   | 1:N:542:LEU:HB2  | 1.83                     | 0.59              |
| 1:B:498:ALA:O    | 1:B:501:VAL:HG12 | 2.03                     | 0.59              |
| 1:B:582:LYS:HE2  | 1:B:586:MET:HE1  | 1.84                     | 0.59              |
| 1:C:497:THR:O    | 1:D:491:SER:HB2  | 2.02                     | 0.59              |
| 1:C:511:THR:HG23 | 1:C:555:VAL:HG21 | 1.84                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:622:MET:HG3  | 1:D:625:GLU:OE2  | 2.02                     | 0.59              |
| 1:E:218:PRO:O    | 1:E:222:ARG:HD3  | 2.02                     | 0.59              |
| 1:E:539:LEU:HA   | 1:E:542:LEU:HB2  | 1.83                     | 0.59              |
| 1:G:511:THR:HG23 | 1:G:555:VAL:HG21 | 1.84                     | 0.59              |
| 1:H:491:SER:H    | 1:N:532:PRO:HB3  | 1.67                     | 0.59              |
| 1:I:511:THR:HG23 | 1:I:555:VAL:HG21 | 1.84                     | 0.59              |
| 1:N:528:GLU:HB3  | 1:N:529:LYS:HA   | 1.84                     | 0.59              |
| 1:D:511:THR:HG23 | 1:D:555:VAL:HG21 | 1.84                     | 0.59              |
| 1:N:423:ALA:HB2  | 1:N:605:ILE:HG21 | 1.83                     | 0.59              |
| 1:F:423:ALA:HB2  | 1:F:605:ILE:HG21 | 1.83                     | 0.59              |
| 1:G:498:ALA:O    | 1:G:501:VAL:HG12 | 2.03                     | 0.59              |
| 1:K:582:LYS:HE2  | 1:K:586:MET:HE1  | 1.84                     | 0.59              |
| 1:L:511:THR:HG23 | 1:L:555:VAL:HG21 | 1.84                     | 0.59              |
| 1:N:218:PRO:O    | 1:N:222:ARG:HD3  | 2.02                     | 0.59              |
| 1:D:668:GLU:OE1  | 1:D:668:GLU:N    | 2.34                     | 0.59              |
| 1:E:528:GLU:HB3  | 1:E:529:LYS:HA   | 1.84                     | 0.59              |
| 1:F:498:ALA:O    | 1:F:501:VAL:HG12 | 2.03                     | 0.59              |
| 1:G:423:ALA:HB2  | 1:G:605:ILE:HG21 | 1.83                     | 0.59              |
| 1:H:423:ALA:HB2  | 1:H:605:ILE:HG21 | 1.83                     | 0.59              |
| 1:H:498:ALA:O    | 1:H:501:VAL:HG12 | 2.03                     | 0.59              |
| 1:I:423:ALA:HB2  | 1:I:605:ILE:HG21 | 1.83                     | 0.59              |
| 1:I:498:ALA:O    | 1:I:501:VAL:HG12 | 2.03                     | 0.59              |
| 1:B:122:ASP:OD1  | 1:B:123:ALA:N    | 2.36                     | 0.59              |
| 1:D:528:GLU:HB3  | 1:D:529:LYS:HA   | 1.84                     | 0.59              |
| 1:F:218:PRO:O    | 1:F:222:ARG:HD3  | 2.02                     | 0.59              |
| 1:F:622:MET:HG3  | 1:F:625:GLU:OE2  | 2.02                     | 0.59              |
| 1:H:622:MET:HG3  | 1:H:625:GLU:OE2  | 2.02                     | 0.59              |
| 1:M:612:LYS:O    | 1:M:652:TYR:OH   | 2.17                     | 0.59              |
| 1:A:285:GLU:H    | 1:A:285:GLU:CD   | 2.11                     | 0.59              |
| 1:B:622:MET:HG3  | 1:B:625:GLU:OE2  | 2.02                     | 0.59              |
| 1:D:411:HIS:HA   | 1:D:414:GLN:HB3  | 1.85                     | 0.59              |
| 1:E:411:HIS:HA   | 1:E:414:GLN:HB3  | 1.85                     | 0.59              |
| 1:E:572:TYR:N    | 1:E:655:VAL:O    | 2.36                     | 0.59              |
| 1:F:668:GLU:OE1  | 1:F:668:GLU:N    | 2.34                     | 0.59              |
| 1:H:218:PRO:O    | 1:H:222:ARG:HD3  | 2.02                     | 0.59              |
| 1:K:122:ASP:OD1  | 1:K:123:ALA:N    | 2.36                     | 0.59              |
| 1:N:498:ALA:O    | 1:N:501:VAL:HG12 | 2.03                     | 0.59              |
| 1:N:572:TYR:N    | 1:N:655:VAL:O    | 2.36                     | 0.59              |
| 1:B:679:ASP:HA   | 1:B:680:HIS:HB2  | 1.85                     | 0.58              |
| 1:C:679:ASP:HA   | 1:C:680:HIS:HB2  | 1.85                     | 0.58              |
| 1:E:498:ALA:O    | 1:E:501:VAL:HG12 | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:622:MET:HG3  | 1:E:625:GLU:OE2  | 2.02                     | 0.58              |
| 1:G:572:TYR:N    | 1:G:655:VAL:O    | 2.36                     | 0.58              |
| 1:H:668:GLU:N    | 1:H:668:GLU:OE1  | 2.34                     | 0.58              |
| 1:I:572:TYR:N    | 1:I:655:VAL:O    | 2.36                     | 0.58              |
| 1:L:103:GLN:NE2  | 1:M:321:GLN:OE1  | 2.32                     | 0.58              |
| 3:L:802:AGS:O2G  | 3:L:802:AGS:O3A  | 2.18                     | 0.58              |
| 1:N:622:MET:HG3  | 1:N:625:GLU:OE2  | 2.02                     | 0.58              |
| 1:B:218:PRO:O    | 1:B:222:ARG:HD3  | 2.02                     | 0.58              |
| 1:J:285:GLU:H    | 1:J:285:GLU:CD   | 2.11                     | 0.58              |
| 1:K:285:GLU:H    | 1:K:285:GLU:CD   | 2.11                     | 0.58              |
| 1:K:622:MET:HG3  | 1:K:625:GLU:OE2  | 2.02                     | 0.58              |
| 1:K:679:ASP:HA   | 1:K:680:HIS:HB2  | 1.85                     | 0.58              |
| 1:L:679:ASP:HA   | 1:L:680:HIS:HB2  | 1.85                     | 0.58              |
| 1:M:411:HIS:HA   | 1:M:414:GLN:HB3  | 1.85                     | 0.58              |
| 1:M:528:GLU:HB3  | 1:M:529:LYS:HA   | 1.84                     | 0.58              |
| 1:N:411:HIS:HA   | 1:N:414:GLN:HB3  | 1.85                     | 0.58              |
| 1:A:317:HIS:ND1  | 1:G:107:GLU:OE2  | 2.32                     | 0.58              |
| 1:A:572:TYR:N    | 1:A:655:VAL:O    | 2.36                     | 0.58              |
| 1:A:679:ASP:HA   | 1:A:680:HIS:HB2  | 1.85                     | 0.58              |
| 1:B:285:GLU:H    | 1:B:285:GLU:CD   | 2.11                     | 0.58              |
| 1:B:679:ASP:HB3  | 1:B:680:HIS:C    | 2.29                     | 0.58              |
| 1:D:112:ARG:HD2  | 1:E:274:TYR:HE1  | 1.68                     | 0.58              |
| 1:E:679:ASP:HA   | 1:E:680:HIS:HB2  | 1.85                     | 0.58              |
| 1:G:679:ASP:HA   | 1:G:680:HIS:HB2  | 1.85                     | 0.58              |
| 1:J:572:TYR:N    | 1:J:655:VAL:O    | 2.36                     | 0.58              |
| 1:K:218:PRO:O    | 1:K:222:ARG:HD3  | 2.02                     | 0.58              |
| 1:K:572:TYR:N    | 1:K:655:VAL:O    | 2.36                     | 0.58              |
| 1:L:411:HIS:HA   | 1:L:414:GLN:HB3  | 1.85                     | 0.58              |
| 1:M:668:GLU:OE1  | 1:M:668:GLU:N    | 2.34                     | 0.58              |
| 1:M:679:ASP:HA   | 1:M:680:HIS:HB2  | 1.85                     | 0.58              |
| 1:N:679:ASP:HA   | 1:N:680:HIS:HB2  | 1.85                     | 0.58              |
| 1:A:122:ASP:OD1  | 1:A:123:ALA:N    | 2.36                     | 0.58              |
| 1:C:411:HIS:HA   | 1:C:414:GLN:HB3  | 1.85                     | 0.58              |
| 1:C:456:VAL:HG21 | 1:C:607:PHE:HB3  | 1.86                     | 0.58              |
| 1:C:572:TYR:N    | 1:C:655:VAL:O    | 2.36                     | 0.58              |
| 3:C:802:AGS:O2G  | 3:C:802:AGS:O3A  | 2.18                     | 0.58              |
| 1:D:456:VAL:HG21 | 1:D:607:PHE:HB3  | 1.86                     | 0.58              |
| 1:D:679:ASP:HA   | 1:D:680:HIS:HB2  | 1.85                     | 0.58              |
| 1:L:456:VAL:HG21 | 1:L:607:PHE:HB3  | 1.86                     | 0.58              |
| 1:L:498:ALA:O    | 1:L:501:VAL:HG12 | 2.03                     | 0.58              |
| 1:L:572:TYR:N    | 1:L:655:VAL:O    | 2.36                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:572:TYR:N    | 1:B:655:VAL:O    | 2.36                     | 0.58              |
| 1:C:498:ALA:O    | 1:C:501:VAL:HG12 | 2.03                     | 0.58              |
| 1:F:679:ASP:HA   | 1:F:680:HIS:HB2  | 1.85                     | 0.58              |
| 1:H:572:TYR:N    | 1:H:655:VAL:O    | 2.36                     | 0.58              |
| 1:I:285:GLU:H    | 1:I:285:GLU:CD   | 2.11                     | 0.58              |
| 1:I:679:ASP:HA   | 1:I:680:HIS:HB2  | 1.86                     | 0.58              |
| 1:J:122:ASP:OD1  | 1:J:123:ALA:N    | 2.36                     | 0.58              |
| 1:J:679:ASP:HA   | 1:J:680:HIS:HB2  | 1.85                     | 0.58              |
| 1:D:498:ALA:O    | 1:D:501:VAL:HG12 | 2.03                     | 0.58              |
| 1:D:612:LYS:O    | 1:D:652:TYR:OH   | 2.17                     | 0.58              |
| 1:E:330:VAL:HG21 | 1:E:366:LYS:HZ3  | 1.68                     | 0.58              |
| 1:F:411:HIS:HA   | 1:F:414:GLN:HB3  | 1.85                     | 0.58              |
| 1:F:572:TYR:N    | 1:F:655:VAL:O    | 2.36                     | 0.58              |
| 1:G:285:GLU:H    | 1:G:285:GLU:CD   | 2.11                     | 0.58              |
| 1:G:679:ASP:HB3  | 1:G:680:HIS:C    | 2.29                     | 0.58              |
| 1:H:411:HIS:HA   | 1:H:414:GLN:HB3  | 1.85                     | 0.58              |
| 1:H:679:ASP:HA   | 1:H:680:HIS:HB2  | 1.85                     | 0.58              |
| 1:I:679:ASP:HB3  | 1:I:680:HIS:C    | 2.28                     | 0.58              |
| 1:J:679:ASP:HB3  | 1:J:680:HIS:C    | 2.28                     | 0.58              |
| 1:K:679:ASP:HB3  | 1:K:680:HIS:C    | 2.29                     | 0.58              |
| 1:M:498:ALA:O    | 1:M:501:VAL:HG12 | 2.03                     | 0.58              |
| 1:N:330:VAL:HG21 | 1:N:366:LYS:HZ3  | 1.68                     | 0.58              |
| 1:A:461:LEU:HD13 | 1:A:465:LEU:HD22 | 1.86                     | 0.58              |
| 1:F:461:LEU:HD13 | 1:F:465:LEU:HD22 | 1.86                     | 0.58              |
| 1:G:461:LEU:HD13 | 1:G:465:LEU:HD22 | 1.86                     | 0.58              |
| 1:I:461:LEU:HD13 | 1:I:465:LEU:HD22 | 1.86                     | 0.58              |
| 1:L:612:LYS:O    | 1:L:652:TYR:OH   | 2.17                     | 0.58              |
| 1:N:461:LEU:HD13 | 1:N:465:LEU:HD22 | 1.86                     | 0.58              |
| 1:A:679:ASP:HB3  | 1:A:680:HIS:C    | 2.28                     | 0.58              |
| 1:G:122:ASP:OD1  | 1:G:123:ALA:N    | 2.36                     | 0.58              |
| 1:H:461:LEU:HD13 | 1:H:465:LEU:HD22 | 1.86                     | 0.58              |
| 1:M:456:VAL:HG21 | 1:M:607:PHE:HB3  | 1.86                     | 0.58              |
| 1:B:668:GLU:OE1  | 1:B:668:GLU:N    | 2.34                     | 0.58              |
| 1:E:461:LEU:HD13 | 1:E:465:LEU:HD22 | 1.86                     | 0.58              |
| 1:J:461:LEU:HD13 | 1:J:465:LEU:HD22 | 1.86                     | 0.58              |
| 1:M:572:TYR:N    | 1:M:655:VAL:O    | 2.36                     | 0.58              |
| 1:D:461:LEU:HD13 | 1:D:465:LEU:HD22 | 1.86                     | 0.58              |
| 1:L:679:ASP:HB3  | 1:L:680:HIS:C    | 2.29                     | 0.58              |
| 1:M:461:LEU:HD13 | 1:M:465:LEU:HD22 | 1.86                     | 0.58              |
| 1:C:679:ASP:HB3  | 1:C:680:HIS:C    | 2.29                     | 0.57              |
| 1:D:210:LYS:NZ   | 1:D:214:ASP:OD2  | 2.36                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:210:LYS:NZ   | 1:E:214:ASP:OD2  | 2.36                     | 0.57              |
| 1:I:122:ASP:OD1  | 1:I:123:ALA:N    | 2.36                     | 0.57              |
| 1:K:411:HIS:HA   | 1:K:414:GLN:HB3  | 1.85                     | 0.57              |
| 1:N:210:LYS:NZ   | 1:N:214:ASP:OD2  | 2.36                     | 0.57              |
| 1:C:612:LYS:O    | 1:C:652:TYR:OH   | 2.17                     | 0.57              |
| 1:B:461:LEU:HD13 | 1:B:465:LEU:HD22 | 1.86                     | 0.57              |
| 1:D:572:TYR:N    | 1:D:655:VAL:O    | 2.36                     | 0.57              |
| 1:I:330:VAL:HG21 | 1:I:366:LYS:HZ3  | 1.69                     | 0.57              |
| 1:K:456:VAL:HG21 | 1:K:607:PHE:HB3  | 1.86                     | 0.57              |
| 1:M:210:LYS:NZ   | 1:M:214:ASP:OD2  | 2.36                     | 0.57              |
| 1:N:285:GLU:H    | 1:N:285:GLU:CD   | 2.11                     | 0.57              |
| 1:B:411:HIS:HA   | 1:B:414:GLN:HB3  | 1.85                     | 0.57              |
| 1:B:456:VAL:HG21 | 1:B:607:PHE:HB3  | 1.86                     | 0.57              |
| 1:D:679:ASP:HB3  | 1:D:680:HIS:C    | 2.28                     | 0.57              |
| 1:E:668:GLU:N    | 1:E:668:GLU:OE1  | 2.34                     | 0.57              |
| 1:F:679:ASP:HB3  | 1:F:680:HIS:C    | 2.28                     | 0.57              |
| 1:K:668:GLU:N    | 1:K:668:GLU:OE1  | 2.34                     | 0.57              |
| 1:N:668:GLU:OE1  | 1:N:668:GLU:N    | 2.34                     | 0.57              |
| 1:E:679:ASP:HB3  | 1:E:680:HIS:C    | 2.28                     | 0.57              |
| 1:F:121:GLY:O    | 1:F:127:LYS:NZ   | 2.34                     | 0.57              |
| 1:F:573:GLU:N    | 1:F:574:ALA:HA   | 2.20                     | 0.57              |
| 1:H:121:GLY:O    | 1:H:127:LYS:NZ   | 2.34                     | 0.57              |
| 1:H:679:ASP:HB3  | 1:H:680:HIS:C    | 2.29                     | 0.57              |
| 1:K:461:LEU:HD13 | 1:K:465:LEU:HD22 | 1.86                     | 0.57              |
| 1:L:330:VAL:HG21 | 1:L:366:LYS:HZ3  | 1.68                     | 0.57              |
| 1:M:679:ASP:HB3  | 1:M:680:HIS:C    | 2.28                     | 0.57              |
| 1:N:573:GLU:N    | 1:N:574:ALA:HA   | 2.20                     | 0.57              |
| 1:H:573:GLU:N    | 1:H:574:ALA:HA   | 2.20                     | 0.57              |
| 1:N:679:ASP:HB3  | 1:N:680:HIS:C    | 2.28                     | 0.57              |
| 1:A:111:ARG:HB3  | 1:B:312:ASP:OD2  | 2.05                     | 0.57              |
| 1:C:330:VAL:HG21 | 1:C:366:LYS:HZ3  | 1.68                     | 0.57              |
| 1:C:461:LEU:HD13 | 1:C:465:LEU:HD22 | 1.86                     | 0.57              |
| 1:D:122:ASP:OD1  | 1:D:123:ALA:N    | 2.36                     | 0.57              |
| 1:E:573:GLU:N    | 1:E:574:ALA:HA   | 2.20                     | 0.57              |
| 1:G:573:GLU:N    | 1:G:574:ALA:HA   | 2.20                     | 0.57              |
| 1:M:122:ASP:OD1  | 1:M:123:ALA:N    | 2.36                     | 0.57              |
| 1:E:285:GLU:H    | 1:E:285:GLU:CD   | 2.11                     | 0.57              |
| 1:F:122:ASP:OD1  | 1:F:123:ALA:N    | 2.36                     | 0.57              |
| 1:G:121:GLY:O    | 1:G:127:LYS:NZ   | 2.34                     | 0.57              |
| 1:G:549:ASP:OD1  | 1:G:553:ASN:N    | 2.38                     | 0.57              |
| 1:I:121:GLY:O    | 1:I:127:LYS:NZ   | 2.34                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:549:ASP:OD1  | 1:I:553:ASN:N    | 2.38                     | 0.57              |
| 1:I:573:GLU:N    | 1:I:574:ALA:HA   | 2.20                     | 0.57              |
| 1:L:461:LEU:HD13 | 1:L:465:LEU:HD22 | 1.86                     | 0.57              |
| 1:A:549:ASP:OD1  | 1:A:553:ASN:N    | 2.38                     | 0.57              |
| 1:D:485:SER:HB2  | 1:D:497:THR:HG23 | 1.87                     | 0.57              |
| 1:D:573:GLU:N    | 1:D:574:ALA:HA   | 2.20                     | 0.57              |
| 1:E:456:VAL:HG21 | 1:E:607:PHE:HB3  | 1.86                     | 0.57              |
| 1:F:549:ASP:OD1  | 1:F:553:ASN:N    | 2.38                     | 0.57              |
| 1:H:549:ASP:OD1  | 1:H:553:ASN:N    | 2.38                     | 0.57              |
| 1:J:549:ASP:OD1  | 1:J:553:ASN:N    | 2.38                     | 0.57              |
| 1:M:485:SER:HB2  | 1:M:497:THR:HG23 | 1.87                     | 0.57              |
| 1:C:485:SER:HB2  | 1:C:497:THR:HG23 | 1.87                     | 0.57              |
| 1:E:485:SER:HB2  | 1:E:497:THR:HG23 | 1.87                     | 0.57              |
| 1:G:411:HIS:HA   | 1:G:414:GLN:HB3  | 1.85                     | 0.57              |
| 1:L:534:VAL:HG22 | 1:M:492:LYS:HB3  | 1.86                     | 0.57              |
| 1:L:549:ASP:OD1  | 1:L:553:ASN:N    | 2.38                     | 0.57              |
| 1:M:573:GLU:N    | 1:M:574:ALA:HA   | 2.20                     | 0.57              |
| 1:A:411:HIS:HA   | 1:A:414:GLN:HB3  | 1.85                     | 0.56              |
| 1:D:549:ASP:OD1  | 1:D:553:ASN:N    | 2.38                     | 0.56              |
| 1:H:122:ASP:OD1  | 1:H:123:ALA:N    | 2.36                     | 0.56              |
| 1:J:411:HIS:HA   | 1:J:414:GLN:HB3  | 1.85                     | 0.56              |
| 1:C:549:ASP:OD1  | 1:C:553:ASN:N    | 2.38                     | 0.56              |
| 1:I:411:HIS:HA   | 1:I:414:GLN:HB3  | 1.85                     | 0.56              |
| 1:A:365:ARG:HG3  | 1:A:365:ARG:NH1  | 2.09                     | 0.56              |
| 1:A:485:SER:HB2  | 1:A:497:THR:HG23 | 1.87                     | 0.56              |
| 1:B:485:SER:HB2  | 1:B:497:THR:HG23 | 1.87                     | 0.56              |
| 1:B:498:ALA:HB1  | 1:C:494:ILE:HA   | 1.86                     | 0.56              |
| 1:H:456:VAL:HG21 | 1:H:607:PHE:HB3  | 1.86                     | 0.56              |
| 1:I:456:VAL:HG21 | 1:I:607:PHE:HB3  | 1.86                     | 0.56              |
| 1:J:365:ARG:HG3  | 1:J:365:ARG:NH1  | 2.09                     | 0.56              |
| 1:J:485:SER:HB2  | 1:J:497:THR:HG23 | 1.87                     | 0.56              |
| 1:L:485:SER:HB2  | 1:L:497:THR:HG23 | 1.87                     | 0.56              |
| 1:L:573:GLU:N    | 1:L:574:ALA:HA   | 2.20                     | 0.56              |
| 1:M:549:ASP:OD1  | 1:M:553:ASN:N    | 2.38                     | 0.56              |
| 1:N:485:SER:HB2  | 1:N:497:THR:HG23 | 1.87                     | 0.56              |
| 1:A:121:GLY:O    | 1:A:127:LYS:NZ   | 2.34                     | 0.56              |
| 1:A:191:PHE:CG   | 1:A:197:ILE:HD11 | 2.41                     | 0.56              |
| 1:B:549:ASP:OD1  | 1:B:553:ASN:N    | 2.38                     | 0.56              |
| 1:G:485:SER:HB2  | 1:G:497:THR:HG23 | 1.87                     | 0.56              |
| 1:J:191:PHE:CG   | 1:J:197:ILE:HD11 | 2.41                     | 0.56              |
| 1:J:456:VAL:HG21 | 1:J:607:PHE:HB3  | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:532:PRO:HA   | 1:L:490:VAL:HB   | 1.87                     | 0.56              |
| 1:L:122:ASP:OD1  | 1:L:123:ALA:N    | 2.36                     | 0.56              |
| 1:N:456:VAL:HG21 | 1:N:607:PHE:HB3  | 1.86                     | 0.56              |
| 1:N:612:LYS:O    | 1:N:652:TYR:OH   | 2.17                     | 0.56              |
| 1:A:456:VAL:HG21 | 1:A:607:PHE:HB3  | 1.86                     | 0.56              |
| 1:C:573:GLU:N    | 1:C:574:ALA:HA   | 2.20                     | 0.56              |
| 1:C:623:LEU:HD22 | 1:C:639:VAL:HG21 | 1.88                     | 0.56              |
| 1:F:456:VAL:HG21 | 1:F:607:PHE:HB3  | 1.86                     | 0.56              |
| 1:G:456:VAL:HG21 | 1:G:607:PHE:HB3  | 1.86                     | 0.56              |
| 1:G:668:GLU:OE1  | 1:G:668:GLU:N    | 2.34                     | 0.56              |
| 1:H:274:TYR:CE1  | 1:N:112:ARG:HD2  | 2.41                     | 0.56              |
| 1:I:485:SER:HB2  | 1:I:497:THR:HG23 | 1.87                     | 0.56              |
| 1:K:549:ASP:OD1  | 1:K:553:ASN:N    | 2.38                     | 0.56              |
| 1:L:285:GLU:H    | 1:L:285:GLU:CD   | 2.11                     | 0.56              |
| 1:L:623:LEU:HD22 | 1:L:639:VAL:HG21 | 1.88                     | 0.56              |
| 1:C:122:ASP:OD1  | 1:C:123:ALA:N    | 2.36                     | 0.56              |
| 1:F:485:SER:HB2  | 1:F:497:THR:HG23 | 1.87                     | 0.56              |
| 1:H:490:VAL:HB   | 1:N:532:PRO:HA   | 1.86                     | 0.56              |
| 1:J:121:GLY:O    | 1:J:127:LYS:NZ   | 2.34                     | 0.56              |
| 1:K:485:SER:HB2  | 1:K:497:THR:HG23 | 1.87                     | 0.56              |
| 1:K:623:LEU:HD22 | 1:K:639:VAL:HG21 | 1.88                     | 0.56              |
| 1:F:327:VAL:HG23 | 1:F:367:ILE:HG12 | 1.88                     | 0.56              |
| 1:H:485:SER:HB2  | 1:H:497:THR:HG23 | 1.87                     | 0.56              |
| 1:I:668:GLU:OE1  | 1:I:668:GLU:N    | 2.34                     | 0.56              |
| 1:N:549:ASP:OD1  | 1:N:553:ASN:N    | 2.38                     | 0.56              |
| 1:F:532:PRO:HA   | 1:G:490:VAL:HB   | 1.88                     | 0.56              |
| 1:J:573:GLU:N    | 1:J:574:ALA:HA   | 2.20                     | 0.56              |
| 1:N:177:LEU:HD21 | 1:N:189:LEU:HD21 | 1.88                     | 0.56              |
| 1:A:573:GLU:N    | 1:A:574:ALA:HA   | 2.20                     | 0.56              |
| 1:A:668:GLU:OE1  | 1:A:668:GLU:N    | 2.34                     | 0.56              |
| 1:B:573:GLU:N    | 1:B:574:ALA:HA   | 2.20                     | 0.56              |
| 1:B:623:LEU:HD22 | 1:B:639:VAL:HG21 | 1.88                     | 0.56              |
| 1:C:191:PHE:CG   | 1:C:197:ILE:HD11 | 2.41                     | 0.56              |
| 1:C:285:GLU:H    | 1:C:285:GLU:CD   | 2.11                     | 0.56              |
| 1:E:177:LEU:HD21 | 1:E:189:LEU:HD21 | 1.88                     | 0.56              |
| 1:E:612:LYS:O    | 1:E:652:TYR:OH   | 2.17                     | 0.56              |
| 1:H:327:VAL:HG23 | 1:H:367:ILE:HG12 | 1.88                     | 0.56              |
| 1:I:112:ARG:HD2  | 1:J:274:TYR:CE1  | 2.40                     | 0.56              |
| 1:A:107:GLU:OE2  | 1:B:317:HIS:ND1  | 2.32                     | 0.56              |
| 1:C:343:LYS:HA   | 1:C:343:LYS:HE3  | 1.88                     | 0.56              |
| 1:D:327:VAL:HG23 | 1:D:367:ILE:HG12 | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:549:ASP:OD1  | 1:E:553:ASN:N    | 2.38                     | 0.56              |
| 1:G:280:VAL:HB   | 1:G:376:VAL:HA   | 1.88                     | 0.56              |
| 1:L:191:PHE:CG   | 1:L:197:ILE:HD11 | 2.41                     | 0.56              |
| 1:M:327:VAL:HG23 | 1:M:367:ILE:HG12 | 1.88                     | 0.56              |
| 1:A:104:GLU:HA   | 1:B:321:GLN:NE2  | 2.22                     | 0.55              |
| 1:B:478:ARG:HG3  | 1:B:523:LEU:CB   | 2.37                     | 0.55              |
| 1:C:177:LEU:HD21 | 1:C:189:LEU:HD21 | 1.88                     | 0.55              |
| 1:C:478:ARG:HG3  | 1:C:523:LEU:CB   | 2.36                     | 0.55              |
| 1:D:450:PHE:HB3  | 1:D:607:PHE:CE2  | 2.42                     | 0.55              |
| 1:E:285:GLU:OE1  | 1:E:285:GLU:N    | 2.26                     | 0.55              |
| 1:F:177:LEU:HD21 | 1:F:189:LEU:HD21 | 1.88                     | 0.55              |
| 1:F:623:LEU:HD22 | 1:F:639:VAL:HG21 | 1.88                     | 0.55              |
| 1:I:280:VAL:HB   | 1:I:376:VAL:HA   | 1.88                     | 0.55              |
| 1:J:537:LEU:HD13 | 1:K:492:LYS:HA   | 1.88                     | 0.55              |
| 1:J:668:GLU:OE1  | 1:J:668:GLU:N    | 2.34                     | 0.55              |
| 1:K:478:ARG:HG3  | 1:K:523:LEU:CB   | 2.37                     | 0.55              |
| 1:K:573:GLU:N    | 1:K:574:ALA:HA   | 2.20                     | 0.55              |
| 1:M:177:LEU:HD21 | 1:M:189:LEU:HD21 | 1.88                     | 0.55              |
| 1:A:280:VAL:HB   | 1:A:376:VAL:HA   | 1.88                     | 0.55              |
| 1:A:481:MET:HE3  | 1:A:527:ILE:HA   | 1.87                     | 0.55              |
| 1:B:403:ILE:HG23 | 1:C:678:LEU:HD22 | 1.89                     | 0.55              |
| 1:D:343:LYS:HA   | 1:D:343:LYS:HE3  | 1.89                     | 0.55              |
| 1:D:623:LEU:HD22 | 1:D:639:VAL:HG21 | 1.88                     | 0.55              |
| 1:E:122:ASP:OD1  | 1:E:123:ALA:N    | 2.36                     | 0.55              |
| 1:F:280:VAL:HB   | 1:F:376:VAL:HA   | 1.88                     | 0.55              |
| 1:F:536:THR:HG21 | 1:G:483:GLU:HG3  | 1.87                     | 0.55              |
| 1:G:481:MET:HE3  | 1:G:527:ILE:HA   | 1.87                     | 0.55              |
| 1:H:177:LEU:HD21 | 1:H:189:LEU:HD21 | 1.88                     | 0.55              |
| 1:I:481:MET:HE3  | 1:I:527:ILE:HA   | 1.88                     | 0.55              |
| 1:J:481:MET:HE3  | 1:J:527:ILE:HA   | 1.88                     | 0.55              |
| 1:K:450:PHE:HB3  | 1:K:607:PHE:CE2  | 2.42                     | 0.55              |
| 1:L:177:LEU:HD21 | 1:L:189:LEU:HD21 | 1.88                     | 0.55              |
| 1:L:343:LYS:HA   | 1:L:343:LYS:HE3  | 1.89                     | 0.55              |
| 1:L:478:ARG:HG3  | 1:L:523:LEU:CB   | 2.37                     | 0.55              |
| 1:M:191:PHE:CG   | 1:M:197:ILE:HD11 | 2.41                     | 0.55              |
| 1:B:450:PHE:HB3  | 1:B:607:PHE:CE2  | 2.42                     | 0.55              |
| 1:D:177:LEU:HD21 | 1:D:189:LEU:HD21 | 1.88                     | 0.55              |
| 1:E:450:PHE:O    | 1:E:565:THR:HA   | 2.07                     | 0.55              |
| 1:H:280:VAL:HB   | 1:H:376:VAL:HA   | 1.88                     | 0.55              |
| 1:H:623:LEU:HD22 | 1:H:639:VAL:HG21 | 1.88                     | 0.55              |
| 1:J:280:VAL:HB   | 1:J:376:VAL:HA   | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:450:PHE:O    | 1:K:565:THR:HA   | 2.07                     | 0.55              |
| 1:K:481:MET:HE3  | 1:K:527:ILE:HA   | 1.87                     | 0.55              |
| 1:L:532:PRO:HA   | 1:M:490:VAL:HB   | 1.88                     | 0.55              |
| 1:M:450:PHE:HB3  | 1:M:607:PHE:CE2  | 2.42                     | 0.55              |
| 1:A:478:ARG:HG3  | 1:A:523:LEU:CB   | 2.37                     | 0.55              |
| 1:E:280:VAL:HB   | 1:E:376:VAL:HA   | 1.88                     | 0.55              |
| 1:F:191:PHE:CG   | 1:F:197:ILE:HD11 | 2.41                     | 0.55              |
| 1:J:478:ARG:HG3  | 1:J:523:LEU:CB   | 2.36                     | 0.55              |
| 1:J:558:LYS:HA   | 1:J:558:LYS:HE2  | 1.89                     | 0.55              |
| 1:K:191:PHE:CG   | 1:K:197:ILE:HD11 | 2.41                     | 0.55              |
| 1:M:623:LEU:HD22 | 1:M:639:VAL:HG21 | 1.88                     | 0.55              |
| 1:N:122:ASP:OD1  | 1:N:123:ALA:N    | 2.36                     | 0.55              |
| 1:N:285:GLU:OE1  | 1:N:285:GLU:N    | 2.26                     | 0.55              |
| 1:N:343:LYS:HA   | 1:N:343:LYS:HE3  | 1.88                     | 0.55              |
| 1:N:450:PHE:O    | 1:N:565:THR:HA   | 2.07                     | 0.55              |
| 1:A:142:ASP:O    | 1:B:323:PRO:HA   | 2.05                     | 0.55              |
| 1:A:558:LYS:HE2  | 1:A:558:LYS:HA   | 1.89                     | 0.55              |
| 1:A:623:LEU:HD22 | 1:A:639:VAL:HG21 | 1.88                     | 0.55              |
| 1:B:450:PHE:O    | 1:B:565:THR:HA   | 2.07                     | 0.55              |
| 1:C:450:PHE:O    | 1:C:565:THR:HA   | 2.07                     | 0.55              |
| 1:D:330:VAL:HG21 | 1:D:366:LYS:HZ3  | 1.71                     | 0.55              |
| 1:E:103:GLN:NE2  | 1:F:321:GLN:OE1  | 2.36                     | 0.55              |
| 1:E:191:PHE:CG   | 1:E:197:ILE:HD11 | 2.41                     | 0.55              |
| 1:E:343:LYS:HA   | 1:E:343:LYS:HE3  | 1.88                     | 0.55              |
| 1:E:450:PHE:HB3  | 1:E:607:PHE:CE2  | 2.41                     | 0.55              |
| 1:F:515:ARG:HG2  | 1:F:516:ARG:HH22 | 1.71                     | 0.55              |
| 1:H:191:PHE:CG   | 1:H:197:ILE:HD11 | 2.41                     | 0.55              |
| 1:I:515:ARG:HG2  | 1:I:516:ARG:HH22 | 1.71                     | 0.55              |
| 1:M:343:LYS:HA   | 1:M:343:LYS:HE3  | 1.89                     | 0.55              |
| 1:N:191:PHE:CG   | 1:N:197:ILE:HD11 | 2.41                     | 0.55              |
| 1:N:450:PHE:HB3  | 1:N:607:PHE:CE2  | 2.42                     | 0.55              |
| 1:A:450:PHE:O    | 1:A:565:THR:HA   | 2.07                     | 0.55              |
| 1:A:450:PHE:HB3  | 1:A:607:PHE:CE2  | 2.42                     | 0.55              |
| 1:B:177:LEU:HD21 | 1:B:189:LEU:HD21 | 1.88                     | 0.55              |
| 1:B:191:PHE:CG   | 1:B:197:ILE:HD11 | 2.41                     | 0.55              |
| 1:D:191:PHE:CG   | 1:D:197:ILE:HD11 | 2.41                     | 0.55              |
| 1:E:623:LEU:HD22 | 1:E:639:VAL:HG21 | 1.88                     | 0.55              |
| 1:G:515:ARG:HG2  | 1:G:516:ARG:HH22 | 1.71                     | 0.55              |
| 1:H:515:ARG:HG2  | 1:H:516:ARG:HH22 | 1.71                     | 0.55              |
| 1:H:612:LYS:O    | 1:H:652:TYR:OH   | 2.17                     | 0.55              |
| 1:J:450:PHE:O    | 1:J:565:THR:HA   | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:450:PHE:HB3  | 1:J:607:PHE:CE2  | 2.42                     | 0.55              |
| 1:J:623:LEU:HD22 | 1:J:639:VAL:HG21 | 1.88                     | 0.55              |
| 1:K:177:LEU:HD21 | 1:K:189:LEU:HD21 | 1.88                     | 0.55              |
| 1:N:280:VAL:HB   | 1:N:376:VAL:HA   | 1.88                     | 0.55              |
| 1:B:481:MET:HE3  | 1:B:527:ILE:HA   | 1.88                     | 0.55              |
| 1:L:450:PHE:HB3  | 1:L:607:PHE:CE2  | 2.41                     | 0.55              |
| 1:L:450:PHE:O    | 1:L:565:THR:HA   | 2.07                     | 0.55              |
| 1:N:623:LEU:HD22 | 1:N:639:VAL:HG21 | 1.88                     | 0.55              |
| 1:B:280:VAL:HB   | 1:B:376:VAL:HA   | 1.88                     | 0.55              |
| 1:E:327:VAL:HG23 | 1:E:367:ILE:HG12 | 1.88                     | 0.55              |
| 1:F:612:LYS:O    | 1:F:652:TYR:OH   | 2.17                     | 0.55              |
| 1:G:558:LYS:HA   | 1:G:558:LYS:HE2  | 1.89                     | 0.55              |
| 1:H:343:LYS:HA   | 1:H:343:LYS:HE3  | 1.88                     | 0.55              |
| 1:I:558:LYS:HE2  | 1:I:558:LYS:HA   | 1.89                     | 0.55              |
| 1:K:210:LYS:NZ   | 1:K:214:ASP:OD2  | 2.36                     | 0.55              |
| 1:N:327:VAL:HG23 | 1:N:367:ILE:HG12 | 1.88                     | 0.55              |
| 1:A:177:LEU:HD21 | 1:A:189:LEU:HD21 | 1.88                     | 0.55              |
| 1:A:461:LEU:O    | 1:A:465:LEU:HB3  | 2.07                     | 0.55              |
| 1:B:343:LYS:HE3  | 1:B:343:LYS:HA   | 1.88                     | 0.55              |
| 1:B:461:LEU:O    | 1:B:465:LEU:HB3  | 2.07                     | 0.55              |
| 1:B:558:LYS:HA   | 1:B:558:LYS:HE2  | 1.89                     | 0.55              |
| 1:C:450:PHE:HB3  | 1:C:607:PHE:CE2  | 2.42                     | 0.55              |
| 1:C:481:MET:HE3  | 1:C:527:ILE:HA   | 1.88                     | 0.55              |
| 1:D:615:LEU:HD23 | 1:D:661:LEU:HD12 | 1.89                     | 0.55              |
| 1:F:343:LYS:HA   | 1:F:343:LYS:HE3  | 1.89                     | 0.55              |
| 1:F:481:MET:HE3  | 1:F:527:ILE:HA   | 1.87                     | 0.55              |
| 1:F:558:LYS:HE2  | 1:F:558:LYS:HA   | 1.89                     | 0.55              |
| 1:G:177:LEU:HD21 | 1:G:189:LEU:HD21 | 1.88                     | 0.55              |
| 1:G:478:ARG:HG3  | 1:G:523:LEU:CB   | 2.36                     | 0.55              |
| 1:G:623:LEU:HD22 | 1:G:639:VAL:HG21 | 1.88                     | 0.55              |
| 1:H:481:MET:HE3  | 1:H:527:ILE:HA   | 1.88                     | 0.55              |
| 1:H:537:LEU:HD13 | 1:I:492:LYS:HA   | 1.88                     | 0.55              |
| 1:H:558:LYS:HE2  | 1:H:558:LYS:HA   | 1.89                     | 0.55              |
| 1:I:327:VAL:HG23 | 1:I:367:ILE:HG12 | 1.88                     | 0.55              |
| 1:I:478:ARG:HG3  | 1:I:523:LEU:CB   | 2.37                     | 0.55              |
| 1:I:623:LEU:HD22 | 1:I:639:VAL:HG21 | 1.88                     | 0.55              |
| 1:J:177:LEU:HD21 | 1:J:189:LEU:HD21 | 1.88                     | 0.55              |
| 1:K:343:LYS:HA   | 1:K:343:LYS:HE3  | 1.89                     | 0.55              |
| 1:K:461:LEU:O    | 1:K:465:LEU:HB3  | 2.07                     | 0.55              |
| 1:K:558:LYS:HE2  | 1:K:558:LYS:HA   | 1.89                     | 0.55              |
| 1:L:481:MET:HE3  | 1:L:527:ILE:HA   | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:615:LEU:HD23 | 1:M:661:LEU:HD12 | 1.89                     | 0.55              |
| 1:D:285:GLU:OE1  | 1:D:285:GLU:N    | 2.26                     | 0.55              |
| 1:E:515:ARG:HG2  | 1:E:516:ARG:HH22 | 1.71                     | 0.55              |
| 1:G:191:PHE:CG   | 1:G:197:ILE:HD11 | 2.41                     | 0.55              |
| 1:G:327:VAL:HG23 | 1:G:367:ILE:HG12 | 1.88                     | 0.55              |
| 1:I:177:LEU:HD21 | 1:I:189:LEU:HD21 | 1.88                     | 0.55              |
| 1:I:191:PHE:CG   | 1:I:197:ILE:HD11 | 2.41                     | 0.55              |
| 1:I:461:LEU:O    | 1:I:465:LEU:HB3  | 2.07                     | 0.55              |
| 1:J:461:LEU:O    | 1:J:465:LEU:HB3  | 2.07                     | 0.55              |
| 1:K:280:VAL:HB   | 1:K:376:VAL:HA   | 1.88                     | 0.55              |
| 1:A:489:ALA:O    | 1:G:497:THR:HB   | 2.08                     | 0.54              |
| 1:C:461:LEU:O    | 1:C:465:LEU:HB3  | 2.07                     | 0.54              |
| 1:D:280:VAL:HB   | 1:D:376:VAL:HA   | 1.88                     | 0.54              |
| 1:G:361:ALA:O    | 1:G:365:ARG:HG2  | 2.07                     | 0.54              |
| 1:G:450:PHE:O    | 1:G:565:THR:HA   | 2.07                     | 0.54              |
| 1:G:461:LEU:O    | 1:G:465:LEU:HB3  | 2.08                     | 0.54              |
| 1:I:536:THR:HG21 | 1:J:483:GLU:HG3  | 1.88                     | 0.54              |
| 1:J:515:ARG:HG2  | 1:J:516:ARG:HH22 | 1.71                     | 0.54              |
| 1:A:112:ARG:HD2  | 1:B:274:TYR:HE1  | 1.73                     | 0.54              |
| 1:A:459:THR:OG1  | 1:A:463:LYS:NZ   | 2.41                     | 0.54              |
| 1:B:210:LYS:NZ   | 1:B:214:ASP:OD2  | 2.36                     | 0.54              |
| 1:B:251:ASN:OD1  | 1:B:252:GLU:N    | 2.41                     | 0.54              |
| 1:C:361:ALA:O    | 1:C:365:ARG:HG2  | 2.07                     | 0.54              |
| 1:D:361:ALA:O    | 1:D:365:ARG:HG2  | 2.07                     | 0.54              |
| 1:E:121:GLY:O    | 1:E:127:LYS:NZ   | 2.34                     | 0.54              |
| 1:E:558:LYS:HE2  | 1:E:558:LYS:HA   | 1.89                     | 0.54              |
| 1:F:450:PHE:HB3  | 1:F:607:PHE:CE2  | 2.42                     | 0.54              |
| 1:H:450:PHE:HB3  | 1:H:607:PHE:CE2  | 2.42                     | 0.54              |
| 1:I:361:ALA:O    | 1:I:365:ARG:HG2  | 2.07                     | 0.54              |
| 1:I:450:PHE:O    | 1:I:565:THR:HA   | 2.07                     | 0.54              |
| 1:J:361:ALA:O    | 1:J:365:ARG:HG2  | 2.07                     | 0.54              |
| 1:J:459:THR:OG1  | 1:J:463:LYS:NZ   | 2.41                     | 0.54              |
| 1:L:361:ALA:O    | 1:L:365:ARG:HG2  | 2.07                     | 0.54              |
| 1:N:515:ARG:HG2  | 1:N:516:ARG:HH22 | 1.71                     | 0.54              |
| 1:A:361:ALA:O    | 1:A:365:ARG:HG2  | 2.07                     | 0.54              |
| 1:A:515:ARG:HG2  | 1:A:516:ARG:HH22 | 1.71                     | 0.54              |
| 1:F:361:ALA:O    | 1:F:365:ARG:HG2  | 2.07                     | 0.54              |
| 1:F:461:LEU:O    | 1:F:465:LEU:HB3  | 2.08                     | 0.54              |
| 1:H:461:LEU:O    | 1:H:465:LEU:HB3  | 2.07                     | 0.54              |
| 1:L:537:LEU:HD13 | 1:M:492:LYS:HA   | 1.89                     | 0.54              |
| 1:N:251:ASN:OD1  | 1:N:252:GLU:N    | 2.41                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:481:MET:HE3  | 1:D:527:ILE:HA   | 1.88                     | 0.54              |
| 1:E:251:ASN:OD1  | 1:E:252:GLU:N    | 2.41                     | 0.54              |
| 1:F:478:ARG:HG3  | 1:F:523:LEU:CB   | 2.37                     | 0.54              |
| 1:H:478:ARG:HG3  | 1:H:523:LEU:CB   | 2.37                     | 0.54              |
| 1:K:251:ASN:OD1  | 1:K:252:GLU:N    | 2.41                     | 0.54              |
| 1:K:501:VAL:HB   | 1:L:491:SER:C    | 2.32                     | 0.54              |
| 1:L:461:LEU:O    | 1:L:465:LEU:HB3  | 2.08                     | 0.54              |
| 1:L:615:LEU:HD23 | 1:L:661:LEU:HD12 | 1.89                     | 0.54              |
| 1:M:280:VAL:HB   | 1:M:376:VAL:HA   | 1.88                     | 0.54              |
| 1:M:285:GLU:H    | 1:M:285:GLU:CD   | 2.11                     | 0.54              |
| 1:M:461:LEU:O    | 1:M:465:LEU:HB3  | 2.07                     | 0.54              |
| 1:N:558:LYS:HE2  | 1:N:558:LYS:HA   | 1.89                     | 0.54              |
| 1:C:327:VAL:HG23 | 1:C:367:ILE:HG12 | 1.88                     | 0.54              |
| 1:C:615:LEU:HD23 | 1:C:661:LEU:HD12 | 1.89                     | 0.54              |
| 1:D:450:PHE:O    | 1:D:565:THR:HA   | 2.07                     | 0.54              |
| 1:D:461:LEU:O    | 1:D:465:LEU:HB3  | 2.07                     | 0.54              |
| 1:G:450:PHE:HB3  | 1:G:607:PHE:CE2  | 2.42                     | 0.54              |
| 1:I:450:PHE:HB3  | 1:I:607:PHE:CE2  | 2.42                     | 0.54              |
| 1:J:327:VAL:HG23 | 1:J:367:ILE:HG12 | 1.88                     | 0.54              |
| 1:K:327:VAL:HG23 | 1:K:367:ILE:HG12 | 1.88                     | 0.54              |
| 1:L:327:VAL:HG23 | 1:L:367:ILE:HG12 | 1.88                     | 0.54              |
| 1:L:515:ARG:HG2  | 1:L:516:ARG:HH22 | 1.71                     | 0.54              |
| 1:M:361:ALA:O    | 1:M:365:ARG:HG2  | 2.07                     | 0.54              |
| 1:B:327:VAL:HG23 | 1:B:367:ILE:HG12 | 1.88                     | 0.54              |
| 1:C:515:ARG:HG2  | 1:C:516:ARG:HH22 | 1.71                     | 0.54              |
| 1:E:535:ILE:HG23 | 1:E:597:PHE:HD1  | 1.73                     | 0.54              |
| 1:E:615:LEU:HD23 | 1:E:661:LEU:HD12 | 1.89                     | 0.54              |
| 1:H:361:ALA:O    | 1:H:365:ARG:HG2  | 2.07                     | 0.54              |
| 1:I:532:PRO:HB3  | 1:J:491:SER:H    | 1.72                     | 0.54              |
| 1:K:361:ALA:O    | 1:K:365:ARG:HG2  | 2.07                     | 0.54              |
| 1:K:515:ARG:HG2  | 1:K:516:ARG:HH22 | 1.71                     | 0.54              |
| 1:M:481:MET:HE3  | 1:M:527:ILE:HA   | 1.88                     | 0.54              |
| 1:M:515:ARG:HG2  | 1:M:516:ARG:HH22 | 1.71                     | 0.54              |
| 1:N:481:MET:HE3  | 1:N:527:ILE:HA   | 1.88                     | 0.54              |
| 1:N:535:ILE:HG23 | 1:N:597:PHE:HD1  | 1.73                     | 0.54              |
| 1:A:343:LYS:HA   | 1:A:343:LYS:HE3  | 1.89                     | 0.54              |
| 1:B:515:ARG:HG2  | 1:B:516:ARG:HH22 | 1.71                     | 0.54              |
| 1:C:280:VAL:HB   | 1:C:376:VAL:HA   | 1.88                     | 0.54              |
| 1:D:515:ARG:HG2  | 1:D:516:ARG:HH22 | 1.71                     | 0.54              |
| 1:E:461:LEU:O    | 1:E:465:LEU:HB3  | 2.07                     | 0.54              |
| 1:E:481:MET:HE3  | 1:E:527:ILE:HA   | 1.87                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:535:ILE:HG23 | 1:F:597:PHE:HD1  | 1.73                     | 0.54              |
| 1:G:343:LYS:HA   | 1:G:343:LYS:HE3  | 1.88                     | 0.54              |
| 1:H:535:ILE:HG23 | 1:H:597:PHE:HD1  | 1.73                     | 0.54              |
| 1:K:192:ASP:N    | 1:K:192:ASP:OD1  | 2.41                     | 0.54              |
| 1:L:280:VAL:HB   | 1:L:376:VAL:HA   | 1.88                     | 0.54              |
| 1:M:366:LYS:HD2  | 1:M:366:LYS:C    | 2.33                     | 0.54              |
| 1:N:461:LEU:O    | 1:N:465:LEU:HB3  | 2.07                     | 0.54              |
| 1:B:361:ALA:O    | 1:B:365:ARG:HG2  | 2.07                     | 0.54              |
| 1:C:622:MET:HA   | 1:C:625:GLU:HG2  | 1.89                     | 0.54              |
| 1:D:285:GLU:H    | 1:D:285:GLU:CD   | 2.11                     | 0.54              |
| 1:E:361:ALA:O    | 1:E:365:ARG:HG2  | 2.07                     | 0.54              |
| 1:G:535:ILE:HG23 | 1:G:597:PHE:HD1  | 1.73                     | 0.54              |
| 1:H:285:GLU:H    | 1:H:285:GLU:CD   | 2.11                     | 0.54              |
| 1:I:343:LYS:HA   | 1:I:343:LYS:HE3  | 1.89                     | 0.54              |
| 1:I:535:ILE:HG23 | 1:I:597:PHE:HD1  | 1.73                     | 0.54              |
| 1:J:343:LYS:HE3  | 1:J:343:LYS:HA   | 1.89                     | 0.54              |
| 1:L:366:LYS:HD2  | 1:L:366:LYS:C    | 2.33                     | 0.54              |
| 1:M:450:PHE:O    | 1:M:565:THR:HA   | 2.07                     | 0.54              |
| 1:A:327:VAL:HG23 | 1:A:367:ILE:HG12 | 1.88                     | 0.54              |
| 1:B:192:ASP:OD1  | 1:B:192:ASP:N    | 2.41                     | 0.54              |
| 1:C:558:LYS:HE2  | 1:C:558:LYS:HA   | 1.89                     | 0.54              |
| 1:H:489:ALA:O    | 1:N:497:THR:HB   | 2.08                     | 0.54              |
| 1:N:615:LEU:HD23 | 1:N:661:LEU:HD12 | 1.89                     | 0.54              |
| 1:C:366:LYS:HD2  | 1:C:366:LYS:C    | 2.33                     | 0.54              |
| 1:D:366:LYS:HD2  | 1:D:366:LYS:C    | 2.33                     | 0.54              |
| 1:D:403:ILE:HG23 | 1:E:678:LEU:HD22 | 1.88                     | 0.54              |
| 1:D:535:ILE:HG23 | 1:D:597:PHE:HD1  | 1.73                     | 0.54              |
| 1:F:285:GLU:H    | 1:F:285:GLU:CD   | 2.11                     | 0.54              |
| 1:J:251:ASN:OD1  | 1:J:252:GLU:N    | 2.40                     | 0.54              |
| 1:K:366:LYS:HD2  | 1:K:366:LYS:C    | 2.33                     | 0.54              |
| 1:A:251:ASN:OD1  | 1:A:252:GLU:N    | 2.41                     | 0.53              |
| 1:D:622:MET:HA   | 1:D:625:GLU:HG2  | 1.89                     | 0.53              |
| 1:F:251:ASN:OD1  | 1:F:252:GLU:N    | 2.41                     | 0.53              |
| 1:H:251:ASN:OD1  | 1:H:252:GLU:N    | 2.41                     | 0.53              |
| 1:L:558:LYS:HE2  | 1:L:558:LYS:HA   | 1.89                     | 0.53              |
| 1:M:285:GLU:OE1  | 1:M:285:GLU:N    | 2.26                     | 0.53              |
| 1:M:558:LYS:HE2  | 1:M:558:LYS:HA   | 1.89                     | 0.53              |
| 1:N:361:ALA:O    | 1:N:365:ARG:HG2  | 2.07                     | 0.53              |
| 1:B:121:GLY:O    | 1:B:127:LYS:NZ   | 2.34                     | 0.53              |
| 1:B:366:LYS:HD2  | 1:B:366:LYS:C    | 2.33                     | 0.53              |
| 1:D:104:GLU:HA   | 1:E:321:GLN:NE2  | 2.23                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:558:LYS:HE2  | 1:D:558:LYS:HA   | 1.89                     | 0.53              |
| 1:E:487:ARG:NH2  | 1:E:530:ALA:HA   | 2.24                     | 0.53              |
| 1:F:450:PHE:O    | 1:F:565:THR:HA   | 2.07                     | 0.53              |
| 1:F:622:MET:HA   | 1:F:625:GLU:HG2  | 1.89                     | 0.53              |
| 1:H:450:PHE:O    | 1:H:565:THR:HA   | 2.07                     | 0.53              |
| 1:H:622:MET:HA   | 1:H:625:GLU:HG2  | 1.89                     | 0.53              |
| 1:K:121:GLY:O    | 1:K:127:LYS:NZ   | 2.34                     | 0.53              |
| 1:M:535:ILE:HG23 | 1:M:597:PHE:HD1  | 1.73                     | 0.53              |
| 1:M:594:ARG:NH2  | 1:M:596:GLU:OE2  | 2.42                     | 0.53              |
| 1:N:366:LYS:HD2  | 1:N:366:LYS:C    | 2.33                     | 0.53              |
| 1:C:668:GLU:OE1  | 1:C:668:GLU:N    | 2.34                     | 0.53              |
| 1:D:594:ARG:NH2  | 1:D:596:GLU:OE2  | 2.42                     | 0.53              |
| 1:E:366:LYS:HD2  | 1:E:366:LYS:C    | 2.33                     | 0.53              |
| 1:F:487:ARG:NH2  | 1:F:530:ALA:HA   | 2.24                     | 0.53              |
| 1:L:487:ARG:NH2  | 1:L:530:ALA:HA   | 2.24                     | 0.53              |
| 1:L:622:MET:HA   | 1:L:625:GLU:HG2  | 1.89                     | 0.53              |
| 1:M:487:ARG:NH2  | 1:M:530:ALA:HA   | 2.24                     | 0.53              |
| 1:N:487:ARG:NH2  | 1:N:530:ALA:HA   | 2.24                     | 0.53              |
| 1:B:615:LEU:O    | 1:B:619:VAL:HG23 | 2.09                     | 0.53              |
| 1:D:487:ARG:NH2  | 1:D:530:ALA:HA   | 2.24                     | 0.53              |
| 1:H:487:ARG:NH2  | 1:H:530:ALA:HA   | 2.24                     | 0.53              |
| 1:J:487:ARG:NH2  | 1:J:530:ALA:HA   | 2.24                     | 0.53              |
| 1:L:615:LEU:O    | 1:L:619:VAL:HG23 | 2.09                     | 0.53              |
| 1:L:668:GLU:OE1  | 1:L:668:GLU:N    | 2.34                     | 0.53              |
| 1:N:478:ARG:HG3  | 1:N:523:LEU:CB   | 2.37                     | 0.53              |
| 1:A:487:ARG:NH2  | 1:A:530:ALA:HA   | 2.24                     | 0.53              |
| 1:B:487:ARG:NH2  | 1:B:530:ALA:HA   | 2.24                     | 0.53              |
| 1:B:535:ILE:HG23 | 1:B:597:PHE:HD1  | 1.73                     | 0.53              |
| 1:C:487:ARG:NH2  | 1:C:530:ALA:HA   | 2.24                     | 0.53              |
| 1:C:615:LEU:O    | 1:C:619:VAL:HG23 | 2.09                     | 0.53              |
| 1:E:622:MET:HA   | 1:E:625:GLU:HG2  | 1.89                     | 0.53              |
| 1:G:487:ARG:NH2  | 1:G:530:ALA:HA   | 2.24                     | 0.53              |
| 1:G:615:LEU:HD23 | 1:G:661:LEU:HD12 | 1.89                     | 0.53              |
| 1:I:210:LYS:NZ   | 1:I:214:ASP:OD2  | 2.36                     | 0.53              |
| 1:I:487:ARG:NH2  | 1:I:530:ALA:HA   | 2.24                     | 0.53              |
| 1:I:615:LEU:HD23 | 1:I:661:LEU:HD12 | 1.89                     | 0.53              |
| 1:K:535:ILE:HG23 | 1:K:597:PHE:HD1  | 1.73                     | 0.53              |
| 1:M:622:MET:HA   | 1:M:625:GLU:HG2  | 1.89                     | 0.53              |
| 1:A:285:GLU:OE1  | 1:A:285:GLU:N    | 2.26                     | 0.53              |
| 1:A:615:LEU:HD23 | 1:A:661:LEU:HD12 | 1.89                     | 0.53              |
| 1:B:538:LEU:O    | 1:B:542:LEU:HG   | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:594:ARG:NH2  | 1:C:596:GLU:OE2  | 2.42                     | 0.53              |
| 1:G:210:LYS:NZ   | 1:G:214:ASP:OD2  | 2.36                     | 0.53              |
| 1:K:487:ARG:NH2  | 1:K:530:ALA:HA   | 2.24                     | 0.53              |
| 1:K:538:LEU:O    | 1:K:542:LEU:HG   | 2.09                     | 0.53              |
| 1:K:615:LEU:O    | 1:K:619:VAL:HG23 | 2.09                     | 0.53              |
| 1:L:594:ARG:NH2  | 1:L:596:GLU:OE2  | 2.42                     | 0.53              |
| 1:M:615:LEU:O    | 1:M:619:VAL:HG23 | 2.09                     | 0.53              |
| 1:N:622:MET:HA   | 1:N:625:GLU:HG2  | 1.89                     | 0.53              |
| 1:A:366:LYS:HD2  | 1:A:366:LYS:C    | 2.33                     | 0.53              |
| 1:A:538:LEU:O    | 1:A:542:LEU:HG   | 2.09                     | 0.53              |
| 1:A:622:MET:HA   | 1:A:625:GLU:HG2  | 1.89                     | 0.53              |
| 1:B:429:ARG:HD3  | 1:C:671:ASP:CG   | 2.34                     | 0.53              |
| 1:G:485:SER:OG   | 1:G:530:ALA:HB1  | 2.09                     | 0.53              |
| 1:I:485:SER:OG   | 1:I:530:ALA:HB1  | 2.09                     | 0.53              |
| 1:J:366:LYS:C    | 1:J:366:LYS:HD2  | 2.33                     | 0.53              |
| 1:J:538:LEU:O    | 1:J:542:LEU:HG   | 2.09                     | 0.53              |
| 1:J:622:MET:HA   | 1:J:625:GLU:HG2  | 1.89                     | 0.53              |
| 1:A:485:SER:OG   | 1:A:530:ALA:HB1  | 2.09                     | 0.53              |
| 1:B:622:MET:HA   | 1:B:625:GLU:HG2  | 1.89                     | 0.53              |
| 1:E:478:ARG:HG3  | 1:E:523:LEU:CB   | 2.37                     | 0.53              |
| 1:F:366:LYS:HD2  | 1:F:366:LYS:C    | 2.33                     | 0.53              |
| 1:G:594:ARG:NH2  | 1:G:596:GLU:OE2  | 2.42                     | 0.53              |
| 1:H:615:LEU:O    | 1:H:619:VAL:HG23 | 2.09                     | 0.53              |
| 1:I:501:VAL:HB   | 1:J:491:SER:C    | 2.33                     | 0.53              |
| 1:J:615:LEU:HD23 | 1:J:661:LEU:HD12 | 1.89                     | 0.53              |
| 1:J:645:ASP:O    | 1:J:648:THR:OG1  | 2.27                     | 0.53              |
| 1:K:594:ARG:NH2  | 1:K:596:GLU:OE2  | 2.42                     | 0.53              |
| 1:K:615:LEU:HD23 | 1:K:661:LEU:HD12 | 1.89                     | 0.53              |
| 1:L:538:LEU:O    | 1:L:542:LEU:HG   | 2.09                     | 0.53              |
| 1:N:192:ASP:OD1  | 1:N:192:ASP:N    | 2.41                     | 0.53              |
| 1:A:594:ARG:NH2  | 1:A:596:GLU:OE2  | 2.42                     | 0.53              |
| 1:B:285:GLU:OE1  | 1:B:285:GLU:N    | 2.26                     | 0.53              |
| 1:D:615:LEU:O    | 1:D:619:VAL:HG23 | 2.09                     | 0.53              |
| 1:F:594:ARG:NH2  | 1:F:596:GLU:OE2  | 2.42                     | 0.53              |
| 1:F:615:LEU:O    | 1:F:619:VAL:HG23 | 2.09                     | 0.53              |
| 1:G:606:GLU:OE1  | 1:G:606:GLU:N    | 2.42                     | 0.53              |
| 1:G:615:LEU:O    | 1:G:619:VAL:HG23 | 2.09                     | 0.53              |
| 1:H:366:LYS:HD2  | 1:H:366:LYS:C    | 2.33                     | 0.53              |
| 1:H:538:LEU:O    | 1:H:542:LEU:HG   | 2.09                     | 0.53              |
| 1:I:594:ARG:NH2  | 1:I:596:GLU:OE2  | 2.42                     | 0.53              |
| 1:I:606:GLU:N    | 1:I:606:GLU:OE1  | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:615:LEU:O    | 1:I:619:VAL:HG23 | 2.09                     | 0.53              |
| 1:J:594:ARG:NH2  | 1:J:596:GLU:OE2  | 2.42                     | 0.53              |
| 1:N:594:ARG:NH2  | 1:N:596:GLU:OE2  | 2.42                     | 0.53              |
| 1:A:321:GLN:NE2  | 1:G:104:GLU:HA   | 2.24                     | 0.53              |
| 1:C:538:LEU:O    | 1:C:542:LEU:HG   | 2.09                     | 0.53              |
| 1:F:538:LEU:O    | 1:F:542:LEU:HG   | 2.09                     | 0.53              |
| 1:G:251:ASN:OD1  | 1:G:252:GLU:N    | 2.41                     | 0.53              |
| 1:H:594:ARG:NH2  | 1:H:596:GLU:OE2  | 2.42                     | 0.53              |
| 1:I:366:LYS:HD2  | 1:I:366:LYS:C    | 2.33                     | 0.53              |
| 1:J:285:GLU:OE1  | 1:J:285:GLU:N    | 2.26                     | 0.53              |
| 1:J:485:SER:OG   | 1:J:530:ALA:HB1  | 2.09                     | 0.53              |
| 1:K:622:MET:HA   | 1:K:625:GLU:HG2  | 1.89                     | 0.53              |
| 1:K:681:LEU:HD21 | 1:K:686:LEU:HD11 | 1.91                     | 0.53              |
| 1:L:192:ASP:OD1  | 1:L:192:ASP:N    | 2.41                     | 0.53              |
| 1:L:536:THR:HG21 | 1:M:483:GLU:HG3  | 1.91                     | 0.53              |
| 1:M:606:GLU:OE1  | 1:M:606:GLU:N    | 2.42                     | 0.53              |
| 1:A:274:TYR:HE1  | 1:G:112:ARG:HD2  | 1.74                     | 0.52              |
| 1:A:515:ARG:HG2  | 1:A:516:ARG:NH2  | 2.24                     | 0.52              |
| 1:A:532:PRO:HA   | 1:B:490:VAL:HB   | 1.90                     | 0.52              |
| 1:B:594:ARG:NH2  | 1:B:596:GLU:OE2  | 2.42                     | 0.52              |
| 1:B:615:LEU:HD23 | 1:B:661:LEU:HD12 | 1.89                     | 0.52              |
| 1:B:681:LEU:HD21 | 1:B:686:LEU:HD11 | 1.91                     | 0.52              |
| 1:D:478:ARG:HG3  | 1:D:523:LEU:CB   | 2.36                     | 0.52              |
| 1:E:594:ARG:NH2  | 1:E:596:GLU:OE2  | 2.42                     | 0.52              |
| 1:G:459:THR:OG1  | 1:G:463:LYS:NZ   | 2.41                     | 0.52              |
| 1:G:515:ARG:HG2  | 1:G:516:ARG:NH2  | 2.24                     | 0.52              |
| 1:G:538:LEU:O    | 1:G:542:LEU:HG   | 2.09                     | 0.52              |
| 1:H:485:SER:OG   | 1:H:530:ALA:HB1  | 2.09                     | 0.52              |
| 1:I:515:ARG:HG2  | 1:I:516:ARG:NH2  | 2.24                     | 0.52              |
| 1:L:535:ILE:HG23 | 1:L:597:PHE:HD1  | 1.73                     | 0.52              |
| 1:M:485:SER:OG   | 1:M:530:ALA:HB1  | 2.09                     | 0.52              |
| 1:B:485:SER:OG   | 1:B:530:ALA:HB1  | 2.09                     | 0.52              |
| 1:C:528:GLU:N    | 1:C:529:LYS:HB2  | 2.24                     | 0.52              |
| 1:C:583:PRO:HA   | 1:C:586:MET:HG2  | 1.91                     | 0.52              |
| 1:C:681:LEU:HD21 | 1:C:686:LEU:HD11 | 1.91                     | 0.52              |
| 1:D:485:SER:OG   | 1:D:530:ALA:HB1  | 2.09                     | 0.52              |
| 1:D:538:LEU:O    | 1:D:542:LEU:HG   | 2.09                     | 0.52              |
| 1:D:606:GLU:N    | 1:D:606:GLU:OE1  | 2.42                     | 0.52              |
| 1:E:485:SER:OG   | 1:E:530:ALA:HB1  | 2.09                     | 0.52              |
| 1:E:515:ARG:HG2  | 1:E:516:ARG:NH2  | 2.24                     | 0.52              |
| 1:F:485:SER:OG   | 1:F:530:ALA:HB1  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:212:LEU:O    | 1:G:216:LEU:N    | 2.33                     | 0.52              |
| 1:G:366:LYS:HD2  | 1:G:366:LYS:C    | 2.33                     | 0.52              |
| 1:G:528:GLU:N    | 1:G:529:LYS:HB2  | 2.24                     | 0.52              |
| 1:G:622:MET:HA   | 1:G:625:GLU:HG2  | 1.89                     | 0.52              |
| 1:H:111:ARG:HB3  | 1:I:312:ASP:OD2  | 2.09                     | 0.52              |
| 1:I:251:ASN:OD1  | 1:I:252:GLU:N    | 2.41                     | 0.52              |
| 1:I:528:GLU:N    | 1:I:529:LYS:HB2  | 2.24                     | 0.52              |
| 1:I:538:LEU:O    | 1:I:542:LEU:HG   | 2.09                     | 0.52              |
| 1:I:612:LYS:O    | 1:I:652:TYR:OH   | 2.17                     | 0.52              |
| 1:I:622:MET:HA   | 1:I:625:GLU:HG2  | 1.89                     | 0.52              |
| 1:K:285:GLU:OE1  | 1:K:285:GLU:N    | 2.26                     | 0.52              |
| 1:L:681:LEU:HD21 | 1:L:686:LEU:HD11 | 1.91                     | 0.52              |
| 1:A:536:THR:HG21 | 1:B:483:GLU:HG3  | 1.92                     | 0.52              |
| 1:A:681:LEU:HD21 | 1:A:686:LEU:HD11 | 1.91                     | 0.52              |
| 1:B:583:PRO:HA   | 1:B:586:MET:HG2  | 1.91                     | 0.52              |
| 1:C:192:ASP:N    | 1:C:192:ASP:OD1  | 2.41                     | 0.52              |
| 1:C:409:MET:HA   | 1:C:412:ARG:HB2  | 1.91                     | 0.52              |
| 1:D:534:VAL:HG22 | 1:E:492:LYS:CB   | 2.30                     | 0.52              |
| 1:E:536:THR:HG21 | 1:F:483:GLU:HG3  | 1.90                     | 0.52              |
| 1:H:112:ARG:HD2  | 1:I:274:TYR:CE1  | 2.44                     | 0.52              |
| 1:I:212:LEU:O    | 1:I:216:LEU:N    | 2.33                     | 0.52              |
| 1:J:515:ARG:HG2  | 1:J:516:ARG:NH2  | 2.24                     | 0.52              |
| 1:J:681:LEU:HD21 | 1:J:686:LEU:HD11 | 1.91                     | 0.52              |
| 1:K:485:SER:OG   | 1:K:530:ALA:HB1  | 2.09                     | 0.52              |
| 1:L:409:MET:HA   | 1:L:412:ARG:HB2  | 1.91                     | 0.52              |
| 1:L:528:GLU:N    | 1:L:529:LYS:HB2  | 2.24                     | 0.52              |
| 1:M:527:ILE:HD13 | 1:M:564:ALA:HB1  | 1.91                     | 0.52              |
| 1:M:538:LEU:O    | 1:M:542:LEU:HG   | 2.09                     | 0.52              |
| 1:N:485:SER:OG   | 1:N:530:ALA:HB1  | 2.09                     | 0.52              |
| 1:N:515:ARG:HG2  | 1:N:516:ARG:NH2  | 2.24                     | 0.52              |
| 1:N:615:LEU:O    | 1:N:619:VAL:HG23 | 2.09                     | 0.52              |
| 1:C:535:ILE:HG23 | 1:C:597:PHE:HD1  | 1.73                     | 0.52              |
| 1:D:409:MET:HA   | 1:D:412:ARG:HB2  | 1.91                     | 0.52              |
| 1:D:515:ARG:HG2  | 1:D:516:ARG:NH2  | 2.24                     | 0.52              |
| 1:E:606:GLU:OE1  | 1:E:606:GLU:N    | 2.42                     | 0.52              |
| 1:F:583:PRO:HA   | 1:F:586:MET:HG2  | 1.91                     | 0.52              |
| 1:F:606:GLU:OE1  | 1:F:606:GLU:N    | 2.42                     | 0.52              |
| 1:F:615:LEU:HD23 | 1:F:661:LEU:HD12 | 1.89                     | 0.52              |
| 1:H:583:PRO:HA   | 1:H:586:MET:HG2  | 1.91                     | 0.52              |
| 1:H:606:GLU:OE1  | 1:H:606:GLU:N    | 2.42                     | 0.52              |
| 1:H:615:LEU:HD23 | 1:H:661:LEU:HD12 | 1.89                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:802:AGS:O3G  | 3:I:802:AGS:O1A  | 2.27                     | 0.52              |
| 1:J:606:GLU:OE1  | 1:J:606:GLU:N    | 2.42                     | 0.52              |
| 1:K:497:THR:HB   | 1:L:489:ALA:O    | 2.09                     | 0.52              |
| 1:K:583:PRO:HA   | 1:K:586:MET:HG2  | 1.91                     | 0.52              |
| 1:K:596:GLU:HG2  | 1:K:597:PHE:N    | 2.25                     | 0.52              |
| 1:L:583:PRO:HA   | 1:L:586:MET:HG2  | 1.91                     | 0.52              |
| 1:M:409:MET:HA   | 1:M:412:ARG:HB2  | 1.91                     | 0.52              |
| 1:M:478:ARG:HG3  | 1:M:523:LEU:CB   | 2.37                     | 0.52              |
| 1:M:515:ARG:HG2  | 1:M:516:ARG:NH2  | 2.24                     | 0.52              |
| 1:N:527:ILE:HD13 | 1:N:564:ALA:HB1  | 1.91                     | 0.52              |
| 1:A:606:GLU:N    | 1:A:606:GLU:OE1  | 2.42                     | 0.52              |
| 1:B:596:GLU:HG2  | 1:B:597:PHE:N    | 2.25                     | 0.52              |
| 1:C:515:ARG:HG2  | 1:C:516:ARG:NH2  | 2.24                     | 0.52              |
| 1:D:527:ILE:HD13 | 1:D:564:ALA:HB1  | 1.91                     | 0.52              |
| 1:G:612:LYS:O    | 1:G:652:TYR:OH   | 2.17                     | 0.52              |
| 1:G:681:LEU:HD21 | 1:G:686:LEU:HD11 | 1.91                     | 0.52              |
| 3:G:802:AGS:O1A  | 3:G:802:AGS:O3G  | 2.27                     | 0.52              |
| 1:H:528:GLU:N    | 1:H:529:LYS:HB2  | 2.24                     | 0.52              |
| 1:H:681:LEU:HD21 | 1:H:686:LEU:HD11 | 1.91                     | 0.52              |
| 1:I:681:LEU:HD21 | 1:I:686:LEU:HD11 | 1.91                     | 0.52              |
| 1:J:528:GLU:N    | 1:J:529:LYS:HB2  | 2.24                     | 0.52              |
| 3:M:802:AGS:O3G  | 3:M:802:AGS:O1A  | 2.27                     | 0.52              |
| 1:A:528:GLU:N    | 1:A:529:LYS:HB2  | 2.24                     | 0.52              |
| 1:A:583:PRO:HA   | 1:A:586:MET:HG2  | 1.91                     | 0.52              |
| 1:D:681:LEU:HD21 | 1:D:686:LEU:HD11 | 1.91                     | 0.52              |
| 3:D:802:AGS:O1A  | 3:D:802:AGS:O3G  | 2.27                     | 0.52              |
| 1:E:615:LEU:O    | 1:E:619:VAL:HG23 | 2.09                     | 0.52              |
| 1:F:528:GLU:N    | 1:F:529:LYS:HB2  | 2.24                     | 0.52              |
| 1:J:583:PRO:HA   | 1:J:586:MET:HG2  | 1.91                     | 0.52              |
| 1:J:596:GLU:HG2  | 1:J:597:PHE:N    | 2.25                     | 0.52              |
| 3:J:802:AGS:O3G  | 3:J:802:AGS:O1A  | 2.27                     | 0.52              |
| 1:M:406:LEU:HA   | 1:M:409:MET:HE3  | 1.92                     | 0.52              |
| 1:N:606:GLU:OE1  | 1:N:606:GLU:N    | 2.42                     | 0.52              |
| 1:A:535:ILE:HG23 | 1:A:597:PHE:HD1  | 1.73                     | 0.52              |
| 3:A:802:AGS:O3G  | 3:A:802:AGS:O1A  | 2.27                     | 0.52              |
| 1:C:501:VAL:HB   | 1:D:491:SER:C    | 2.35                     | 0.52              |
| 3:C:802:AGS:O3G  | 3:C:802:AGS:O1A  | 2.27                     | 0.52              |
| 1:F:515:ARG:HG2  | 1:F:516:ARG:NH2  | 2.24                     | 0.52              |
| 1:I:463:LYS:HG3  | 1:I:464:GLN:HG2  | 1.92                     | 0.52              |
| 1:J:112:ARG:HD2  | 1:K:274:TYR:CE1  | 2.45                     | 0.52              |
| 1:K:606:GLU:OE1  | 1:K:606:GLU:N    | 2.42                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:463:LYS:HG3  | 1:L:464:GLN:HG2  | 1.92                     | 0.52              |
| 1:L:515:ARG:HG2  | 1:L:516:ARG:NH2  | 2.24                     | 0.52              |
| 3:L:802:AGS:O1A  | 3:L:802:AGS:O3G  | 2.27                     | 0.52              |
| 1:B:350:PHE:HB3  | 1:N:350:PHE:HB3  | 1.91                     | 0.52              |
| 1:B:606:GLU:OE1  | 1:B:606:GLU:N    | 2.42                     | 0.52              |
| 1:D:98:ARG:NH2   | 1:D:125:VAL:O    | 2.43                     | 0.52              |
| 1:D:463:LYS:HG3  | 1:D:464:GLN:HG2  | 1.92                     | 0.52              |
| 1:E:213:ALA:O    | 1:E:217:LYS:HG3  | 2.10                     | 0.52              |
| 1:E:527:ILE:HD13 | 1:E:564:ALA:HB1  | 1.91                     | 0.52              |
| 1:E:538:LEU:O    | 1:E:542:LEU:HG   | 2.09                     | 0.52              |
| 1:F:112:ARG:HD2  | 1:G:274:TYR:CE1  | 2.45                     | 0.52              |
| 1:F:681:LEU:HD21 | 1:F:686:LEU:HD11 | 1.91                     | 0.52              |
| 1:G:645:ASP:O    | 1:G:648:THR:OG1  | 2.27                     | 0.52              |
| 1:H:515:ARG:HG2  | 1:H:516:ARG:NH2  | 2.24                     | 0.52              |
| 1:H:527:ILE:HD13 | 1:H:564:ALA:HB1  | 1.91                     | 0.52              |
| 1:L:527:ILE:HD13 | 1:L:564:ALA:HB1  | 1.91                     | 0.52              |
| 1:M:463:LYS:HG3  | 1:M:464:GLN:HG2  | 1.92                     | 0.52              |
| 1:M:681:LEU:HD21 | 1:M:686:LEU:HD11 | 1.91                     | 0.52              |
| 1:N:213:ALA:O    | 1:N:217:LYS:HG3  | 2.10                     | 0.52              |
| 1:A:596:GLU:HG2  | 1:A:597:PHE:N    | 2.25                     | 0.52              |
| 1:A:615:LEU:O    | 1:A:619:VAL:HG23 | 2.09                     | 0.52              |
| 1:C:98:ARG:NH2   | 1:C:125:VAL:O    | 2.43                     | 0.52              |
| 1:C:463:LYS:HG3  | 1:C:464:GLN:HG2  | 1.92                     | 0.52              |
| 1:C:606:GLU:OE1  | 1:C:606:GLU:N    | 2.42                     | 0.52              |
| 1:D:406:LEU:HA   | 1:D:409:MET:HE3  | 1.92                     | 0.52              |
| 3:E:802:AGS:O3G  | 3:E:802:AGS:O1A  | 2.28                     | 0.52              |
| 1:F:463:LYS:HG3  | 1:F:464:GLN:HG2  | 1.92                     | 0.52              |
| 1:F:527:ILE:HD13 | 1:F:564:ALA:HB1  | 1.91                     | 0.52              |
| 1:G:463:LYS:HG3  | 1:G:464:GLN:HG2  | 1.92                     | 0.52              |
| 1:H:463:LYS:HG3  | 1:H:464:GLN:HG2  | 1.92                     | 0.52              |
| 1:I:645:ASP:O    | 1:I:648:THR:OG1  | 2.27                     | 0.52              |
| 1:J:535:ILE:HG23 | 1:J:597:PHE:HD1  | 1.73                     | 0.52              |
| 1:J:615:LEU:O    | 1:J:619:VAL:HG23 | 2.09                     | 0.52              |
| 1:K:515:ARG:HG2  | 1:K:516:ARG:NH2  | 2.24                     | 0.52              |
| 1:M:528:GLU:N    | 1:M:529:LYS:HB2  | 2.24                     | 0.52              |
| 1:M:596:GLU:HG2  | 1:M:597:PHE:N    | 2.25                     | 0.52              |
| 1:N:528:GLU:N    | 1:N:529:LYS:HB2  | 2.24                     | 0.52              |
| 1:N:538:LEU:O    | 1:N:542:LEU:HG   | 2.09                     | 0.52              |
| 1:N:583:PRO:HA   | 1:N:586:MET:HG2  | 1.91                     | 0.52              |
| 1:A:463:LYS:HG3  | 1:A:464:GLN:HG2  | 1.92                     | 0.52              |
| 1:C:485:SER:OG   | 1:C:530:ALA:HB1  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:527:ILE:HD13 | 1:C:564:ALA:HB1  | 1.91                     | 0.52              |
| 1:E:528:GLU:N    | 1:E:529:LYS:HB2  | 2.24                     | 0.52              |
| 1:E:583:PRO:HA   | 1:E:586:MET:HG2  | 1.91                     | 0.52              |
| 1:F:213:ALA:O    | 1:F:217:LYS:HG3  | 2.10                     | 0.52              |
| 1:L:98:ARG:NH2   | 1:L:125:VAL:O    | 2.43                     | 0.52              |
| 1:L:485:SER:OG   | 1:L:530:ALA:HB1  | 2.09                     | 0.52              |
| 1:M:98:ARG:NH2   | 1:M:125:VAL:O    | 2.43                     | 0.52              |
| 1:N:406:LEU:HA   | 1:N:409:MET:HE3  | 1.92                     | 0.52              |
| 1:N:409:MET:HA   | 1:N:412:ARG:HB2  | 1.91                     | 0.52              |
| 3:N:802:AGS:O3G  | 3:N:802:AGS:O1A  | 2.27                     | 0.52              |
| 1:B:515:ARG:HG2  | 1:B:516:ARG:NH2  | 2.24                     | 0.51              |
| 3:B:803:AGS:O1B  | 3:B:803:AGS:O2G  | 2.29                     | 0.51              |
| 1:C:406:LEU:HA   | 1:C:409:MET:HE3  | 1.92                     | 0.51              |
| 1:C:596:GLU:HG2  | 1:C:597:PHE:N    | 2.25                     | 0.51              |
| 1:E:98:ARG:NH2   | 1:E:125:VAL:O    | 2.43                     | 0.51              |
| 1:E:406:LEU:HA   | 1:E:409:MET:HE3  | 1.92                     | 0.51              |
| 1:E:409:MET:HA   | 1:E:412:ARG:HB2  | 1.91                     | 0.51              |
| 1:G:583:PRO:HA   | 1:G:586:MET:HG2  | 1.91                     | 0.51              |
| 3:H:802:AGS:O3G  | 3:H:802:AGS:O1A  | 2.27                     | 0.51              |
| 1:I:406:LEU:HA   | 1:I:409:MET:HE3  | 1.92                     | 0.51              |
| 1:I:532:PRO:HA   | 1:J:490:VAL:HB   | 1.91                     | 0.51              |
| 1:I:583:PRO:HA   | 1:I:586:MET:HG2  | 1.91                     | 0.51              |
| 1:J:463:LYS:HG3  | 1:J:464:GLN:HG2  | 1.92                     | 0.51              |
| 1:L:606:GLU:N    | 1:L:606:GLU:OE1  | 2.42                     | 0.51              |
| 1:N:98:ARG:NH2   | 1:N:125:VAL:O    | 2.43                     | 0.51              |
| 1:A:406:LEU:HA   | 1:A:409:MET:HE3  | 1.92                     | 0.51              |
| 1:D:583:PRO:HA   | 1:D:586:MET:HG2  | 1.91                     | 0.51              |
| 1:E:681:LEU:HD21 | 1:E:686:LEU:HD11 | 1.91                     | 0.51              |
| 3:F:802:AGS:O3G  | 3:F:802:AGS:O1A  | 2.27                     | 0.51              |
| 1:G:192:ASP:OD1  | 1:G:192:ASP:N    | 2.41                     | 0.51              |
| 1:G:406:LEU:HA   | 1:G:409:MET:HE3  | 1.92                     | 0.51              |
| 1:G:527:ILE:HD13 | 1:G:564:ALA:HB1  | 1.91                     | 0.51              |
| 1:H:213:ALA:O    | 1:H:217:LYS:HG3  | 2.10                     | 0.51              |
| 1:I:527:ILE:HD13 | 1:I:564:ALA:HB1  | 1.91                     | 0.51              |
| 1:K:409:MET:HA   | 1:K:412:ARG:HB2  | 1.91                     | 0.51              |
| 1:K:528:GLU:N    | 1:K:529:LYS:HB2  | 2.24                     | 0.51              |
| 3:K:803:AGS:O1B  | 3:K:803:AGS:O2G  | 2.29                     | 0.51              |
| 1:L:406:LEU:HA   | 1:L:409:MET:HE3  | 1.92                     | 0.51              |
| 1:B:362:GLU:CD   | 1:B:365:ARG:HH12 | 2.19                     | 0.51              |
| 1:B:528:GLU:N    | 1:B:529:LYS:HB2  | 2.24                     | 0.51              |
| 1:C:213:ALA:O    | 1:C:217:LYS:HG3  | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:803:AGS:O1B  | 3:C:803:AGS:O2G  | 2.29                     | 0.51              |
| 1:D:528:GLU:N    | 1:D:529:LYS:HB2  | 2.24                     | 0.51              |
| 1:E:463:LYS:HG3  | 1:E:464:GLN:HG2  | 1.92                     | 0.51              |
| 1:E:596:GLU:HG2  | 1:E:597:PHE:N    | 2.25                     | 0.51              |
| 1:J:406:LEU:HA   | 1:J:409:MET:HE3  | 1.92                     | 0.51              |
| 1:K:213:ALA:O    | 1:K:217:LYS:HG3  | 2.10                     | 0.51              |
| 1:K:463:LYS:HG3  | 1:K:464:GLN:HG2  | 1.92                     | 0.51              |
| 1:K:527:ILE:HD13 | 1:K:564:ALA:HB1  | 1.91                     | 0.51              |
| 1:L:213:ALA:O    | 1:L:217:LYS:HG3  | 2.10                     | 0.51              |
| 3:L:803:AGS:O1B  | 3:L:803:AGS:O2G  | 2.29                     | 0.51              |
| 1:M:192:ASP:OD1  | 1:M:192:ASP:N    | 2.41                     | 0.51              |
| 1:B:409:MET:HA   | 1:B:412:ARG:HB2  | 1.91                     | 0.51              |
| 1:B:463:LYS:HG3  | 1:B:464:GLN:HG2  | 1.92                     | 0.51              |
| 1:C:103:GLN:NE2  | 1:D:321:GLN:OE1  | 2.39                     | 0.51              |
| 1:D:213:ALA:O    | 1:D:217:LYS:HG3  | 2.10                     | 0.51              |
| 1:E:452:GLY:HA3  | 1:E:607:PHE:HB2  | 1.92                     | 0.51              |
| 1:F:210:LYS:NZ   | 1:F:214:ASP:OD2  | 2.36                     | 0.51              |
| 1:F:212:LEU:O    | 1:F:216:LEU:N    | 2.33                     | 0.51              |
| 1:F:452:GLY:HA3  | 1:F:607:PHE:HB2  | 1.92                     | 0.51              |
| 1:G:409:MET:HA   | 1:G:412:ARG:HB2  | 1.91                     | 0.51              |
| 1:H:212:LEU:O    | 1:H:216:LEU:N    | 2.33                     | 0.51              |
| 1:H:452:GLY:HA3  | 1:H:607:PHE:HB2  | 1.92                     | 0.51              |
| 1:I:192:ASP:OD1  | 1:I:192:ASP:N    | 2.41                     | 0.51              |
| 1:J:527:ILE:HD13 | 1:J:564:ALA:HB1  | 1.91                     | 0.51              |
| 1:K:362:GLU:CD   | 1:K:365:ARG:HH12 | 2.19                     | 0.51              |
| 3:K:802:AGS:O3G  | 3:K:802:AGS:O1A  | 2.27                     | 0.51              |
| 1:N:452:GLY:HA3  | 1:N:607:PHE:HB2  | 1.92                     | 0.51              |
| 1:N:463:LYS:HG3  | 1:N:464:GLN:HG2  | 1.92                     | 0.51              |
| 1:A:527:ILE:HD13 | 1:A:564:ALA:HB1  | 1.91                     | 0.51              |
| 1:B:213:ALA:O    | 1:B:217:LYS:HG3  | 2.10                     | 0.51              |
| 3:B:802:AGS:O3G  | 3:B:802:AGS:O1A  | 2.27                     | 0.51              |
| 1:D:111:ARG:HB3  | 1:E:312:ASP:OD2  | 2.11                     | 0.51              |
| 1:D:362:GLU:CD   | 1:D:365:ARG:HH12 | 2.19                     | 0.51              |
| 1:G:596:GLU:HG2  | 1:G:597:PHE:N    | 2.25                     | 0.51              |
| 1:I:409:MET:HA   | 1:I:412:ARG:HB2  | 1.91                     | 0.51              |
| 1:I:596:GLU:HG2  | 1:I:597:PHE:N    | 2.25                     | 0.51              |
| 1:L:596:GLU:HG2  | 1:L:597:PHE:N    | 2.25                     | 0.51              |
| 1:M:213:ALA:O    | 1:M:217:LYS:HG3  | 2.10                     | 0.51              |
| 1:M:459:THR:OG1  | 1:M:463:LYS:NZ   | 2.41                     | 0.51              |
| 1:M:583:PRO:HA   | 1:M:586:MET:HG2  | 1.91                     | 0.51              |
| 1:N:108:ILE:HA   | 1:N:111:ARG:CZ   | 2.41                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:596:GLU:HG2  | 1:N:597:PHE:N    | 2.25                     | 0.51              |
| 1:N:681:LEU:HD21 | 1:N:686:LEU:HD11 | 1.91                     | 0.51              |
| 1:B:452:GLY:HA3  | 1:B:607:PHE:HB2  | 1.92                     | 0.51              |
| 1:B:527:ILE:HD13 | 1:B:564:ALA:HB1  | 1.91                     | 0.51              |
| 1:C:108:ILE:HA   | 1:C:111:ARG:CZ   | 2.41                     | 0.51              |
| 1:C:645:ASP:O    | 1:C:648:THR:OG1  | 2.27                     | 0.51              |
| 1:E:108:ILE:HA   | 1:E:111:ARG:CZ   | 2.41                     | 0.51              |
| 1:F:365:ARG:HG3  | 1:F:365:ARG:NH1  | 2.09                     | 0.51              |
| 1:H:210:LYS:NZ   | 1:H:214:ASP:OD2  | 2.36                     | 0.51              |
| 1:H:365:ARG:HG3  | 1:H:365:ARG:NH1  | 2.09                     | 0.51              |
| 1:I:112:ARG:HD2  | 1:J:274:TYR:HE1  | 1.76                     | 0.51              |
| 1:N:362:GLU:CD   | 1:N:365:ARG:HH12 | 2.19                     | 0.51              |
| 1:D:596:GLU:HG2  | 1:D:597:PHE:N    | 2.25                     | 0.51              |
| 1:E:362:GLU:CD   | 1:E:365:ARG:HH12 | 2.19                     | 0.51              |
| 1:F:596:GLU:HG2  | 1:F:597:PHE:N    | 2.25                     | 0.51              |
| 1:H:596:GLU:HG2  | 1:H:597:PHE:N    | 2.25                     | 0.51              |
| 1:A:409:MET:HA   | 1:A:412:ARG:HB2  | 1.91                     | 0.51              |
| 1:B:406:LEU:HA   | 1:B:409:MET:HE3  | 1.92                     | 0.51              |
| 1:D:402:ASP:OD1  | 1:D:402:ASP:N    | 2.44                     | 0.51              |
| 1:G:98:ARG:NH2   | 1:G:125:VAL:O    | 2.43                     | 0.51              |
| 1:G:213:ALA:O    | 1:G:217:LYS:HG3  | 2.10                     | 0.51              |
| 1:G:362:GLU:CD   | 1:G:365:ARG:HH12 | 2.19                     | 0.51              |
| 1:I:213:ALA:O    | 1:I:217:LYS:HG3  | 2.10                     | 0.51              |
| 1:I:362:GLU:CD   | 1:I:365:ARG:HH12 | 2.19                     | 0.51              |
| 1:K:98:ARG:NH2   | 1:K:125:VAL:O    | 2.43                     | 0.51              |
| 1:K:452:GLY:HA3  | 1:K:607:PHE:HB2  | 1.92                     | 0.51              |
| 1:L:108:ILE:HA   | 1:L:111:ARG:CZ   | 2.41                     | 0.51              |
| 1:M:362:GLU:CD   | 1:M:365:ARG:HH12 | 2.19                     | 0.51              |
| 3:A:803:AGS:O1B  | 3:A:803:AGS:O2G  | 2.29                     | 0.51              |
| 1:D:459:THR:OG1  | 1:D:463:LYS:NZ   | 2.41                     | 0.51              |
| 1:E:402:ASP:N    | 1:E:402:ASP:OD1  | 2.44                     | 0.51              |
| 1:F:98:ARG:NH2   | 1:F:125:VAL:O    | 2.43                     | 0.51              |
| 1:F:362:GLU:CD   | 1:F:365:ARG:HH12 | 2.19                     | 0.51              |
| 1:H:98:ARG:NH2   | 1:H:125:VAL:O    | 2.43                     | 0.51              |
| 1:H:491:SER:C    | 1:N:501:VAL:HB   | 2.35                     | 0.51              |
| 1:I:98:ARG:NH2   | 1:I:125:VAL:O    | 2.43                     | 0.51              |
| 1:J:108:ILE:HA   | 1:J:111:ARG:CZ   | 2.41                     | 0.51              |
| 3:J:803:AGS:O1B  | 3:J:803:AGS:O2G  | 2.29                     | 0.51              |
| 1:K:406:LEU:HA   | 1:K:409:MET:HE3  | 1.92                     | 0.51              |
| 1:L:362:GLU:CD   | 1:L:365:ARG:HH12 | 2.19                     | 0.51              |
| 1:L:645:ASP:O    | 1:L:648:THR:OG1  | 2.27                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:402:ASP:N    | 1:M:402:ASP:OD1  | 2.44                     | 0.51              |
| 1:M:452:GLY:HA3  | 1:M:607:PHE:HB2  | 1.92                     | 0.51              |
| 1:A:312:ASP:OD2  | 1:G:111:ARG:HB3  | 2.11                     | 0.51              |
| 1:A:452:GLY:HA3  | 1:A:607:PHE:HB2  | 1.92                     | 0.51              |
| 1:B:108:ILE:HA   | 1:B:111:ARG:CZ   | 2.40                     | 0.51              |
| 1:D:192:ASP:OD1  | 1:D:192:ASP:N    | 2.41                     | 0.51              |
| 1:D:452:GLY:HA3  | 1:D:607:PHE:HB2  | 1.92                     | 0.51              |
| 1:F:409:MET:HA   | 1:F:412:ARG:HB2  | 1.91                     | 0.51              |
| 1:H:409:MET:HA   | 1:H:412:ARG:HB2  | 1.91                     | 0.51              |
| 1:K:108:ILE:HA   | 1:K:111:ARG:CZ   | 2.41                     | 0.51              |
| 1:M:108:ILE:HA   | 1:M:111:ARG:CZ   | 2.41                     | 0.51              |
| 1:M:137:ALA:HB1  | 1:M:142:ASP:HB3  | 1.93                     | 0.51              |
| 1:N:402:ASP:OD1  | 1:N:402:ASP:N    | 2.44                     | 0.51              |
| 1:A:108:ILE:HA   | 1:A:111:ARG:CZ   | 2.41                     | 0.50              |
| 1:A:192:ASP:OD1  | 1:A:192:ASP:N    | 2.41                     | 0.50              |
| 1:B:98:ARG:NH2   | 1:B:125:VAL:O    | 2.43                     | 0.50              |
| 1:C:362:GLU:CD   | 1:C:365:ARG:HH12 | 2.19                     | 0.50              |
| 1:D:108:ILE:HA   | 1:D:111:ARG:CZ   | 2.41                     | 0.50              |
| 1:F:108:ILE:HA   | 1:F:111:ARG:CZ   | 2.41                     | 0.50              |
| 1:F:406:LEU:HA   | 1:F:409:MET:HE3  | 1.92                     | 0.50              |
| 1:G:108:ILE:HA   | 1:G:111:ARG:CZ   | 2.41                     | 0.50              |
| 1:H:108:ILE:HA   | 1:H:111:ARG:CZ   | 2.41                     | 0.50              |
| 1:H:406:LEU:HA   | 1:H:409:MET:HE3  | 1.92                     | 0.50              |
| 1:I:108:ILE:HA   | 1:I:111:ARG:CZ   | 2.41                     | 0.50              |
| 1:J:452:GLY:HA3  | 1:J:607:PHE:HB2  | 1.92                     | 0.50              |
| 1:A:494:ILE:HA   | 1:G:498:ALA:HB1  | 1.94                     | 0.50              |
| 1:A:672:LYS:HE3  | 1:A:695:LEU:HB3  | 1.94                     | 0.50              |
| 1:D:137:ALA:HB1  | 1:D:142:ASP:HB3  | 1.93                     | 0.50              |
| 1:G:452:GLY:HA3  | 1:G:607:PHE:HB2  | 1.92                     | 0.50              |
| 1:H:362:GLU:CD   | 1:H:365:ARG:HH12 | 2.19                     | 0.50              |
| 1:H:536:THR:HG21 | 1:I:483:GLU:CG   | 2.38                     | 0.50              |
| 1:J:409:MET:HA   | 1:J:412:ARG:HB2  | 1.91                     | 0.50              |
| 1:K:672:LYS:HE3  | 1:K:695:LEU:HB3  | 1.94                     | 0.50              |
| 1:A:213:ALA:O    | 1:A:217:LYS:HG3  | 2.10                     | 0.50              |
| 1:B:672:LYS:HE3  | 1:B:695:LEU:HB3  | 1.94                     | 0.50              |
| 1:C:137:ALA:HB1  | 1:C:142:ASP:HB3  | 1.93                     | 0.50              |
| 1:E:137:ALA:HB1  | 1:E:142:ASP:HB3  | 1.93                     | 0.50              |
| 1:F:192:ASP:OD1  | 1:F:192:ASP:N    | 2.41                     | 0.50              |
| 1:F:672:LYS:HE3  | 1:F:695:LEU:HB3  | 1.94                     | 0.50              |
| 3:F:803:AGS:O1B  | 3:F:803:AGS:O2G  | 2.29                     | 0.50              |
| 1:G:622:MET:O    | 1:G:626:VAL:HG23 | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:672:LYS:HE3  | 1:H:695:LEU:HB3  | 1.94                     | 0.50              |
| 3:H:803:AGS:O1B  | 3:H:803:AGS:O2G  | 2.29                     | 0.50              |
| 1:I:452:GLY:HA3  | 1:I:607:PHE:HB2  | 1.92                     | 0.50              |
| 1:J:192:ASP:OD1  | 1:J:192:ASP:N    | 2.41                     | 0.50              |
| 1:L:452:GLY:HA3  | 1:L:607:PHE:HB2  | 1.92                     | 0.50              |
| 3:M:803:AGS:O1B  | 3:M:803:AGS:O2G  | 2.29                     | 0.50              |
| 1:C:452:GLY:HA3  | 1:C:607:PHE:HB2  | 1.92                     | 0.50              |
| 1:D:532:PRO:HB3  | 1:E:491:SER:N    | 2.20                     | 0.50              |
| 1:E:672:LYS:HE3  | 1:E:695:LEU:HB3  | 1.94                     | 0.50              |
| 1:F:645:ASP:O    | 1:F:648:THR:OG1  | 2.27                     | 0.50              |
| 1:H:192:ASP:N    | 1:H:192:ASP:OD1  | 2.41                     | 0.50              |
| 1:I:622:MET:O    | 1:I:626:VAL:HG23 | 2.11                     | 0.50              |
| 1:I:672:LYS:HE3  | 1:I:695:LEU:HB3  | 1.94                     | 0.50              |
| 1:J:286:VAL:HG21 | 1:J:378:ALA:HB1  | 1.94                     | 0.50              |
| 1:J:672:LYS:HE3  | 1:J:695:LEU:HB3  | 1.94                     | 0.50              |
| 1:K:691:GLU:CD   | 1:K:696:VAL:HG21 | 2.37                     | 0.50              |
| 1:L:285:GLU:OE1  | 1:L:285:GLU:N    | 2.26                     | 0.50              |
| 1:N:137:ALA:HB1  | 1:N:142:ASP:HB3  | 1.93                     | 0.50              |
| 1:N:672:LYS:HE3  | 1:N:695:LEU:HB3  | 1.94                     | 0.50              |
| 1:A:286:VAL:HG21 | 1:A:378:ALA:HB1  | 1.94                     | 0.50              |
| 1:A:691:GLU:CD   | 1:A:696:VAL:HG21 | 2.37                     | 0.50              |
| 1:B:286:VAL:HG21 | 1:B:378:ALA:HB1  | 1.94                     | 0.50              |
| 1:C:285:GLU:OE1  | 1:C:285:GLU:N    | 2.26                     | 0.50              |
| 1:D:251:ASN:OD1  | 1:D:252:GLU:N    | 2.41                     | 0.50              |
| 1:E:160:LEU:HB3  | 1:E:170:PHE:HE1  | 1.77                     | 0.50              |
| 3:E:803:AGS:O1B  | 3:E:803:AGS:O2G  | 2.29                     | 0.50              |
| 1:F:622:MET:O    | 1:F:626:VAL:HG23 | 2.11                     | 0.50              |
| 1:G:286:VAL:HG21 | 1:G:378:ALA:HB1  | 1.94                     | 0.50              |
| 1:G:672:LYS:HE3  | 1:G:695:LEU:HB3  | 1.94                     | 0.50              |
| 1:H:622:MET:O    | 1:H:626:VAL:HG23 | 2.11                     | 0.50              |
| 1:H:645:ASP:O    | 1:H:648:THR:OG1  | 2.27                     | 0.50              |
| 1:I:286:VAL:HG21 | 1:I:378:ALA:HB1  | 1.94                     | 0.50              |
| 3:I:803:AGS:O1B  | 3:I:803:AGS:O2G  | 2.29                     | 0.50              |
| 1:J:213:ALA:O    | 1:J:217:LYS:HG3  | 2.10                     | 0.50              |
| 1:J:691:GLU:CD   | 1:J:696:VAL:HG21 | 2.37                     | 0.50              |
| 1:L:137:ALA:HB1  | 1:L:142:ASP:HB3  | 1.93                     | 0.50              |
| 1:L:672:LYS:HE3  | 1:L:695:LEU:HB3  | 1.94                     | 0.50              |
| 1:L:691:GLU:CD   | 1:L:696:VAL:HG21 | 2.37                     | 0.50              |
| 1:B:691:GLU:CD   | 1:B:696:VAL:HG21 | 2.37                     | 0.50              |
| 1:C:672:LYS:HE3  | 1:C:695:LEU:HB3  | 1.94                     | 0.50              |
| 1:C:691:GLU:CD   | 1:C:696:VAL:HG21 | 2.37                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:286:VAL:HG21 | 1:F:378:ALA:HB1  | 1.94                     | 0.50              |
| 1:F:534:VAL:HG13 | 1:F:537:LEU:HB3  | 1.94                     | 0.50              |
| 3:G:803:AGS:O2G  | 3:G:803:AGS:O1B  | 2.29                     | 0.50              |
| 1:H:275:GLN:HA   | 1:H:281:ILE:HD11 | 1.94                     | 0.50              |
| 1:K:286:VAL:HG21 | 1:K:378:ALA:HB1  | 1.94                     | 0.50              |
| 1:N:459:THR:OG1  | 1:N:463:LYS:NZ   | 2.41                     | 0.50              |
| 1:A:622:MET:O    | 1:A:626:VAL:HG23 | 2.11                     | 0.50              |
| 1:D:128:THR:O    | 1:D:131:VAL:HG12 | 2.12                     | 0.50              |
| 1:D:672:LYS:HE3  | 1:D:695:LEU:HB3  | 1.94                     | 0.50              |
| 1:D:691:GLU:CD   | 1:D:696:VAL:HG21 | 2.37                     | 0.50              |
| 3:D:803:AGS:O1B  | 3:D:803:AGS:O2G  | 2.29                     | 0.50              |
| 1:E:128:THR:O    | 1:E:131:VAL:HG12 | 2.12                     | 0.50              |
| 1:F:128:THR:O    | 1:F:131:VAL:HG12 | 2.12                     | 0.50              |
| 1:F:275:GLN:HA   | 1:F:281:ILE:HD11 | 1.94                     | 0.50              |
| 1:F:402:ASP:OD1  | 1:F:402:ASP:N    | 2.44                     | 0.50              |
| 1:G:365:ARG:HG3  | 1:G:365:ARG:NH1  | 2.09                     | 0.50              |
| 1:H:286:VAL:HG21 | 1:H:378:ALA:HB1  | 1.94                     | 0.50              |
| 1:H:402:ASP:N    | 1:H:402:ASP:OD1  | 2.44                     | 0.50              |
| 1:I:365:ARG:HG3  | 1:I:365:ARG:NH1  | 2.09                     | 0.50              |
| 1:J:402:ASP:N    | 1:J:402:ASP:OD1  | 2.44                     | 0.50              |
| 1:M:112:ARG:HD2  | 1:N:274:TYR:CE1  | 2.47                     | 0.50              |
| 1:M:251:ASN:OD1  | 1:M:252:GLU:N    | 2.41                     | 0.50              |
| 3:N:803:AGS:O1B  | 3:N:803:AGS:O2G  | 2.29                     | 0.50              |
| 1:C:275:GLN:HA   | 1:C:281:ILE:HD11 | 1.94                     | 0.50              |
| 1:E:459:THR:OG1  | 1:E:463:LYS:NZ   | 2.41                     | 0.50              |
| 1:E:534:VAL:HG13 | 1:E:537:LEU:HB3  | 1.94                     | 0.50              |
| 1:E:589:LEU:HA   | 1:E:592:PHE:HB2  | 1.94                     | 0.50              |
| 1:H:128:THR:O    | 1:H:131:VAL:HG12 | 2.12                     | 0.50              |
| 1:H:534:VAL:HG13 | 1:H:537:LEU:HB3  | 1.94                     | 0.50              |
| 1:I:497:THR:HB   | 1:J:489:ALA:O    | 2.12                     | 0.50              |
| 1:I:691:GLU:CD   | 1:I:696:VAL:HG21 | 2.37                     | 0.50              |
| 1:J:528:GLU:HA   | 1:J:593:PHE:HE1  | 1.77                     | 0.50              |
| 1:J:622:MET:O    | 1:J:626:VAL:HG23 | 2.11                     | 0.50              |
| 1:K:402:ASP:OD1  | 1:K:402:ASP:N    | 2.44                     | 0.50              |
| 1:M:128:THR:O    | 1:M:131:VAL:HG12 | 2.12                     | 0.50              |
| 1:M:672:LYS:HE3  | 1:M:695:LEU:HB3  | 1.94                     | 0.50              |
| 1:M:691:GLU:CD   | 1:M:696:VAL:HG21 | 2.37                     | 0.50              |
| 1:N:128:THR:O    | 1:N:131:VAL:HG12 | 2.12                     | 0.50              |
| 1:N:160:LEU:HB3  | 1:N:170:PHE:HE1  | 1.77                     | 0.50              |
| 1:N:534:VAL:HG13 | 1:N:537:LEU:HB3  | 1.94                     | 0.50              |
| 1:A:362:GLU:CD   | 1:A:365:ARG:HH12 | 2.19                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:402:ASP:OD1  | 1:A:402:ASP:N    | 2.44                     | 0.50              |
| 1:A:528:GLU:HA   | 1:A:593:PHE:HE1  | 1.77                     | 0.50              |
| 1:C:160:LEU:HB3  | 1:C:170:PHE:HE1  | 1.77                     | 0.50              |
| 1:G:691:GLU:CD   | 1:G:696:VAL:HG21 | 2.37                     | 0.50              |
| 1:L:275:GLN:HA   | 1:L:281:ILE:HD11 | 1.94                     | 0.50              |
| 1:B:275:GLN:HA   | 1:B:281:ILE:HD11 | 1.94                     | 0.49              |
| 1:F:589:LEU:O    | 1:F:593:PHE:N    | 2.33                     | 0.49              |
| 1:F:589:LEU:HA   | 1:F:592:PHE:HB2  | 1.94                     | 0.49              |
| 1:G:160:LEU:HB3  | 1:G:170:PHE:HE1  | 1.77                     | 0.49              |
| 1:I:402:ASP:OD1  | 1:I:402:ASP:N    | 2.44                     | 0.49              |
| 1:J:137:ALA:HB1  | 1:J:142:ASP:HB3  | 1.93                     | 0.49              |
| 1:J:362:GLU:CD   | 1:J:365:ARG:HH12 | 2.19                     | 0.49              |
| 1:L:160:LEU:HB3  | 1:L:170:PHE:HE1  | 1.77                     | 0.49              |
| 1:L:534:VAL:HA   | 1:M:492:LYS:HD2  | 1.93                     | 0.49              |
| 1:M:160:LEU:HB3  | 1:M:170:PHE:HE1  | 1.77                     | 0.49              |
| 1:A:98:ARG:NH2   | 1:A:125:VAL:O    | 2.43                     | 0.49              |
| 1:A:137:ALA:HB1  | 1:A:142:ASP:HB3  | 1.93                     | 0.49              |
| 1:A:535:ILE:HG23 | 1:A:597:PHE:CD1  | 2.47                     | 0.49              |
| 1:B:402:ASP:N    | 1:B:402:ASP:OD1  | 2.44                     | 0.49              |
| 1:B:528:GLU:HA   | 1:B:593:PHE:HE1  | 1.77                     | 0.49              |
| 1:E:622:MET:O    | 1:E:626:VAL:HG23 | 2.11                     | 0.49              |
| 1:G:402:ASP:N    | 1:G:402:ASP:OD1  | 2.44                     | 0.49              |
| 1:H:589:LEU:HA   | 1:H:592:PHE:HB2  | 1.94                     | 0.49              |
| 1:I:137:ALA:HB1  | 1:I:142:ASP:HB3  | 1.93                     | 0.49              |
| 1:I:160:LEU:HB3  | 1:I:170:PHE:HE1  | 1.77                     | 0.49              |
| 1:J:98:ARG:NH2   | 1:J:125:VAL:O    | 2.43                     | 0.49              |
| 1:J:535:ILE:HG23 | 1:J:597:PHE:CD1  | 2.47                     | 0.49              |
| 1:K:275:GLN:HA   | 1:K:281:ILE:HD11 | 1.94                     | 0.49              |
| 1:K:528:GLU:HA   | 1:K:593:PHE:HE1  | 1.77                     | 0.49              |
| 1:L:170:PHE:O    | 1:L:174:VAL:HG23 | 2.12                     | 0.49              |
| 1:L:528:GLU:HA   | 1:L:593:PHE:HE1  | 1.77                     | 0.49              |
| 1:N:589:LEU:HA   | 1:N:592:PHE:HB2  | 1.95                     | 0.49              |
| 1:B:170:PHE:O    | 1:B:174:VAL:HG23 | 2.12                     | 0.49              |
| 1:C:170:PHE:O    | 1:C:174:VAL:HG23 | 2.13                     | 0.49              |
| 1:C:251:ASN:OD1  | 1:C:252:GLU:N    | 2.41                     | 0.49              |
| 1:D:170:PHE:O    | 1:D:174:VAL:HG23 | 2.13                     | 0.49              |
| 1:F:170:PHE:O    | 1:F:174:VAL:HG23 | 2.13                     | 0.49              |
| 1:G:128:THR:O    | 1:G:131:VAL:HG12 | 2.12                     | 0.49              |
| 1:G:137:ALA:HB1  | 1:G:142:ASP:HB3  | 1.93                     | 0.49              |
| 1:G:275:GLN:HA   | 1:G:281:ILE:HD11 | 1.94                     | 0.49              |
| 1:H:170:PHE:O    | 1:H:174:VAL:HG23 | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:589:LEU:O    | 1:H:593:PHE:N    | 2.33                     | 0.49              |
| 1:I:128:THR:O    | 1:I:131:VAL:HG12 | 2.12                     | 0.49              |
| 1:I:275:GLN:HA   | 1:I:281:ILE:HD11 | 1.94                     | 0.49              |
| 1:I:528:GLU:HA   | 1:I:593:PHE:HE1  | 1.77                     | 0.49              |
| 1:L:425:GLU:OE2  | 1:L:429:ARG:NE   | 2.38                     | 0.49              |
| 1:L:459:THR:OG1  | 1:L:463:LYS:NZ   | 2.41                     | 0.49              |
| 1:M:170:PHE:O    | 1:M:174:VAL:HG23 | 2.13                     | 0.49              |
| 1:N:212:LEU:O    | 1:N:216:LEU:N    | 2.33                     | 0.49              |
| 1:N:275:GLN:HA   | 1:N:281:ILE:HD11 | 1.94                     | 0.49              |
| 1:N:622:MET:O    | 1:N:626:VAL:HG23 | 2.11                     | 0.49              |
| 1:A:275:GLN:HA   | 1:A:281:ILE:HD11 | 1.94                     | 0.49              |
| 1:A:549:ASP:OD2  | 1:A:553:ASN:HB2  | 2.13                     | 0.49              |
| 1:B:160:LEU:HB3  | 1:B:170:PHE:HE1  | 1.77                     | 0.49              |
| 1:B:535:ILE:HG23 | 1:B:597:PHE:CD1  | 2.47                     | 0.49              |
| 1:C:286:VAL:HG21 | 1:C:378:ALA:HB1  | 1.94                     | 0.49              |
| 1:C:459:THR:OG1  | 1:C:463:LYS:NZ   | 2.41                     | 0.49              |
| 1:C:490:VAL:HG23 | 1:C:492:LYS:HG2  | 1.95                     | 0.49              |
| 1:C:528:GLU:HA   | 1:C:593:PHE:HE1  | 1.77                     | 0.49              |
| 1:D:160:LEU:HB3  | 1:D:170:PHE:HE1  | 1.77                     | 0.49              |
| 1:D:622:MET:O    | 1:D:626:VAL:HG23 | 2.11                     | 0.49              |
| 1:F:549:ASP:OD2  | 1:F:553:ASN:HB2  | 2.13                     | 0.49              |
| 1:G:528:GLU:HA   | 1:G:593:PHE:HE1  | 1.78                     | 0.49              |
| 1:H:549:ASP:OD2  | 1:H:553:ASN:HB2  | 2.13                     | 0.49              |
| 1:I:459:THR:OG1  | 1:I:463:LYS:NZ   | 2.41                     | 0.49              |
| 1:J:275:GLN:HA   | 1:J:281:ILE:HD11 | 1.94                     | 0.49              |
| 1:K:160:LEU:HB3  | 1:K:170:PHE:HE1  | 1.77                     | 0.49              |
| 1:K:490:VAL:HG23 | 1:K:492:LYS:HG2  | 1.95                     | 0.49              |
| 1:L:128:THR:O    | 1:L:131:VAL:HG12 | 2.12                     | 0.49              |
| 1:L:490:VAL:HG23 | 1:L:492:LYS:HG2  | 1.95                     | 0.49              |
| 1:M:549:ASP:OD2  | 1:M:553:ASN:HB2  | 2.13                     | 0.49              |
| 1:N:365:ARG:HG3  | 1:N:365:ARG:NH1  | 2.09                     | 0.49              |
| 1:A:128:THR:O    | 1:A:131:VAL:HG12 | 2.12                     | 0.49              |
| 1:B:137:ALA:HB1  | 1:B:142:ASP:HB3  | 1.93                     | 0.49              |
| 1:B:537:LEU:HD13 | 1:C:492:LYS:HA   | 1.94                     | 0.49              |
| 1:C:128:THR:O    | 1:C:131:VAL:HG12 | 2.12                     | 0.49              |
| 1:D:284:ASP:HA   | 1:D:287:LEU:HD12 | 1.95                     | 0.49              |
| 1:E:212:LEU:O    | 1:E:216:LEU:N    | 2.33                     | 0.49              |
| 1:E:284:ASP:HA   | 1:E:287:LEU:HD12 | 1.95                     | 0.49              |
| 1:E:691:GLU:CD   | 1:E:696:VAL:HG21 | 2.37                     | 0.49              |
| 1:F:691:GLU:CD   | 1:F:696:VAL:HG21 | 2.37                     | 0.49              |
| 1:G:285:GLU:OE1  | 1:G:285:GLU:N    | 2.26                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:534:VAL:HG13 | 1:G:537:LEU:HB3  | 1.94                     | 0.49              |
| 1:H:160:LEU:HB3  | 1:H:170:PHE:HE1  | 1.77                     | 0.49              |
| 1:J:128:THR:O    | 1:J:131:VAL:HG12 | 2.12                     | 0.49              |
| 1:K:137:ALA:HB1  | 1:K:142:ASP:HB3  | 1.93                     | 0.49              |
| 1:K:170:PHE:O    | 1:K:174:VAL:HG23 | 2.13                     | 0.49              |
| 1:K:534:VAL:HG13 | 1:K:537:LEU:HB3  | 1.94                     | 0.49              |
| 1:K:535:ILE:HG23 | 1:K:597:PHE:CD1  | 2.47                     | 0.49              |
| 1:L:251:ASN:OD1  | 1:L:252:GLU:N    | 2.41                     | 0.49              |
| 1:L:286:VAL:HG21 | 1:L:378:ALA:HB1  | 1.94                     | 0.49              |
| 1:M:284:ASP:HA   | 1:M:287:LEU:HD12 | 1.95                     | 0.49              |
| 1:A:490:VAL:HG23 | 1:A:492:LYS:HG2  | 1.95                     | 0.49              |
| 1:D:549:ASP:OD2  | 1:D:553:ASN:HB2  | 2.13                     | 0.49              |
| 1:E:275:GLN:HA   | 1:E:281:ILE:HD11 | 1.94                     | 0.49              |
| 1:E:549:ASP:OD2  | 1:E:553:ASN:HB2  | 2.13                     | 0.49              |
| 1:F:160:LEU:HB3  | 1:F:170:PHE:HE1  | 1.77                     | 0.49              |
| 1:G:535:ILE:HG23 | 1:G:597:PHE:CD1  | 2.47                     | 0.49              |
| 1:H:691:GLU:CD   | 1:H:696:VAL:HG21 | 2.37                     | 0.49              |
| 1:I:285:GLU:OE1  | 1:I:285:GLU:N    | 2.26                     | 0.49              |
| 1:I:535:ILE:HG23 | 1:I:597:PHE:CD1  | 2.47                     | 0.49              |
| 1:J:490:VAL:HG23 | 1:J:492:LYS:HG2  | 1.95                     | 0.49              |
| 1:J:549:ASP:OD2  | 1:J:553:ASN:HB2  | 2.13                     | 0.49              |
| 1:K:549:ASP:OD2  | 1:K:553:ASN:HB2  | 2.13                     | 0.49              |
| 1:M:534:VAL:HG13 | 1:M:537:LEU:HB3  | 1.94                     | 0.49              |
| 1:M:589:LEU:HA   | 1:M:592:PHE:HB2  | 1.94                     | 0.49              |
| 1:N:284:ASP:HA   | 1:N:287:LEU:HD12 | 1.95                     | 0.49              |
| 1:N:691:GLU:CD   | 1:N:696:VAL:HG21 | 2.37                     | 0.49              |
| 1:B:490:VAL:HG23 | 1:B:492:LYS:HG2  | 1.95                     | 0.49              |
| 1:B:622:MET:O    | 1:B:626:VAL:HG23 | 2.11                     | 0.49              |
| 1:E:528:GLU:HA   | 1:E:593:PHE:HE1  | 1.77                     | 0.49              |
| 1:F:284:ASP:HA   | 1:F:287:LEU:HD12 | 1.95                     | 0.49              |
| 1:H:274:TYR:HE1  | 1:N:112:ARG:HD2  | 1.78                     | 0.49              |
| 1:H:284:ASP:HA   | 1:H:287:LEU:HD12 | 1.95                     | 0.49              |
| 1:H:535:ILE:HG23 | 1:H:597:PHE:CD1  | 2.47                     | 0.49              |
| 1:K:128:THR:O    | 1:K:131:VAL:HG12 | 2.12                     | 0.49              |
| 1:L:402:ASP:OD1  | 1:L:402:ASP:N    | 2.44                     | 0.49              |
| 1:M:535:ILE:HG23 | 1:M:597:PHE:CD1  | 2.47                     | 0.49              |
| 1:M:622:MET:O    | 1:M:626:VAL:HG23 | 2.11                     | 0.49              |
| 1:N:170:PHE:O    | 1:N:174:VAL:HG23 | 2.13                     | 0.49              |
| 1:N:549:ASP:OD2  | 1:N:553:ASN:HB2  | 2.13                     | 0.49              |
| 1:A:160:LEU:HB3  | 1:A:170:PHE:HE1  | 1.77                     | 0.49              |
| 1:A:310:LEU:O    | 1:A:314:THR:OG1  | 2.30                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:128:THR:O    | 1:B:131:VAL:HG12 | 2.12                     | 0.49              |
| 1:B:534:VAL:HG13 | 1:B:537:LEU:HB3  | 1.94                     | 0.49              |
| 1:B:549:ASP:OD2  | 1:B:553:ASN:HB2  | 2.13                     | 0.49              |
| 1:C:425:GLU:OE2  | 1:C:429:ARG:NE   | 2.38                     | 0.49              |
| 1:D:99:ASN:O     | 1:D:102:ILE:HG12 | 2.13                     | 0.49              |
| 1:D:534:VAL:HG13 | 1:D:537:LEU:HB3  | 1.94                     | 0.49              |
| 1:D:589:LEU:HA   | 1:D:592:PHE:HB2  | 1.94                     | 0.49              |
| 1:E:170:PHE:O    | 1:E:174:VAL:HG23 | 2.13                     | 0.49              |
| 1:E:365:ARG:HG3  | 1:E:365:ARG:NH1  | 2.09                     | 0.49              |
| 1:F:535:ILE:HG23 | 1:F:597:PHE:CD1  | 2.47                     | 0.49              |
| 1:G:589:LEU:HA   | 1:G:592:PHE:HB2  | 1.94                     | 0.49              |
| 1:I:170:PHE:O    | 1:I:174:VAL:HG23 | 2.12                     | 0.49              |
| 1:I:534:VAL:HG13 | 1:I:537:LEU:HB3  | 1.94                     | 0.49              |
| 1:K:615:LEU:O    | 1:K:618:ILE:HG22 | 2.13                     | 0.49              |
| 1:L:622:MET:O    | 1:L:626:VAL:HG23 | 2.11                     | 0.49              |
| 1:N:286:VAL:HG21 | 1:N:378:ALA:HB1  | 1.94                     | 0.49              |
| 1:N:528:GLU:HA   | 1:N:593:PHE:HE1  | 1.77                     | 0.49              |
| 1:N:535:ILE:HG23 | 1:N:597:PHE:CD1  | 2.47                     | 0.49              |
| 1:A:212:LEU:O    | 1:A:216:LEU:N    | 2.33                     | 0.49              |
| 1:A:534:VAL:HG13 | 1:A:537:LEU:HB3  | 1.94                     | 0.49              |
| 1:B:102:ILE:HG13 | 1:B:103:GLN:N    | 2.28                     | 0.49              |
| 1:B:615:LEU:O    | 1:B:618:ILE:HG22 | 2.13                     | 0.49              |
| 1:D:275:GLN:HA   | 1:D:281:ILE:HD11 | 1.94                     | 0.49              |
| 1:D:535:ILE:HG23 | 1:D:597:PHE:CD1  | 2.47                     | 0.49              |
| 1:E:192:ASP:N    | 1:E:192:ASP:OD1  | 2.41                     | 0.49              |
| 1:F:137:ALA:HB1  | 1:F:142:ASP:HB3  | 1.93                     | 0.49              |
| 1:G:170:PHE:O    | 1:G:174:VAL:HG23 | 2.13                     | 0.49              |
| 1:G:615:LEU:O    | 1:G:618:ILE:HG22 | 2.13                     | 0.49              |
| 1:H:312:ASP:OD2  | 1:N:111:ARG:HB3  | 2.13                     | 0.49              |
| 1:I:490:VAL:HG23 | 1:I:492:LYS:HG2  | 1.95                     | 0.49              |
| 1:J:310:LEU:O    | 1:J:314:THR:OG1  | 2.30                     | 0.49              |
| 1:J:534:VAL:HG13 | 1:J:537:LEU:HB3  | 1.94                     | 0.49              |
| 1:L:534:VAL:HG13 | 1:L:537:LEU:HB3  | 1.94                     | 0.49              |
| 1:L:535:ILE:HG23 | 1:L:597:PHE:CD1  | 2.47                     | 0.49              |
| 1:M:99:ASN:O     | 1:M:102:ILE:HG12 | 2.13                     | 0.49              |
| 1:A:615:LEU:O    | 1:A:618:ILE:HG22 | 2.13                     | 0.49              |
| 1:C:535:ILE:HG23 | 1:C:597:PHE:CD1  | 2.47                     | 0.49              |
| 1:C:622:MET:O    | 1:C:626:VAL:HG23 | 2.11                     | 0.49              |
| 1:D:490:VAL:HG23 | 1:D:492:LYS:HG2  | 1.95                     | 0.49              |
| 1:E:112:ARG:HD2  | 1:F:274:TYR:CE1  | 2.48                     | 0.49              |
| 1:E:535:ILE:HG23 | 1:E:597:PHE:CD1  | 2.47                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:615:LEU:O    | 1:F:618:ILE:HG22 | 2.13                     | 0.49              |
| 1:G:490:VAL:HG23 | 1:G:492:LYS:HG2  | 1.95                     | 0.49              |
| 1:H:137:ALA:HB1  | 1:H:142:ASP:HB3  | 1.93                     | 0.49              |
| 1:H:492:LYS:HD2  | 1:N:534:VAL:HA   | 1.95                     | 0.49              |
| 1:I:589:LEU:HA   | 1:I:592:PHE:HB2  | 1.94                     | 0.49              |
| 1:I:615:LEU:O    | 1:I:618:ILE:HG22 | 2.13                     | 0.49              |
| 1:J:615:LEU:O    | 1:J:618:ILE:HG22 | 2.13                     | 0.49              |
| 1:K:102:ILE:HG13 | 1:K:103:GLN:N    | 2.28                     | 0.49              |
| 1:K:622:MET:O    | 1:K:626:VAL:HG23 | 2.11                     | 0.49              |
| 1:N:114:LYS:NZ   | 1:N:250:PHE:O    | 2.43                     | 0.49              |
| 1:C:534:VAL:HG13 | 1:C:537:LEU:HB3  | 1.94                     | 0.48              |
| 1:E:286:VAL:HG21 | 1:E:378:ALA:HB1  | 1.94                     | 0.48              |
| 1:E:350:PHE:HB3  | 1:K:350:PHE:HB3  | 1.95                     | 0.48              |
| 1:E:615:LEU:O    | 1:E:618:ILE:HG22 | 2.13                     | 0.48              |
| 1:I:177:LEU:O    | 1:I:181:VAL:HG23 | 2.13                     | 0.48              |
| 1:J:160:LEU:HB3  | 1:J:170:PHE:HE1  | 1.77                     | 0.48              |
| 1:K:476:ILE:HA   | 1:K:521:ILE:O    | 2.14                     | 0.48              |
| 1:K:645:ASP:O    | 1:K:648:THR:OG1  | 2.27                     | 0.48              |
| 1:M:490:VAL:HG23 | 1:M:492:LYS:HG2  | 1.95                     | 0.48              |
| 1:B:476:ILE:HA   | 1:B:521:ILE:O    | 2.14                     | 0.48              |
| 1:C:284:ASP:HA   | 1:C:287:LEU:HD12 | 1.95                     | 0.48              |
| 1:C:402:ASP:OD1  | 1:C:402:ASP:N    | 2.44                     | 0.48              |
| 1:E:534:VAL:HA   | 1:F:492:LYS:HD2  | 1.95                     | 0.48              |
| 1:G:177:LEU:O    | 1:G:181:VAL:HG23 | 2.14                     | 0.48              |
| 1:H:615:LEU:O    | 1:H:618:ILE:HG22 | 2.13                     | 0.48              |
| 1:I:284:ASP:HA   | 1:I:287:LEU:HD12 | 1.95                     | 0.48              |
| 1:K:99:ASN:O     | 1:K:102:ILE:HG12 | 2.13                     | 0.48              |
| 1:K:425:GLU:OE2  | 1:K:429:ARG:NE   | 2.39                     | 0.48              |
| 1:M:177:LEU:O    | 1:M:181:VAL:HG23 | 2.14                     | 0.48              |
| 1:M:476:ILE:HA   | 1:M:521:ILE:O    | 2.13                     | 0.48              |
| 1:B:589:LEU:HA   | 1:B:592:PHE:HB2  | 1.94                     | 0.48              |
| 1:B:645:ASP:O    | 1:B:648:THR:OG1  | 2.27                     | 0.48              |
| 1:C:589:LEU:HA   | 1:C:592:PHE:HB2  | 1.94                     | 0.48              |
| 1:D:177:LEU:O    | 1:D:181:VAL:HG23 | 2.14                     | 0.48              |
| 1:D:476:ILE:HA   | 1:D:521:ILE:O    | 2.14                     | 0.48              |
| 1:J:212:LEU:O    | 1:J:216:LEU:N    | 2.33                     | 0.48              |
| 1:L:284:ASP:HA   | 1:L:287:LEU:HD12 | 1.95                     | 0.48              |
| 1:M:275:GLN:HA   | 1:M:281:ILE:HD11 | 1.94                     | 0.48              |
| 1:N:615:LEU:O    | 1:N:618:ILE:HG22 | 2.13                     | 0.48              |
| 1:B:99:ASN:O     | 1:B:102:ILE:HG12 | 2.13                     | 0.48              |
| 1:G:284:ASP:HA   | 1:G:287:LEU:HD12 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:549:ASP:OD2  | 1:G:553:ASN:HB2  | 2.13                     | 0.48              |
| 1:I:102:ILE:HG13 | 1:I:103:GLN:N    | 2.28                     | 0.48              |
| 1:J:99:ASN:O     | 1:J:102:ILE:HG12 | 2.13                     | 0.48              |
| 1:L:99:ASN:O     | 1:L:102:ILE:HG12 | 2.13                     | 0.48              |
| 1:L:177:LEU:O    | 1:L:181:VAL:HG23 | 2.14                     | 0.48              |
| 1:A:99:ASN:O     | 1:A:102:ILE:HG12 | 2.13                     | 0.48              |
| 1:A:170:PHE:O    | 1:A:174:VAL:HG23 | 2.12                     | 0.48              |
| 1:A:589:LEU:HA   | 1:A:592:PHE:HB2  | 1.94                     | 0.48              |
| 1:B:460:GLU:OE2  | 3:B:803:AGS:H8   | 2.14                     | 0.48              |
| 1:C:99:ASN:O     | 1:C:102:ILE:HG12 | 2.13                     | 0.48              |
| 1:C:177:LEU:O    | 1:C:181:VAL:HG23 | 2.14                     | 0.48              |
| 1:D:102:ILE:HG13 | 1:D:103:GLN:N    | 2.28                     | 0.48              |
| 1:D:286:VAL:HG21 | 1:D:378:ALA:HB1  | 1.94                     | 0.48              |
| 1:E:645:ASP:O    | 1:E:648:THR:OG1  | 2.27                     | 0.48              |
| 1:H:425:GLU:OE2  | 1:H:429:ARG:NE   | 2.38                     | 0.48              |
| 1:I:549:ASP:OD2  | 1:I:553:ASN:HB2  | 2.13                     | 0.48              |
| 1:J:589:LEU:HA   | 1:J:592:PHE:HB2  | 1.94                     | 0.48              |
| 1:K:589:LEU:HA   | 1:K:592:PHE:HB2  | 1.94                     | 0.48              |
| 1:M:645:ASP:O    | 1:M:648:THR:OG1  | 2.27                     | 0.48              |
| 1:A:177:LEU:O    | 1:A:181:VAL:HG23 | 2.14                     | 0.48              |
| 1:A:481:MET:SD   | 1:A:530:ALA:HB3  | 2.54                     | 0.48              |
| 1:B:425:GLU:OE2  | 1:B:429:ARG:NE   | 2.38                     | 0.48              |
| 1:B:501:VAL:HB   | 1:C:491:SER:C    | 2.38                     | 0.48              |
| 1:C:549:ASP:OD2  | 1:C:553:ASN:HB2  | 2.13                     | 0.48              |
| 1:C:615:LEU:O    | 1:C:618:ILE:HG22 | 2.13                     | 0.48              |
| 1:D:615:LEU:O    | 1:D:618:ILE:HG22 | 2.13                     | 0.48              |
| 1:E:102:ILE:HG13 | 1:E:103:GLN:N    | 2.28                     | 0.48              |
| 1:E:300:GLN:HA   | 1:E:519:TYR:CE2  | 2.49                     | 0.48              |
| 1:E:481:MET:SD   | 1:E:530:ALA:HB3  | 2.54                     | 0.48              |
| 1:E:571:GLY:HA3  | 1:E:572:TYR:HA   | 1.57                     | 0.48              |
| 1:F:177:LEU:O    | 1:F:181:VAL:HG23 | 2.14                     | 0.48              |
| 1:G:102:ILE:HG13 | 1:G:103:GLN:N    | 2.28                     | 0.48              |
| 1:G:572:TYR:C    | 1:G:574:ALA:HA   | 2.39                     | 0.48              |
| 1:H:177:LEU:O    | 1:H:181:VAL:HG23 | 2.13                     | 0.48              |
| 1:H:528:GLU:HA   | 1:H:593:PHE:HE1  | 1.77                     | 0.48              |
| 1:I:99:ASN:O     | 1:I:102:ILE:HG12 | 2.13                     | 0.48              |
| 1:I:572:TYR:C    | 1:I:574:ALA:HA   | 2.39                     | 0.48              |
| 1:J:170:PHE:O    | 1:J:174:VAL:HG23 | 2.12                     | 0.48              |
| 1:K:365:ARG:HG3  | 1:K:365:ARG:NH1  | 2.09                     | 0.48              |
| 1:L:549:ASP:OD2  | 1:L:553:ASN:HB2  | 2.13                     | 0.48              |
| 1:M:300:GLN:HA   | 1:M:519:TYR:CE2  | 2.49                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:615:LEU:O    | 1:M:618:ILE:HG22 | 2.13                     | 0.48              |
| 1:N:300:GLN:HA   | 1:N:519:TYR:CE2  | 2.49                     | 0.48              |
| 1:N:481:MET:SD   | 1:N:530:ALA:HB3  | 2.54                     | 0.48              |
| 1:F:403:ILE:HD12 | 1:F:403:ILE:H    | 1.79                     | 0.48              |
| 1:F:528:GLU:HA   | 1:F:593:PHE:HE1  | 1.77                     | 0.48              |
| 1:G:99:ASN:O     | 1:G:102:ILE:HG12 | 2.13                     | 0.48              |
| 1:G:452:GLY:HA2  | 1:G:568:ALA:HB3  | 1.96                     | 0.48              |
| 1:H:99:ASN:O     | 1:H:102:ILE:HG12 | 2.13                     | 0.48              |
| 1:J:300:GLN:HA   | 1:J:519:TYR:CE2  | 2.49                     | 0.48              |
| 1:J:481:MET:SD   | 1:J:530:ALA:HB3  | 2.54                     | 0.48              |
| 1:K:460:GLU:OE2  | 3:K:803:AGS:H8   | 2.14                     | 0.48              |
| 1:L:589:LEU:HA   | 1:L:592:PHE:HB2  | 1.94                     | 0.48              |
| 1:N:102:ILE:HG13 | 1:N:103:GLN:N    | 2.28                     | 0.48              |
| 1:A:300:GLN:HA   | 1:A:519:TYR:CE2  | 2.49                     | 0.48              |
| 1:A:403:ILE:H    | 1:A:403:ILE:HD12 | 1.79                     | 0.48              |
| 1:D:300:GLN:HA   | 1:D:519:TYR:CE2  | 2.49                     | 0.48              |
| 1:D:571:GLY:HA3  | 1:D:572:TYR:HA   | 1.57                     | 0.48              |
| 1:E:490:VAL:HG23 | 1:E:492:LYS:HG2  | 1.95                     | 0.48              |
| 1:F:99:ASN:O     | 1:F:102:ILE:HG12 | 2.13                     | 0.48              |
| 1:F:476:ILE:HA   | 1:F:521:ILE:O    | 2.14                     | 0.48              |
| 1:G:300:GLN:HA   | 1:G:519:TYR:CE2  | 2.49                     | 0.48              |
| 1:G:460:GLU:OE2  | 3:G:803:AGS:H8   | 2.14                     | 0.48              |
| 1:G:476:ILE:HA   | 1:G:521:ILE:O    | 2.13                     | 0.48              |
| 1:H:300:GLN:HA   | 1:H:519:TYR:CE2  | 2.49                     | 0.48              |
| 1:I:460:GLU:OE2  | 3:I:803:AGS:H8   | 2.14                     | 0.48              |
| 1:J:177:LEU:O    | 1:J:181:VAL:HG23 | 2.14                     | 0.48              |
| 1:J:403:ILE:H    | 1:J:403:ILE:HD12 | 1.79                     | 0.48              |
| 1:L:160:LEU:HB3  | 1:L:170:PHE:CE1  | 2.49                     | 0.48              |
| 1:L:481:MET:SD   | 1:L:530:ALA:HB3  | 2.54                     | 0.48              |
| 1:L:615:LEU:O    | 1:L:618:ILE:HG22 | 2.13                     | 0.48              |
| 1:M:102:ILE:HG13 | 1:M:103:GLN:N    | 2.28                     | 0.48              |
| 1:N:490:VAL:HG23 | 1:N:492:LYS:HG2  | 1.95                     | 0.48              |
| 1:A:102:ILE:HG13 | 1:A:103:GLN:N    | 2.28                     | 0.48              |
| 1:A:284:ASP:HA   | 1:A:287:LEU:HD12 | 1.95                     | 0.48              |
| 1:C:160:LEU:HB3  | 1:C:170:PHE:CE1  | 2.49                     | 0.48              |
| 1:C:300:GLN:HA   | 1:C:519:TYR:CE2  | 2.49                     | 0.48              |
| 1:C:476:ILE:HA   | 1:C:521:ILE:O    | 2.13                     | 0.48              |
| 1:D:528:GLU:HA   | 1:D:593:PHE:HE1  | 1.78                     | 0.48              |
| 1:D:589:LEU:O    | 1:D:593:PHE:N    | 2.33                     | 0.48              |
| 1:D:645:ASP:O    | 1:D:648:THR:OG1  | 2.27                     | 0.48              |
| 1:F:102:ILE:HG13 | 1:F:103:GLN:N    | 2.28                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:490:VAL:HG23 | 1:F:492:LYS:HG2  | 1.95                     | 0.48              |
| 1:G:310:LEU:O    | 1:G:314:THR:OG1  | 2.30                     | 0.48              |
| 1:H:403:ILE:H    | 1:H:403:ILE:HD12 | 1.79                     | 0.48              |
| 1:H:476:ILE:HA   | 1:H:521:ILE:O    | 2.14                     | 0.48              |
| 1:H:490:VAL:HG23 | 1:H:492:LYS:HG2  | 1.95                     | 0.48              |
| 1:I:300:GLN:HA   | 1:I:519:TYR:CE2  | 2.49                     | 0.48              |
| 1:I:452:GLY:HA2  | 1:I:568:ALA:HB3  | 1.96                     | 0.48              |
| 1:J:102:ILE:HG13 | 1:J:103:GLN:N    | 2.28                     | 0.48              |
| 1:L:300:GLN:HA   | 1:L:519:TYR:CE2  | 2.49                     | 0.48              |
| 1:B:365:ARG:HG3  | 1:B:365:ARG:NH1  | 2.09                     | 0.48              |
| 1:C:572:TYR:C    | 1:C:574:ALA:HA   | 2.39                     | 0.48              |
| 1:D:160:LEU:HB3  | 1:D:170:PHE:CE1  | 2.49                     | 0.48              |
| 1:D:212:LEU:O    | 1:D:216:LEU:N    | 2.33                     | 0.48              |
| 1:E:177:LEU:O    | 1:E:181:VAL:HG23 | 2.14                     | 0.48              |
| 1:F:300:GLN:HA   | 1:F:519:TYR:CE2  | 2.49                     | 0.48              |
| 1:F:425:GLU:OE2  | 1:F:429:ARG:NE   | 2.39                     | 0.48              |
| 1:G:481:MET:SD   | 1:G:530:ALA:HB3  | 2.54                     | 0.48              |
| 1:H:102:ILE:HG13 | 1:H:103:GLN:N    | 2.28                     | 0.48              |
| 1:I:476:ILE:HA   | 1:I:521:ILE:O    | 2.14                     | 0.48              |
| 1:K:160:LEU:HB3  | 1:K:170:PHE:CE1  | 2.49                     | 0.48              |
| 1:L:572:TYR:C    | 1:L:574:ALA:HA   | 2.39                     | 0.48              |
| 1:N:177:LEU:O    | 1:N:181:VAL:HG23 | 2.14                     | 0.48              |
| 1:N:645:ASP:O    | 1:N:648:THR:OG1  | 2.27                     | 0.48              |
| 1:B:160:LEU:HB3  | 1:B:170:PHE:CE1  | 2.49                     | 0.47              |
| 1:C:102:ILE:HG13 | 1:C:103:GLN:N    | 2.28                     | 0.47              |
| 1:C:403:ILE:HD12 | 1:C:403:ILE:H    | 1.79                     | 0.47              |
| 1:C:481:MET:SD   | 1:C:530:ALA:HB3  | 2.54                     | 0.47              |
| 1:D:572:TYR:C    | 1:D:574:ALA:HA   | 2.39                     | 0.47              |
| 1:I:481:MET:SD   | 1:I:530:ALA:HB3  | 2.54                     | 0.47              |
| 1:J:284:ASP:HA   | 1:J:287:LEU:HD12 | 1.95                     | 0.47              |
| 1:K:177:LEU:O    | 1:K:181:VAL:HG23 | 2.14                     | 0.47              |
| 1:L:403:ILE:H    | 1:L:403:ILE:HD12 | 1.79                     | 0.47              |
| 1:L:476:ILE:HA   | 1:L:521:ILE:O    | 2.13                     | 0.47              |
| 1:M:286:VAL:HG21 | 1:M:378:ALA:HB1  | 1.94                     | 0.47              |
| 1:M:572:TYR:C    | 1:M:574:ALA:HA   | 2.39                     | 0.47              |
| 1:A:572:TYR:C    | 1:A:574:ALA:HA   | 2.39                     | 0.47              |
| 1:B:284:ASP:HA   | 1:B:287:LEU:HD12 | 1.95                     | 0.47              |
| 1:B:465:LEU:O    | 1:B:469:MET:HG2  | 2.14                     | 0.47              |
| 1:C:465:LEU:O    | 1:C:469:MET:HG2  | 2.14                     | 0.47              |
| 1:E:99:ASN:O     | 1:E:102:ILE:HG12 | 2.13                     | 0.47              |
| 1:F:452:GLY:HA2  | 1:F:568:ALA:HB3  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:452:GLY:HA2  | 1:H:568:ALA:HB3  | 1.96                     | 0.47              |
| 1:H:481:MET:SD   | 1:H:530:ALA:HB3  | 2.54                     | 0.47              |
| 1:J:572:TYR:C    | 1:J:574:ALA:HA   | 2.39                     | 0.47              |
| 1:K:284:ASP:HA   | 1:K:287:LEU:HD12 | 1.95                     | 0.47              |
| 1:K:465:LEU:O    | 1:K:469:MET:HG2  | 2.14                     | 0.47              |
| 1:L:460:GLU:OE2  | 3:L:803:AGS:H8   | 2.14                     | 0.47              |
| 1:L:465:LEU:O    | 1:L:469:MET:HG2  | 2.14                     | 0.47              |
| 1:M:160:LEU:HB3  | 1:M:170:PHE:CE1  | 2.49                     | 0.47              |
| 1:M:532:PRO:HB3  | 1:N:491:SER:N    | 2.19                     | 0.47              |
| 1:B:300:GLN:HA   | 1:B:519:TYR:CE2  | 2.49                     | 0.47              |
| 1:C:460:GLU:OE2  | 3:C:803:AGS:H8   | 2.14                     | 0.47              |
| 1:K:300:GLN:HA   | 1:K:519:TYR:CE2  | 2.49                     | 0.47              |
| 1:L:102:ILE:HG13 | 1:L:103:GLN:N    | 2.28                     | 0.47              |
| 1:N:452:GLY:HA2  | 1:N:568:ALA:HB3  | 1.96                     | 0.47              |
| 1:A:160:LEU:HB3  | 1:A:170:PHE:CE1  | 2.49                     | 0.47              |
| 1:B:177:LEU:O    | 1:B:181:VAL:HG23 | 2.14                     | 0.47              |
| 1:B:530:ALA:HB3  | 1:B:532:PRO:HD2  | 1.97                     | 0.47              |
| 1:D:403:ILE:H    | 1:D:403:ILE:HD12 | 1.79                     | 0.47              |
| 1:D:465:LEU:O    | 1:D:469:MET:HG2  | 2.14                     | 0.47              |
| 1:D:481:MET:SD   | 1:D:530:ALA:HB3  | 2.54                     | 0.47              |
| 1:F:267:LEU:HD21 | 1:F:287:LEU:HD22 | 1.96                     | 0.47              |
| 1:F:481:MET:SD   | 1:F:530:ALA:HB3  | 2.54                     | 0.47              |
| 1:H:492:LYS:HA   | 1:N:537:LEU:HD13 | 1.95                     | 0.47              |
| 1:J:160:LEU:HB3  | 1:J:170:PHE:CE1  | 2.49                     | 0.47              |
| 1:J:452:GLY:HA2  | 1:J:568:ALA:HB3  | 1.96                     | 0.47              |
| 1:M:528:GLU:HA   | 1:M:593:PHE:HE1  | 1.78                     | 0.47              |
| 1:N:99:ASN:O     | 1:N:102:ILE:HG12 | 2.13                     | 0.47              |
| 1:N:476:ILE:HA   | 1:N:521:ILE:O    | 2.13                     | 0.47              |
| 1:A:452:GLY:HA2  | 1:A:568:ALA:HB3  | 1.96                     | 0.47              |
| 1:A:476:ILE:HA   | 1:A:521:ILE:O    | 2.13                     | 0.47              |
| 1:B:453:SER:O    | 1:B:458:LYS:HD2  | 2.15                     | 0.47              |
| 1:B:572:TYR:C    | 1:B:574:ALA:HA   | 2.39                     | 0.47              |
| 1:D:497:THR:HG22 | 1:E:491:SER:N    | 2.29                     | 0.47              |
| 1:E:452:GLY:HA2  | 1:E:568:ALA:HB3  | 1.96                     | 0.47              |
| 1:E:460:GLU:OE2  | 3:E:803:AGS:H8   | 2.14                     | 0.47              |
| 1:E:476:ILE:HA   | 1:E:521:ILE:O    | 2.14                     | 0.47              |
| 1:F:460:GLU:OE2  | 3:F:803:AGS:H8   | 2.14                     | 0.47              |
| 1:F:572:TYR:C    | 1:F:574:ALA:HA   | 2.39                     | 0.47              |
| 1:G:160:LEU:HB3  | 1:G:170:PHE:CE1  | 2.49                     | 0.47              |
| 1:G:571:GLY:HA3  | 1:G:572:TYR:HA   | 1.57                     | 0.47              |
| 1:H:460:GLU:OE2  | 3:H:803:AGS:H8   | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:572:TYR:C    | 1:H:574:ALA:HA   | 2.39                     | 0.47              |
| 1:J:476:ILE:HA   | 1:J:521:ILE:O    | 2.13                     | 0.47              |
| 1:J:530:ALA:HB3  | 1:J:532:PRO:HD2  | 1.96                     | 0.47              |
| 1:K:572:TYR:C    | 1:K:574:ALA:HA   | 2.39                     | 0.47              |
| 1:N:403:ILE:HD12 | 1:N:403:ILE:H    | 1.79                     | 0.47              |
| 1:N:460:GLU:OE2  | 3:N:803:AGS:H8   | 2.14                     | 0.47              |
| 1:A:460:GLU:OE2  | 3:A:803:AGS:H8   | 2.14                     | 0.47              |
| 1:A:530:ALA:HB3  | 1:A:532:PRO:HD2  | 1.97                     | 0.47              |
| 1:C:453:SER:O    | 1:C:458:LYS:HD2  | 2.15                     | 0.47              |
| 1:E:160:LEU:HB3  | 1:E:170:PHE:CE1  | 2.49                     | 0.47              |
| 1:E:267:LEU:HD21 | 1:E:287:LEU:HD22 | 1.96                     | 0.47              |
| 1:F:453:SER:O    | 1:F:458:LYS:HD2  | 2.15                     | 0.47              |
| 1:F:571:GLY:HA3  | 1:F:572:TYR:HA   | 1.57                     | 0.47              |
| 1:H:267:LEU:HD21 | 1:H:287:LEU:HD22 | 1.96                     | 0.47              |
| 1:H:453:SER:O    | 1:H:458:LYS:HD2  | 2.15                     | 0.47              |
| 1:I:160:LEU:HB3  | 1:I:170:PHE:CE1  | 2.49                     | 0.47              |
| 1:J:460:GLU:OE2  | 3:J:803:AGS:H8   | 2.14                     | 0.47              |
| 1:J:465:LEU:O    | 1:J:469:MET:HG2  | 2.14                     | 0.47              |
| 1:K:481:MET:SD   | 1:K:530:ALA:HB3  | 2.54                     | 0.47              |
| 1:K:530:ALA:HB3  | 1:K:532:PRO:HD2  | 1.96                     | 0.47              |
| 1:L:530:ALA:HB3  | 1:L:532:PRO:HD2  | 1.96                     | 0.47              |
| 1:N:267:LEU:HD21 | 1:N:287:LEU:HD22 | 1.96                     | 0.47              |
| 1:A:465:LEU:O    | 1:A:469:MET:HG2  | 2.14                     | 0.47              |
| 1:B:212:LEU:O    | 1:B:216:LEU:N    | 2.33                     | 0.47              |
| 1:B:481:MET:SD   | 1:B:530:ALA:HB3  | 2.54                     | 0.47              |
| 1:C:530:ALA:HB3  | 1:C:532:PRO:HD2  | 1.96                     | 0.47              |
| 1:D:460:GLU:OE2  | 3:D:803:AGS:H8   | 2.14                     | 0.47              |
| 1:E:403:ILE:H    | 1:E:403:ILE:HD12 | 1.79                     | 0.47              |
| 1:E:572:TYR:C    | 1:E:574:ALA:HA   | 2.39                     | 0.47              |
| 1:G:453:SER:O    | 1:G:458:LYS:HD2  | 2.15                     | 0.47              |
| 1:G:589:LEU:O    | 1:G:593:PHE:N    | 2.33                     | 0.47              |
| 1:K:212:LEU:O    | 1:K:216:LEU:N    | 2.33                     | 0.47              |
| 1:K:453:SER:O    | 1:K:458:LYS:HD2  | 2.15                     | 0.47              |
| 1:L:453:SER:O    | 1:L:458:LYS:HD2  | 2.15                     | 0.47              |
| 1:M:403:ILE:H    | 1:M:403:ILE:HD12 | 1.79                     | 0.47              |
| 1:M:465:LEU:O    | 1:M:469:MET:HG2  | 2.14                     | 0.47              |
| 1:N:571:GLY:HA3  | 1:N:572:TYR:HA   | 1.57                     | 0.47              |
| 1:C:267:LEU:HD21 | 1:C:287:LEU:HD22 | 1.96                     | 0.47              |
| 1:C:534:VAL:HG22 | 1:D:492:LYS:HB3  | 1.96                     | 0.47              |
| 1:I:453:SER:O    | 1:I:458:LYS:HD2  | 2.15                     | 0.47              |
| 1:I:571:GLY:HA3  | 1:I:572:TYR:HA   | 1.57                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:589:LEU:O    | 1:I:593:PHE:N    | 2.33                     | 0.47              |
| 1:M:460:GLU:OE2  | 3:M:803:AGS:H8   | 2.14                     | 0.47              |
| 1:M:481:MET:SD   | 1:M:530:ALA:HB3  | 2.54                     | 0.47              |
| 1:M:589:LEU:O    | 1:M:593:PHE:N    | 2.33                     | 0.47              |
| 1:N:160:LEU:HB3  | 1:N:170:PHE:CE1  | 2.49                     | 0.47              |
| 1:N:572:TYR:C    | 1:N:574:ALA:HA   | 2.39                     | 0.47              |
| 1:D:669:ILE:HD13 | 1:D:695:LEU:HD22 | 1.97                     | 0.47              |
| 1:E:453:SER:O    | 1:E:458:LYS:HD2  | 2.15                     | 0.47              |
| 1:E:537:LEU:HD13 | 1:F:492:LYS:HA   | 1.97                     | 0.47              |
| 1:H:160:LEU:HB3  | 1:H:170:PHE:CE1  | 2.49                     | 0.47              |
| 1:I:425:GLU:OE2  | 1:I:429:ARG:NE   | 2.38                     | 0.47              |
| 1:J:470:PHE:CZ   | 1:J:519:TYR:HB3  | 2.50                     | 0.47              |
| 1:M:530:ALA:HB3  | 1:M:532:PRO:HD2  | 1.96                     | 0.47              |
| 1:N:453:SER:O    | 1:N:458:LYS:HD2  | 2.15                     | 0.47              |
| 1:A:470:PHE:CZ   | 1:A:519:TYR:HB3  | 2.50                     | 0.47              |
| 1:B:267:LEU:HD21 | 1:B:287:LEU:HD22 | 1.96                     | 0.47              |
| 1:C:669:ILE:HD13 | 1:C:695:LEU:HD22 | 1.97                     | 0.47              |
| 1:F:160:LEU:HB3  | 1:F:170:PHE:CE1  | 2.49                     | 0.47              |
| 1:H:459:THR:OG1  | 1:H:463:LYS:NZ   | 2.41                     | 0.47              |
| 1:H:571:GLY:HA3  | 1:H:572:TYR:HA   | 1.57                     | 0.47              |
| 1:K:452:GLY:HA2  | 1:K:568:ALA:HB3  | 1.96                     | 0.47              |
| 1:L:267:LEU:HD21 | 1:L:287:LEU:HD22 | 1.96                     | 0.47              |
| 1:B:452:GLY:HA2  | 1:B:568:ALA:HB3  | 1.96                     | 0.46              |
| 1:D:452:GLY:HA2  | 1:D:568:ALA:HB3  | 1.96                     | 0.46              |
| 1:D:530:ALA:HB3  | 1:D:532:PRO:HD2  | 1.97                     | 0.46              |
| 1:E:470:PHE:CZ   | 1:E:519:TYR:HB3  | 2.50                     | 0.46              |
| 1:F:107:GLU:OE2  | 1:G:317:HIS:ND1  | 2.41                     | 0.46              |
| 1:F:112:ARG:HD2  | 1:G:274:TYR:HE1  | 1.80                     | 0.46              |
| 1:F:459:THR:OG1  | 1:F:463:LYS:NZ   | 2.41                     | 0.46              |
| 1:G:425:GLU:OE2  | 1:G:429:ARG:NE   | 2.38                     | 0.46              |
| 1:I:530:ALA:HB3  | 1:I:532:PRO:HD2  | 1.96                     | 0.46              |
| 1:J:267:LEU:HD21 | 1:J:287:LEU:HD22 | 1.96                     | 0.46              |
| 1:K:267:LEU:HD21 | 1:K:287:LEU:HD22 | 1.96                     | 0.46              |
| 1:M:212:LEU:O    | 1:M:216:LEU:N    | 2.33                     | 0.46              |
| 1:M:452:GLY:HA2  | 1:M:568:ALA:HB3  | 1.96                     | 0.46              |
| 1:A:267:LEU:HD21 | 1:A:287:LEU:HD22 | 1.96                     | 0.46              |
| 1:B:403:ILE:H    | 1:B:403:ILE:HD12 | 1.79                     | 0.46              |
| 1:C:470:PHE:CZ   | 1:C:519:TYR:HB3  | 2.50                     | 0.46              |
| 1:I:403:ILE:H    | 1:I:403:ILE:HD12 | 1.79                     | 0.46              |
| 1:L:470:PHE:CZ   | 1:L:519:TYR:HB3  | 2.50                     | 0.46              |
| 1:L:669:ILE:HD13 | 1:L:695:LEU:HD22 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:470:PHE:CZ   | 1:N:519:TYR:HB3  | 2.50                     | 0.46              |
| 1:A:645:ASP:O    | 1:A:648:THR:OG1  | 2.27                     | 0.46              |
| 1:B:470:PHE:CZ   | 1:B:519:TYR:HB3  | 2.51                     | 0.46              |
| 1:E:465:LEU:O    | 1:E:469:MET:HG2  | 2.14                     | 0.46              |
| 1:F:530:ALA:HB3  | 1:F:532:PRO:HD2  | 1.96                     | 0.46              |
| 1:G:272:ASP:O    | 1:G:275:GLN:HG3  | 2.16                     | 0.46              |
| 1:G:403:ILE:H    | 1:G:403:ILE:HD12 | 1.79                     | 0.46              |
| 1:G:530:ALA:HB3  | 1:G:532:PRO:HD2  | 1.96                     | 0.46              |
| 1:H:272:ASP:O    | 1:H:275:GLN:HG3  | 2.16                     | 0.46              |
| 1:H:533:GLN:O    | 1:I:492:LYS:NZ   | 2.36                     | 0.46              |
| 1:I:272:ASP:O    | 1:I:275:GLN:HG3  | 2.16                     | 0.46              |
| 1:K:403:ILE:HD12 | 1:K:403:ILE:H    | 1.79                     | 0.46              |
| 1:K:470:PHE:CZ   | 1:K:519:TYR:HB3  | 2.50                     | 0.46              |
| 1:M:669:ILE:HD13 | 1:M:695:LEU:HD22 | 1.97                     | 0.46              |
| 1:N:272:ASP:O    | 1:N:275:GLN:HG3  | 2.16                     | 0.46              |
| 1:A:272:ASP:O    | 1:A:275:GLN:HG3  | 2.16                     | 0.46              |
| 1:F:272:ASP:O    | 1:F:275:GLN:HG3  | 2.16                     | 0.46              |
| 1:F:470:PHE:CZ   | 1:F:519:TYR:HB3  | 2.50                     | 0.46              |
| 1:H:470:PHE:CZ   | 1:H:519:TYR:HB3  | 2.50                     | 0.46              |
| 1:I:465:LEU:O    | 1:I:469:MET:HG2  | 2.14                     | 0.46              |
| 1:J:272:ASP:O    | 1:J:275:GLN:HG3  | 2.16                     | 0.46              |
| 1:J:453:SER:O    | 1:J:458:LYS:HD2  | 2.15                     | 0.46              |
| 1:K:214:ASP:HA   | 1:K:217:LYS:HZ1  | 1.79                     | 0.46              |
| 1:A:453:SER:O    | 1:A:458:LYS:HD2  | 2.15                     | 0.46              |
| 1:B:663:ARG:HA   | 1:B:666:GLU:HB2  | 1.98                     | 0.46              |
| 1:D:267:LEU:HD21 | 1:D:287:LEU:HD22 | 1.96                     | 0.46              |
| 1:E:272:ASP:O    | 1:E:275:GLN:HG3  | 2.16                     | 0.46              |
| 1:E:530:ALA:HB3  | 1:E:532:PRO:HD2  | 1.96                     | 0.46              |
| 1:G:465:LEU:O    | 1:G:469:MET:HG2  | 2.14                     | 0.46              |
| 1:H:310:LEU:HD12 | 1:H:310:LEU:HA   | 1.74                     | 0.46              |
| 1:H:530:ALA:HB3  | 1:H:532:PRO:HD2  | 1.97                     | 0.46              |
| 1:I:537:LEU:HD13 | 1:J:492:LYS:HA   | 1.97                     | 0.46              |
| 1:K:663:ARG:HA   | 1:K:666:GLU:HB2  | 1.98                     | 0.46              |
| 1:L:663:ARG:HA   | 1:L:666:GLU:HB2  | 1.98                     | 0.46              |
| 1:M:267:LEU:HD21 | 1:M:287:LEU:HD22 | 1.96                     | 0.46              |
| 1:M:365:ARG:HG3  | 1:M:365:ARG:NH1  | 2.09                     | 0.46              |
| 1:M:453:SER:O    | 1:M:458:LYS:HD2  | 2.15                     | 0.46              |
| 1:B:669:ILE:HD13 | 1:B:695:LEU:HD22 | 1.97                     | 0.46              |
| 1:C:272:ASP:O    | 1:C:275:GLN:HG3  | 2.16                     | 0.46              |
| 1:C:663:ARG:HA   | 1:C:666:GLU:HB2  | 1.98                     | 0.46              |
| 1:D:453:SER:O    | 1:D:458:LYS:HD2  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:532:PRO:CA   | 1:E:490:VAL:HB   | 2.37                     | 0.46              |
| 1:F:214:ASP:HA   | 1:F:217:LYS:HZ1  | 1.80                     | 0.46              |
| 1:G:267:LEU:HD21 | 1:G:287:LEU:HD22 | 1.96                     | 0.46              |
| 1:G:341:GLN:NE2  | 1:G:357:LYS:HE2  | 2.31                     | 0.46              |
| 1:H:465:LEU:O    | 1:H:469:MET:HG2  | 2.14                     | 0.46              |
| 1:I:341:GLN:NE2  | 1:I:357:LYS:HE2  | 2.31                     | 0.46              |
| 1:M:403:ILE:HG23 | 1:N:678:LEU:HD22 | 1.97                     | 0.46              |
| 1:M:571:GLY:HA3  | 1:M:572:TYR:HA   | 1.57                     | 0.46              |
| 1:E:669:ILE:HD13 | 1:E:695:LEU:HD22 | 1.97                     | 0.46              |
| 1:F:465:LEU:O    | 1:F:469:MET:HG2  | 2.14                     | 0.46              |
| 1:G:669:ILE:HD13 | 1:G:695:LEU:HD22 | 1.97                     | 0.46              |
| 1:I:114:LYS:NZ   | 1:I:250:PHE:O    | 2.43                     | 0.46              |
| 1:I:267:LEU:HD21 | 1:I:287:LEU:HD22 | 1.96                     | 0.46              |
| 1:I:669:ILE:HD13 | 1:I:695:LEU:HD22 | 1.97                     | 0.46              |
| 1:J:112:ARG:HD2  | 1:K:274:TYR:HE1  | 1.81                     | 0.46              |
| 1:L:272:ASP:O    | 1:L:275:GLN:HG3  | 2.16                     | 0.46              |
| 1:L:452:GLY:HA2  | 1:L:568:ALA:HB3  | 1.96                     | 0.46              |
| 1:M:663:ARG:HA   | 1:M:666:GLU:HB2  | 1.98                     | 0.46              |
| 1:N:465:LEU:O    | 1:N:469:MET:HG2  | 2.14                     | 0.46              |
| 1:A:491:SER:C    | 1:G:501:VAL:HB   | 2.41                     | 0.46              |
| 1:B:272:ASP:O    | 1:B:275:GLN:HG3  | 2.16                     | 0.46              |
| 1:C:571:GLY:HA3  | 1:C:572:TYR:HA   | 1.56                     | 0.46              |
| 1:G:114:LYS:NZ   | 1:G:250:PHE:O    | 2.43                     | 0.46              |
| 1:I:111:ARG:HB3  | 1:J:312:ASP:OD2  | 2.16                     | 0.46              |
| 1:K:669:ILE:HD13 | 1:K:695:LEU:HD22 | 1.97                     | 0.46              |
| 1:M:470:PHE:CZ   | 1:M:519:TYR:HB3  | 2.50                     | 0.46              |
| 1:N:530:ALA:HB3  | 1:N:532:PRO:HD2  | 1.97                     | 0.46              |
| 1:A:447:ASN:N    | 1:A:602:ASN:OD1  | 2.43                     | 0.46              |
| 1:C:452:GLY:HA2  | 1:C:568:ALA:HB3  | 1.96                     | 0.46              |
| 1:D:470:PHE:CZ   | 1:D:519:TYR:HB3  | 2.50                     | 0.46              |
| 1:D:663:ARG:HA   | 1:D:666:GLU:HB2  | 1.98                     | 0.46              |
| 1:H:669:ILE:HD13 | 1:H:695:LEU:HD22 | 1.97                     | 0.46              |
| 1:I:108:ILE:HD13 | 1:I:251:ASN:HB3  | 1.98                     | 0.46              |
| 1:I:310:LEU:HA   | 1:I:310:LEU:HD12 | 1.74                     | 0.46              |
| 1:J:447:ASN:N    | 1:J:602:ASN:OD1  | 2.43                     | 0.46              |
| 1:A:492:LYS:NZ   | 1:G:533:GLN:O    | 2.32                     | 0.46              |
| 1:B:341:GLN:NE2  | 1:B:357:LYS:HE2  | 2.31                     | 0.46              |
| 1:F:310:LEU:HD12 | 1:F:310:LEU:HA   | 1.74                     | 0.46              |
| 1:F:669:ILE:HD13 | 1:F:695:LEU:HD22 | 1.97                     | 0.46              |
| 1:G:108:ILE:HD13 | 1:G:251:ASN:HB3  | 1.98                     | 0.46              |
| 1:J:108:ILE:HD13 | 1:J:251:ASN:HB3  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:341:GLN:NE2  | 1:J:357:LYS:HE2  | 2.31                     | 0.46              |
| 1:J:522:ILE:HB   | 1:J:562:ILE:CD1  | 2.46                     | 0.46              |
| 1:K:272:ASP:O    | 1:K:275:GLN:HG3  | 2.16                     | 0.46              |
| 1:K:341:GLN:NE2  | 1:K:357:LYS:HE2  | 2.31                     | 0.46              |
| 1:L:108:ILE:HD13 | 1:L:251:ASN:HB3  | 1.98                     | 0.46              |
| 1:M:272:ASP:O    | 1:M:275:GLN:HG3  | 2.16                     | 0.46              |
| 1:N:669:ILE:HD13 | 1:N:695:LEU:HD22 | 1.97                     | 0.46              |
| 1:A:522:ILE:HB   | 1:A:562:ILE:CD1  | 2.46                     | 0.45              |
| 1:A:540:GLN:OE1  | 1:A:547:LEU:HG   | 2.17                     | 0.45              |
| 1:A:663:ARG:HA   | 1:A:666:GLU:HB2  | 1.98                     | 0.45              |
| 1:C:164:THR:HG21 | 1:C:170:PHE:HB2  | 1.98                     | 0.45              |
| 1:F:108:ILE:HD13 | 1:F:251:ASN:HB3  | 1.98                     | 0.45              |
| 1:F:522:ILE:HB   | 1:F:562:ILE:CD1  | 2.46                     | 0.45              |
| 1:G:540:GLN:OE1  | 1:G:547:LEU:HG   | 2.17                     | 0.45              |
| 1:H:108:ILE:HD13 | 1:H:251:ASN:HB3  | 1.98                     | 0.45              |
| 1:I:540:GLN:OE1  | 1:I:547:LEU:HG   | 2.17                     | 0.45              |
| 1:J:497:THR:HB   | 1:K:489:ALA:O    | 2.16                     | 0.45              |
| 1:M:537:LEU:HD13 | 1:N:492:LYS:HA   | 1.98                     | 0.45              |
| 1:A:108:ILE:HD13 | 1:A:251:ASN:HB3  | 1.98                     | 0.45              |
| 1:A:341:GLN:NE2  | 1:A:357:LYS:HE2  | 2.31                     | 0.45              |
| 1:B:540:GLN:OE1  | 1:B:547:LEU:HG   | 2.17                     | 0.45              |
| 1:C:108:ILE:HD13 | 1:C:251:ASN:HB3  | 1.98                     | 0.45              |
| 1:C:341:GLN:NE2  | 1:C:357:LYS:HE2  | 2.31                     | 0.45              |
| 1:D:272:ASP:O    | 1:D:275:GLN:HG3  | 2.16                     | 0.45              |
| 1:E:310:LEU:O    | 1:E:314:THR:OG1  | 2.30                     | 0.45              |
| 1:F:341:GLN:NE2  | 1:F:357:LYS:HE2  | 2.31                     | 0.45              |
| 1:G:470:PHE:CZ   | 1:G:519:TYR:HB3  | 2.50                     | 0.45              |
| 1:H:522:ILE:HB   | 1:H:562:ILE:CD1  | 2.47                     | 0.45              |
| 1:J:540:GLN:OE1  | 1:J:547:LEU:HG   | 2.17                     | 0.45              |
| 1:K:108:ILE:HD13 | 1:K:251:ASN:HB3  | 1.98                     | 0.45              |
| 1:K:164:THR:HG21 | 1:K:170:PHE:HB2  | 1.99                     | 0.45              |
| 1:L:164:THR:HG21 | 1:L:170:PHE:HB2  | 1.99                     | 0.45              |
| 1:L:341:GLN:NE2  | 1:L:357:LYS:HE2  | 2.31                     | 0.45              |
| 1:B:108:ILE:HD13 | 1:B:251:ASN:HB3  | 1.98                     | 0.45              |
| 1:B:164:THR:HG21 | 1:B:170:PHE:HB2  | 1.99                     | 0.45              |
| 1:D:540:GLN:OE1  | 1:D:547:LEU:HG   | 2.17                     | 0.45              |
| 1:H:330:VAL:HG21 | 1:H:366:LYS:NZ   | 2.32                     | 0.45              |
| 1:I:470:PHE:CZ   | 1:I:519:TYR:HB3  | 2.50                     | 0.45              |
| 1:J:425:GLU:OE2  | 1:J:429:ARG:NE   | 2.38                     | 0.45              |
| 1:J:663:ARG:HA   | 1:J:666:GLU:HB2  | 1.98                     | 0.45              |
| 1:K:403:ILE:HG23 | 1:L:678:LEU:HD22 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:540:GLN:OE1  | 1:K:547:LEU:HG   | 2.17                     | 0.45              |
| 1:L:280:VAL:HB   | 1:L:376:VAL:CA   | 2.47                     | 0.45              |
| 1:B:214:ASP:HA   | 1:B:217:LYS:HZ1  | 1.80                     | 0.45              |
| 1:E:540:GLN:OE1  | 1:E:547:LEU:HG   | 2.17                     | 0.45              |
| 1:F:663:ARG:HA   | 1:F:666:GLU:HB2  | 1.98                     | 0.45              |
| 1:G:310:LEU:HA   | 1:G:310:LEU:HD12 | 1.74                     | 0.45              |
| 1:H:341:GLN:NE2  | 1:H:357:LYS:HE2  | 2.31                     | 0.45              |
| 1:I:164:THR:HG21 | 1:I:170:PHE:HB2  | 1.99                     | 0.45              |
| 1:J:164:THR:HG21 | 1:J:170:PHE:HB2  | 1.99                     | 0.45              |
| 1:K:280:VAL:HB   | 1:K:376:VAL:CA   | 2.47                     | 0.45              |
| 1:M:108:ILE:HD13 | 1:M:251:ASN:HB3  | 1.98                     | 0.45              |
| 1:N:108:ILE:HD13 | 1:N:251:ASN:HB3  | 1.98                     | 0.45              |
| 1:A:425:GLU:OE2  | 1:A:429:ARG:NE   | 2.38                     | 0.45              |
| 1:A:669:ILE:HD13 | 1:A:695:LEU:HD22 | 1.97                     | 0.45              |
| 1:B:280:VAL:HB   | 1:B:376:VAL:CA   | 2.47                     | 0.45              |
| 1:C:280:VAL:HB   | 1:C:376:VAL:CA   | 2.47                     | 0.45              |
| 1:C:540:GLN:OE1  | 1:C:547:LEU:HG   | 2.17                     | 0.45              |
| 1:D:108:ILE:HD13 | 1:D:251:ASN:HB3  | 1.98                     | 0.45              |
| 1:D:365:ARG:HG3  | 1:D:365:ARG:NH1  | 2.09                     | 0.45              |
| 1:E:447:ASN:N    | 1:E:602:ASN:OD1  | 2.43                     | 0.45              |
| 1:G:164:THR:HG21 | 1:G:170:PHE:HB2  | 1.99                     | 0.45              |
| 1:H:663:ARG:HA   | 1:H:666:GLU:HB2  | 1.98                     | 0.45              |
| 1:J:669:ILE:HD13 | 1:J:695:LEU:HD22 | 1.97                     | 0.45              |
| 1:M:382:ASP:HA   | 1:M:385:GLU:OE1  | 2.17                     | 0.45              |
| 1:M:540:GLN:OE1  | 1:M:547:LEU:HG   | 2.17                     | 0.45              |
| 1:N:519:TYR:HA   | 1:N:559:ASN:O    | 2.17                     | 0.45              |
| 1:N:540:GLN:OE1  | 1:N:547:LEU:HG   | 2.17                     | 0.45              |
| 1:A:164:THR:HG21 | 1:A:170:PHE:HB2  | 1.99                     | 0.45              |
| 1:A:516:ARG:NE   | 1:A:516:ARG:HA   | 2.32                     | 0.45              |
| 1:C:522:ILE:HB   | 1:C:562:ILE:CD1  | 2.46                     | 0.45              |
| 1:D:189:LEU:HD23 | 1:D:191:PHE:HZ   | 1.82                     | 0.45              |
| 1:D:280:VAL:HB   | 1:D:376:VAL:CA   | 2.47                     | 0.45              |
| 1:E:108:ILE:HD13 | 1:E:251:ASN:HB3  | 1.98                     | 0.45              |
| 1:E:519:TYR:HA   | 1:E:559:ASN:O    | 2.17                     | 0.45              |
| 1:F:519:TYR:HA   | 1:F:559:ASN:O    | 2.17                     | 0.45              |
| 1:F:540:GLN:OE1  | 1:F:547:LEU:HG   | 2.17                     | 0.45              |
| 1:H:532:PRO:HB3  | 1:I:491:SER:N    | 2.17                     | 0.45              |
| 1:H:540:GLN:OE1  | 1:H:547:LEU:HG   | 2.17                     | 0.45              |
| 1:K:382:ASP:HA   | 1:K:385:GLU:OE1  | 2.17                     | 0.45              |
| 1:K:459:THR:OG1  | 1:K:463:LYS:NZ   | 2.41                     | 0.45              |
| 1:K:516:ARG:HA   | 1:K:516:ARG:NE   | 2.32                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:659:ARG:HB3  | 1:K:660:PRO:HD3  | 1.99                     | 0.45              |
| 1:L:540:GLN:OE1  | 1:L:547:LEU:HG   | 2.17                     | 0.45              |
| 1:M:164:THR:HG21 | 1:M:170:PHE:HB2  | 1.99                     | 0.45              |
| 1:M:189:LEU:HD23 | 1:M:191:PHE:HZ   | 1.82                     | 0.45              |
| 1:M:280:VAL:HB   | 1:M:376:VAL:CA   | 2.47                     | 0.45              |
| 1:A:280:VAL:HB   | 1:A:376:VAL:CA   | 2.47                     | 0.45              |
| 1:A:382:ASP:HA   | 1:A:385:GLU:OE1  | 2.17                     | 0.45              |
| 1:A:516:ARG:HG2  | 1:A:516:ARG:HH11 | 1.82                     | 0.45              |
| 1:A:589:LEU:O    | 1:A:593:PHE:N    | 2.33                     | 0.45              |
| 1:B:200:ALA:HA   | 1:B:210:LYS:HA   | 1.99                     | 0.45              |
| 1:B:382:ASP:HA   | 1:B:385:GLU:OE1  | 2.17                     | 0.45              |
| 1:B:516:ARG:NE   | 1:B:516:ARG:HA   | 2.32                     | 0.45              |
| 1:B:659:ARG:HB3  | 1:B:660:PRO:HD3  | 1.99                     | 0.45              |
| 1:C:210:LYS:NZ   | 1:C:214:ASP:OD2  | 2.36                     | 0.45              |
| 1:C:519:TYR:HA   | 1:C:559:ASN:O    | 2.17                     | 0.45              |
| 1:D:164:THR:HG21 | 1:D:170:PHE:HB2  | 1.99                     | 0.45              |
| 1:D:341:GLN:NE2  | 1:D:357:LYS:HE2  | 2.31                     | 0.45              |
| 1:D:382:ASP:HA   | 1:D:385:GLU:OE1  | 2.17                     | 0.45              |
| 1:E:200:ALA:HA   | 1:E:210:LYS:HA   | 1.99                     | 0.45              |
| 1:E:382:ASP:HA   | 1:E:385:GLU:OE1  | 2.17                     | 0.45              |
| 1:G:330:VAL:HG21 | 1:G:366:LYS:NZ   | 2.32                     | 0.45              |
| 1:H:470:PHE:HZ   | 1:H:519:TYR:HB3  | 1.82                     | 0.45              |
| 1:I:107:GLU:OE2  | 1:J:317:HIS:ND1  | 2.41                     | 0.45              |
| 1:I:330:VAL:HG21 | 1:I:366:LYS:NZ   | 2.32                     | 0.45              |
| 1:J:280:VAL:HB   | 1:J:376:VAL:CA   | 2.47                     | 0.45              |
| 1:J:382:ASP:HA   | 1:J:385:GLU:OE1  | 2.17                     | 0.45              |
| 1:J:516:ARG:NE   | 1:J:516:ARG:HA   | 2.32                     | 0.45              |
| 1:L:214:ASP:HA   | 1:L:217:LYS:HZ1  | 1.82                     | 0.45              |
| 1:M:341:GLN:NE2  | 1:M:357:LYS:HE2  | 2.31                     | 0.45              |
| 1:M:522:ILE:HB   | 1:M:562:ILE:CD1  | 2.46                     | 0.45              |
| 1:N:310:LEU:O    | 1:N:314:THR:OG1  | 2.30                     | 0.45              |
| 1:N:330:VAL:HG21 | 1:N:366:LYS:NZ   | 2.32                     | 0.45              |
| 1:A:571:GLY:HA3  | 1:A:572:TYR:HA   | 1.57                     | 0.45              |
| 1:B:470:PHE:HZ   | 1:B:519:TYR:HB3  | 1.82                     | 0.45              |
| 1:B:571:GLY:HA3  | 1:B:572:TYR:HA   | 1.57                     | 0.45              |
| 1:C:214:ASP:HA   | 1:C:217:LYS:HZ1  | 1.82                     | 0.45              |
| 1:C:516:ARG:HG2  | 1:C:516:ARG:HH11 | 1.82                     | 0.45              |
| 1:D:486:ASP:HB3  | 1:D:497:THR:N    | 2.32                     | 0.45              |
| 1:E:114:LYS:NZ   | 1:E:250:PHE:O    | 2.43                     | 0.45              |
| 1:E:330:VAL:HG21 | 1:E:366:LYS:NZ   | 2.32                     | 0.45              |
| 1:E:522:ILE:HB   | 1:E:562:ILE:CD1  | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:200:ALA:HA   | 1:F:210:LYS:HA   | 1.99                     | 0.45              |
| 1:F:382:ASP:HA   | 1:F:385:GLU:OE1  | 2.17                     | 0.45              |
| 1:F:470:PHE:HZ   | 1:F:519:TYR:HB3  | 1.82                     | 0.45              |
| 1:G:539:LEU:O    | 1:G:543:ASP:N    | 2.50                     | 0.45              |
| 1:H:200:ALA:HA   | 1:H:210:LYS:HA   | 1.99                     | 0.45              |
| 1:H:382:ASP:HA   | 1:H:385:GLU:OE1  | 2.17                     | 0.45              |
| 1:H:519:TYR:HA   | 1:H:559:ASN:O    | 2.17                     | 0.45              |
| 1:H:596:GLU:O    | 1:H:600:ARG:HG2  | 2.16                     | 0.45              |
| 1:I:539:LEU:O    | 1:I:543:ASP:N    | 2.50                     | 0.45              |
| 1:J:516:ARG:HG2  | 1:J:516:ARG:HH11 | 1.82                     | 0.45              |
| 1:J:596:GLU:O    | 1:J:600:ARG:HG2  | 2.16                     | 0.45              |
| 1:K:200:ALA:HA   | 1:K:210:LYS:HA   | 1.99                     | 0.45              |
| 1:L:470:PHE:HZ   | 1:L:519:TYR:HB3  | 1.82                     | 0.45              |
| 1:L:519:TYR:HA   | 1:L:559:ASN:O    | 2.17                     | 0.45              |
| 1:L:522:ILE:HB   | 1:L:562:ILE:CD1  | 2.46                     | 0.45              |
| 1:L:539:LEU:O    | 1:L:543:ASP:N    | 2.50                     | 0.45              |
| 1:M:486:ASP:HB3  | 1:M:497:THR:N    | 2.32                     | 0.45              |
| 1:N:200:ALA:HA   | 1:N:210:LYS:HA   | 1.99                     | 0.45              |
| 1:N:382:ASP:HA   | 1:N:385:GLU:OE1  | 2.17                     | 0.45              |
| 1:A:596:GLU:O    | 1:A:600:ARG:HG2  | 2.16                     | 0.45              |
| 1:C:470:PHE:HZ   | 1:C:519:TYR:HB3  | 1.82                     | 0.45              |
| 1:D:522:ILE:HB   | 1:D:562:ILE:CD1  | 2.46                     | 0.45              |
| 1:E:280:VAL:HB   | 1:E:376:VAL:CA   | 2.47                     | 0.45              |
| 1:E:486:ASP:HB3  | 1:E:497:THR:N    | 2.32                     | 0.45              |
| 1:E:596:GLU:O    | 1:E:600:ARG:HG2  | 2.16                     | 0.45              |
| 1:G:519:TYR:HA   | 1:G:559:ASN:O    | 2.17                     | 0.45              |
| 1:H:317:HIS:ND1  | 1:N:107:GLU:OE2  | 2.42                     | 0.45              |
| 1:I:516:ARG:NE   | 1:I:516:ARG:HA   | 2.32                     | 0.45              |
| 1:I:519:TYR:HA   | 1:I:559:ASN:O    | 2.17                     | 0.45              |
| 1:I:596:GLU:O    | 1:I:600:ARG:HG2  | 2.16                     | 0.45              |
| 1:J:589:LEU:O    | 1:J:593:PHE:N    | 2.33                     | 0.45              |
| 1:K:189:LEU:HD23 | 1:K:191:PHE:HZ   | 1.82                     | 0.45              |
| 1:K:470:PHE:HZ   | 1:K:519:TYR:HB3  | 1.82                     | 0.45              |
| 1:K:486:ASP:HB3  | 1:K:497:THR:N    | 2.32                     | 0.45              |
| 1:K:519:TYR:HA   | 1:K:559:ASN:O    | 2.17                     | 0.45              |
| 1:L:210:LYS:NZ   | 1:L:214:ASP:OD2  | 2.36                     | 0.45              |
| 1:L:571:GLY:HA3  | 1:L:572:TYR:HA   | 1.57                     | 0.45              |
| 1:L:659:ARG:HB3  | 1:L:660:PRO:HD3  | 1.99                     | 0.45              |
| 1:M:470:PHE:HZ   | 1:M:519:TYR:HB3  | 1.82                     | 0.45              |
| 1:N:447:ASN:N    | 1:N:602:ASN:OD1  | 2.43                     | 0.45              |
| 1:N:596:GLU:O    | 1:N:600:ARG:HG2  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:519:TYR:HA   | 1:A:559:ASN:O   | 2.17                     | 0.45              |
| 1:B:486:ASP:HB3  | 1:B:497:THR:N   | 2.32                     | 0.45              |
| 1:C:200:ALA:HA   | 1:C:210:LYS:HA  | 1.99                     | 0.45              |
| 1:C:659:ARG:HB3  | 1:C:660:PRO:HD3 | 1.99                     | 0.45              |
| 1:D:516:ARG:NE   | 1:D:516:ARG:HA  | 2.32                     | 0.45              |
| 1:D:519:TYR:HA   | 1:D:559:ASN:O   | 2.17                     | 0.45              |
| 1:D:534:VAL:CA   | 1:E:492:LYS:HD2 | 2.46                     | 0.45              |
| 1:E:456:VAL:HG21 | 1:E:607:PHE:CB  | 2.47                     | 0.45              |
| 1:E:470:PHE:HZ   | 1:E:519:TYR:HB3 | 1.82                     | 0.45              |
| 1:F:596:GLU:O    | 1:F:600:ARG:HG2 | 2.16                     | 0.45              |
| 1:G:482:SER:HB3  | 1:G:529:LYS:HB3 | 1.99                     | 0.45              |
| 1:H:164:THR:HG21 | 1:H:170:PHE:HB2 | 1.99                     | 0.45              |
| 1:I:482:SER:HB3  | 1:I:529:LYS:HB3 | 1.99                     | 0.45              |
| 1:I:486:ASP:HB3  | 1:I:497:THR:N   | 2.32                     | 0.45              |
| 1:K:330:VAL:HG21 | 1:K:366:LYS:NZ  | 2.32                     | 0.45              |
| 1:L:200:ALA:HA   | 1:L:210:LYS:HA  | 1.99                     | 0.45              |
| 1:L:447:ASN:N    | 1:L:602:ASN:OD1 | 2.43                     | 0.45              |
| 1:L:456:VAL:HG21 | 1:L:607:PHE:CB  | 2.47                     | 0.45              |
| 1:M:516:ARG:NE   | 1:M:516:ARG:HA  | 2.32                     | 0.45              |
| 1:N:280:VAL:HB   | 1:N:376:VAL:CA  | 2.47                     | 0.45              |
| 1:N:516:ARG:HA   | 1:N:516:ARG:NE  | 2.32                     | 0.45              |
| 1:N:522:ILE:HB   | 1:N:562:ILE:CD1 | 2.46                     | 0.45              |
| 1:A:140:ASN:O    | 1:B:325:THR:OG1 | 2.34                     | 0.44              |
| 1:A:482:SER:HB3  | 1:A:529:LYS:HB3 | 1.99                     | 0.44              |
| 1:A:655:VAL:HG23 | 1:A:656:MET:HG2 | 1.99                     | 0.44              |
| 1:B:189:LEU:HD23 | 1:B:191:PHE:HZ  | 1.82                     | 0.44              |
| 1:C:456:VAL:HG21 | 1:C:607:PHE:CB  | 2.47                     | 0.44              |
| 1:C:486:ASP:HB3  | 1:C:497:THR:N   | 2.32                     | 0.44              |
| 1:C:539:LEU:O    | 1:C:543:ASP:N   | 2.50                     | 0.44              |
| 1:D:200:ALA:HA   | 1:D:210:LYS:HA  | 1.99                     | 0.44              |
| 1:D:214:ASP:HA   | 1:D:217:LYS:HZ1 | 1.82                     | 0.44              |
| 1:F:164:THR:HG21 | 1:F:170:PHE:HB2 | 1.99                     | 0.44              |
| 1:F:454:THR:HA   | 1:F:458:LYS:HD2 | 2.00                     | 0.44              |
| 1:F:486:ASP:HB3  | 1:F:497:THR:N   | 2.32                     | 0.44              |
| 1:G:280:VAL:HB   | 1:G:376:VAL:CA  | 2.47                     | 0.44              |
| 1:G:486:ASP:HB3  | 1:G:497:THR:N   | 2.32                     | 0.44              |
| 1:G:516:ARG:NE   | 1:G:516:ARG:HA  | 2.32                     | 0.44              |
| 1:G:522:ILE:HB   | 1:G:562:ILE:CD1 | 2.46                     | 0.44              |
| 1:H:486:ASP:HB3  | 1:H:497:THR:N   | 2.32                     | 0.44              |
| 1:I:663:ARG:HA   | 1:I:666:GLU:HB2 | 1.98                     | 0.44              |
| 1:J:470:PHE:HZ   | 1:J:519:TYR:HB3 | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:486:ASP:HB3  | 1:J:497:THR:N    | 2.32                     | 0.44              |
| 1:J:655:VAL:HG23 | 1:J:656:MET:HG2  | 1.99                     | 0.44              |
| 1:K:596:GLU:O    | 1:K:600:ARG:HG2  | 2.16                     | 0.44              |
| 1:L:486:ASP:HB3  | 1:L:497:THR:N    | 2.32                     | 0.44              |
| 1:L:516:ARG:HG2  | 1:L:516:ARG:HH11 | 1.82                     | 0.44              |
| 1:N:486:ASP:HB3  | 1:N:497:THR:N    | 2.32                     | 0.44              |
| 1:A:470:PHE:HZ   | 1:A:519:TYR:HB3  | 1.82                     | 0.44              |
| 1:A:486:ASP:HB3  | 1:A:497:THR:N    | 2.32                     | 0.44              |
| 1:B:456:VAL:HG21 | 1:B:607:PHE:CB   | 2.47                     | 0.44              |
| 1:B:459:THR:OG1  | 1:B:463:LYS:NZ   | 2.41                     | 0.44              |
| 1:B:519:TYR:HA   | 1:B:559:ASN:O    | 2.17                     | 0.44              |
| 1:B:522:ILE:HB   | 1:B:562:ILE:CD1  | 2.47                     | 0.44              |
| 1:B:566:SER:OG   | 1:B:567:ASN:N    | 2.50                     | 0.44              |
| 1:B:655:VAL:HG23 | 1:B:656:MET:HG2  | 1.99                     | 0.44              |
| 1:C:516:ARG:HA   | 1:C:516:ARG:NE   | 2.32                     | 0.44              |
| 1:D:470:PHE:HZ   | 1:D:519:TYR:HB3  | 1.82                     | 0.44              |
| 1:D:596:GLU:O    | 1:D:600:ARG:HG2  | 2.16                     | 0.44              |
| 1:E:112:ARG:HD2  | 1:F:274:TYR:HE1  | 1.81                     | 0.44              |
| 1:E:516:ARG:NE   | 1:E:516:ARG:HA   | 2.32                     | 0.44              |
| 1:F:482:SER:HB3  | 1:F:529:LYS:HB3  | 1.99                     | 0.44              |
| 1:F:516:ARG:HA   | 1:F:516:ARG:NE   | 2.32                     | 0.44              |
| 1:G:596:GLU:O    | 1:G:600:ARG:HG2  | 2.16                     | 0.44              |
| 1:G:663:ARG:HA   | 1:G:666:GLU:HB2  | 1.98                     | 0.44              |
| 1:H:516:ARG:HG2  | 1:H:516:ARG:HH11 | 1.82                     | 0.44              |
| 1:I:280:VAL:HB   | 1:I:376:VAL:CA   | 2.47                     | 0.44              |
| 1:J:137:ALA:HA   | 1:J:140:ASN:HB2  | 2.00                     | 0.44              |
| 1:J:539:LEU:O    | 1:J:543:ASP:N    | 2.50                     | 0.44              |
| 1:J:571:GLY:HA3  | 1:J:572:TYR:HA   | 1.57                     | 0.44              |
| 1:K:539:LEU:O    | 1:K:543:ASP:N    | 2.50                     | 0.44              |
| 1:K:655:VAL:HG23 | 1:K:656:MET:HG2  | 1.99                     | 0.44              |
| 1:M:594:ARG:HB3  | 1:M:596:GLU:OE1  | 2.18                     | 0.44              |
| 1:N:164:THR:HG21 | 1:N:170:PHE:HB2  | 1.98                     | 0.44              |
| 1:N:341:GLN:NE2  | 1:N:357:LYS:HE2  | 2.31                     | 0.44              |
| 1:N:456:VAL:HG21 | 1:N:607:PHE:CB   | 2.47                     | 0.44              |
| 1:A:137:ALA:HA   | 1:A:140:ASN:HB2  | 2.00                     | 0.44              |
| 1:A:200:ALA:HA   | 1:A:210:LYS:HA   | 1.99                     | 0.44              |
| 1:A:438:PHE:CE1  | 1:B:633:LYS:HE3  | 2.52                     | 0.44              |
| 1:A:539:LEU:O    | 1:A:543:ASP:N    | 2.50                     | 0.44              |
| 1:A:572:TYR:CG   | 1:A:610:LEU:HD23 | 2.53                     | 0.44              |
| 1:B:330:VAL:HG21 | 1:B:366:LYS:NZ   | 2.32                     | 0.44              |
| 1:B:596:GLU:O    | 1:B:600:ARG:HG2  | 2.16                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:212:LEU:O    | 1:C:216:LEU:N    | 2.33                     | 0.44              |
| 1:C:655:VAL:HG23 | 1:C:656:MET:HG2  | 1.99                     | 0.44              |
| 1:D:594:ARG:HB3  | 1:D:596:GLU:OE1  | 2.18                     | 0.44              |
| 1:E:164:THR:HG21 | 1:E:170:PHE:HB2  | 1.99                     | 0.44              |
| 1:E:341:GLN:NE2  | 1:E:357:LYS:HE2  | 2.31                     | 0.44              |
| 1:E:393:ILE:HG13 | 1:E:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:E:482:SER:HB3  | 1:E:529:LYS:HB3  | 1.99                     | 0.44              |
| 1:F:516:ARG:HG2  | 1:F:516:ARG:HH11 | 1.82                     | 0.44              |
| 1:G:137:ALA:HA   | 1:G:140:ASN:HB2  | 2.00                     | 0.44              |
| 1:G:470:PHE:HZ   | 1:G:519:TYR:HB3  | 1.82                     | 0.44              |
| 1:H:454:THR:HA   | 1:H:458:LYS:HD2  | 2.00                     | 0.44              |
| 1:I:522:ILE:HB   | 1:I:562:ILE:CD1  | 2.46                     | 0.44              |
| 1:J:200:ALA:HA   | 1:J:210:LYS:HA   | 1.99                     | 0.44              |
| 1:J:482:SER:HB3  | 1:J:529:LYS:HB3  | 1.99                     | 0.44              |
| 1:J:519:TYR:HA   | 1:J:559:ASN:O    | 2.17                     | 0.44              |
| 1:K:137:ALA:HA   | 1:K:140:ASN:HB2  | 2.00                     | 0.44              |
| 1:K:566:SER:OG   | 1:K:567:ASN:N    | 2.50                     | 0.44              |
| 1:L:330:VAL:HG21 | 1:L:366:LYS:NZ   | 2.32                     | 0.44              |
| 1:L:516:ARG:NE   | 1:L:516:ARG:HA   | 2.32                     | 0.44              |
| 1:L:594:ARG:HB3  | 1:L:596:GLU:OE1  | 2.18                     | 0.44              |
| 1:L:655:VAL:HG23 | 1:L:656:MET:HG2  | 2.00                     | 0.44              |
| 1:M:134:LEU:HD12 | 1:M:134:LEU:HA   | 1.78                     | 0.44              |
| 1:M:200:ALA:HA   | 1:M:210:LYS:HA   | 1.99                     | 0.44              |
| 1:M:310:LEU:HD12 | 1:M:310:LEU:HA   | 1.74                     | 0.44              |
| 1:M:330:VAL:HG21 | 1:M:366:LYS:NZ   | 2.32                     | 0.44              |
| 1:M:519:TYR:HA   | 1:M:559:ASN:O    | 2.17                     | 0.44              |
| 1:M:655:VAL:HG23 | 1:M:656:MET:HG2  | 1.99                     | 0.44              |
| 1:N:470:PHE:HZ   | 1:N:519:TYR:HB3  | 1.82                     | 0.44              |
| 1:N:482:SER:HB3  | 1:N:529:LYS:HB3  | 1.99                     | 0.44              |
| 1:A:523:LEU:HA   | 1:A:563:ILE:O    | 2.18                     | 0.44              |
| 1:B:271:ARG:NE   | 1:B:282:LEU:O    | 2.32                     | 0.44              |
| 1:B:539:LEU:O    | 1:B:543:ASP:N    | 2.50                     | 0.44              |
| 1:B:572:TYR:CG   | 1:B:610:LEU:HD23 | 2.53                     | 0.44              |
| 1:C:382:ASP:HA   | 1:C:385:GLU:OE1  | 2.17                     | 0.44              |
| 1:C:523:LEU:HA   | 1:C:563:ILE:O    | 2.18                     | 0.44              |
| 1:D:429:ARG:HD3  | 1:E:671:ASP:CG   | 2.42                     | 0.44              |
| 1:E:516:ARG:HG2  | 1:E:516:ARG:HH11 | 1.82                     | 0.44              |
| 1:E:594:ARG:HB3  | 1:E:596:GLU:OE1  | 2.18                     | 0.44              |
| 1:E:655:VAL:HG23 | 1:E:656:MET:HG2  | 1.99                     | 0.44              |
| 1:F:566:SER:OG   | 1:F:567:ASN:N    | 2.50                     | 0.44              |
| 1:H:482:SER:HB3  | 1:H:529:LYS:HB3  | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:516:ARG:NE   | 1:H:516:ARG:HA   | 2.32                     | 0.44              |
| 1:H:566:SER:OG   | 1:H:567:ASN:N    | 2.50                     | 0.44              |
| 1:I:137:ALA:HA   | 1:I:140:ASN:HB2  | 2.00                     | 0.44              |
| 1:J:523:LEU:HA   | 1:J:563:ILE:O    | 2.18                     | 0.44              |
| 1:J:572:TYR:CG   | 1:J:610:LEU:HD23 | 2.53                     | 0.44              |
| 1:K:454:THR:HA   | 1:K:458:LYS:HD2  | 2.00                     | 0.44              |
| 1:K:522:ILE:HB   | 1:K:562:ILE:CD1  | 2.46                     | 0.44              |
| 1:M:214:ASP:HA   | 1:M:217:LYS:HZ1  | 1.82                     | 0.44              |
| 1:M:393:ILE:HG13 | 1:M:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:M:516:ARG:HG2  | 1:M:516:ARG:HH11 | 1.82                     | 0.44              |
| 1:M:596:GLU:O    | 1:M:600:ARG:HG2  | 2.16                     | 0.44              |
| 1:N:523:LEU:HA   | 1:N:563:ILE:O    | 2.18                     | 0.44              |
| 1:N:655:VAL:HG23 | 1:N:656:MET:HG2  | 1.99                     | 0.44              |
| 1:A:393:ILE:HG13 | 1:A:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:A:454:THR:HA   | 1:A:458:LYS:HD2  | 2.00                     | 0.44              |
| 1:A:573:GLU:N    | 1:A:574:ALA:CA   | 2.81                     | 0.44              |
| 1:A:659:ARG:HB3  | 1:A:660:PRO:HD3  | 1.99                     | 0.44              |
| 1:B:137:ALA:HA   | 1:B:140:ASN:HB2  | 2.00                     | 0.44              |
| 1:B:482:SER:HB3  | 1:B:529:LYS:HB3  | 1.99                     | 0.44              |
| 1:C:566:SER:OG   | 1:C:567:ASN:N    | 2.50                     | 0.44              |
| 1:C:594:ARG:HB3  | 1:C:596:GLU:OE1  | 2.18                     | 0.44              |
| 1:D:393:ILE:HG13 | 1:D:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:D:532:PRO:HA   | 1:E:490:VAL:CB   | 2.37                     | 0.44              |
| 1:D:655:VAL:HG23 | 1:D:656:MET:HG2  | 1.99                     | 0.44              |
| 1:E:523:LEU:HA   | 1:E:563:ILE:O    | 2.18                     | 0.44              |
| 1:E:663:ARG:HA   | 1:E:666:GLU:HB2  | 1.98                     | 0.44              |
| 1:F:280:VAL:HB   | 1:F:376:VAL:CA   | 2.47                     | 0.44              |
| 1:G:393:ILE:HG13 | 1:G:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:G:454:THR:HA   | 1:G:458:LYS:HD2  | 2.00                     | 0.44              |
| 1:G:566:SER:OG   | 1:G:567:ASN:N    | 2.50                     | 0.44              |
| 1:H:280:VAL:HB   | 1:H:376:VAL:CA   | 2.47                     | 0.44              |
| 1:H:393:ILE:HG13 | 1:H:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:I:393:ILE:HG13 | 1:I:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:I:454:THR:HA   | 1:I:458:LYS:HD2  | 2.00                     | 0.44              |
| 1:I:566:SER:OG   | 1:I:567:ASN:N    | 2.50                     | 0.44              |
| 1:J:393:ILE:HG13 | 1:J:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:J:454:THR:HA   | 1:J:458:LYS:HD2  | 2.00                     | 0.44              |
| 1:K:572:TYR:CG   | 1:K:610:LEU:HD23 | 2.53                     | 0.44              |
| 1:K:594:ARG:HB3  | 1:K:596:GLU:OE1  | 2.18                     | 0.44              |
| 1:L:212:LEU:O    | 1:L:216:LEU:N    | 2.33                     | 0.44              |
| 1:M:523:LEU:HA   | 1:M:563:ILE:O    | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:393:ILE:HG13 | 1:N:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:N:454:THR:HA   | 1:N:458:LYS:HD2  | 2.00                     | 0.44              |
| 1:N:594:ARG:HB3  | 1:N:596:GLU:OE1  | 2.18                     | 0.44              |
| 1:N:663:ARG:HA   | 1:N:666:GLU:HB2  | 1.98                     | 0.44              |
| 1:B:151:GLU:N    | 1:B:186:ASN:O    | 2.30                     | 0.44              |
| 1:B:454:THR:HA   | 1:B:458:LYS:HD2  | 2.00                     | 0.44              |
| 1:B:594:ARG:HB3  | 1:B:596:GLU:OE1  | 2.18                     | 0.44              |
| 1:C:330:VAL:HG21 | 1:C:366:LYS:NZ   | 2.32                     | 0.44              |
| 1:C:501:VAL:HB   | 1:D:491:SER:O    | 2.17                     | 0.44              |
| 1:D:330:VAL:HG21 | 1:D:366:LYS:NZ   | 2.32                     | 0.44              |
| 1:D:659:ARG:HB3  | 1:D:660:PRO:HD3  | 1.99                     | 0.44              |
| 1:E:454:THR:HA   | 1:E:458:LYS:HD2  | 2.00                     | 0.44              |
| 1:F:393:ILE:HG13 | 1:F:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:G:382:ASP:HA   | 1:G:385:GLU:OE1  | 2.17                     | 0.44              |
| 1:G:573:GLU:N    | 1:G:574:ALA:CA   | 2.81                     | 0.44              |
| 1:H:456:VAL:HG21 | 1:H:607:PHE:CB   | 2.47                     | 0.44              |
| 1:I:470:PHE:HZ   | 1:I:519:TYR:HB3  | 1.82                     | 0.44              |
| 1:I:573:GLU:N    | 1:I:574:ALA:CA   | 2.81                     | 0.44              |
| 1:I:655:VAL:HG23 | 1:I:656:MET:HG2  | 1.99                     | 0.44              |
| 1:J:456:VAL:HG21 | 1:J:607:PHE:CB   | 2.47                     | 0.44              |
| 1:J:573:GLU:N    | 1:J:574:ALA:CA   | 2.81                     | 0.44              |
| 1:J:659:ARG:HB3  | 1:J:660:PRO:HD3  | 1.99                     | 0.44              |
| 1:K:151:GLU:N    | 1:K:186:ASN:O    | 2.30                     | 0.44              |
| 1:K:482:SER:HB3  | 1:K:529:LYS:HB3  | 1.99                     | 0.44              |
| 1:K:516:ARG:HG2  | 1:K:516:ARG:HH11 | 1.82                     | 0.44              |
| 1:L:523:LEU:HA   | 1:L:563:ILE:O    | 2.18                     | 0.44              |
| 1:L:572:TYR:CG   | 1:L:610:LEU:HD23 | 2.53                     | 0.44              |
| 1:N:516:ARG:HG2  | 1:N:516:ARG:HH11 | 1.82                     | 0.44              |
| 1:A:456:VAL:HG21 | 1:A:607:PHE:CB   | 2.47                     | 0.44              |
| 1:A:491:SER:N    | 1:G:497:THR:HG22 | 2.33                     | 0.44              |
| 1:C:572:TYR:CG   | 1:C:610:LEU:HD23 | 2.53                     | 0.44              |
| 1:C:596:GLU:O    | 1:C:600:ARG:HG2  | 2.16                     | 0.44              |
| 1:D:482:SER:HB3  | 1:D:529:LYS:HB3  | 1.99                     | 0.44              |
| 1:D:516:ARG:HH11 | 1:D:516:ARG:HG2  | 1.82                     | 0.44              |
| 1:D:523:LEU:HA   | 1:D:563:ILE:O    | 2.18                     | 0.44              |
| 1:F:534:VAL:HA   | 1:G:492:LYS:HD2  | 2.00                     | 0.44              |
| 1:G:350:PHE:HB3  | 1:I:350:PHE:HB3  | 1.99                     | 0.44              |
| 1:G:655:VAL:HG23 | 1:G:656:MET:HG2  | 1.99                     | 0.44              |
| 1:H:103:GLN:NE2  | 1:I:321:GLN:HB3  | 2.32                     | 0.44              |
| 1:H:655:VAL:HG23 | 1:H:656:MET:HG2  | 1.99                     | 0.44              |
| 1:I:382:ASP:HA   | 1:I:385:GLU:OE1  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:310:LEU:HD12 | 1:J:310:LEU:HA   | 1.74                     | 0.44              |
| 1:J:594:ARG:HB3  | 1:J:596:GLU:OE1  | 2.18                     | 0.44              |
| 1:K:573:GLU:N    | 1:K:574:ALA:CA   | 2.81                     | 0.44              |
| 1:L:382:ASP:HA   | 1:L:385:GLU:OE1  | 2.17                     | 0.44              |
| 1:L:596:GLU:O    | 1:L:600:ARG:HG2  | 2.16                     | 0.44              |
| 1:A:151:GLU:N    | 1:A:186:ASN:O    | 2.30                     | 0.44              |
| 1:A:594:ARG:HB3  | 1:A:596:GLU:OE1  | 2.18                     | 0.44              |
| 1:B:516:ARG:HG2  | 1:B:516:ARG:HH11 | 1.82                     | 0.44              |
| 1:B:573:GLU:N    | 1:B:574:ALA:CA   | 2.81                     | 0.44              |
| 1:C:454:THR:HA   | 1:C:458:LYS:HD2  | 2.00                     | 0.44              |
| 1:D:537:LEU:HD13 | 1:E:492:LYS:HA   | 1.99                     | 0.44              |
| 1:D:566:SER:OG   | 1:D:567:ASN:N    | 2.50                     | 0.44              |
| 1:F:456:VAL:HG21 | 1:F:607:PHE:CB   | 2.47                     | 0.44              |
| 1:F:655:VAL:HG23 | 1:F:656:MET:HG2  | 1.99                     | 0.44              |
| 1:J:151:GLU:N    | 1:J:186:ASN:O    | 2.30                     | 0.44              |
| 1:J:189:LEU:HD23 | 1:J:191:PHE:HZ   | 1.82                     | 0.44              |
| 1:K:393:ILE:HG13 | 1:K:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:L:393:ILE:HG13 | 1:L:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:L:566:SER:OG   | 1:L:567:ASN:N    | 2.50                     | 0.44              |
| 1:M:456:VAL:HG21 | 1:M:607:PHE:CB   | 2.47                     | 0.44              |
| 1:N:214:ASP:HA   | 1:N:217:LYS:HZ1  | 1.82                     | 0.44              |
| 1:A:167:ARG:HA   | 1:A:170:PHE:HB3  | 2.00                     | 0.44              |
| 1:A:189:LEU:HD23 | 1:A:191:PHE:HZ   | 1.82                     | 0.44              |
| 1:A:323:PRO:HA   | 1:G:142:ASP:O    | 2.17                     | 0.44              |
| 1:B:393:ILE:HG13 | 1:B:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:B:612:LYS:HB2  | 1:B:652:TYR:CZ   | 2.53                     | 0.44              |
| 1:C:167:ARG:HA   | 1:C:170:PHE:HB3  | 2.00                     | 0.44              |
| 1:C:189:LEU:HD23 | 1:C:191:PHE:HZ   | 1.82                     | 0.44              |
| 1:C:393:ILE:HG13 | 1:C:471:GLY:HA2  | 2.00                     | 0.44              |
| 1:D:167:ARG:HA   | 1:D:170:PHE:HB3  | 2.00                     | 0.44              |
| 1:D:454:THR:HA   | 1:D:458:LYS:HD2  | 2.00                     | 0.44              |
| 1:D:612:LYS:HB2  | 1:D:652:TYR:CZ   | 2.53                     | 0.44              |
| 1:E:566:SER:OG   | 1:E:567:ASN:N    | 2.50                     | 0.44              |
| 1:F:137:ALA:HA   | 1:F:140:ASN:HB2  | 2.00                     | 0.44              |
| 1:H:137:ALA:HA   | 1:H:140:ASN:HB2  | 2.00                     | 0.44              |
| 1:H:285:GLU:OE1  | 1:H:285:GLU:N    | 2.26                     | 0.44              |
| 1:I:167:ARG:HA   | 1:I:170:PHE:HB3  | 2.00                     | 0.44              |
| 1:I:534:VAL:HA   | 1:J:492:LYS:HD2  | 2.00                     | 0.44              |
| 1:L:454:THR:HA   | 1:L:458:LYS:HD2  | 2.00                     | 0.44              |
| 1:L:573:GLU:N    | 1:L:574:ALA:CA   | 2.81                     | 0.44              |
| 1:M:482:SER:HB3  | 1:M:529:LYS:HB3  | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:659:ARG:HB3  | 1:M:660:PRO:HD3  | 1.99                     | 0.44              |
| 1:N:189:LEU:HD23 | 1:N:191:PHE:HZ   | 1.82                     | 0.44              |
| 1:C:482:SER:HB3  | 1:C:529:LYS:HB3  | 1.99                     | 0.43              |
| 1:E:167:ARG:HA   | 1:E:170:PHE:HB3  | 2.00                     | 0.43              |
| 1:F:167:ARG:HA   | 1:F:170:PHE:HB3  | 2.00                     | 0.43              |
| 1:F:285:GLU:OE1  | 1:F:285:GLU:N    | 2.26                     | 0.43              |
| 1:G:167:ARG:HA   | 1:G:170:PHE:HB3  | 2.00                     | 0.43              |
| 1:H:167:ARG:HA   | 1:H:170:PHE:HB3  | 2.00                     | 0.43              |
| 1:J:167:ARG:HA   | 1:J:170:PHE:HB3  | 2.00                     | 0.43              |
| 1:K:271:ARG:NE   | 1:K:282:LEU:O    | 2.32                     | 0.43              |
| 1:K:612:LYS:HB2  | 1:K:652:TYR:CZ   | 2.53                     | 0.43              |
| 1:L:482:SER:HB3  | 1:L:529:LYS:HB3  | 1.99                     | 0.43              |
| 1:A:310:LEU:HD12 | 1:A:310:LEU:HA   | 1.74                     | 0.43              |
| 1:B:167:ARG:HA   | 1:B:170:PHE:HB3  | 2.00                     | 0.43              |
| 1:C:137:ALA:HA   | 1:C:140:ASN:HB2  | 2.00                     | 0.43              |
| 1:C:573:GLU:N    | 1:C:574:ALA:CA   | 2.81                     | 0.43              |
| 1:D:456:VAL:HG21 | 1:D:607:PHE:CB   | 2.47                     | 0.43              |
| 1:D:519:TYR:CD1  | 1:D:559:ASN:HB3  | 2.53                     | 0.43              |
| 1:D:573:GLU:N    | 1:D:574:ALA:CA   | 2.81                     | 0.43              |
| 1:F:594:ARG:HB3  | 1:F:596:GLU:OE1  | 2.18                     | 0.43              |
| 1:G:594:ARG:HB3  | 1:G:596:GLU:OE1  | 2.18                     | 0.43              |
| 1:G:659:ARG:HB3  | 1:G:660:PRO:HD3  | 1.99                     | 0.43              |
| 1:I:200:ALA:HA   | 1:I:210:LYS:HA   | 1.99                     | 0.43              |
| 1:I:523:LEU:HA   | 1:I:563:ILE:O    | 2.18                     | 0.43              |
| 1:I:594:ARG:HB3  | 1:I:596:GLU:OE1  | 2.18                     | 0.43              |
| 1:I:659:ARG:HB3  | 1:I:660:PRO:HD3  | 1.99                     | 0.43              |
| 1:K:167:ARG:HA   | 1:K:170:PHE:HB3  | 2.00                     | 0.43              |
| 1:K:267:LEU:HD22 | 1:K:287:LEU:HD13 | 2.00                     | 0.43              |
| 1:L:137:ALA:HA   | 1:L:140:ASN:HB2  | 2.00                     | 0.43              |
| 1:L:167:ARG:HA   | 1:L:170:PHE:HB3  | 2.00                     | 0.43              |
| 1:L:189:LEU:HD23 | 1:L:191:PHE:HZ   | 1.82                     | 0.43              |
| 1:M:167:ARG:HA   | 1:M:170:PHE:HB3  | 2.00                     | 0.43              |
| 1:M:454:THR:HA   | 1:M:458:LYS:HD2  | 2.00                     | 0.43              |
| 1:M:566:SER:OG   | 1:M:567:ASN:N    | 2.50                     | 0.43              |
| 1:M:612:LYS:HB2  | 1:M:652:TYR:CZ   | 2.53                     | 0.43              |
| 1:N:425:GLU:OE2  | 1:N:429:ARG:NE   | 2.38                     | 0.43              |
| 1:A:341:GLN:CD   | 1:A:357:LYS:HE2  | 2.43                     | 0.43              |
| 1:A:519:TYR:CD1  | 1:A:559:ASN:HB3  | 2.53                     | 0.43              |
| 1:B:267:LEU:HD22 | 1:B:287:LEU:HD13 | 2.00                     | 0.43              |
| 1:B:438:PHE:CE1  | 1:C:633:LYS:HE3  | 2.52                     | 0.43              |
| 1:C:271:ARG:HG2  | 1:C:281:ILE:HG22 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:341:GLN:CD   | 1:D:357:LYS:HE2  | 2.43                     | 0.43              |
| 1:D:536:THR:HG21 | 1:E:483:GLU:CG   | 2.41                     | 0.43              |
| 1:F:519:TYR:CD1  | 1:F:559:ASN:HB3  | 2.53                     | 0.43              |
| 1:G:214:ASP:HA   | 1:G:217:LYS:HZ1  | 1.82                     | 0.43              |
| 1:H:189:LEU:HD23 | 1:H:191:PHE:HZ   | 1.82                     | 0.43              |
| 1:H:594:ARG:HB3  | 1:H:596:GLU:OE1  | 2.18                     | 0.43              |
| 1:I:189:LEU:HD23 | 1:I:191:PHE:HZ   | 1.82                     | 0.43              |
| 1:I:516:ARG:HG2  | 1:I:516:ARG:HH11 | 1.82                     | 0.43              |
| 1:J:267:LEU:HD22 | 1:J:287:LEU:HD13 | 2.00                     | 0.43              |
| 1:J:341:GLN:CD   | 1:J:357:LYS:HE2  | 2.43                     | 0.43              |
| 1:K:271:ARG:HG2  | 1:K:281:ILE:HG22 | 2.00                     | 0.43              |
| 1:K:571:GLY:HA3  | 1:K:572:TYR:HA   | 1.57                     | 0.43              |
| 1:L:271:ARG:HG2  | 1:L:281:ILE:HG22 | 2.00                     | 0.43              |
| 1:N:167:ARG:HA   | 1:N:170:PHE:HB3  | 2.00                     | 0.43              |
| 1:N:566:SER:OG   | 1:N:567:ASN:N    | 2.50                     | 0.43              |
| 1:A:267:LEU:HD22 | 1:A:287:LEU:HD13 | 2.01                     | 0.43              |
| 1:A:497:THR:O    | 1:A:500:TYR:HB2  | 2.19                     | 0.43              |
| 1:B:497:THR:HG22 | 1:C:491:SER:N    | 2.33                     | 0.43              |
| 1:B:523:LEU:HA   | 1:B:563:ILE:O    | 2.18                     | 0.43              |
| 1:E:214:ASP:HA   | 1:E:217:LYS:HZ1  | 1.82                     | 0.43              |
| 1:E:425:GLU:OE2  | 1:E:429:ARG:NE   | 2.39                     | 0.43              |
| 1:E:572:TYR:CG   | 1:E:610:LEU:HD23 | 2.53                     | 0.43              |
| 1:E:612:LYS:HB2  | 1:E:652:TYR:CZ   | 2.53                     | 0.43              |
| 1:G:516:ARG:HG2  | 1:G:516:ARG:HH11 | 1.82                     | 0.43              |
| 1:G:519:TYR:CD1  | 1:G:559:ASN:HB3  | 2.53                     | 0.43              |
| 1:G:523:LEU:HA   | 1:G:563:ILE:O    | 2.18                     | 0.43              |
| 1:G:530:ALA:CB   | 1:G:532:PRO:HD2  | 2.49                     | 0.43              |
| 1:G:612:LYS:HB2  | 1:G:652:TYR:CZ   | 2.53                     | 0.43              |
| 1:H:519:TYR:CD1  | 1:H:559:ASN:HB3  | 2.53                     | 0.43              |
| 1:H:612:LYS:HB2  | 1:H:652:TYR:CZ   | 2.53                     | 0.43              |
| 1:I:519:TYR:CD1  | 1:I:559:ASN:HB3  | 2.53                     | 0.43              |
| 1:I:530:ALA:CB   | 1:I:532:PRO:HD2  | 2.49                     | 0.43              |
| 1:I:612:LYS:HB2  | 1:I:652:TYR:CZ   | 2.53                     | 0.43              |
| 1:J:519:TYR:CD1  | 1:J:559:ASN:HB3  | 2.53                     | 0.43              |
| 1:J:566:SER:OG   | 1:J:567:ASN:N    | 2.50                     | 0.43              |
| 1:L:612:LYS:HB2  | 1:L:652:TYR:CZ   | 2.53                     | 0.43              |
| 1:M:519:TYR:CD1  | 1:M:559:ASN:HB3  | 2.54                     | 0.43              |
| 1:M:572:TYR:CG   | 1:M:610:LEU:HD23 | 2.53                     | 0.43              |
| 1:N:612:LYS:HB2  | 1:N:652:TYR:CZ   | 2.53                     | 0.43              |
| 1:B:271:ARG:HG2  | 1:B:281:ILE:HG22 | 2.01                     | 0.43              |
| 1:C:341:GLN:CD   | 1:C:357:LYS:HE2  | 2.43                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:612:LYS:HB2  | 1:C:652:TYR:CZ   | 2.53                     | 0.43              |
| 1:E:189:LEU:HD23 | 1:E:191:PHE:HZ   | 1.82                     | 0.43              |
| 1:E:659:ARG:HB3  | 1:E:660:PRO:HD3  | 1.99                     | 0.43              |
| 1:F:189:LEU:HD23 | 1:F:191:PHE:HZ   | 1.82                     | 0.43              |
| 1:F:271:ARG:NE   | 1:F:282:LEU:O    | 2.32                     | 0.43              |
| 1:F:572:TYR:CG   | 1:F:610:LEU:HD23 | 2.53                     | 0.43              |
| 1:F:573:GLU:N    | 1:F:574:ALA:CA   | 2.81                     | 0.43              |
| 1:F:612:LYS:HB2  | 1:F:652:TYR:CZ   | 2.53                     | 0.43              |
| 1:F:659:ARG:HB3  | 1:F:660:PRO:HD3  | 1.99                     | 0.43              |
| 1:G:189:LEU:HD23 | 1:G:191:PHE:HZ   | 1.82                     | 0.43              |
| 1:H:523:LEU:HA   | 1:H:563:ILE:O    | 2.18                     | 0.43              |
| 1:H:572:TYR:CG   | 1:H:610:LEU:HD23 | 2.53                     | 0.43              |
| 1:J:497:THR:O    | 1:J:500:TYR:HB2  | 2.19                     | 0.43              |
| 1:K:114:LYS:NZ   | 1:K:250:PHE:O    | 2.43                     | 0.43              |
| 1:M:463:LYS:HG3  | 1:M:464:GLN:N    | 2.34                     | 0.43              |
| 1:M:573:GLU:N    | 1:M:574:ALA:CA   | 2.81                     | 0.43              |
| 1:N:519:TYR:CD1  | 1:N:559:ASN:HB3  | 2.53                     | 0.43              |
| 1:A:612:LYS:HB2  | 1:A:652:TYR:CZ   | 2.53                     | 0.43              |
| 1:B:498:ALA:HB2  | 1:C:489:ALA:HA   | 2.00                     | 0.43              |
| 1:C:438:PHE:CE2  | 1:D:674:THR:HA   | 2.53                     | 0.43              |
| 1:D:463:LYS:HG3  | 1:D:464:GLN:N    | 2.34                     | 0.43              |
| 1:D:497:THR:O    | 1:D:500:TYR:HB2  | 2.19                     | 0.43              |
| 1:D:572:TYR:CG   | 1:D:610:LEU:HD23 | 2.53                     | 0.43              |
| 1:D:653:ASP:O    | 1:D:655:VAL:N    | 2.51                     | 0.43              |
| 1:F:523:LEU:HA   | 1:F:563:ILE:O    | 2.18                     | 0.43              |
| 1:F:537:LEU:HD13 | 1:G:492:LYS:HA   | 2.01                     | 0.43              |
| 1:G:200:ALA:HA   | 1:G:210:LYS:HA   | 1.99                     | 0.43              |
| 1:G:572:TYR:CG   | 1:G:610:LEU:HD23 | 2.53                     | 0.43              |
| 1:H:573:GLU:N    | 1:H:574:ALA:CA   | 2.81                     | 0.43              |
| 1:J:612:LYS:HB2  | 1:J:652:TYR:CZ   | 2.53                     | 0.43              |
| 1:K:523:LEU:HA   | 1:K:563:ILE:O    | 2.18                     | 0.43              |
| 1:L:341:GLN:CD   | 1:L:357:LYS:HE2  | 2.43                     | 0.43              |
| 1:L:463:LYS:HG3  | 1:L:464:GLN:N    | 2.34                     | 0.43              |
| 1:M:497:THR:O    | 1:M:500:TYR:HB2  | 2.19                     | 0.43              |
| 1:N:497:THR:O    | 1:N:500:TYR:HB2  | 2.19                     | 0.43              |
| 1:N:572:TYR:CG   | 1:N:610:LEU:HD23 | 2.53                     | 0.43              |
| 1:N:659:ARG:HB3  | 1:N:660:PRO:HD3  | 1.99                     | 0.43              |
| 1:A:114:LYS:NZ   | 1:A:250:PHE:O    | 2.43                     | 0.43              |
| 1:B:463:LYS:HG3  | 1:B:464:GLN:N    | 2.34                     | 0.43              |
| 1:B:519:TYR:CD1  | 1:B:559:ASN:HB3  | 2.54                     | 0.43              |
| 1:C:267:LEU:HD22 | 1:C:287:LEU:HD13 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:432:CYS:SG   | 1:D:674:THR:HG23 | 2.58                     | 0.43              |
| 1:C:463:LYS:HG3  | 1:C:464:GLN:N    | 2.34                     | 0.43              |
| 1:D:108:ILE:HG12 | 1:D:111:ARG:NH2  | 2.34                     | 0.43              |
| 1:D:310:LEU:HD12 | 1:D:310:LEU:HA   | 1.74                     | 0.43              |
| 1:E:365:ARG:HH11 | 1:E:365:ARG:CG   | 2.17                     | 0.43              |
| 1:E:463:LYS:HG3  | 1:E:464:GLN:N    | 2.34                     | 0.43              |
| 1:E:488:THR:O    | 1:E:490:VAL:N    | 2.52                     | 0.43              |
| 1:E:497:THR:O    | 1:E:500:TYR:HB2  | 2.19                     | 0.43              |
| 1:F:497:THR:O    | 1:F:500:TYR:HB2  | 2.19                     | 0.43              |
| 1:F:582:LYS:HG2  | 1:F:586:MET:HE3  | 2.01                     | 0.43              |
| 1:H:112:ARG:HD2  | 1:I:274:TYR:HE1  | 1.83                     | 0.43              |
| 1:H:214:ASP:HA   | 1:H:217:LYS:HZ1  | 1.83                     | 0.43              |
| 1:H:497:THR:O    | 1:H:500:TYR:HB2  | 2.19                     | 0.43              |
| 1:H:582:LYS:HG2  | 1:H:586:MET:HE3  | 2.01                     | 0.43              |
| 1:H:659:ARG:HB3  | 1:H:660:PRO:HD3  | 1.99                     | 0.43              |
| 1:I:572:TYR:CG   | 1:I:610:LEU:HD23 | 2.53                     | 0.43              |
| 1:J:114:LYS:NZ   | 1:J:250:PHE:O    | 2.43                     | 0.43              |
| 1:K:134:LEU:HD12 | 1:K:134:LEU:HA   | 1.78                     | 0.43              |
| 1:K:463:LYS:HG3  | 1:K:464:GLN:N    | 2.34                     | 0.43              |
| 1:K:519:TYR:CD1  | 1:K:559:ASN:HB3  | 2.54                     | 0.43              |
| 1:L:267:LEU:HD22 | 1:L:287:LEU:HD13 | 2.00                     | 0.43              |
| 1:M:341:GLN:CD   | 1:M:357:LYS:HE2  | 2.43                     | 0.43              |
| 1:N:463:LYS:HG3  | 1:N:464:GLN:N    | 2.34                     | 0.43              |
| 1:B:282:LEU:HD23 | 1:B:378:ALA:HB1  | 2.01                     | 0.43              |
| 1:B:341:GLN:CD   | 1:B:357:LYS:HE2  | 2.43                     | 0.43              |
| 1:C:501:VAL:N    | 1:D:491:SER:OG   | 2.52                     | 0.43              |
| 1:D:271:ARG:HG2  | 1:D:281:ILE:HG22 | 2.00                     | 0.43              |
| 1:D:616:SER:O    | 1:D:619:VAL:HB   | 2.19                     | 0.43              |
| 1:E:137:ALA:HA   | 1:E:140:ASN:HB2  | 2.00                     | 0.43              |
| 1:E:341:GLN:CD   | 1:E:357:LYS:HE2  | 2.43                     | 0.43              |
| 1:E:519:TYR:CD1  | 1:E:559:ASN:HB3  | 2.54                     | 0.43              |
| 1:F:341:GLN:CD   | 1:F:357:LYS:HE2  | 2.43                     | 0.43              |
| 1:G:108:ILE:HG12 | 1:G:111:ARG:NH2  | 2.34                     | 0.43              |
| 1:G:447:ASN:N    | 1:G:602:ASN:OD1  | 2.43                     | 0.43              |
| 1:H:271:ARG:NE   | 1:H:282:LEU:O    | 2.32                     | 0.43              |
| 1:I:267:LEU:HD22 | 1:I:287:LEU:HD13 | 2.00                     | 0.43              |
| 1:M:108:ILE:HG12 | 1:M:111:ARG:NH2  | 2.34                     | 0.43              |
| 1:N:488:THR:O    | 1:N:490:VAL:N    | 2.52                     | 0.43              |
| 1:N:530:ALA:CB   | 1:N:532:PRO:HD2  | 2.49                     | 0.43              |
| 1:A:271:ARG:HG2  | 1:A:281:ILE:HG22 | 2.00                     | 0.43              |
| 1:B:589:LEU:O    | 1:B:593:PHE:N    | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:282:LEU:HD23 | 1:C:378:ALA:HB1  | 2.01                     | 0.43              |
| 1:C:497:THR:O    | 1:C:500:TYR:HB2  | 2.19                     | 0.43              |
| 1:D:134:LEU:HD12 | 1:D:134:LEU:HA   | 1.78                     | 0.43              |
| 1:E:530:ALA:CB   | 1:E:532:PRO:HD2  | 2.49                     | 0.43              |
| 1:E:653:ASP:O    | 1:E:655:VAL:N    | 2.51                     | 0.43              |
| 1:F:104:GLU:HA   | 1:G:321:GLN:NE2  | 2.34                     | 0.43              |
| 1:G:267:LEU:HD22 | 1:G:287:LEU:HD13 | 2.00                     | 0.43              |
| 1:H:341:GLN:CD   | 1:H:357:LYS:HE2  | 2.43                     | 0.43              |
| 1:I:108:ILE:HG12 | 1:I:111:ARG:NH2  | 2.34                     | 0.43              |
| 1:J:271:ARG:HG2  | 1:J:281:ILE:HG22 | 2.01                     | 0.43              |
| 1:K:282:LEU:HD23 | 1:K:378:ALA:HB1  | 2.01                     | 0.43              |
| 1:L:108:ILE:HG12 | 1:L:111:ARG:NH2  | 2.34                     | 0.43              |
| 1:L:653:ASP:O    | 1:L:655:VAL:N    | 2.51                     | 0.43              |
| 1:N:137:ALA:HA   | 1:N:140:ASN:HB2  | 2.00                     | 0.43              |
| 1:N:160:LEU:HD23 | 1:N:160:LEU:HA   | 1.90                     | 0.43              |
| 1:N:310:LEU:HD12 | 1:N:310:LEU:HA   | 1.74                     | 0.43              |
| 1:N:573:GLU:N    | 1:N:574:ALA:CA   | 2.81                     | 0.43              |
| 1:N:582:LYS:HG2  | 1:N:586:MET:HE3  | 2.01                     | 0.43              |
| 1:N:616:SER:O    | 1:N:619:VAL:HB   | 2.19                     | 0.43              |
| 1:D:271:ARG:NE   | 1:D:282:LEU:O    | 2.32                     | 0.43              |
| 1:D:452:GLY:O    | 1:D:458:LYS:NZ   | 2.37                     | 0.43              |
| 1:D:530:ALA:CB   | 1:D:532:PRO:HD2  | 2.49                     | 0.43              |
| 1:E:409:MET:HA   | 1:E:412:ARG:HD2  | 2.01                     | 0.43              |
| 1:E:582:LYS:HG2  | 1:E:586:MET:HE3  | 2.01                     | 0.43              |
| 1:E:616:SER:O    | 1:E:619:VAL:HB   | 2.19                     | 0.43              |
| 1:F:108:ILE:HG12 | 1:F:111:ARG:NH2  | 2.34                     | 0.43              |
| 1:F:327:VAL:O    | 1:F:331:GLU:HG2  | 2.19                     | 0.43              |
| 1:H:108:ILE:HG12 | 1:H:111:ARG:NH2  | 2.34                     | 0.43              |
| 1:H:327:VAL:O    | 1:H:331:GLU:HG2  | 2.19                     | 0.43              |
| 1:I:447:ASN:N    | 1:I:602:ASN:OD1  | 2.43                     | 0.43              |
| 1:K:113:THR:OG1  | 1:K:114:LYS:N    | 2.52                     | 0.43              |
| 1:K:341:GLN:CD   | 1:K:357:LYS:HE2  | 2.43                     | 0.43              |
| 1:L:497:THR:O    | 1:L:500:TYR:HB2  | 2.19                     | 0.43              |
| 1:M:137:ALA:HA   | 1:M:140:ASN:HB2  | 2.00                     | 0.43              |
| 1:M:271:ARG:HG2  | 1:M:281:ILE:HG22 | 2.00                     | 0.43              |
| 1:M:327:VAL:O    | 1:M:331:GLU:HG2  | 2.19                     | 0.43              |
| 1:M:616:SER:O    | 1:M:619:VAL:HB   | 2.19                     | 0.43              |
| 1:M:653:ASP:O    | 1:M:655:VAL:N    | 2.51                     | 0.43              |
| 1:N:341:GLN:CD   | 1:N:357:LYS:HE2  | 2.43                     | 0.43              |
| 1:A:112:ARG:NE   | 1:B:273:LEU:HD21 | 2.34                     | 0.42              |
| 1:A:488:THR:O    | 1:A:490:VAL:N    | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:113:THR:OG1  | 1:B:114:LYS:N    | 2.52                     | 0.42              |
| 1:B:534:VAL:HG22 | 1:C:492:LYS:CB   | 2.38                     | 0.42              |
| 1:B:653:ASP:O    | 1:B:655:VAL:N    | 2.51                     | 0.42              |
| 1:C:108:ILE:HD12 | 1:C:117:PRO:HB3  | 2.01                     | 0.42              |
| 1:C:142:ASP:O    | 1:D:323:PRO:HA   | 2.19                     | 0.42              |
| 1:C:365:ARG:HH11 | 1:C:365:ARG:CG   | 2.17                     | 0.42              |
| 1:C:618:ILE:HG12 | 1:C:622:MET:CE   | 2.46                     | 0.42              |
| 1:E:160:LEU:HD23 | 1:E:160:LEU:HA   | 1.90                     | 0.42              |
| 1:E:573:GLU:N    | 1:E:574:ALA:CA   | 2.81                     | 0.42              |
| 1:F:522:ILE:HB   | 1:F:562:ILE:HD13 | 2.01                     | 0.42              |
| 1:H:497:THR:HB   | 1:I:489:ALA:O    | 2.19                     | 0.42              |
| 1:J:488:THR:O    | 1:J:490:VAL:N    | 2.52                     | 0.42              |
| 1:K:409:MET:HA   | 1:K:412:ARG:HD2  | 2.01                     | 0.42              |
| 1:L:114:LYS:NZ   | 1:L:250:PHE:O    | 2.43                     | 0.42              |
| 1:L:282:LEU:HD23 | 1:L:378:ALA:HB1  | 2.01                     | 0.42              |
| 1:A:103:GLN:NE2  | 1:B:321:GLN:HB3  | 2.34                     | 0.42              |
| 1:A:108:ILE:HG12 | 1:A:111:ARG:NH2  | 2.34                     | 0.42              |
| 1:A:282:LEU:HD23 | 1:A:378:ALA:HB1  | 2.01                     | 0.42              |
| 1:B:114:LYS:NZ   | 1:B:250:PHE:O    | 2.43                     | 0.42              |
| 1:C:108:ILE:HG12 | 1:C:111:ARG:NH2  | 2.34                     | 0.42              |
| 1:C:114:LYS:NZ   | 1:C:250:PHE:O    | 2.43                     | 0.42              |
| 1:C:530:ALA:CB   | 1:C:532:PRO:HD2  | 2.49                     | 0.42              |
| 1:C:616:SER:O    | 1:C:619:VAL:HB   | 2.19                     | 0.42              |
| 1:D:160:LEU:HD23 | 1:D:160:LEU:HA   | 1.90                     | 0.42              |
| 1:D:327:VAL:O    | 1:D:331:GLU:HG2  | 2.19                     | 0.42              |
| 1:D:582:LYS:HG2  | 1:D:586:MET:HE3  | 2.01                     | 0.42              |
| 1:E:108:ILE:HG12 | 1:E:111:ARG:NH2  | 2.34                     | 0.42              |
| 1:G:522:ILE:HB   | 1:G:562:ILE:HD13 | 2.01                     | 0.42              |
| 1:H:522:ILE:HB   | 1:H:562:ILE:HD13 | 2.01                     | 0.42              |
| 1:I:463:LYS:HG3  | 1:I:464:GLN:N    | 2.34                     | 0.42              |
| 1:J:108:ILE:HG12 | 1:J:111:ARG:NH2  | 2.34                     | 0.42              |
| 1:K:327:VAL:O    | 1:K:331:GLU:HG2  | 2.19                     | 0.42              |
| 1:L:108:ILE:HD12 | 1:L:117:PRO:HB3  | 2.01                     | 0.42              |
| 1:L:618:ILE:HG12 | 1:L:622:MET:CE   | 2.46                     | 0.42              |
| 1:M:530:ALA:CB   | 1:M:532:PRO:HD2  | 2.49                     | 0.42              |
| 1:N:327:VAL:O    | 1:N:331:GLU:HG2  | 2.19                     | 0.42              |
| 1:N:409:MET:HA   | 1:N:412:ARG:HD2  | 2.01                     | 0.42              |
| 1:N:653:ASP:O    | 1:N:655:VAL:N    | 2.51                     | 0.42              |
| 1:A:113:THR:OG1  | 1:A:114:LYS:N    | 2.52                     | 0.42              |
| 1:A:409:MET:HA   | 1:A:412:ARG:HD2  | 2.01                     | 0.42              |
| 1:B:327:VAL:O    | 1:B:331:GLU:HG2  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:409:MET:HA   | 1:B:412:ARG:HD2  | 2.01                     | 0.42              |
| 1:C:488:THR:O    | 1:C:490:VAL:N    | 2.52                     | 0.42              |
| 1:D:137:ALA:HA   | 1:D:140:ASN:HB2  | 2.00                     | 0.42              |
| 1:E:327:VAL:O    | 1:E:331:GLU:HG2  | 2.19                     | 0.42              |
| 1:F:176:ASN:HA   | 1:F:179:ASN:ND2  | 2.35                     | 0.42              |
| 1:F:488:THR:O    | 1:F:490:VAL:N    | 2.52                     | 0.42              |
| 1:F:616:SER:O    | 1:F:619:VAL:HB   | 2.19                     | 0.42              |
| 1:G:463:LYS:HG3  | 1:G:464:GLN:N    | 2.34                     | 0.42              |
| 1:G:582:LYS:HG2  | 1:G:586:MET:HE3  | 2.01                     | 0.42              |
| 1:H:176:ASN:HA   | 1:H:179:ASN:ND2  | 2.35                     | 0.42              |
| 1:H:488:THR:O    | 1:H:490:VAL:N    | 2.52                     | 0.42              |
| 1:H:539:LEU:O    | 1:H:543:ASP:N    | 2.50                     | 0.42              |
| 1:H:616:SER:O    | 1:H:619:VAL:HB   | 2.19                     | 0.42              |
| 1:I:214:ASP:HA   | 1:I:217:LYS:HZ1  | 1.83                     | 0.42              |
| 1:I:285:GLU:CD   | 1:I:285:GLU:N    | 2.77                     | 0.42              |
| 1:I:522:ILE:HB   | 1:I:562:ILE:HD13 | 2.01                     | 0.42              |
| 1:J:113:THR:OG1  | 1:J:114:LYS:N    | 2.52                     | 0.42              |
| 1:J:282:LEU:HD23 | 1:J:378:ALA:HB1  | 2.01                     | 0.42              |
| 1:J:409:MET:HA   | 1:J:412:ARG:HD2  | 2.01                     | 0.42              |
| 1:L:327:VAL:O    | 1:L:331:GLU:HG2  | 2.19                     | 0.42              |
| 1:L:488:THR:O    | 1:L:490:VAL:N    | 2.52                     | 0.42              |
| 1:L:519:TYR:CD1  | 1:L:559:ASN:HB3  | 2.53                     | 0.42              |
| 1:L:530:ALA:CB   | 1:L:532:PRO:HD2  | 2.49                     | 0.42              |
| 1:M:488:THR:O    | 1:M:490:VAL:N    | 2.52                     | 0.42              |
| 1:M:497:THR:HB   | 1:N:489:ALA:O    | 2.19                     | 0.42              |
| 1:N:108:ILE:HG12 | 1:N:111:ARG:NH2  | 2.34                     | 0.42              |
| 1:A:112:ARG:CZ   | 1:B:273:LEU:HD21 | 2.49                     | 0.42              |
| 1:B:488:THR:O    | 1:B:490:VAL:N    | 2.52                     | 0.42              |
| 1:B:530:ALA:CB   | 1:B:532:PRO:HD2  | 2.49                     | 0.42              |
| 1:C:113:THR:OG1  | 1:C:114:LYS:N    | 2.52                     | 0.42              |
| 1:C:176:ASN:HA   | 1:C:179:ASN:ND2  | 2.34                     | 0.42              |
| 1:C:327:VAL:O    | 1:C:331:GLU:HG2  | 2.19                     | 0.42              |
| 1:D:176:ASN:HA   | 1:D:179:ASN:ND2  | 2.35                     | 0.42              |
| 1:D:618:ILE:HG12 | 1:D:622:MET:CE   | 2.46                     | 0.42              |
| 1:E:267:LEU:HD22 | 1:E:287:LEU:HD13 | 2.00                     | 0.42              |
| 1:F:539:LEU:O    | 1:F:543:ASP:N    | 2.50                     | 0.42              |
| 1:G:285:GLU:CD   | 1:G:285:GLU:N    | 2.77                     | 0.42              |
| 1:G:497:THR:O    | 1:G:500:TYR:HB2  | 2.19                     | 0.42              |
| 1:I:341:GLN:CD   | 1:I:357:LYS:HE2  | 2.43                     | 0.42              |
| 1:I:582:LYS:HG2  | 1:I:586:MET:HE3  | 2.01                     | 0.42              |
| 1:J:528:GLU:H    | 1:J:529:LYS:HB2  | 1.85                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:653:ASP:O    | 1:K:655:VAL:N    | 2.51                     | 0.42              |
| 1:L:113:THR:OG1  | 1:L:114:LYS:N    | 2.52                     | 0.42              |
| 1:L:616:SER:O    | 1:L:619:VAL:HB   | 2.19                     | 0.42              |
| 1:M:582:LYS:HG2  | 1:M:586:MET:HE3  | 2.01                     | 0.42              |
| 1:A:463:LYS:HG3  | 1:A:464:GLN:H    | 1.84                     | 0.42              |
| 1:A:566:SER:OG   | 1:A:567:ASN:N    | 2.50                     | 0.42              |
| 1:C:519:TYR:CD1  | 1:C:559:ASN:HB3  | 2.54                     | 0.42              |
| 1:C:589:LEU:O    | 1:C:593:PHE:N    | 2.33                     | 0.42              |
| 1:D:108:ILE:HD12 | 1:D:117:PRO:HB3  | 2.01                     | 0.42              |
| 1:E:176:ASN:HA   | 1:E:179:ASN:ND2  | 2.34                     | 0.42              |
| 1:F:271:ARG:HG2  | 1:F:281:ILE:HG22 | 2.00                     | 0.42              |
| 1:J:327:VAL:O    | 1:J:331:GLU:HG2  | 2.19                     | 0.42              |
| 1:J:463:LYS:HG3  | 1:J:464:GLN:N    | 2.34                     | 0.42              |
| 1:J:522:ILE:HB   | 1:J:562:ILE:HD13 | 2.01                     | 0.42              |
| 1:K:497:THR:O    | 1:K:500:TYR:HB2  | 2.19                     | 0.42              |
| 1:M:267:LEU:HD22 | 1:M:287:LEU:HD13 | 2.00                     | 0.42              |
| 1:N:176:ASN:HA   | 1:N:179:ASN:ND2  | 2.34                     | 0.42              |
| 1:N:267:LEU:HD22 | 1:N:287:LEU:HD13 | 2.00                     | 0.42              |
| 1:A:327:VAL:O    | 1:A:331:GLU:HG2  | 2.19                     | 0.42              |
| 1:A:528:GLU:H    | 1:A:529:LYS:HB2  | 1.85                     | 0.42              |
| 1:A:530:ALA:CB   | 1:A:532:PRO:HD2  | 2.49                     | 0.42              |
| 1:B:134:LEU:HD12 | 1:B:134:LEU:HA   | 1.78                     | 0.42              |
| 1:E:282:LEU:HD23 | 1:E:378:ALA:HB1  | 2.01                     | 0.42              |
| 1:F:653:ASP:O    | 1:F:655:VAL:N    | 2.51                     | 0.42              |
| 1:G:341:GLN:CD   | 1:G:357:LYS:HE2  | 2.43                     | 0.42              |
| 1:H:271:ARG:HG2  | 1:H:281:ILE:HG22 | 2.00                     | 0.42              |
| 1:H:653:ASP:O    | 1:H:655:VAL:N    | 2.51                     | 0.42              |
| 1:I:463:LYS:HG3  | 1:I:464:GLN:H    | 1.84                     | 0.42              |
| 1:I:497:THR:O    | 1:I:500:TYR:HB2  | 2.19                     | 0.42              |
| 1:J:463:LYS:HG3  | 1:J:464:GLN:H    | 1.84                     | 0.42              |
| 1:J:530:ALA:CB   | 1:J:532:PRO:HD2  | 2.49                     | 0.42              |
| 1:K:488:THR:O    | 1:K:490:VAL:N    | 2.52                     | 0.42              |
| 1:K:589:LEU:O    | 1:K:593:PHE:N    | 2.33                     | 0.42              |
| 1:L:176:ASN:HA   | 1:L:179:ASN:ND2  | 2.35                     | 0.42              |
| 1:L:501:VAL:HB   | 1:M:491:SER:C    | 2.45                     | 0.42              |
| 1:A:214:ASP:HA   | 1:A:217:LYS:HZ1  | 1.84                     | 0.42              |
| 1:A:463:LYS:HG3  | 1:A:464:GLN:N    | 2.34                     | 0.42              |
| 1:A:522:ILE:HB   | 1:A:562:ILE:HD13 | 2.01                     | 0.42              |
| 1:B:497:THR:O    | 1:B:500:TYR:HB2  | 2.19                     | 0.42              |
| 1:C:409:MET:HA   | 1:C:412:ARG:HD2  | 2.01                     | 0.42              |
| 1:C:583:PRO:C    | 1:C:585:LEU:N    | 2.77                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:592:PHE:N    | 1:C:592:PHE:CD1  | 2.88                     | 0.42              |
| 1:D:267:LEU:HD22 | 1:D:287:LEU:HD13 | 2.00                     | 0.42              |
| 1:D:409:MET:HA   | 1:D:412:ARG:HD2  | 2.01                     | 0.42              |
| 1:E:497:THR:HB   | 1:F:489:ALA:O    | 2.19                     | 0.42              |
| 1:F:463:LYS:HG3  | 1:F:464:GLN:N    | 2.34                     | 0.42              |
| 1:F:530:ALA:CB   | 1:F:532:PRO:HD2  | 2.49                     | 0.42              |
| 1:G:176:ASN:HA   | 1:G:179:ASN:ND2  | 2.34                     | 0.42              |
| 1:H:267:LEU:HD22 | 1:H:287:LEU:HD13 | 2.00                     | 0.42              |
| 1:H:463:LYS:HG3  | 1:H:464:GLN:N    | 2.34                     | 0.42              |
| 1:H:528:GLU:H    | 1:H:529:LYS:HB2  | 1.84                     | 0.42              |
| 1:K:108:ILE:HD12 | 1:K:117:PRO:HB3  | 2.01                     | 0.42              |
| 1:K:463:LYS:HG3  | 1:K:464:GLN:H    | 1.84                     | 0.42              |
| 1:K:530:ALA:CB   | 1:K:532:PRO:HD2  | 2.49                     | 0.42              |
| 1:L:409:MET:HA   | 1:L:412:ARG:HD2  | 2.01                     | 0.42              |
| 1:L:528:GLU:H    | 1:L:529:LYS:HB2  | 1.85                     | 0.42              |
| 1:M:176:ASN:HA   | 1:M:179:ASN:ND2  | 2.35                     | 0.42              |
| 1:M:271:ARG:NE   | 1:M:282:LEU:O    | 2.32                     | 0.42              |
| 1:M:452:GLY:O    | 1:M:458:LYS:NZ   | 2.37                     | 0.42              |
| 1:M:618:ILE:HG12 | 1:M:622:MET:CE   | 2.46                     | 0.42              |
| 1:N:113:THR:OG1  | 1:N:114:LYS:N    | 2.52                     | 0.42              |
| 1:B:176:ASN:HA   | 1:B:179:ASN:ND2  | 2.35                     | 0.42              |
| 1:C:285:GLU:CD   | 1:C:285:GLU:N    | 2.77                     | 0.42              |
| 1:D:310:LEU:O    | 1:D:314:THR:OG1  | 2.30                     | 0.42              |
| 1:E:271:ARG:HG2  | 1:E:281:ILE:HG22 | 2.00                     | 0.42              |
| 1:F:463:LYS:HG3  | 1:F:464:GLN:H    | 1.84                     | 0.42              |
| 1:H:409:MET:HA   | 1:H:412:ARG:HD2  | 2.01                     | 0.42              |
| 1:I:653:ASP:O    | 1:I:655:VAL:N    | 2.51                     | 0.42              |
| 1:K:176:ASN:HA   | 1:K:179:ASN:ND2  | 2.35                     | 0.42              |
| 1:L:365:ARG:HH11 | 1:L:365:ARG:CG   | 2.17                     | 0.42              |
| 1:L:582:LYS:HG2  | 1:L:586:MET:HE3  | 2.01                     | 0.42              |
| 1:M:108:ILE:HD12 | 1:M:117:PRO:HB3  | 2.01                     | 0.42              |
| 1:M:112:ARG:HD2  | 1:N:274:TYR:HE1  | 1.83                     | 0.42              |
| 1:N:108:ILE:HD12 | 1:N:117:PRO:HB3  | 2.01                     | 0.42              |
| 1:N:271:ARG:HG2  | 1:N:281:ILE:HG22 | 2.01                     | 0.42              |
| 1:A:176:ASN:HA   | 1:A:179:ASN:ND2  | 2.35                     | 0.42              |
| 1:B:310:LEU:O    | 1:B:314:THR:OG1  | 2.30                     | 0.42              |
| 1:B:463:LYS:HG3  | 1:B:464:GLN:H    | 1.84                     | 0.42              |
| 1:C:528:GLU:H    | 1:C:529:LYS:HB2  | 1.85                     | 0.42              |
| 1:D:282:LEU:HD23 | 1:D:378:ALA:HB1  | 2.01                     | 0.42              |
| 1:D:586:MET:HG3  | 1:D:587:ASP:OD1  | 2.20                     | 0.42              |
| 1:E:108:ILE:HD12 | 1:E:117:PRO:HB3  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:113:THR:OG1  | 1:E:114:LYS:N    | 2.52                     | 0.42              |
| 1:F:267:LEU:HD22 | 1:F:287:LEU:HD13 | 2.00                     | 0.42              |
| 1:F:528:GLU:H    | 1:F:529:LYS:HB2  | 1.85                     | 0.42              |
| 1:G:271:ARG:HG2  | 1:G:281:ILE:HG22 | 2.00                     | 0.42              |
| 1:G:463:LYS:HG3  | 1:G:464:GLN:H    | 1.84                     | 0.42              |
| 1:G:488:THR:O    | 1:G:490:VAL:N    | 2.52                     | 0.42              |
| 1:G:616:SER:O    | 1:G:619:VAL:HB   | 2.19                     | 0.42              |
| 1:G:653:ASP:O    | 1:G:655:VAL:N    | 2.51                     | 0.42              |
| 1:H:108:ILE:HD12 | 1:H:117:PRO:HB3  | 2.01                     | 0.42              |
| 1:H:463:LYS:HG3  | 1:H:464:GLN:H    | 1.84                     | 0.42              |
| 1:H:530:ALA:CB   | 1:H:532:PRO:HD2  | 2.49                     | 0.42              |
| 1:I:176:ASN:HA   | 1:I:179:ASN:ND2  | 2.35                     | 0.42              |
| 1:J:176:ASN:HA   | 1:J:179:ASN:ND2  | 2.34                     | 0.42              |
| 1:K:522:ILE:HB   | 1:K:562:ILE:HD13 | 2.01                     | 0.42              |
| 1:L:285:GLU:CD   | 1:L:285:GLU:N    | 2.77                     | 0.42              |
| 1:L:583:PRO:C    | 1:L:585:LEU:N    | 2.77                     | 0.42              |
| 1:L:592:PHE:N    | 1:L:592:PHE:CD1  | 2.88                     | 0.42              |
| 1:M:401:SER:OG   | 1:M:404:GLU:HG3  | 2.20                     | 0.42              |
| 1:M:586:MET:HG3  | 1:M:587:ASP:OD1  | 2.20                     | 0.42              |
| 1:N:282:LEU:HD23 | 1:N:378:ALA:HB1  | 2.01                     | 0.42              |
| 1:N:522:ILE:HB   | 1:N:562:ILE:HD13 | 2.01                     | 0.42              |
| 1:B:108:ILE:HD12 | 1:B:117:PRO:HB3  | 2.01                     | 0.42              |
| 1:B:583:PRO:C    | 1:B:585:LEU:N    | 2.77                     | 0.42              |
| 1:F:108:ILE:HD12 | 1:F:117:PRO:HB3  | 2.01                     | 0.42              |
| 1:F:113:THR:OG1  | 1:F:114:LYS:N    | 2.52                     | 0.42              |
| 1:F:282:LEU:HD23 | 1:F:378:ALA:HB1  | 2.01                     | 0.42              |
| 1:F:409:MET:HA   | 1:F:412:ARG:HD2  | 2.01                     | 0.42              |
| 1:G:282:LEU:HD23 | 1:G:378:ALA:HB1  | 2.01                     | 0.42              |
| 1:G:586:MET:HG3  | 1:G:587:ASP:OD1  | 2.20                     | 0.42              |
| 1:H:113:THR:OG1  | 1:H:114:LYS:N    | 2.52                     | 0.42              |
| 1:H:282:LEU:HD23 | 1:H:378:ALA:HB1  | 2.01                     | 0.42              |
| 1:I:271:ARG:HG2  | 1:I:281:ILE:HG22 | 2.01                     | 0.42              |
| 1:I:488:THR:O    | 1:I:490:VAL:N    | 2.52                     | 0.42              |
| 1:I:586:MET:HG3  | 1:I:587:ASP:OD1  | 2.20                     | 0.42              |
| 1:J:214:ASP:HA   | 1:J:217:LYS:HZ1  | 1.84                     | 0.42              |
| 1:K:108:ILE:HG12 | 1:K:111:ARG:NH2  | 2.34                     | 0.42              |
| 1:K:456:VAL:HG21 | 1:K:607:PHE:CB   | 2.47                     | 0.42              |
| 1:K:583:PRO:C    | 1:K:585:LEU:N    | 2.77                     | 0.42              |
| 1:L:388:GLU:OE2  | 1:L:394:PRO:HA   | 2.20                     | 0.42              |
| 1:M:282:LEU:HD23 | 1:M:378:ALA:HB1  | 2.01                     | 0.42              |
| 1:M:283:PRO:HB2  | 1:M:285:GLU:OE1  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:492:LYS:HD2  | 1:G:534:VAL:HA   | 2.02                     | 0.41              |
| 1:B:108:ILE:HG12 | 1:B:111:ARG:NH2  | 2.34                     | 0.41              |
| 1:C:388:GLU:OE2  | 1:C:394:PRO:HA   | 2.20                     | 0.41              |
| 1:C:582:LYS:HG2  | 1:C:586:MET:HE3  | 2.01                     | 0.41              |
| 1:D:283:PRO:HB2  | 1:D:285:GLU:OE1  | 2.20                     | 0.41              |
| 1:D:401:SER:OG   | 1:D:404:GLU:HG3  | 2.20                     | 0.41              |
| 1:E:134:LEU:O    | 1:E:138:ILE:HG13 | 2.21                     | 0.41              |
| 1:E:310:LEU:HD12 | 1:E:310:LEU:HA   | 1.74                     | 0.41              |
| 1:E:522:ILE:HB   | 1:E:562:ILE:HD13 | 2.01                     | 0.41              |
| 1:F:401:SER:OG   | 1:F:404:GLU:HG3  | 2.21                     | 0.41              |
| 1:F:586:MET:HG3  | 1:F:587:ASP:OD1  | 2.20                     | 0.41              |
| 1:G:134:LEU:O    | 1:G:138:ILE:HG13 | 2.20                     | 0.41              |
| 1:G:327:VAL:O    | 1:G:331:GLU:HG2  | 2.19                     | 0.41              |
| 1:G:454:THR:O    | 1:G:456:VAL:N    | 2.50                     | 0.41              |
| 1:H:401:SER:OG   | 1:H:404:GLU:HG3  | 2.20                     | 0.41              |
| 1:I:282:LEU:HD23 | 1:I:378:ALA:HB1  | 2.01                     | 0.41              |
| 1:I:283:PRO:HB2  | 1:I:285:GLU:OE1  | 2.20                     | 0.41              |
| 1:I:616:SER:O    | 1:I:619:VAL:HB   | 2.19                     | 0.41              |
| 1:J:401:SER:OG   | 1:J:404:GLU:HG3  | 2.20                     | 0.41              |
| 1:K:582:LYS:HG2  | 1:K:586:MET:HE3  | 2.01                     | 0.41              |
| 1:L:589:LEU:O    | 1:L:593:PHE:N    | 2.33                     | 0.41              |
| 1:M:409:MET:HA   | 1:M:412:ARG:HD2  | 2.01                     | 0.41              |
| 1:N:134:LEU:O    | 1:N:138:ILE:HG13 | 2.20                     | 0.41              |
| 1:A:108:ILE:HD12 | 1:A:117:PRO:HB3  | 2.01                     | 0.41              |
| 1:A:283:PRO:HB2  | 1:A:285:GLU:OE1  | 2.20                     | 0.41              |
| 1:B:582:LYS:HG2  | 1:B:586:MET:HE3  | 2.01                     | 0.41              |
| 1:B:615:LEU:HD23 | 1:B:661:LEU:CD1  | 2.51                     | 0.41              |
| 1:E:283:PRO:HB2  | 1:E:285:GLU:OE1  | 2.20                     | 0.41              |
| 1:G:283:PRO:HB2  | 1:G:285:GLU:OE1  | 2.20                     | 0.41              |
| 1:H:586:MET:HG3  | 1:H:587:ASP:OD1  | 2.20                     | 0.41              |
| 1:I:134:LEU:O    | 1:I:138:ILE:HG13 | 2.21                     | 0.41              |
| 1:I:454:THR:O    | 1:I:456:VAL:N    | 2.50                     | 0.41              |
| 1:J:283:PRO:HB2  | 1:J:285:GLU:OE1  | 2.20                     | 0.41              |
| 1:L:118:VAL:HG22 | 1:L:251:ASN:O    | 2.20                     | 0.41              |
| 1:M:522:ILE:HB   | 1:M:562:ILE:HD13 | 2.01                     | 0.41              |
| 1:A:401:SER:OG   | 1:A:404:GLU:HG3  | 2.20                     | 0.41              |
| 1:A:616:SER:O    | 1:A:619:VAL:HB   | 2.19                     | 0.41              |
| 1:B:285:GLU:CD   | 1:B:285:GLU:N    | 2.77                     | 0.41              |
| 1:B:522:ILE:HB   | 1:B:562:ILE:HD13 | 2.01                     | 0.41              |
| 1:D:388:GLU:OE2  | 1:D:394:PRO:HA   | 2.20                     | 0.41              |
| 1:D:522:ILE:HB   | 1:D:562:ILE:HD13 | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:615:LEU:HD23 | 1:F:661:LEU:CD1  | 2.51                     | 0.41              |
| 1:G:108:ILE:HD12 | 1:G:117:PRO:HB3  | 2.01                     | 0.41              |
| 1:G:113:THR:OG1  | 1:G:114:LYS:N    | 2.52                     | 0.41              |
| 1:G:409:MET:HA   | 1:G:412:ARG:HD2  | 2.01                     | 0.41              |
| 1:I:108:ILE:HD12 | 1:I:117:PRO:HB3  | 2.01                     | 0.41              |
| 1:I:113:THR:OG1  | 1:I:114:LYS:N    | 2.52                     | 0.41              |
| 1:I:327:VAL:O    | 1:I:331:GLU:HG2  | 2.19                     | 0.41              |
| 1:I:409:MET:HA   | 1:I:412:ARG:HD2  | 2.01                     | 0.41              |
| 1:J:616:SER:O    | 1:J:619:VAL:HB   | 2.19                     | 0.41              |
| 1:K:310:LEU:O    | 1:K:314:THR:OG1  | 2.30                     | 0.41              |
| 1:K:615:LEU:HD23 | 1:K:661:LEU:CD1  | 2.51                     | 0.41              |
| 1:N:283:PRO:HB2  | 1:N:285:GLU:OE1  | 2.20                     | 0.41              |
| 1:N:463:LYS:HG3  | 1:N:464:GLN:H    | 1.84                     | 0.41              |
| 1:N:586:MET:HG3  | 1:N:587:ASP:OD1  | 2.20                     | 0.41              |
| 1:A:376:VAL:HG23 | 1:A:376:VAL:O    | 2.21                     | 0.41              |
| 1:A:388:GLU:OE2  | 1:A:394:PRO:HA   | 2.20                     | 0.41              |
| 1:B:401:SER:OG   | 1:B:404:GLU:HG3  | 2.20                     | 0.41              |
| 1:B:616:SER:O    | 1:B:619:VAL:HB   | 2.19                     | 0.41              |
| 1:B:618:ILE:HG12 | 1:B:622:MET:CE   | 2.46                     | 0.41              |
| 1:C:118:VAL:HG22 | 1:C:251:ASN:O    | 2.20                     | 0.41              |
| 1:D:113:THR:OG1  | 1:D:114:LYS:N    | 2.52                     | 0.41              |
| 1:H:109:LEU:HD23 | 1:H:109:LEU:HA   | 1.88                     | 0.41              |
| 1:H:429:ARG:HD3  | 1:I:671:ASP:CG   | 2.46                     | 0.41              |
| 1:H:615:LEU:HD23 | 1:H:661:LEU:CD1  | 2.51                     | 0.41              |
| 1:I:456:VAL:HG21 | 1:I:607:PHE:CB   | 2.47                     | 0.41              |
| 1:J:108:ILE:HD12 | 1:J:117:PRO:HB3  | 2.01                     | 0.41              |
| 1:J:381:ASN:O    | 1:J:384:ALA:HB3  | 2.21                     | 0.41              |
| 1:J:388:GLU:OE2  | 1:J:394:PRO:HA   | 2.20                     | 0.41              |
| 1:K:401:SER:OG   | 1:K:404:GLU:HG3  | 2.20                     | 0.41              |
| 1:L:216:LEU:HD12 | 1:L:217:LYS:N    | 2.36                     | 0.41              |
| 1:L:271:ARG:NH2  | 1:L:281:ILE:O    | 2.54                     | 0.41              |
| 1:L:283:PRO:HB2  | 1:L:285:GLU:OE1  | 2.20                     | 0.41              |
| 1:M:118:VAL:HG22 | 1:M:251:ASN:O    | 2.20                     | 0.41              |
| 1:M:310:LEU:O    | 1:M:314:THR:OG1  | 2.30                     | 0.41              |
| 1:M:583:PRO:C    | 1:M:585:LEU:N    | 2.78                     | 0.41              |
| 1:A:381:ASN:O    | 1:A:384:ALA:HB3  | 2.21                     | 0.41              |
| 1:C:216:LEU:HD12 | 1:C:217:LYS:N    | 2.36                     | 0.41              |
| 1:C:271:ARG:NH2  | 1:C:281:ILE:O    | 2.54                     | 0.41              |
| 1:C:283:PRO:HB2  | 1:C:285:GLU:OE1  | 2.20                     | 0.41              |
| 1:C:522:ILE:HB   | 1:C:562:ILE:HD13 | 2.01                     | 0.41              |
| 1:D:271:ARG:NH2  | 1:D:281:ILE:O    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:285:GLU:N    | 1:D:285:GLU:CD   | 2.77                     | 0.41              |
| 1:D:463:LYS:HG3  | 1:D:464:GLN:H    | 1.84                     | 0.41              |
| 1:D:615:LEU:HD23 | 1:D:661:LEU:CD1  | 2.51                     | 0.41              |
| 1:E:114:LYS:NZ   | 1:E:251:ASN:HB2  | 2.36                     | 0.41              |
| 1:E:463:LYS:HG3  | 1:E:464:GLN:H    | 1.84                     | 0.41              |
| 1:E:586:MET:HG3  | 1:E:587:ASP:OD1  | 2.20                     | 0.41              |
| 1:F:160:LEU:HD23 | 1:F:160:LEU:HA   | 1.90                     | 0.41              |
| 1:G:388:GLU:OE2  | 1:G:394:PRO:HA   | 2.20                     | 0.41              |
| 1:G:456:VAL:HG21 | 1:G:607:PHE:CB   | 2.47                     | 0.41              |
| 1:H:160:LEU:HD23 | 1:H:160:LEU:HA   | 1.90                     | 0.41              |
| 1:H:494:ILE:HA   | 1:N:498:ALA:HB1  | 2.03                     | 0.41              |
| 1:I:212:LEU:CB   | 1:I:216:LEU:HD23 | 2.51                     | 0.41              |
| 1:I:388:GLU:OE2  | 1:I:394:PRO:HA   | 2.20                     | 0.41              |
| 1:J:376:VAL:HG23 | 1:J:376:VAL:O    | 2.21                     | 0.41              |
| 1:K:285:GLU:CD   | 1:K:285:GLU:N    | 2.77                     | 0.41              |
| 1:K:592:PHE:CD1  | 1:K:592:PHE:N    | 2.88                     | 0.41              |
| 1:K:618:ILE:HG12 | 1:K:622:MET:CE   | 2.46                     | 0.41              |
| 1:L:160:LEU:HD23 | 1:L:160:LEU:HA   | 1.90                     | 0.41              |
| 1:M:388:GLU:OE2  | 1:M:394:PRO:HA   | 2.20                     | 0.41              |
| 1:M:615:LEU:HD23 | 1:M:661:LEU:CD1  | 2.51                     | 0.41              |
| 1:M:684:LYS:HD3  | 1:M:684:LYS:N    | 2.36                     | 0.41              |
| 1:N:114:LYS:NZ   | 1:N:251:ASN:HB2  | 2.36                     | 0.41              |
| 1:N:212:LEU:CB   | 1:N:216:LEU:HD23 | 2.51                     | 0.41              |
| 1:A:582:LYS:HG2  | 1:A:586:MET:HE3  | 2.01                     | 0.41              |
| 1:B:271:ARG:NH2  | 1:B:281:ILE:O    | 2.54                     | 0.41              |
| 1:B:376:VAL:HG23 | 1:B:376:VAL:O    | 2.21                     | 0.41              |
| 1:B:381:ASN:O    | 1:B:385:GLU:OE1  | 2.39                     | 0.41              |
| 1:B:592:PHE:N    | 1:B:592:PHE:CD1  | 2.88                     | 0.41              |
| 1:D:118:VAL:HG22 | 1:D:251:ASN:O    | 2.20                     | 0.41              |
| 1:D:583:PRO:C    | 1:D:585:LEU:N    | 2.78                     | 0.41              |
| 1:E:212:LEU:CB   | 1:E:216:LEU:HD23 | 2.51                     | 0.41              |
| 1:E:528:GLU:H    | 1:E:529:LYS:HB2  | 1.85                     | 0.41              |
| 1:F:109:LEU:HD23 | 1:F:109:LEU:HA   | 1.88                     | 0.41              |
| 1:G:212:LEU:CB   | 1:G:216:LEU:HD23 | 2.51                     | 0.41              |
| 1:G:592:PHE:N    | 1:G:592:PHE:CD1  | 2.88                     | 0.41              |
| 1:H:678:LEU:HD22 | 1:N:403:ILE:HG23 | 2.02                     | 0.41              |
| 1:I:216:LEU:HD12 | 1:I:217:LYS:N    | 2.36                     | 0.41              |
| 1:I:401:SER:OG   | 1:I:404:GLU:HG3  | 2.20                     | 0.41              |
| 1:I:592:PHE:N    | 1:I:592:PHE:CD1  | 2.88                     | 0.41              |
| 1:J:508:ASN:HA   | 1:J:512:GLU:HB2  | 2.02                     | 0.41              |
| 1:K:271:ARG:NH2  | 1:K:281:ILE:O    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:376:VAL:HG23 | 1:K:376:VAL:O    | 2.21                     | 0.41              |
| 1:K:381:ASN:O    | 1:K:385:GLU:OE1  | 2.39                     | 0.41              |
| 1:L:365:ARG:HG3  | 1:L:365:ARG:NH1  | 2.09                     | 0.41              |
| 1:L:463:LYS:HG3  | 1:L:464:GLN:H    | 1.84                     | 0.41              |
| 1:M:113:THR:OG1  | 1:M:114:LYS:N    | 2.52                     | 0.41              |
| 1:M:271:ARG:NH2  | 1:M:281:ILE:O    | 2.54                     | 0.41              |
| 1:M:285:GLU:CD   | 1:M:285:GLU:N    | 2.77                     | 0.41              |
| 1:A:212:LEU:CB   | 1:A:216:LEU:HD23 | 2.51                     | 0.41              |
| 1:A:216:LEU:HD12 | 1:A:217:LYS:N    | 2.36                     | 0.41              |
| 1:A:271:ARG:CZ   | 1:A:281:ILE:HG22 | 2.51                     | 0.41              |
| 1:A:508:ASN:HA   | 1:A:512:GLU:HB2  | 2.02                     | 0.41              |
| 1:B:381:ASN:O    | 1:B:384:ALA:HB3  | 2.21                     | 0.41              |
| 1:B:388:GLU:OE2  | 1:B:394:PRO:HA   | 2.20                     | 0.41              |
| 1:D:114:LYS:NZ   | 1:D:251:ASN:HB2  | 2.36                     | 0.41              |
| 1:D:286:VAL:HG21 | 1:D:378:ALA:CB   | 2.51                     | 0.41              |
| 1:D:381:ASN:O    | 1:D:385:GLU:OE1  | 2.39                     | 0.41              |
| 1:D:684:LYS:N    | 1:D:684:LYS:HD3  | 2.36                     | 0.41              |
| 1:E:583:PRO:C    | 1:E:585:LEU:N    | 2.78                     | 0.41              |
| 1:E:618:ILE:HG12 | 1:E:622:MET:CE   | 2.46                     | 0.41              |
| 1:G:401:SER:OG   | 1:G:404:GLU:HG3  | 2.20                     | 0.41              |
| 1:H:450:PHE:HB3  | 1:H:607:PHE:CZ   | 2.56                     | 0.41              |
| 1:H:488:THR:O    | 1:H:490:VAL:HG22 | 2.21                     | 0.41              |
| 1:J:271:ARG:CZ   | 1:J:281:ILE:HG22 | 2.51                     | 0.41              |
| 1:J:512:GLU:C    | 1:J:512:GLU:OE1  | 2.64                     | 0.41              |
| 1:J:582:LYS:HG2  | 1:J:586:MET:HE3  | 2.01                     | 0.41              |
| 1:J:586:MET:HG3  | 1:J:587:ASP:OD1  | 2.20                     | 0.41              |
| 1:K:134:LEU:O    | 1:K:138:ILE:HG13 | 2.21                     | 0.41              |
| 1:K:381:ASN:O    | 1:K:384:ALA:HB3  | 2.21                     | 0.41              |
| 1:K:616:SER:O    | 1:K:619:VAL:HB   | 2.19                     | 0.41              |
| 1:L:376:VAL:O    | 1:L:376:VAL:HG23 | 2.21                     | 0.41              |
| 1:L:522:ILE:HB   | 1:L:562:ILE:HD13 | 2.01                     | 0.41              |
| 1:M:381:ASN:O    | 1:M:385:GLU:OE1  | 2.39                     | 0.41              |
| 1:M:425:GLU:OE2  | 1:M:429:ARG:NE   | 2.38                     | 0.41              |
| 1:M:463:LYS:HG3  | 1:M:464:GLN:H    | 1.84                     | 0.41              |
| 1:N:376:VAL:O    | 1:N:376:VAL:HG23 | 2.21                     | 0.41              |
| 1:N:381:ASN:O    | 1:N:385:GLU:OE1  | 2.39                     | 0.41              |
| 1:N:488:THR:O    | 1:N:490:VAL:HG22 | 2.21                     | 0.41              |
| 1:N:528:GLU:H    | 1:N:529:LYS:HB2  | 1.85                     | 0.41              |
| 1:N:583:PRO:C    | 1:N:585:LEU:N    | 2.77                     | 0.41              |
| 1:A:512:GLU:C    | 1:A:512:GLU:OE1  | 2.64                     | 0.41              |
| 1:A:653:ASP:O    | 1:A:655:VAL:N    | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:286:VAL:HG21 | 1:B:378:ALA:CB   | 2.51                     | 0.41              |
| 1:C:114:LYS:NZ   | 1:C:251:ASN:HB2  | 2.36                     | 0.41              |
| 1:C:376:VAL:O    | 1:C:376:VAL:HG23 | 2.21                     | 0.41              |
| 1:C:586:MET:HG3  | 1:C:587:ASP:OD1  | 2.20                     | 0.41              |
| 1:D:541:VAL:HA   | 1:D:545:GLY:H    | 1.86                     | 0.41              |
| 1:E:376:VAL:O    | 1:E:376:VAL:HG23 | 2.21                     | 0.41              |
| 1:E:381:ASN:O    | 1:E:385:GLU:OE1  | 2.39                     | 0.41              |
| 1:E:488:THR:O    | 1:E:490:VAL:HG22 | 2.21                     | 0.41              |
| 1:F:212:LEU:CB   | 1:F:216:LEU:HD23 | 2.51                     | 0.41              |
| 1:F:329:ALA:HA   | 1:F:332:ARG:CZ   | 2.51                     | 0.41              |
| 1:F:488:THR:O    | 1:F:490:VAL:HG22 | 2.21                     | 0.41              |
| 1:G:216:LEU:HD12 | 1:G:217:LYS:N    | 2.36                     | 0.41              |
| 1:G:376:VAL:HG23 | 1:G:376:VAL:O    | 2.21                     | 0.41              |
| 1:G:528:GLU:H    | 1:G:529:LYS:HB2  | 1.85                     | 0.41              |
| 1:H:212:LEU:CB   | 1:H:216:LEU:HD23 | 2.51                     | 0.41              |
| 1:H:329:ALA:HA   | 1:H:332:ARG:CZ   | 2.51                     | 0.41              |
| 1:H:534:VAL:CA   | 1:I:492:LYS:HD2  | 2.47                     | 0.41              |
| 1:I:376:VAL:HG23 | 1:I:376:VAL:O    | 2.21                     | 0.41              |
| 1:I:528:GLU:H    | 1:I:529:LYS:HB2  | 1.85                     | 0.41              |
| 1:J:216:LEU:HD12 | 1:J:217:LYS:N    | 2.36                     | 0.41              |
| 1:J:653:ASP:O    | 1:J:655:VAL:N    | 2.51                     | 0.41              |
| 1:K:283:PRO:HB2  | 1:K:285:GLU:OE1  | 2.20                     | 0.41              |
| 1:L:134:LEU:O    | 1:L:138:ILE:HG13 | 2.20                     | 0.41              |
| 1:N:271:ARG:CZ   | 1:N:281:ILE:HG22 | 2.51                     | 0.41              |
| 1:A:118:VAL:HG22 | 1:A:251:ASN:O    | 2.20                     | 0.41              |
| 1:A:450:PHE:HB3  | 1:A:607:PHE:CZ   | 2.56                     | 0.41              |
| 1:A:586:MET:HG3  | 1:A:587:ASP:OD1  | 2.20                     | 0.41              |
| 1:B:134:LEU:O    | 1:B:138:ILE:HG13 | 2.21                     | 0.41              |
| 1:B:329:ALA:HA   | 1:B:332:ARG:CZ   | 2.51                     | 0.41              |
| 1:B:508:ASN:HA   | 1:B:512:GLU:HB2  | 2.03                     | 0.41              |
| 1:B:541:VAL:HA   | 1:B:545:GLY:H    | 1.86                     | 0.41              |
| 1:C:134:LEU:O    | 1:C:138:ILE:HG13 | 2.21                     | 0.41              |
| 1:C:454:THR:O    | 1:C:456:VAL:N    | 2.50                     | 0.41              |
| 1:C:463:LYS:HG3  | 1:C:464:GLN:H    | 1.84                     | 0.41              |
| 1:D:425:GLU:OE2  | 1:D:429:ARG:NE   | 2.38                     | 0.41              |
| 1:D:450:PHE:HB3  | 1:D:607:PHE:CZ   | 2.56                     | 0.41              |
| 1:E:271:ARG:CZ   | 1:E:281:ILE:HG22 | 2.51                     | 0.41              |
| 1:E:381:ASN:O    | 1:E:384:ALA:HB3  | 2.21                     | 0.41              |
| 1:E:401:SER:OG   | 1:E:404:GLU:HG3  | 2.20                     | 0.41              |
| 1:E:450:PHE:HB3  | 1:E:607:PHE:CZ   | 2.56                     | 0.41              |
| 1:E:512:GLU:OE1  | 1:E:512:GLU:C    | 2.64                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:541:VAL:HA   | 1:E:545:GLY:H    | 1.86                     | 0.41              |
| 1:E:589:LEU:O    | 1:E:593:PHE:N    | 2.33                     | 0.41              |
| 1:E:684:LYS:HD3  | 1:E:684:LYS:N    | 2.36                     | 0.41              |
| 1:F:376:VAL:O    | 1:F:376:VAL:HG23 | 2.21                     | 0.41              |
| 1:F:381:ASN:O    | 1:F:385:GLU:OE1  | 2.39                     | 0.41              |
| 1:F:447:ASN:N    | 1:F:602:ASN:OD1  | 2.43                     | 0.41              |
| 1:F:450:PHE:HB3  | 1:F:607:PHE:CZ   | 2.56                     | 0.41              |
| 1:G:118:VAL:HG22 | 1:G:251:ASN:O    | 2.20                     | 0.41              |
| 1:G:271:ARG:CZ   | 1:G:281:ILE:HG22 | 2.51                     | 0.41              |
| 1:G:286:VAL:HG21 | 1:G:378:ALA:CB   | 2.51                     | 0.41              |
| 1:G:450:PHE:HB3  | 1:G:607:PHE:CZ   | 2.56                     | 0.41              |
| 1:G:488:THR:O    | 1:G:490:VAL:HG22 | 2.21                     | 0.41              |
| 1:G:512:GLU:C    | 1:G:512:GLU:OE1  | 2.64                     | 0.41              |
| 1:G:615:LEU:HD23 | 1:G:661:LEU:CD1  | 2.51                     | 0.41              |
| 1:H:283:PRO:HB2  | 1:H:285:GLU:OE1  | 2.20                     | 0.41              |
| 1:H:381:ASN:O    | 1:H:385:GLU:OE1  | 2.39                     | 0.41              |
| 1:H:447:ASN:N    | 1:H:602:ASN:OD1  | 2.43                     | 0.41              |
| 1:H:684:LYS:N    | 1:H:684:LYS:HD3  | 2.36                     | 0.41              |
| 1:I:118:VAL:HG22 | 1:I:251:ASN:O    | 2.20                     | 0.41              |
| 1:I:271:ARG:CZ   | 1:I:281:ILE:HG22 | 2.51                     | 0.41              |
| 1:I:300:GLN:OE1  | 1:I:300:GLN:N    | 2.32                     | 0.41              |
| 1:I:450:PHE:HB3  | 1:I:607:PHE:CZ   | 2.56                     | 0.41              |
| 1:I:512:GLU:C    | 1:I:512:GLU:OE1  | 2.64                     | 0.41              |
| 1:I:615:LEU:HD23 | 1:I:661:LEU:CD1  | 2.51                     | 0.41              |
| 1:J:111:ARG:HB3  | 1:K:312:ASP:OD2  | 2.21                     | 0.41              |
| 1:J:118:VAL:HG22 | 1:J:251:ASN:O    | 2.20                     | 0.41              |
| 1:J:160:LEU:HD23 | 1:J:160:LEU:HA   | 1.90                     | 0.41              |
| 1:J:212:LEU:CB   | 1:J:216:LEU:HD23 | 2.51                     | 0.41              |
| 1:J:450:PHE:HB3  | 1:J:607:PHE:CZ   | 2.56                     | 0.41              |
| 1:K:118:VAL:HG22 | 1:K:251:ASN:O    | 2.20                     | 0.41              |
| 1:K:286:VAL:HG21 | 1:K:378:ALA:CB   | 2.51                     | 0.41              |
| 1:K:329:ALA:HA   | 1:K:332:ARG:CZ   | 2.51                     | 0.41              |
| 1:K:388:GLU:OE2  | 1:K:394:PRO:HA   | 2.20                     | 0.41              |
| 1:K:508:ASN:HA   | 1:K:512:GLU:HB2  | 2.02                     | 0.41              |
| 1:K:541:VAL:HA   | 1:K:545:GLY:H    | 1.86                     | 0.41              |
| 1:L:114:LYS:NZ   | 1:L:251:ASN:HB2  | 2.36                     | 0.41              |
| 1:L:381:ASN:O    | 1:L:385:GLU:OE1  | 2.39                     | 0.41              |
| 1:L:381:ASN:O    | 1:L:384:ALA:HB3  | 2.21                     | 0.41              |
| 1:L:586:MET:HG3  | 1:L:587:ASP:OD1  | 2.20                     | 0.41              |
| 1:M:114:LYS:NZ   | 1:M:251:ASN:HB2  | 2.36                     | 0.41              |
| 1:M:286:VAL:HG21 | 1:M:378:ALA:CB   | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:528:GLU:H    | 1:M:529:LYS:HB2  | 1.84                     | 0.41              |
| 1:M:541:VAL:HA   | 1:M:545:GLY:H    | 1.86                     | 0.41              |
| 1:N:329:ALA:HA   | 1:N:332:ARG:CZ   | 2.51                     | 0.41              |
| 1:N:381:ASN:O    | 1:N:384:ALA:HB3  | 2.21                     | 0.41              |
| 1:N:450:PHE:HB3  | 1:N:607:PHE:CZ   | 2.56                     | 0.41              |
| 1:N:512:GLU:OE1  | 1:N:512:GLU:C    | 2.64                     | 0.41              |
| 1:N:541:VAL:HA   | 1:N:545:GLY:H    | 1.86                     | 0.41              |
| 1:N:618:ILE:HG12 | 1:N:622:MET:CE   | 2.46                     | 0.41              |
| 1:A:160:LEU:HD23 | 1:A:160:LEU:HA   | 1.90                     | 0.41              |
| 1:A:271:ARG:NH2  | 1:A:281:ILE:O    | 2.54                     | 0.41              |
| 1:A:329:ALA:HA   | 1:A:332:ARG:CZ   | 2.51                     | 0.41              |
| 1:A:381:ASN:O    | 1:A:385:GLU:OE1  | 2.39                     | 0.41              |
| 1:A:583:PRO:C    | 1:A:585:LEU:N    | 2.78                     | 0.41              |
| 1:A:684:LYS:N    | 1:A:684:LYS:HD3  | 2.36                     | 0.41              |
| 1:B:118:VAL:HG22 | 1:B:251:ASN:O    | 2.20                     | 0.41              |
| 1:B:684:LYS:HD3  | 1:B:684:LYS:N    | 2.36                     | 0.41              |
| 1:C:160:LEU:HD23 | 1:C:160:LEU:HA   | 1.90                     | 0.41              |
| 1:C:212:LEU:CB   | 1:C:216:LEU:HD23 | 2.51                     | 0.41              |
| 1:C:286:VAL:HG21 | 1:C:378:ALA:CB   | 2.51                     | 0.41              |
| 1:C:381:ASN:O    | 1:C:384:ALA:HB3  | 2.21                     | 0.41              |
| 1:C:381:ASN:O    | 1:C:385:GLU:OE1  | 2.39                     | 0.41              |
| 1:D:376:VAL:O    | 1:D:376:VAL:HG23 | 2.21                     | 0.41              |
| 1:D:447:ASN:N    | 1:D:602:ASN:OD1  | 2.43                     | 0.41              |
| 1:D:488:THR:O    | 1:D:490:VAL:HG22 | 2.21                     | 0.41              |
| 1:D:528:GLU:H    | 1:D:529:LYS:HB2  | 1.85                     | 0.41              |
| 1:E:329:ALA:HA   | 1:E:332:ARG:CZ   | 2.51                     | 0.41              |
| 1:E:388:GLU:OE2  | 1:E:394:PRO:HA   | 2.20                     | 0.41              |
| 1:E:592:PHE:CD1  | 1:E:592:PHE:N    | 2.88                     | 0.41              |
| 1:F:114:LYS:NZ   | 1:F:251:ASN:HB2  | 2.36                     | 0.41              |
| 1:F:283:PRO:HB2  | 1:F:285:GLU:OE1  | 2.20                     | 0.41              |
| 1:F:512:GLU:OE1  | 1:F:512:GLU:C    | 2.64                     | 0.41              |
| 1:F:684:LYS:N    | 1:F:684:LYS:HD3  | 2.36                     | 0.41              |
| 1:G:508:ASN:HA   | 1:G:512:GLU:HB2  | 2.03                     | 0.41              |
| 1:H:114:LYS:NZ   | 1:H:251:ASN:HB2  | 2.36                     | 0.41              |
| 1:H:134:LEU:O    | 1:H:138:ILE:HG13 | 2.21                     | 0.41              |
| 1:H:376:VAL:O    | 1:H:376:VAL:HG23 | 2.21                     | 0.41              |
| 1:H:541:VAL:HA   | 1:H:545:GLY:H    | 1.86                     | 0.41              |
| 1:I:286:VAL:HG21 | 1:I:378:ALA:CB   | 2.51                     | 0.41              |
| 1:I:488:THR:O    | 1:I:490:VAL:HG22 | 2.21                     | 0.41              |
| 1:I:508:ASN:HA   | 1:I:512:GLU:HB2  | 2.03                     | 0.41              |
| 1:J:271:ARG:NH2  | 1:J:281:ILE:O    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:329:ALA:HA   | 1:J:332:ARG:CZ   | 2.51                     | 0.41              |
| 1:J:381:ASN:O    | 1:J:385:GLU:OE1  | 2.39                     | 0.41              |
| 1:J:583:PRO:C    | 1:J:585:LEU:N    | 2.78                     | 0.41              |
| 1:K:557:PHE:O    | 1:K:560:THR:HG22 | 2.21                     | 0.41              |
| 1:L:454:THR:O    | 1:L:456:VAL:N    | 2.50                     | 0.41              |
| 1:M:212:LEU:CB   | 1:M:216:LEU:HD23 | 2.51                     | 0.41              |
| 1:M:450:PHE:HB3  | 1:M:607:PHE:CZ   | 2.56                     | 0.41              |
| 1:M:488:THR:O    | 1:M:490:VAL:HG22 | 2.21                     | 0.41              |
| 1:N:684:LYS:HD3  | 1:N:684:LYS:N    | 2.36                     | 0.41              |
| 1:A:134:LEU:O    | 1:A:138:ILE:HG13 | 2.21                     | 0.40              |
| 1:B:283:PRO:HB2  | 1:B:285:GLU:OE1  | 2.20                     | 0.40              |
| 1:B:359:ARG:NE   | 1:B:359:ARG:HA   | 2.36                     | 0.40              |
| 1:B:557:PHE:O    | 1:B:560:THR:HG22 | 2.22                     | 0.40              |
| 1:C:248:ARG:HG2  | 1:C:249:ARG:NH1  | 2.37                     | 0.40              |
| 1:C:310:LEU:HD12 | 1:C:310:LEU:HA   | 1.74                     | 0.40              |
| 1:D:216:LEU:HD12 | 1:D:217:LYS:N    | 2.36                     | 0.40              |
| 1:E:549:ASP:OD1  | 1:E:552:GLY:N    | 2.55                     | 0.40              |
| 1:E:557:PHE:O    | 1:E:560:THR:HG22 | 2.21                     | 0.40              |
| 1:F:134:LEU:O    | 1:F:138:ILE:HG13 | 2.21                     | 0.40              |
| 1:F:381:ASN:O    | 1:F:384:ALA:HB3  | 2.21                     | 0.40              |
| 1:F:541:VAL:HA   | 1:F:545:GLY:H    | 1.86                     | 0.40              |
| 1:G:329:ALA:HA   | 1:G:332:ARG:CZ   | 2.51                     | 0.40              |
| 1:G:541:VAL:HA   | 1:G:545:GLY:H    | 1.86                     | 0.40              |
| 1:H:76:LEU:HD22  | 1:H:82:ASN:HB2   | 2.03                     | 0.40              |
| 1:H:381:ASN:O    | 1:H:384:ALA:HB3  | 2.21                     | 0.40              |
| 1:H:512:GLU:C    | 1:H:512:GLU:OE1  | 2.64                     | 0.40              |
| 1:H:532:PRO:HA   | 1:I:490:VAL:CB   | 2.42                     | 0.40              |
| 1:I:329:ALA:HA   | 1:I:332:ARG:CZ   | 2.51                     | 0.40              |
| 1:I:583:PRO:C    | 1:I:585:LEU:N    | 2.77                     | 0.40              |
| 1:J:134:LEU:O    | 1:J:138:ILE:HG13 | 2.21                     | 0.40              |
| 1:J:684:LYS:N    | 1:J:684:LYS:HD3  | 2.36                     | 0.40              |
| 1:K:271:ARG:CZ   | 1:K:281:ILE:HG22 | 2.51                     | 0.40              |
| 1:K:684:LYS:HD3  | 1:K:684:LYS:N    | 2.36                     | 0.40              |
| 1:L:212:LEU:CB   | 1:L:216:LEU:HD23 | 2.51                     | 0.40              |
| 1:L:286:VAL:HG21 | 1:L:378:ALA:CB   | 2.51                     | 0.40              |
| 1:L:329:ALA:HA   | 1:L:332:ARG:CZ   | 2.51                     | 0.40              |
| 1:L:359:ARG:NE   | 1:L:359:ARG:HA   | 2.37                     | 0.40              |
| 1:L:401:SER:OG   | 1:L:404:GLU:HG3  | 2.20                     | 0.40              |
| 1:M:271:ARG:CZ   | 1:M:281:ILE:HG22 | 2.51                     | 0.40              |
| 1:N:76:LEU:HD22  | 1:N:82:ASN:HB2   | 2.03                     | 0.40              |
| 1:N:388:GLU:OE2  | 1:N:394:PRO:HA   | 2.20                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:592:PHE:CD1  | 1:N:592:PHE:N    | 2.88                     | 0.40              |
| 1:B:114:LYS:NZ   | 1:B:251:ASN:HB2  | 2.36                     | 0.40              |
| 1:B:271:ARG:CZ   | 1:B:281:ILE:HG22 | 2.51                     | 0.40              |
| 1:C:359:ARG:HA   | 1:C:359:ARG:NE   | 2.37                     | 0.40              |
| 1:C:365:ARG:HG3  | 1:C:365:ARG:NH1  | 2.09                     | 0.40              |
| 1:C:557:PHE:O    | 1:C:560:THR:HG22 | 2.21                     | 0.40              |
| 1:C:684:LYS:HD3  | 1:C:684:LYS:N    | 2.36                     | 0.40              |
| 1:D:248:ARG:HG2  | 1:D:249:ARG:NH1  | 2.37                     | 0.40              |
| 1:D:488:THR:O    | 1:D:490:VAL:N    | 2.52                     | 0.40              |
| 1:E:76:LEU:HD22  | 1:E:82:ASN:HB2   | 2.03                     | 0.40              |
| 1:E:109:LEU:HA   | 1:E:109:LEU:HD23 | 1.88                     | 0.40              |
| 1:E:216:LEU:HD12 | 1:E:217:LYS:N    | 2.36                     | 0.40              |
| 1:E:248:ARG:HG2  | 1:E:249:ARG:NH1  | 2.37                     | 0.40              |
| 1:F:76:LEU:HD22  | 1:F:82:ASN:HB2   | 2.03                     | 0.40              |
| 1:F:286:VAL:HG21 | 1:F:378:ALA:CB   | 2.51                     | 0.40              |
| 1:G:679:ASP:CA   | 1:G:680:HIS:HB2  | 2.52                     | 0.40              |
| 1:H:438:PHE:CE1  | 1:I:633:LYS:HE3  | 2.57                     | 0.40              |
| 1:K:359:ARG:HA   | 1:K:359:ARG:NE   | 2.37                     | 0.40              |
| 1:L:248:ARG:HG2  | 1:L:249:ARG:NH1  | 2.37                     | 0.40              |
| 1:L:271:ARG:CZ   | 1:L:281:ILE:HG22 | 2.51                     | 0.40              |
| 1:M:376:VAL:O    | 1:M:376:VAL:HG23 | 2.21                     | 0.40              |
| 1:M:445:ILE:HB   | 1:M:560:THR:O    | 2.22                     | 0.40              |
| 1:M:508:ASN:HA   | 1:M:512:GLU:HB2  | 2.03                     | 0.40              |
| 1:M:549:ASP:OD1  | 1:M:552:GLY:N    | 2.54                     | 0.40              |
| 1:N:216:LEU:HD12 | 1:N:217:LYS:N    | 2.36                     | 0.40              |
| 1:N:285:GLU:CD   | 1:N:285:GLU:N    | 2.77                     | 0.40              |
| 1:N:445:ILE:HB   | 1:N:560:THR:O    | 2.22                     | 0.40              |
| 1:N:549:ASP:OD1  | 1:N:552:GLY:N    | 2.54                     | 0.40              |
| 1:N:585:LEU:HD23 | 1:N:589:LEU:HD13 | 2.03                     | 0.40              |
| 1:N:615:LEU:HD23 | 1:N:661:LEU:CD1  | 2.51                     | 0.40              |
| 1:A:102:ILE:O    | 1:A:105:ALA:HB3  | 2.22                     | 0.40              |
| 1:B:575:ASN:HA   | 1:B:578:GLU:HB3  | 2.04                     | 0.40              |
| 1:C:271:ARG:CZ   | 1:C:281:ILE:HG22 | 2.51                     | 0.40              |
| 1:C:329:ALA:HA   | 1:C:332:ARG:CZ   | 2.51                     | 0.40              |
| 1:C:401:SER:OG   | 1:C:404:GLU:HG3  | 2.20                     | 0.40              |
| 1:C:512:GLU:OE1  | 1:C:512:GLU:C    | 2.64                     | 0.40              |
| 1:D:212:LEU:CB   | 1:D:216:LEU:HD23 | 2.51                     | 0.40              |
| 1:D:271:ARG:CZ   | 1:D:281:ILE:HG22 | 2.51                     | 0.40              |
| 1:D:557:PHE:O    | 1:D:560:THR:HG22 | 2.21                     | 0.40              |
| 1:D:613:GLU:H    | 1:D:613:GLU:CD   | 2.30                     | 0.40              |
| 1:D:617:LYS:O    | 1:D:621:LEU:HG   | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:279:ASN:HD21 | 1:E:315:ALA:HB1  | 1.87                     | 0.40              |
| 1:E:585:LEU:HD23 | 1:E:589:LEU:HD13 | 2.03                     | 0.40              |
| 1:E:615:LEU:HD23 | 1:E:661:LEU:CD1  | 2.51                     | 0.40              |
| 1:G:381:ASN:O    | 1:G:385:GLU:OE1  | 2.39                     | 0.40              |
| 1:G:583:PRO:C    | 1:G:585:LEU:N    | 2.78                     | 0.40              |
| 1:H:112:ARG:NE   | 1:I:273:LEU:HD21 | 2.36                     | 0.40              |
| 1:H:286:VAL:HG21 | 1:H:378:ALA:CB   | 2.51                     | 0.40              |
| 1:I:381:ASN:O    | 1:I:385:GLU:OE1  | 2.39                     | 0.40              |
| 1:I:541:VAL:HA   | 1:I:545:GLY:H    | 1.86                     | 0.40              |
| 1:I:549:ASP:OD1  | 1:I:552:GLY:N    | 2.54                     | 0.40              |
| 1:J:102:ILE:O    | 1:J:105:ALA:HB3  | 2.22                     | 0.40              |
| 1:K:114:LYS:NZ   | 1:K:251:ASN:HB2  | 2.36                     | 0.40              |
| 1:K:212:LEU:CB   | 1:K:216:LEU:HD23 | 2.51                     | 0.40              |
| 1:K:216:LEU:HD12 | 1:K:217:LYS:N    | 2.36                     | 0.40              |
| 1:K:248:ARG:HG2  | 1:K:249:ARG:NH1  | 2.36                     | 0.40              |
| 1:K:575:ASN:HA   | 1:K:578:GLU:HB3  | 2.04                     | 0.40              |
| 1:K:586:MET:HG3  | 1:K:587:ASP:OD1  | 2.20                     | 0.40              |
| 1:K:617:LYS:O    | 1:K:621:LEU:HG   | 2.22                     | 0.40              |
| 1:L:512:GLU:C    | 1:L:512:GLU:OE1  | 2.64                     | 0.40              |
| 1:L:557:PHE:O    | 1:L:560:THR:HG22 | 2.21                     | 0.40              |
| 1:L:684:LYS:N    | 1:L:684:LYS:HD3  | 2.36                     | 0.40              |
| 1:M:134:LEU:O    | 1:M:138:ILE:HG13 | 2.20                     | 0.40              |
| 1:M:216:LEU:HD12 | 1:M:217:LYS:N    | 2.36                     | 0.40              |
| 1:M:248:ARG:HG2  | 1:M:249:ARG:NH1  | 2.37                     | 0.40              |
| 1:M:329:ALA:HA   | 1:M:332:ARG:CZ   | 2.51                     | 0.40              |
| 1:M:557:PHE:O    | 1:M:560:THR:HG22 | 2.21                     | 0.40              |
| 1:N:248:ARG:HG2  | 1:N:249:ARG:NH1  | 2.37                     | 0.40              |
| 1:N:279:ASN:HD21 | 1:N:315:ALA:HB1  | 1.87                     | 0.40              |
| 1:N:401:SER:OG   | 1:N:404:GLU:HG3  | 2.20                     | 0.40              |
| 1:N:557:PHE:O    | 1:N:560:THR:HG22 | 2.21                     | 0.40              |
| 1:A:557:PHE:O    | 1:A:560:THR:HG22 | 2.21                     | 0.40              |
| 1:A:615:LEU:HD23 | 1:A:661:LEU:CD1  | 2.51                     | 0.40              |
| 1:B:248:ARG:HG2  | 1:B:249:ARG:NH1  | 2.37                     | 0.40              |
| 1:B:450:PHE:HB3  | 1:B:607:PHE:CZ   | 2.56                     | 0.40              |
| 1:B:512:GLU:C    | 1:B:512:GLU:OE1  | 2.64                     | 0.40              |
| 1:C:102:ILE:O    | 1:C:105:ALA:HB3  | 2.22                     | 0.40              |
| 1:C:575:ASN:HA   | 1:C:578:GLU:HB3  | 2.04                     | 0.40              |
| 1:D:445:ILE:HB   | 1:D:560:THR:O    | 2.22                     | 0.40              |
| 1:D:508:ASN:HA   | 1:D:512:GLU:HB2  | 2.02                     | 0.40              |
| 1:E:118:VAL:HG22 | 1:E:251:ASN:O    | 2.20                     | 0.40              |
| 1:F:271:ARG:CZ   | 1:F:281:ILE:HG22 | 2.51                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:365:ARG:HH11 | 1:F:365:ARG:CG   | 2.17                     | 0.40              |
| 1:F:403:ILE:HG23 | 1:G:678:LEU:HD22 | 2.03                     | 0.40              |
| 1:F:592:PHE:N    | 1:F:592:PHE:CD1  | 2.88                     | 0.40              |
| 1:G:279:ASN:HD21 | 1:G:315:ALA:HB1  | 1.87                     | 0.40              |
| 1:G:300:GLN:OE1  | 1:G:300:GLN:N    | 2.32                     | 0.40              |
| 1:G:549:ASP:OD1  | 1:G:552:GLY:N    | 2.54                     | 0.40              |
| 1:H:271:ARG:CZ   | 1:H:281:ILE:HG22 | 2.51                     | 0.40              |
| 1:H:285:GLU:CD   | 1:H:285:GLU:N    | 2.77                     | 0.40              |
| 1:H:592:PHE:N    | 1:H:592:PHE:CD1  | 2.88                     | 0.40              |
| 1:I:248:ARG:HG2  | 1:I:249:ARG:NH1  | 2.36                     | 0.40              |
| 1:I:279:ASN:HD21 | 1:I:315:ALA:HB1  | 1.87                     | 0.40              |
| 1:I:679:ASP:CA   | 1:I:680:HIS:HB2  | 2.52                     | 0.40              |
| 1:J:359:ARG:HA   | 1:J:359:ARG:NE   | 2.36                     | 0.40              |
| 1:J:615:LEU:HD23 | 1:J:661:LEU:CD1  | 2.51                     | 0.40              |
| 1:K:102:ILE:O    | 1:K:105:ALA:HB3  | 2.22                     | 0.40              |
| 1:K:450:PHE:HB3  | 1:K:607:PHE:CZ   | 2.56                     | 0.40              |
| 1:K:454:THR:HB   | 3:K:803:AGS:O2G  | 2.22                     | 0.40              |
| 1:K:512:GLU:C    | 1:K:512:GLU:OE1  | 2.64                     | 0.40              |
| 1:L:96:ILE:H     | 3:L:802:AGS:HN62 | 1.70                     | 0.40              |
| 1:L:102:ILE:O    | 1:L:105:ALA:HB3  | 2.22                     | 0.40              |
| 1:L:541:VAL:HA   | 1:L:545:GLY:H    | 1.86                     | 0.40              |
| 1:L:575:ASN:HA   | 1:L:578:GLU:HB3  | 2.04                     | 0.40              |
| 1:L:613:GLU:H    | 1:L:613:GLU:CD   | 2.30                     | 0.40              |
| 1:M:613:GLU:H    | 1:M:613:GLU:CD   | 2.29                     | 0.40              |
| 1:M:617:LYS:O    | 1:M:621:LEU:HG   | 2.22                     | 0.40              |
| 1:N:118:VAL:HG22 | 1:N:251:ASN:O    | 2.20                     | 0.40              |
| 1:N:121:GLY:O    | 1:N:232:THR:HA   | 2.21                     | 0.40              |
| 1:A:575:ASN:HA   | 1:A:578:GLU:HB3  | 2.04                     | 0.40              |
| 1:B:212:LEU:CB   | 1:B:216:LEU:HD23 | 2.51                     | 0.40              |
| 1:B:341:GLN:HB2  | 1:B:356:TYR:HB3  | 2.03                     | 0.40              |
| 1:B:447:ASN:N    | 1:B:602:ASN:OD1  | 2.43                     | 0.40              |
| 1:B:454:THR:HB   | 3:B:803:AGS:O2G  | 2.22                     | 0.40              |
| 1:B:586:MET:HG3  | 1:B:587:ASP:OD1  | 2.20                     | 0.40              |
| 1:B:617:LYS:O    | 1:B:621:LEU:HG   | 2.22                     | 0.40              |
| 1:C:450:PHE:HB3  | 1:C:607:PHE:CZ   | 2.56                     | 0.40              |
| 1:C:541:VAL:HA   | 1:C:545:GLY:H    | 1.86                     | 0.40              |
| 1:C:613:GLU:H    | 1:C:613:GLU:CD   | 2.30                     | 0.40              |
| 1:D:96:ILE:H     | 3:D:802:AGS:HN62 | 1.70                     | 0.40              |
| 1:D:102:ILE:O    | 1:D:105:ALA:HB3  | 2.22                     | 0.40              |
| 1:D:329:ALA:HA   | 1:D:332:ARG:CZ   | 2.51                     | 0.40              |
| 1:D:549:ASP:OD1  | 1:D:552:GLY:N    | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:585:LEU:HD23 | 1:D:589:LEU:HD13 | 2.03                     | 0.40              |
| 1:E:121:GLY:O    | 1:E:232:THR:HA   | 2.21                     | 0.40              |
| 1:E:271:ARG:NH2  | 1:E:281:ILE:O    | 2.54                     | 0.40              |
| 1:E:285:GLU:CD   | 1:E:285:GLU:N    | 2.77                     | 0.40              |
| 1:E:445:ILE:HB   | 1:E:560:THR:O    | 2.22                     | 0.40              |
| 1:F:118:VAL:HG22 | 1:F:251:ASN:O    | 2.20                     | 0.40              |
| 1:F:285:GLU:CD   | 1:F:285:GLU:N    | 2.77                     | 0.40              |
| 1:F:388:GLU:OE2  | 1:F:394:PRO:HA   | 2.20                     | 0.40              |
| 1:F:445:ILE:HB   | 1:F:560:THR:O    | 2.22                     | 0.40              |
| 1:F:613:GLU:H    | 1:F:613:GLU:CD   | 2.30                     | 0.40              |
| 1:G:102:ILE:O    | 1:G:105:ALA:HB3  | 2.22                     | 0.40              |
| 1:G:248:ARG:HG2  | 1:G:249:ARG:NH1  | 2.37                     | 0.40              |
| 1:G:271:ARG:NH2  | 1:G:281:ILE:O    | 2.54                     | 0.40              |
| 1:G:381:ASN:O    | 1:G:384:ALA:HB3  | 2.21                     | 0.40              |
| 1:H:118:VAL:HG22 | 1:H:251:ASN:O    | 2.20                     | 0.40              |
| 1:H:388:GLU:OE2  | 1:H:394:PRO:HA   | 2.20                     | 0.40              |
| 1:H:613:GLU:H    | 1:H:613:GLU:CD   | 2.30                     | 0.40              |
| 1:I:102:ILE:O    | 1:I:105:ALA:HB3  | 2.22                     | 0.40              |
| 1:I:151:GLU:N    | 1:I:186:ASN:O    | 2.30                     | 0.40              |
| 1:I:271:ARG:NH2  | 1:I:281:ILE:O    | 2.54                     | 0.40              |
| 1:J:114:LYS:NZ   | 1:J:251:ASN:HB2  | 2.36                     | 0.40              |
| 1:J:557:PHE:O    | 1:J:560:THR:HG22 | 2.21                     | 0.40              |
| 1:J:575:ASN:HA   | 1:J:578:GLU:HB3  | 2.04                     | 0.40              |
| 1:J:585:LEU:HD23 | 1:J:589:LEU:HD13 | 2.03                     | 0.40              |
| 1:K:341:GLN:HB2  | 1:K:356:TYR:HB3  | 2.03                     | 0.40              |
| 1:L:450:PHE:HB3  | 1:L:607:PHE:CZ   | 2.56                     | 0.40              |
| 1:M:102:ILE:O    | 1:M:105:ALA:HB3  | 2.22                     | 0.40              |
| 1:M:104:GLU:HA   | 1:N:321:GLN:NE2  | 2.36                     | 0.40              |
| 1:M:114:LYS:NZ   | 1:M:250:PHE:O    | 2.43                     | 0.40              |
| 1:M:575:ASN:HA   | 1:M:578:GLU:HB3  | 2.04                     | 0.40              |
| 1:M:585:LEU:HD23 | 1:M:589:LEU:HD13 | 2.03                     | 0.40              |
| 1:N:76:LEU:HB3   | 1:N:77:ALA:H     | 1.68                     | 0.40              |
| 1:N:286:VAL:HG21 | 1:N:378:ALA:CB   | 2.51                     | 0.40              |
| 1:N:613:GLU:H    | 1:N:613:GLU:CD   | 2.29                     | 0.40              |
| 1:N:617:LYS:O    | 1:N:621:LEU:HG   | 2.22                     | 0.40              |

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 621/701 (89%)   | 574 (92%)  | 47 (8%)  | 0        | 100         | 100 |
| 1   | B     | 621/701 (89%)   | 574 (92%)  | 47 (8%)  | 0        | 100         | 100 |
| 1   | C     | 621/701 (89%)   | 573 (92%)  | 48 (8%)  | 0        | 100         | 100 |
| 1   | D     | 621/701 (89%)   | 573 (92%)  | 48 (8%)  | 0        | 100         | 100 |
| 1   | E     | 621/701 (89%)   | 573 (92%)  | 48 (8%)  | 0        | 100         | 100 |
| 1   | F     | 621/701 (89%)   | 573 (92%)  | 48 (8%)  | 0        | 100         | 100 |
| 1   | G     | 621/701 (89%)   | 574 (92%)  | 47 (8%)  | 0        | 100         | 100 |
| 1   | H     | 621/701 (89%)   | 574 (92%)  | 47 (8%)  | 0        | 100         | 100 |
| 1   | I     | 621/701 (89%)   | 574 (92%)  | 47 (8%)  | 0        | 100         | 100 |
| 1   | J     | 621/701 (89%)   | 573 (92%)  | 48 (8%)  | 0        | 100         | 100 |
| 1   | K     | 621/701 (89%)   | 573 (92%)  | 48 (8%)  | 0        | 100         | 100 |
| 1   | L     | 621/701 (89%)   | 573 (92%)  | 48 (8%)  | 0        | 100         | 100 |
| 1   | M     | 621/701 (89%)   | 573 (92%)  | 48 (8%)  | 0        | 100         | 100 |
| 1   | N     | 621/701 (89%)   | 572 (92%)  | 49 (8%)  | 0        | 100         | 100 |
| All | All   | 8694/9814 (89%) | 8026 (92%) | 668 (8%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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



| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| 1   | B     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| 1   | C     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| 1   | D     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| 1   | E     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| 1   | F     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| 1   | G     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| 1   | H     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| 1   | I     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| 1   | J     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| 1   | K     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| 1   | L     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| 1   | M     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| 1   | N     | 520/586 (89%)   | 512 (98%)  | 8 (2%)   | 57          | 70 |
| All | All   | 7280/8204 (89%) | 7168 (98%) | 112 (2%) | 55          | 70 |

All (112) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 222 | ARG  |
| 1   | A     | 225 | LEU  |
| 1   | A     | 233 | GLN  |
| 1   | A     | 365 | ARG  |
| 1   | A     | 377 | THR  |
| 1   | A     | 461 | LEU  |
| 1   | A     | 473 | GLN  |
| 1   | A     | 690 | MET  |
| 1   | B     | 222 | ARG  |
| 1   | B     | 225 | LEU  |
| 1   | B     | 233 | GLN  |
| 1   | B     | 365 | ARG  |
| 1   | B     | 377 | THR  |
| 1   | B     | 461 | LEU  |
| 1   | B     | 473 | GLN  |
| 1   | B     | 690 | MET  |
| 1   | C     | 222 | ARG  |
| 1   | C     | 225 | LEU  |
| 1   | C     | 233 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 365 | ARG  |
| 1   | C     | 377 | THR  |
| 1   | C     | 461 | LEU  |
| 1   | C     | 473 | GLN  |
| 1   | C     | 690 | MET  |
| 1   | D     | 222 | ARG  |
| 1   | D     | 225 | LEU  |
| 1   | D     | 233 | GLN  |
| 1   | D     | 365 | ARG  |
| 1   | D     | 377 | THR  |
| 1   | D     | 461 | LEU  |
| 1   | D     | 473 | GLN  |
| 1   | D     | 690 | MET  |
| 1   | E     | 222 | ARG  |
| 1   | E     | 225 | LEU  |
| 1   | E     | 233 | GLN  |
| 1   | E     | 365 | ARG  |
| 1   | E     | 377 | THR  |
| 1   | E     | 461 | LEU  |
| 1   | E     | 473 | GLN  |
| 1   | E     | 690 | MET  |
| 1   | F     | 222 | ARG  |
| 1   | F     | 225 | LEU  |
| 1   | F     | 233 | GLN  |
| 1   | F     | 365 | ARG  |
| 1   | F     | 377 | THR  |
| 1   | F     | 461 | LEU  |
| 1   | F     | 473 | GLN  |
| 1   | F     | 690 | MET  |
| 1   | G     | 222 | ARG  |
| 1   | G     | 225 | LEU  |
| 1   | G     | 233 | GLN  |
| 1   | G     | 365 | ARG  |
| 1   | G     | 377 | THR  |
| 1   | G     | 461 | LEU  |
| 1   | G     | 473 | GLN  |
| 1   | G     | 690 | MET  |
| 1   | H     | 222 | ARG  |
| 1   | H     | 225 | LEU  |
| 1   | H     | 233 | GLN  |
| 1   | H     | 365 | ARG  |
| 1   | H     | 377 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 461 | LEU  |
| 1   | H     | 473 | GLN  |
| 1   | H     | 690 | MET  |
| 1   | I     | 222 | ARG  |
| 1   | I     | 225 | LEU  |
| 1   | I     | 233 | GLN  |
| 1   | I     | 365 | ARG  |
| 1   | I     | 377 | THR  |
| 1   | I     | 461 | LEU  |
| 1   | I     | 473 | GLN  |
| 1   | I     | 690 | MET  |
| 1   | J     | 222 | ARG  |
| 1   | J     | 225 | LEU  |
| 1   | J     | 233 | GLN  |
| 1   | J     | 365 | ARG  |
| 1   | J     | 377 | THR  |
| 1   | J     | 461 | LEU  |
| 1   | J     | 473 | GLN  |
| 1   | J     | 690 | MET  |
| 1   | K     | 222 | ARG  |
| 1   | K     | 225 | LEU  |
| 1   | K     | 233 | GLN  |
| 1   | K     | 365 | ARG  |
| 1   | K     | 377 | THR  |
| 1   | K     | 461 | LEU  |
| 1   | K     | 473 | GLN  |
| 1   | K     | 690 | MET  |
| 1   | L     | 222 | ARG  |
| 1   | L     | 225 | LEU  |
| 1   | L     | 233 | GLN  |
| 1   | L     | 365 | ARG  |
| 1   | L     | 377 | THR  |
| 1   | L     | 461 | LEU  |
| 1   | L     | 473 | GLN  |
| 1   | L     | 690 | MET  |
| 1   | M     | 222 | ARG  |
| 1   | M     | 225 | LEU  |
| 1   | M     | 233 | GLN  |
| 1   | M     | 365 | ARG  |
| 1   | M     | 377 | THR  |
| 1   | M     | 461 | LEU  |
| 1   | M     | 473 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 690 | MET  |
| 1   | N     | 222 | ARG  |
| 1   | N     | 225 | LEU  |
| 1   | N     | 233 | GLN  |
| 1   | N     | 365 | ARG  |
| 1   | N     | 377 | THR  |
| 1   | N     | 461 | LEU  |
| 1   | N     | 473 | GLN  |
| 1   | N     | 690 | MET  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 175 | GLN  |
| 1   | A     | 176 | ASN  |
| 1   | A     | 179 | ASN  |
| 1   | A     | 414 | GLN  |
| 1   | A     | 599 | ASN  |
| 1   | A     | 680 | HIS  |
| 1   | B     | 175 | GLN  |
| 1   | B     | 176 | ASN  |
| 1   | B     | 179 | ASN  |
| 1   | B     | 414 | GLN  |
| 1   | C     | 175 | GLN  |
| 1   | C     | 176 | ASN  |
| 1   | C     | 179 | ASN  |
| 1   | C     | 414 | GLN  |
| 1   | D     | 175 | GLN  |
| 1   | D     | 176 | ASN  |
| 1   | D     | 179 | ASN  |
| 1   | D     | 414 | GLN  |
| 1   | E     | 175 | GLN  |
| 1   | E     | 176 | ASN  |
| 1   | E     | 179 | ASN  |
| 1   | E     | 414 | GLN  |
| 1   | E     | 680 | HIS  |
| 1   | F     | 175 | GLN  |
| 1   | F     | 176 | ASN  |
| 1   | F     | 179 | ASN  |
| 1   | F     | 414 | GLN  |
| 1   | G     | 175 | GLN  |
| 1   | G     | 176 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 179 | ASN  |
| 1   | G     | 414 | GLN  |
| 1   | H     | 175 | GLN  |
| 1   | H     | 176 | ASN  |
| 1   | H     | 179 | ASN  |
| 1   | H     | 414 | GLN  |
| 1   | I     | 175 | GLN  |
| 1   | I     | 176 | ASN  |
| 1   | I     | 179 | ASN  |
| 1   | I     | 414 | GLN  |
| 1   | J     | 175 | GLN  |
| 1   | J     | 176 | ASN  |
| 1   | J     | 179 | ASN  |
| 1   | J     | 296 | GLN  |
| 1   | J     | 414 | GLN  |
| 1   | J     | 680 | HIS  |
| 1   | K     | 175 | GLN  |
| 1   | K     | 176 | ASN  |
| 1   | K     | 179 | ASN  |
| 1   | K     | 414 | GLN  |
| 1   | L     | 175 | GLN  |
| 1   | L     | 176 | ASN  |
| 1   | L     | 179 | ASN  |
| 1   | L     | 414 | GLN  |
| 1   | M     | 175 | GLN  |
| 1   | M     | 176 | ASN  |
| 1   | M     | 179 | ASN  |
| 1   | M     | 414 | GLN  |
| 1   | N     | 175 | GLN  |
| 1   | N     | 176 | ASN  |
| 1   | N     | 179 | ASN  |
| 1   | N     | 414 | GLN  |
| 1   | N     | 680 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 28 are monoatomic - leaving 28 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | AGS  | H     | 802 | 2    | 32,33,33     | 0.81 | 4 (12%)  | 45,52,52    | 0.83 | 1 (2%)   |
| 3   | AGS  | G     | 803 | 2    | 32,33,33     | 0.50 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | A     | 802 | 2    | 32,33,33     | 0.81 | 3 (9%)   | 45,52,52    | 0.83 | 1 (2%)   |
| 3   | AGS  | H     | 803 | 2    | 32,33,33     | 0.50 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | E     | 802 | 2    | 32,33,33     | 0.81 | 4 (12%)  | 45,52,52    | 0.83 | 1 (2%)   |
| 3   | AGS  | J     | 802 | 2    | 32,33,33     | 0.81 | 3 (9%)   | 45,52,52    | 0.83 | 1 (2%)   |
| 3   | AGS  | M     | 802 | 2    | 32,33,33     | 0.81 | 3 (9%)   | 45,52,52    | 0.83 | 1 (2%)   |
| 3   | AGS  | M     | 803 | 2    | 32,33,33     | 0.50 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | L     | 802 | 2    | 32,33,33     | 0.81 | 4 (12%)  | 45,52,52    | 0.83 | 1 (2%)   |
| 3   | AGS  | D     | 803 | 2    | 32,33,33     | 0.49 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | F     | 803 | 2    | 32,33,33     | 0.49 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | N     | 802 | 2    | 32,33,33     | 0.81 | 3 (9%)   | 45,52,52    | 0.83 | 1 (2%)   |
| 3   | AGS  | I     | 802 | 2    | 32,33,33     | 0.81 | 4 (12%)  | 45,52,52    | 0.83 | 1 (2%)   |
| 3   | AGS  | K     | 802 | 2    | 32,33,33     | 0.80 | 3 (9%)   | 45,52,52    | 0.83 | 1 (2%)   |
| 3   | AGS  | L     | 803 | 2    | 32,33,33     | 0.50 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | N     | 803 | 2    | 32,33,33     | 0.49 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | K     | 803 | 2    | 32,33,33     | 0.50 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | I     | 803 | 2    | 32,33,33     | 0.49 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | A     | 803 | 2    | 32,33,33     | 0.50 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | J     | 803 | 2    | 32,33,33     | 0.50 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | C     | 803 | 2    | 32,33,33     | 0.50 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | B     | 802 | 2    | 32,33,33     | 0.81 | 3 (9%)   | 45,52,52    | 0.83 | 1 (2%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | AGS  | D     | 802 | 2    | 32,33,33     | 0.81 | 4 (12%)  | 45,52,52    | 0.83 | 1 (2%)   |
| 3   | AGS  | F     | 802 | 2    | 32,33,33     | 0.81 | 3 (9%)   | 45,52,52    | 0.83 | 1 (2%)   |
| 3   | AGS  | E     | 803 | 2    | 32,33,33     | 0.49 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | B     | 803 | 2    | 32,33,33     | 0.50 | 0        | 45,52,52    | 0.79 | 1 (2%)   |
| 3   | AGS  | C     | 802 | 2    | 32,33,33     | 0.81 | 3 (9%)   | 45,52,52    | 0.83 | 1 (2%)   |
| 3   | AGS  | G     | 802 | 2    | 32,33,33     | 0.80 | 3 (9%)   | 45,52,52    | 0.83 | 1 (2%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 3   | AGS  | H     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |
| 3   | AGS  | G     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | A     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |
| 3   | AGS  | H     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | E     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |
| 3   | AGS  | J     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |
| 3   | AGS  | M     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |
| 3   | AGS  | M     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | L     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |
| 3   | AGS  | D     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | F     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | N     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |
| 3   | AGS  | I     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |
| 3   | AGS  | K     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |
| 3   | AGS  | L     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | N     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | K     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | I     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | A     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | J     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | C     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | B     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |
| 3   | AGS  | D     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 3   | AGS  | F     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |
| 3   | AGS  | E     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | B     | 803 | 2    | -       | 10/21/38/38 | 0/3/3/3 |
| 3   | AGS  | C     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |
| 3   | AGS  | G     | 802 | 2    | -       | 6/21/38/38  | 0/3/3/3 |

All (47) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | I     | 802 | AGS  | PB-O3B | -2.32 | 1.57        | 1.59     |
| 3   | D     | 802 | AGS  | PB-O3B | -2.31 | 1.57        | 1.59     |
| 3   | E     | 802 | AGS  | PB-O3B | -2.31 | 1.57        | 1.59     |
| 3   | F     | 802 | AGS  | PB-O3B | -2.29 | 1.57        | 1.59     |
| 3   | G     | 802 | AGS  | PB-O3B | -2.29 | 1.57        | 1.59     |
| 3   | L     | 802 | AGS  | PB-O3B | -2.28 | 1.57        | 1.59     |
| 3   | A     | 802 | AGS  | PB-O3B | -2.28 | 1.57        | 1.59     |
| 3   | N     | 802 | AGS  | PB-O3B | -2.28 | 1.57        | 1.59     |
| 3   | J     | 802 | AGS  | PB-O3B | -2.27 | 1.57        | 1.59     |
| 3   | C     | 802 | AGS  | PB-O3B | -2.27 | 1.57        | 1.59     |
| 3   | B     | 802 | AGS  | PB-O3B | -2.26 | 1.57        | 1.59     |
| 3   | H     | 802 | AGS  | PB-O3B | -2.26 | 1.57        | 1.59     |
| 3   | K     | 802 | AGS  | PB-O3B | -2.25 | 1.57        | 1.59     |
| 3   | M     | 802 | AGS  | PB-O3B | -2.25 | 1.57        | 1.59     |
| 3   | M     | 802 | AGS  | PA-O3A | -2.21 | 1.57        | 1.59     |
| 3   | L     | 802 | AGS  | PB-O3A | -2.21 | 1.57        | 1.59     |
| 3   | A     | 802 | AGS  | PB-O3A | -2.20 | 1.57        | 1.59     |
| 3   | N     | 802 | AGS  | PA-O3A | -2.20 | 1.57        | 1.59     |
| 3   | E     | 802 | AGS  | PA-O3A | -2.19 | 1.57        | 1.59     |
| 3   | J     | 802 | AGS  | PB-O3A | -2.18 | 1.57        | 1.59     |
| 3   | B     | 802 | AGS  | PA-O3A | -2.18 | 1.57        | 1.59     |
| 3   | C     | 802 | AGS  | PA-O3A | -2.17 | 1.57        | 1.59     |
| 3   | B     | 802 | AGS  | PB-O3A | -2.17 | 1.57        | 1.59     |
| 3   | G     | 802 | AGS  | PA-O3A | -2.17 | 1.57        | 1.59     |
| 3   | L     | 802 | AGS  | PA-O3A | -2.16 | 1.57        | 1.59     |
| 3   | N     | 802 | AGS  | PB-O3A | -2.16 | 1.57        | 1.59     |
| 3   | H     | 802 | AGS  | PA-O3A | -2.15 | 1.57        | 1.59     |
| 3   | D     | 802 | AGS  | PA-O3A | -2.15 | 1.57        | 1.59     |
| 3   | F     | 802 | AGS  | PB-O3A | -2.15 | 1.57        | 1.59     |
| 3   | F     | 802 | AGS  | PA-O3A | -2.14 | 1.57        | 1.59     |
| 3   | H     | 802 | AGS  | PB-O3A | -2.14 | 1.57        | 1.59     |
| 3   | K     | 802 | AGS  | PA-O3A | -2.14 | 1.57        | 1.59     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | I     | 802 | AGS  | PB-O3A | -2.14 | 1.57        | 1.59     |
| 3   | I     | 802 | AGS  | PA-O3A | -2.13 | 1.57        | 1.59     |
| 3   | M     | 802 | AGS  | PB-O3A | -2.13 | 1.57        | 1.59     |
| 3   | A     | 802 | AGS  | PA-O3A | -2.13 | 1.57        | 1.59     |
| 3   | C     | 802 | AGS  | PB-O3A | -2.13 | 1.57        | 1.59     |
| 3   | K     | 802 | AGS  | PB-O3A | -2.13 | 1.57        | 1.59     |
| 3   | J     | 802 | AGS  | PA-O3A | -2.13 | 1.57        | 1.59     |
| 3   | E     | 802 | AGS  | PB-O3A | -2.11 | 1.57        | 1.59     |
| 3   | G     | 802 | AGS  | PB-O3A | -2.11 | 1.57        | 1.59     |
| 3   | D     | 802 | AGS  | PB-O3A | -2.08 | 1.57        | 1.59     |
| 3   | D     | 802 | AGS  | PG-S1G | 2.03  | 1.95        | 1.90     |
| 3   | E     | 802 | AGS  | PG-S1G | 2.02  | 1.95        | 1.90     |
| 3   | H     | 802 | AGS  | PG-S1G | 2.01  | 1.95        | 1.90     |
| 3   | L     | 802 | AGS  | PG-S1G | 2.01  | 1.95        | 1.90     |
| 3   | I     | 802 | AGS  | PG-S1G | 2.01  | 1.95        | 1.90     |

All (28) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | M     | 802 | AGS  | PB-O3B-PG | -4.92 | 115.16      | 133.17   |
| 3   | N     | 802 | AGS  | PB-O3B-PG | -4.91 | 115.19      | 133.17   |
| 3   | A     | 802 | AGS  | PB-O3B-PG | -4.91 | 115.19      | 133.17   |
| 3   | H     | 802 | AGS  | PB-O3B-PG | -4.91 | 115.20      | 133.17   |
| 3   | E     | 802 | AGS  | PB-O3B-PG | -4.91 | 115.20      | 133.17   |
| 3   | I     | 802 | AGS  | PB-O3B-PG | -4.91 | 115.21      | 133.17   |
| 3   | K     | 802 | AGS  | PB-O3B-PG | -4.91 | 115.21      | 133.17   |
| 3   | B     | 802 | AGS  | PB-O3B-PG | -4.90 | 115.22      | 133.17   |
| 3   | G     | 802 | AGS  | PB-O3B-PG | -4.90 | 115.22      | 133.17   |
| 3   | L     | 802 | AGS  | PB-O3B-PG | -4.90 | 115.23      | 133.17   |
| 3   | C     | 802 | AGS  | PB-O3B-PG | -4.90 | 115.23      | 133.17   |
| 3   | J     | 802 | AGS  | PB-O3B-PG | -4.90 | 115.24      | 133.17   |
| 3   | F     | 802 | AGS  | PB-O3B-PG | -4.90 | 115.24      | 133.17   |
| 3   | D     | 802 | AGS  | PB-O3B-PG | -4.90 | 115.25      | 133.17   |
| 3   | F     | 803 | AGS  | PB-O3B-PG | -4.28 | 117.52      | 133.17   |
| 3   | N     | 803 | AGS  | PB-O3B-PG | -4.28 | 117.52      | 133.17   |
| 3   | H     | 803 | AGS  | PB-O3B-PG | -4.27 | 117.53      | 133.17   |
| 3   | A     | 803 | AGS  | PB-O3B-PG | -4.27 | 117.55      | 133.17   |
| 3   | L     | 803 | AGS  | PB-O3B-PG | -4.27 | 117.56      | 133.17   |
| 3   | J     | 803 | AGS  | PB-O3B-PG | -4.26 | 117.57      | 133.17   |
| 3   | K     | 803 | AGS  | PB-O3B-PG | -4.26 | 117.57      | 133.17   |
| 3   | C     | 803 | AGS  | PB-O3B-PG | -4.26 | 117.57      | 133.17   |
| 3   | G     | 803 | AGS  | PB-O3B-PG | -4.26 | 117.57      | 133.17   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | D     | 803 | AGS  | PB-O3B-PG | -4.26 | 117.58      | 133.17   |
| 3   | M     | 803 | AGS  | PB-O3B-PG | -4.26 | 117.58      | 133.17   |
| 3   | B     | 803 | AGS  | PB-O3B-PG | -4.26 | 117.58      | 133.17   |
| 3   | I     | 803 | AGS  | PB-O3B-PG | -4.26 | 117.59      | 133.17   |
| 3   | E     | 803 | AGS  | PB-O3B-PG | -4.26 | 117.60      | 133.17   |

There are no chirality outliers.

All (224) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | A     | 802 | AGS  | PB-O3B-PG-O2G  |
| 3   | A     | 802 | AGS  | C5'-O5'-PA-O2A |
| 3   | A     | 802 | AGS  | C5'-O5'-PA-O3A |
| 3   | A     | 803 | AGS  | PB-O3B-PG-O2G  |
| 3   | A     | 803 | AGS  | PB-O3B-PG-O3G  |
| 3   | A     | 803 | AGS  | C5'-O5'-PA-O1A |
| 3   | B     | 802 | AGS  | PB-O3B-PG-O2G  |
| 3   | B     | 802 | AGS  | C5'-O5'-PA-O2A |
| 3   | B     | 802 | AGS  | C5'-O5'-PA-O3A |
| 3   | B     | 803 | AGS  | PB-O3B-PG-O2G  |
| 3   | B     | 803 | AGS  | PB-O3B-PG-O3G  |
| 3   | B     | 803 | AGS  | C5'-O5'-PA-O1A |
| 3   | C     | 802 | AGS  | PB-O3B-PG-O2G  |
| 3   | C     | 802 | AGS  | C5'-O5'-PA-O2A |
| 3   | C     | 802 | AGS  | C5'-O5'-PA-O3A |
| 3   | C     | 803 | AGS  | PB-O3B-PG-O2G  |
| 3   | C     | 803 | AGS  | PB-O3B-PG-O3G  |
| 3   | C     | 803 | AGS  | C5'-O5'-PA-O1A |
| 3   | D     | 802 | AGS  | PB-O3B-PG-O2G  |
| 3   | D     | 802 | AGS  | C5'-O5'-PA-O2A |
| 3   | D     | 802 | AGS  | C5'-O5'-PA-O3A |
| 3   | D     | 803 | AGS  | PB-O3B-PG-O2G  |
| 3   | D     | 803 | AGS  | PB-O3B-PG-O3G  |
| 3   | D     | 803 | AGS  | C5'-O5'-PA-O1A |
| 3   | E     | 802 | AGS  | PB-O3B-PG-O2G  |
| 3   | E     | 802 | AGS  | C5'-O5'-PA-O2A |
| 3   | E     | 802 | AGS  | C5'-O5'-PA-O3A |
| 3   | E     | 803 | AGS  | PB-O3B-PG-O2G  |
| 3   | E     | 803 | AGS  | PB-O3B-PG-O3G  |
| 3   | E     | 803 | AGS  | C5'-O5'-PA-O1A |
| 3   | F     | 802 | AGS  | PB-O3B-PG-O2G  |
| 3   | F     | 802 | AGS  | C5'-O5'-PA-O2A |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | F     | 802 | AGS  | C5'-O5'-PA-O3A |
| 3   | F     | 803 | AGS  | PB-O3B-PG-O2G  |
| 3   | F     | 803 | AGS  | PB-O3B-PG-O3G  |
| 3   | F     | 803 | AGS  | C5'-O5'-PA-O1A |
| 3   | G     | 802 | AGS  | PB-O3B-PG-O2G  |
| 3   | G     | 802 | AGS  | C5'-O5'-PA-O2A |
| 3   | G     | 802 | AGS  | C5'-O5'-PA-O3A |
| 3   | G     | 803 | AGS  | PB-O3B-PG-O2G  |
| 3   | G     | 803 | AGS  | PB-O3B-PG-O3G  |
| 3   | G     | 803 | AGS  | C5'-O5'-PA-O1A |
| 3   | H     | 802 | AGS  | PB-O3B-PG-O2G  |
| 3   | H     | 802 | AGS  | C5'-O5'-PA-O2A |
| 3   | H     | 802 | AGS  | C5'-O5'-PA-O3A |
| 3   | H     | 803 | AGS  | PB-O3B-PG-O2G  |
| 3   | H     | 803 | AGS  | PB-O3B-PG-O3G  |
| 3   | H     | 803 | AGS  | C5'-O5'-PA-O1A |
| 3   | I     | 802 | AGS  | PB-O3B-PG-O2G  |
| 3   | I     | 802 | AGS  | C5'-O5'-PA-O2A |
| 3   | I     | 802 | AGS  | C5'-O5'-PA-O3A |
| 3   | I     | 803 | AGS  | PB-O3B-PG-O2G  |
| 3   | I     | 803 | AGS  | PB-O3B-PG-O3G  |
| 3   | I     | 803 | AGS  | C5'-O5'-PA-O1A |
| 3   | J     | 802 | AGS  | PB-O3B-PG-O2G  |
| 3   | J     | 802 | AGS  | C5'-O5'-PA-O2A |
| 3   | J     | 802 | AGS  | C5'-O5'-PA-O3A |
| 3   | J     | 803 | AGS  | PB-O3B-PG-O2G  |
| 3   | J     | 803 | AGS  | PB-O3B-PG-O3G  |
| 3   | J     | 803 | AGS  | C5'-O5'-PA-O1A |
| 3   | K     | 802 | AGS  | PB-O3B-PG-O2G  |
| 3   | K     | 802 | AGS  | C5'-O5'-PA-O2A |
| 3   | K     | 802 | AGS  | C5'-O5'-PA-O3A |
| 3   | K     | 803 | AGS  | PB-O3B-PG-O2G  |
| 3   | K     | 803 | AGS  | PB-O3B-PG-O3G  |
| 3   | K     | 803 | AGS  | C5'-O5'-PA-O1A |
| 3   | L     | 802 | AGS  | PB-O3B-PG-O2G  |
| 3   | L     | 802 | AGS  | C5'-O5'-PA-O2A |
| 3   | L     | 802 | AGS  | C5'-O5'-PA-O3A |
| 3   | L     | 803 | AGS  | PB-O3B-PG-O2G  |
| 3   | L     | 803 | AGS  | PB-O3B-PG-O3G  |
| 3   | L     | 803 | AGS  | C5'-O5'-PA-O1A |
| 3   | M     | 802 | AGS  | PB-O3B-PG-O2G  |
| 3   | M     | 802 | AGS  | C5'-O5'-PA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | M     | 802 | AGS  | C5'-O5'-PA-O3A  |
| 3   | M     | 803 | AGS  | PB-O3B-PG-O2G   |
| 3   | M     | 803 | AGS  | PB-O3B-PG-O3G   |
| 3   | M     | 803 | AGS  | C5'-O5'-PA-O1A  |
| 3   | N     | 802 | AGS  | PB-O3B-PG-O2G   |
| 3   | N     | 802 | AGS  | C5'-O5'-PA-O2A  |
| 3   | N     | 802 | AGS  | C5'-O5'-PA-O3A  |
| 3   | N     | 803 | AGS  | PB-O3B-PG-O2G   |
| 3   | N     | 803 | AGS  | PB-O3B-PG-O3G   |
| 3   | N     | 803 | AGS  | C5'-O5'-PA-O1A  |
| 3   | A     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | B     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | C     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | D     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | E     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | F     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | G     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | H     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | I     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | J     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | K     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | L     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | M     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | N     | 802 | AGS  | O4'-C4'-C5'-O5' |
| 3   | A     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | B     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | C     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | D     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | E     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | F     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | G     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | H     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | I     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | J     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | K     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | L     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | M     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | N     | 803 | AGS  | O4'-C4'-C5'-O5' |
| 3   | A     | 802 | AGS  | PB-O3A-PA-O5'   |
| 3   | B     | 802 | AGS  | PB-O3A-PA-O5'   |
| 3   | C     | 802 | AGS  | PB-O3A-PA-O5'   |
| 3   | D     | 802 | AGS  | PB-O3A-PA-O5'   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | E     | 802 | AGS  | PB-O3A-PA-O5'   |
| 3   | F     | 802 | AGS  | PB-O3A-PA-O5'   |
| 3   | G     | 802 | AGS  | PB-O3A-PA-O5'   |
| 3   | H     | 802 | AGS  | PB-O3A-PA-O5'   |
| 3   | I     | 802 | AGS  | PB-O3A-PA-O5'   |
| 3   | J     | 802 | AGS  | PB-O3A-PA-O5'   |
| 3   | K     | 802 | AGS  | PB-O3A-PA-O5'   |
| 3   | L     | 802 | AGS  | PB-O3A-PA-O5'   |
| 3   | M     | 802 | AGS  | PB-O3A-PA-O5'   |
| 3   | N     | 802 | AGS  | PB-O3A-PA-O5'   |
| 3   | A     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | B     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | C     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | D     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | E     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | F     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | G     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | H     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | I     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | J     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | K     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | L     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | M     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | N     | 803 | AGS  | C2'-C1'-N9-C8   |
| 3   | C     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | A     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | B     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | C     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | D     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | E     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | F     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | G     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | H     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | I     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | J     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | K     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | L     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | M     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | N     | 803 | AGS  | O4'-C1'-N9-C8   |
| 3   | A     | 803 | AGS  | C4'-C5'-O5'-PA  |
| 3   | B     | 803 | AGS  | C4'-C5'-O5'-PA  |
| 3   | C     | 803 | AGS  | C4'-C5'-O5'-PA  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | D     | 803 | AGS  | C4'-C5'-O5'-PA  |
| 3   | E     | 803 | AGS  | C4'-C5'-O5'-PA  |
| 3   | F     | 803 | AGS  | C4'-C5'-O5'-PA  |
| 3   | G     | 803 | AGS  | C4'-C5'-O5'-PA  |
| 3   | H     | 803 | AGS  | C4'-C5'-O5'-PA  |
| 3   | I     | 803 | AGS  | C4'-C5'-O5'-PA  |
| 3   | J     | 803 | AGS  | C4'-C5'-O5'-PA  |
| 3   | K     | 803 | AGS  | C4'-C5'-O5'-PA  |
| 3   | L     | 803 | AGS  | C4'-C5'-O5'-PA  |
| 3   | M     | 803 | AGS  | C4'-C5'-O5'-PA  |
| 3   | N     | 803 | AGS  | C4'-C5'-O5'-PA  |
| 3   | A     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | B     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | D     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | E     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | F     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | G     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | H     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | I     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | J     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | K     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | L     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | M     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | N     | 803 | AGS  | C3'-C4'-C5'-O5' |
| 3   | A     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | B     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | C     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | D     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | E     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | F     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | G     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | H     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | I     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | J     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | K     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | L     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | M     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | N     | 803 | AGS  | O4'-C1'-N9-C4   |
| 3   | G     | 803 | AGS  | C2'-C1'-N9-C4   |
| 3   | K     | 803 | AGS  | C2'-C1'-N9-C4   |
| 3   | L     | 803 | AGS  | C2'-C1'-N9-C4   |
| 3   | A     | 802 | AGS  | PB-O3A-PA-O2A   |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 3   | B     | 802 | AGS  | PB-O3A-PA-O2A |
| 3   | C     | 802 | AGS  | PB-O3A-PA-O2A |
| 3   | D     | 802 | AGS  | PB-O3A-PA-O2A |
| 3   | E     | 802 | AGS  | PB-O3A-PA-O2A |
| 3   | F     | 802 | AGS  | PB-O3A-PA-O2A |
| 3   | G     | 802 | AGS  | PB-O3A-PA-O2A |
| 3   | H     | 802 | AGS  | PB-O3A-PA-O2A |
| 3   | I     | 802 | AGS  | PB-O3A-PA-O2A |
| 3   | J     | 802 | AGS  | PB-O3A-PA-O2A |
| 3   | K     | 802 | AGS  | PB-O3A-PA-O2A |
| 3   | L     | 802 | AGS  | PB-O3A-PA-O2A |
| 3   | M     | 802 | AGS  | PB-O3A-PA-O2A |
| 3   | N     | 802 | AGS  | PB-O3A-PA-O2A |
| 3   | A     | 803 | AGS  | C2'-C1'-N9-C4 |
| 3   | B     | 803 | AGS  | C2'-C1'-N9-C4 |
| 3   | C     | 803 | AGS  | C2'-C1'-N9-C4 |
| 3   | D     | 803 | AGS  | C2'-C1'-N9-C4 |
| 3   | E     | 803 | AGS  | C2'-C1'-N9-C4 |
| 3   | F     | 803 | AGS  | C2'-C1'-N9-C4 |
| 3   | H     | 803 | AGS  | C2'-C1'-N9-C4 |
| 3   | I     | 803 | AGS  | C2'-C1'-N9-C4 |
| 3   | J     | 803 | AGS  | C2'-C1'-N9-C4 |
| 3   | M     | 803 | AGS  | C2'-C1'-N9-C4 |
| 3   | N     | 803 | AGS  | C2'-C1'-N9-C4 |

There are no ring outliers.

28 monomers are involved in 88 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | H     | 802 | AGS  | 3       | 0            |
| 3   | G     | 803 | AGS  | 3       | 0            |
| 3   | A     | 802 | AGS  | 3       | 0            |
| 3   | H     | 803 | AGS  | 3       | 0            |
| 3   | E     | 802 | AGS  | 3       | 0            |
| 3   | J     | 802 | AGS  | 3       | 0            |
| 3   | M     | 802 | AGS  | 3       | 0            |
| 3   | M     | 803 | AGS  | 3       | 0            |
| 3   | L     | 802 | AGS  | 4       | 0            |
| 3   | D     | 803 | AGS  | 3       | 0            |
| 3   | F     | 803 | AGS  | 3       | 0            |
| 3   | N     | 802 | AGS  | 3       | 0            |
| 3   | I     | 802 | AGS  | 3       | 0            |

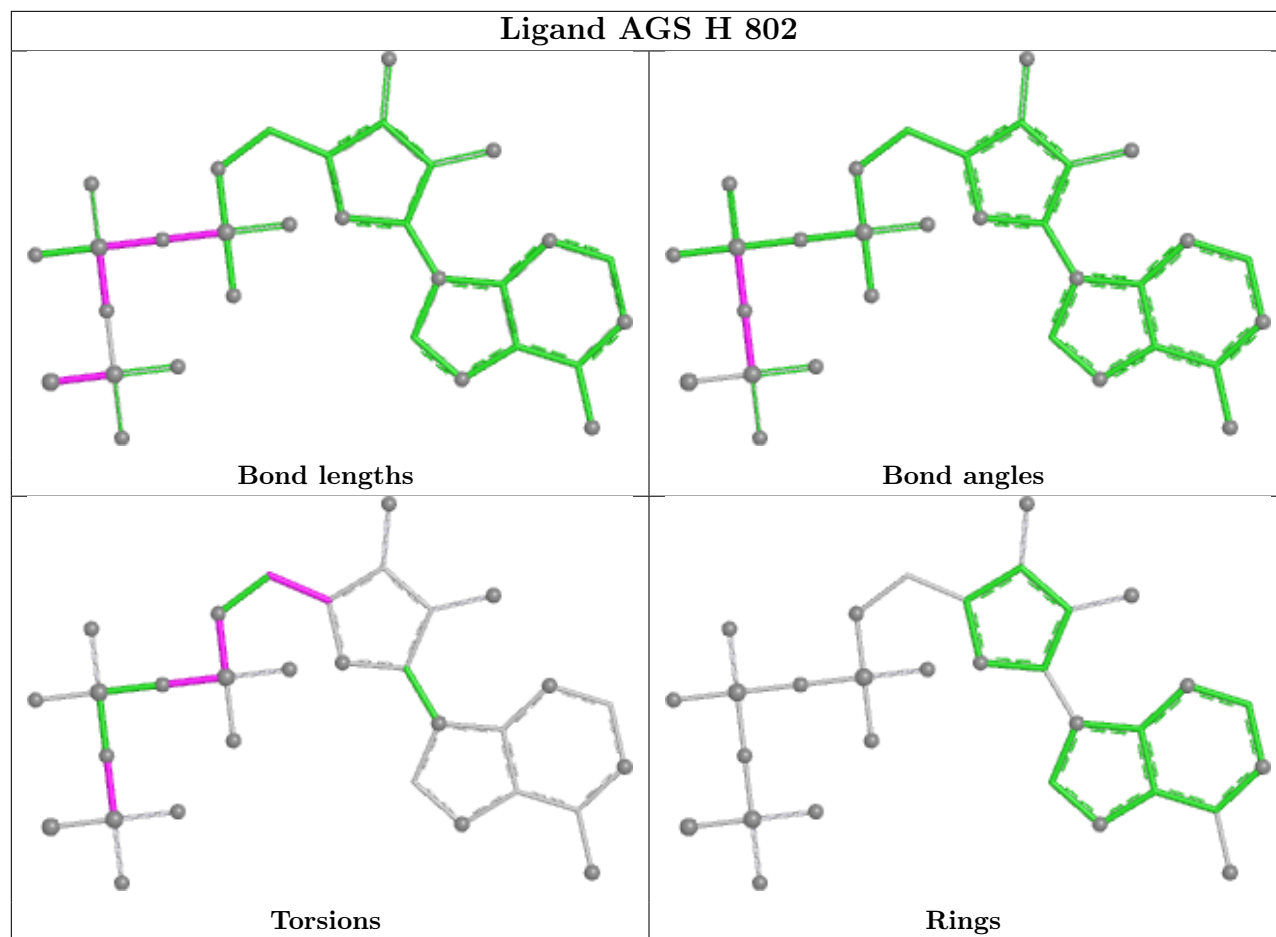
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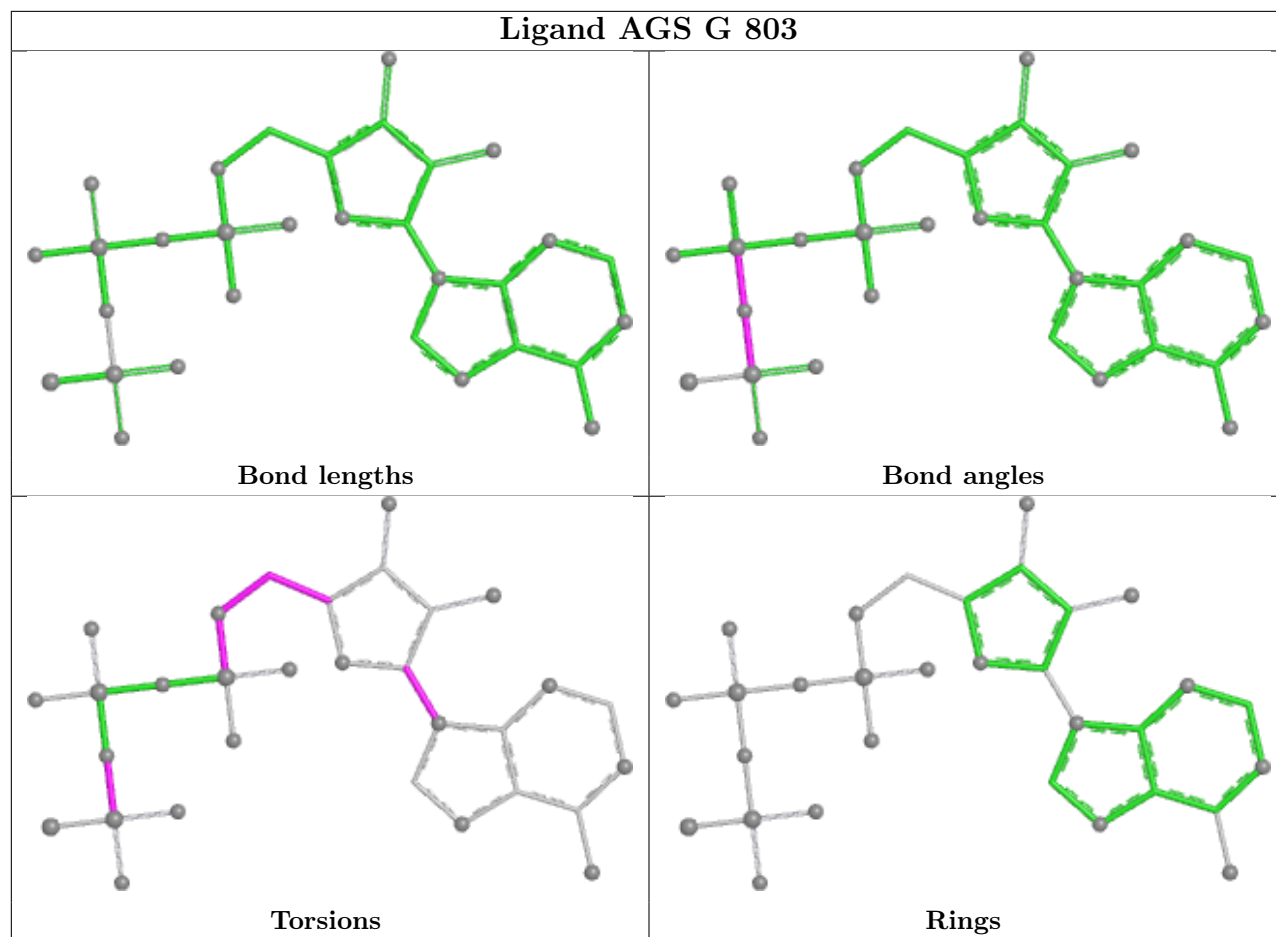


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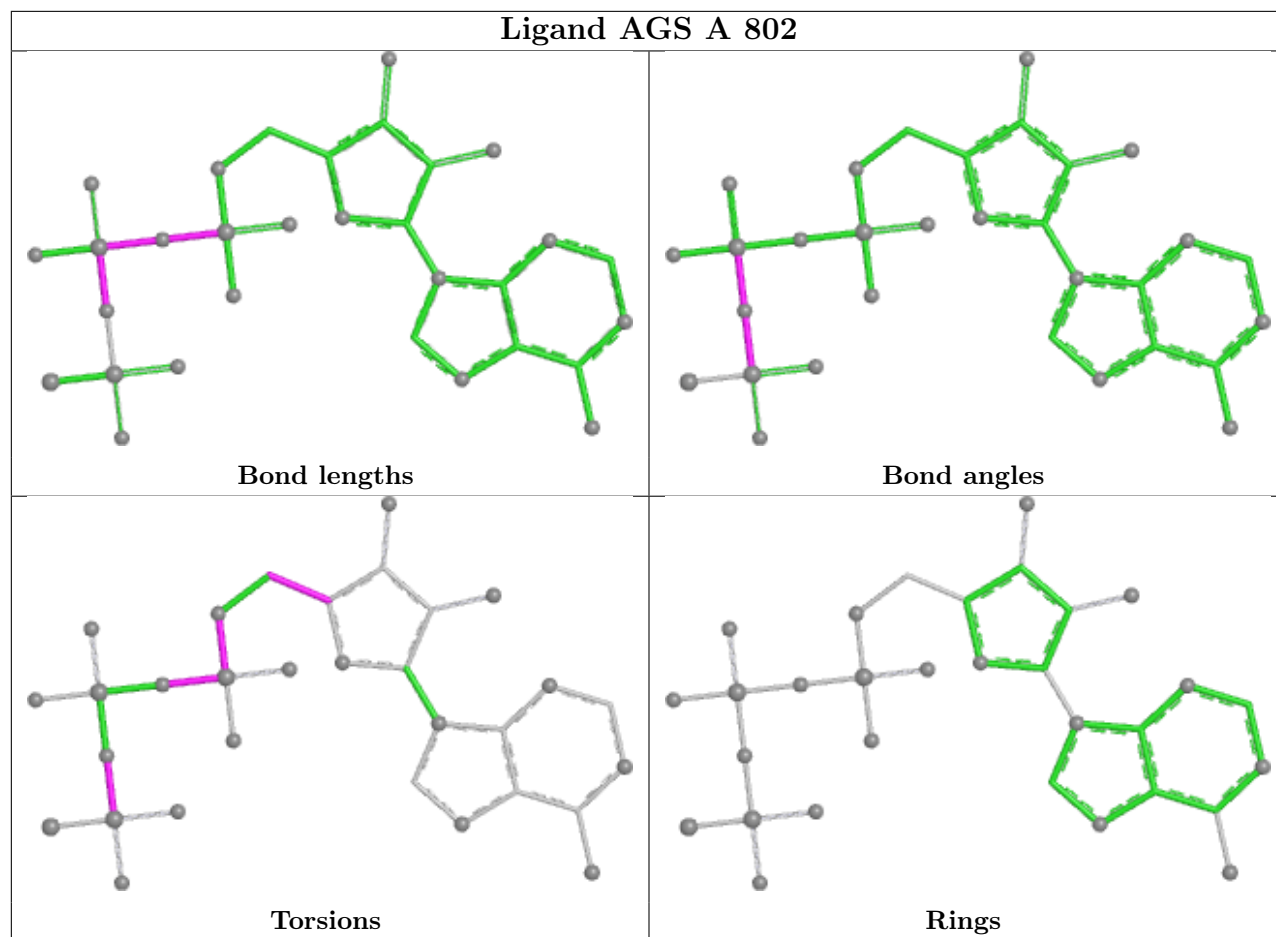
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | K     | 802 | AGS  | 3       | 0            |
| 3   | L     | 803 | AGS  | 3       | 0            |
| 3   | N     | 803 | AGS  | 3       | 0            |
| 3   | K     | 803 | AGS  | 4       | 0            |
| 3   | I     | 803 | AGS  | 3       | 0            |
| 3   | A     | 803 | AGS  | 3       | 0            |
| 3   | J     | 803 | AGS  | 3       | 0            |
| 3   | C     | 803 | AGS  | 3       | 0            |
| 3   | B     | 802 | AGS  | 3       | 0            |
| 3   | D     | 802 | AGS  | 4       | 0            |
| 3   | F     | 802 | AGS  | 3       | 0            |
| 3   | E     | 803 | AGS  | 3       | 0            |
| 3   | B     | 803 | AGS  | 4       | 0            |
| 3   | C     | 802 | AGS  | 3       | 0            |
| 3   | G     | 802 | AGS  | 3       | 0            |

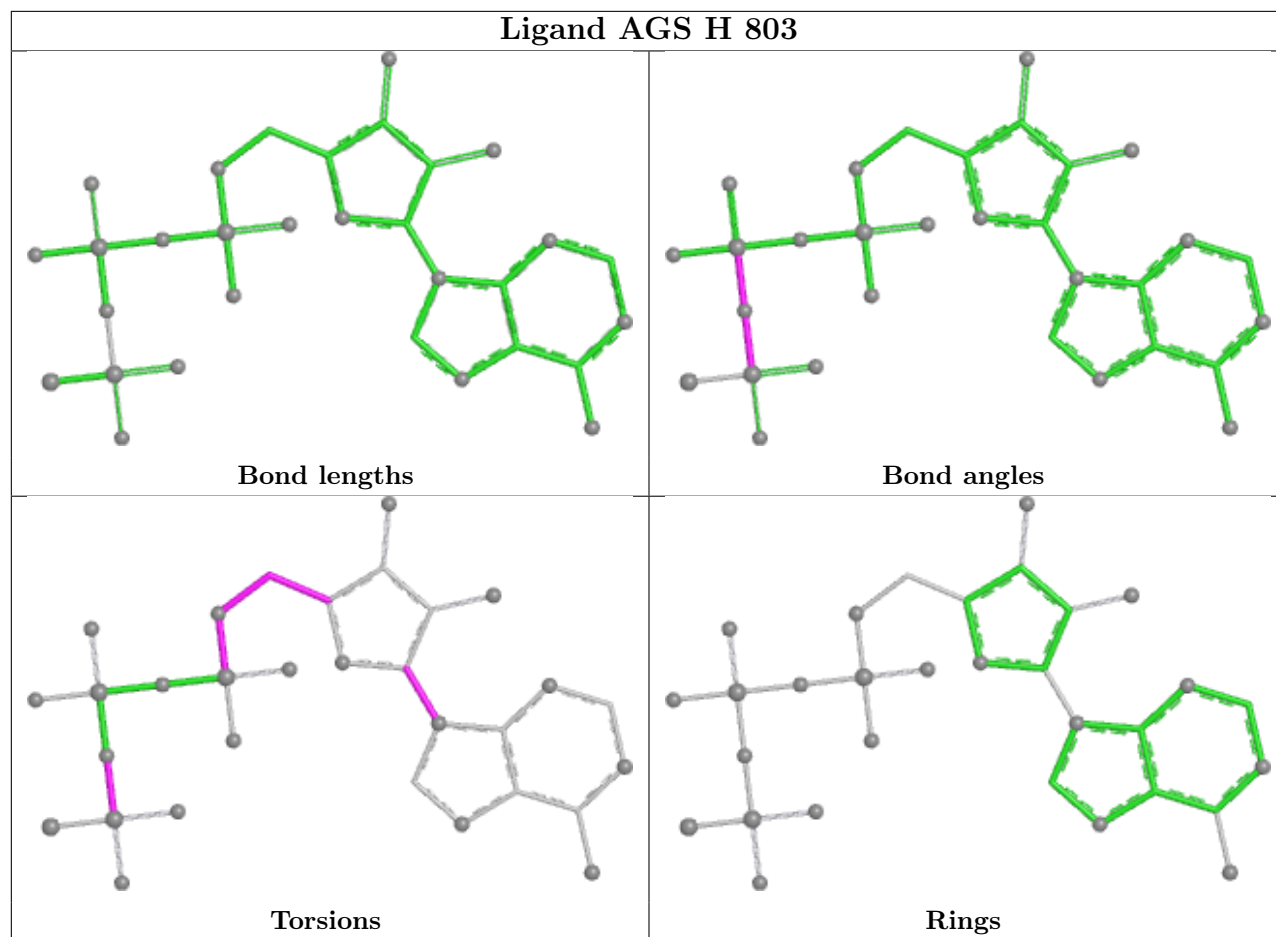
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



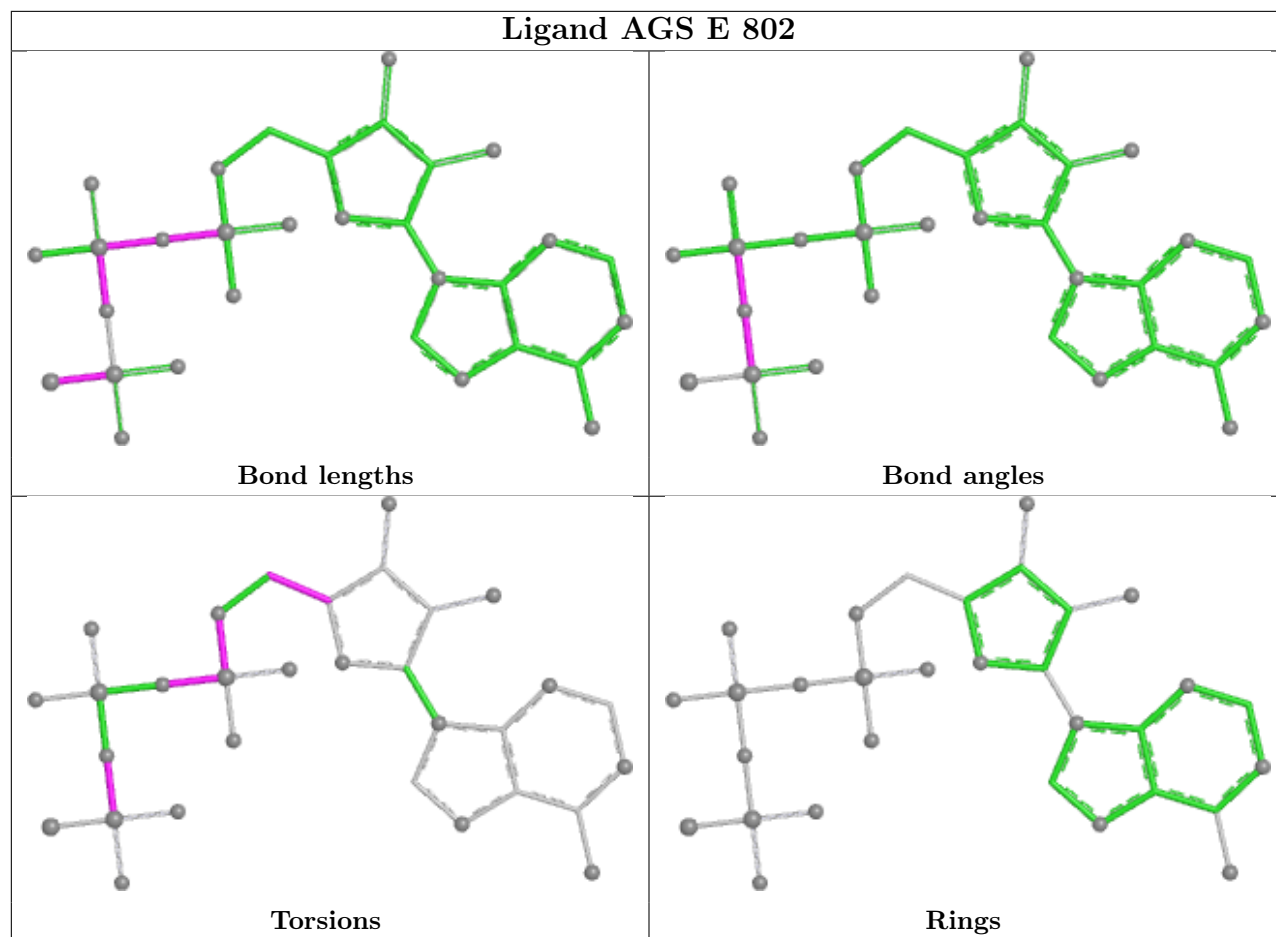


## Ligand AGS A 802

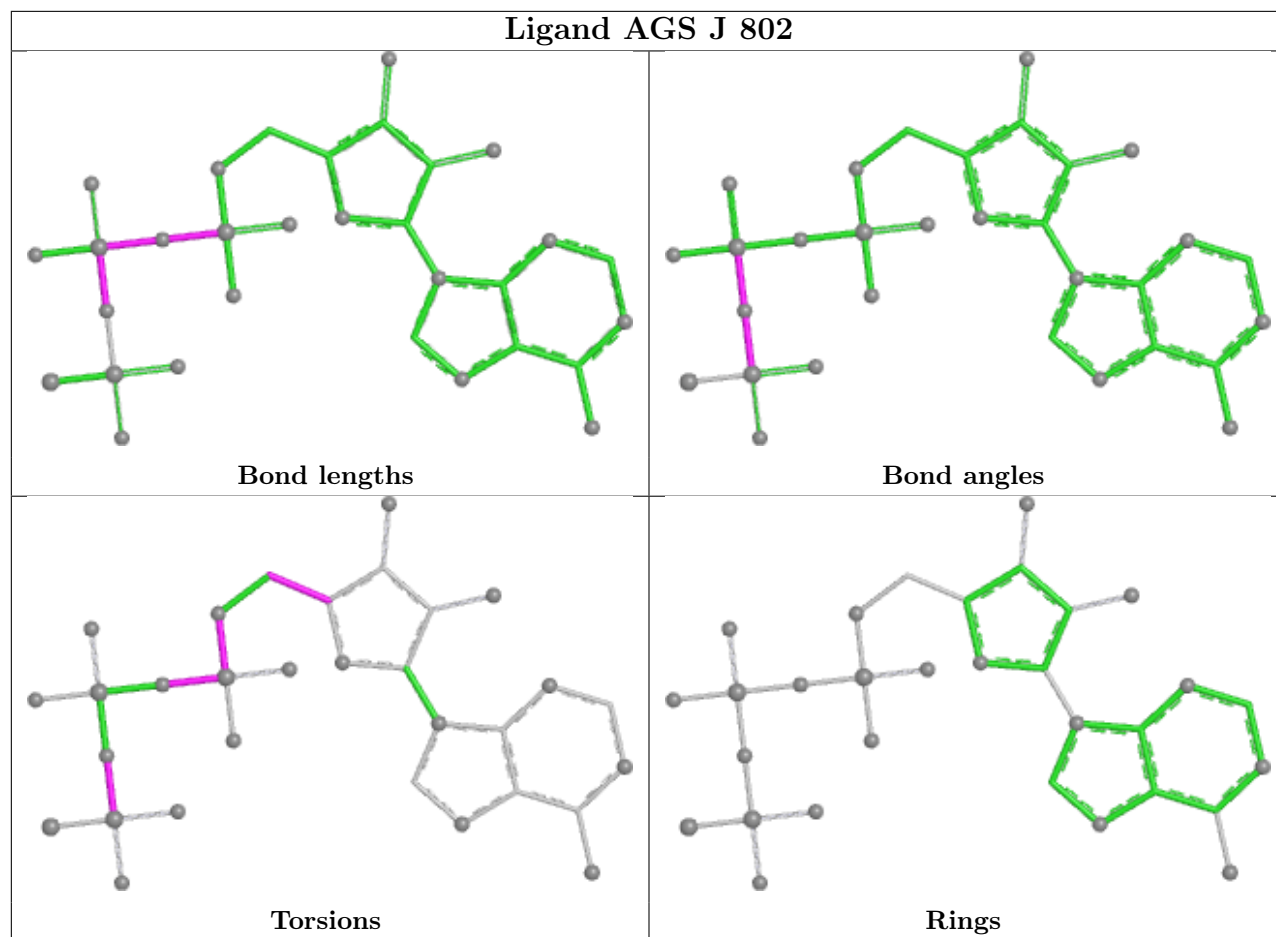


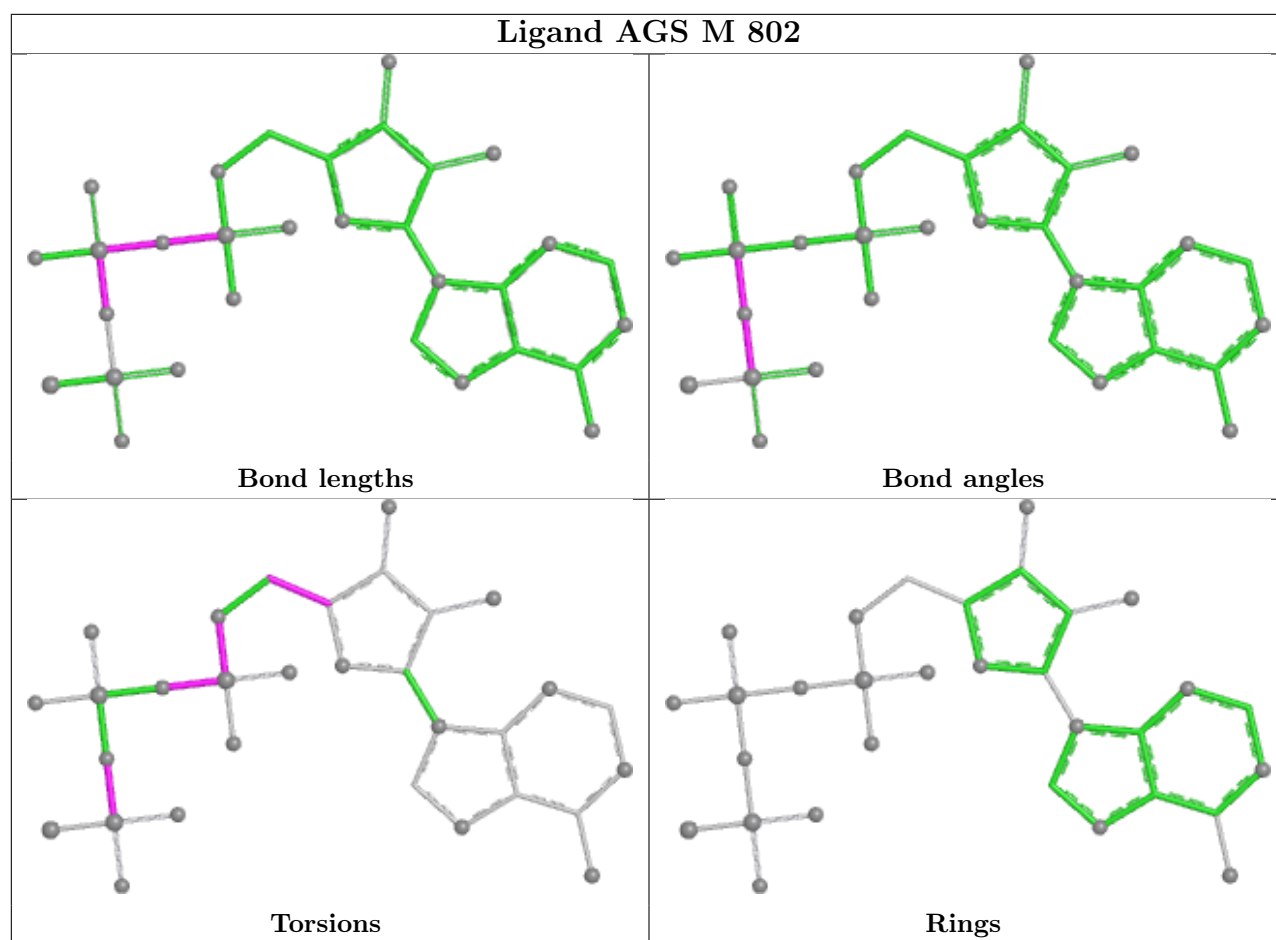


## Ligand AGS E 802

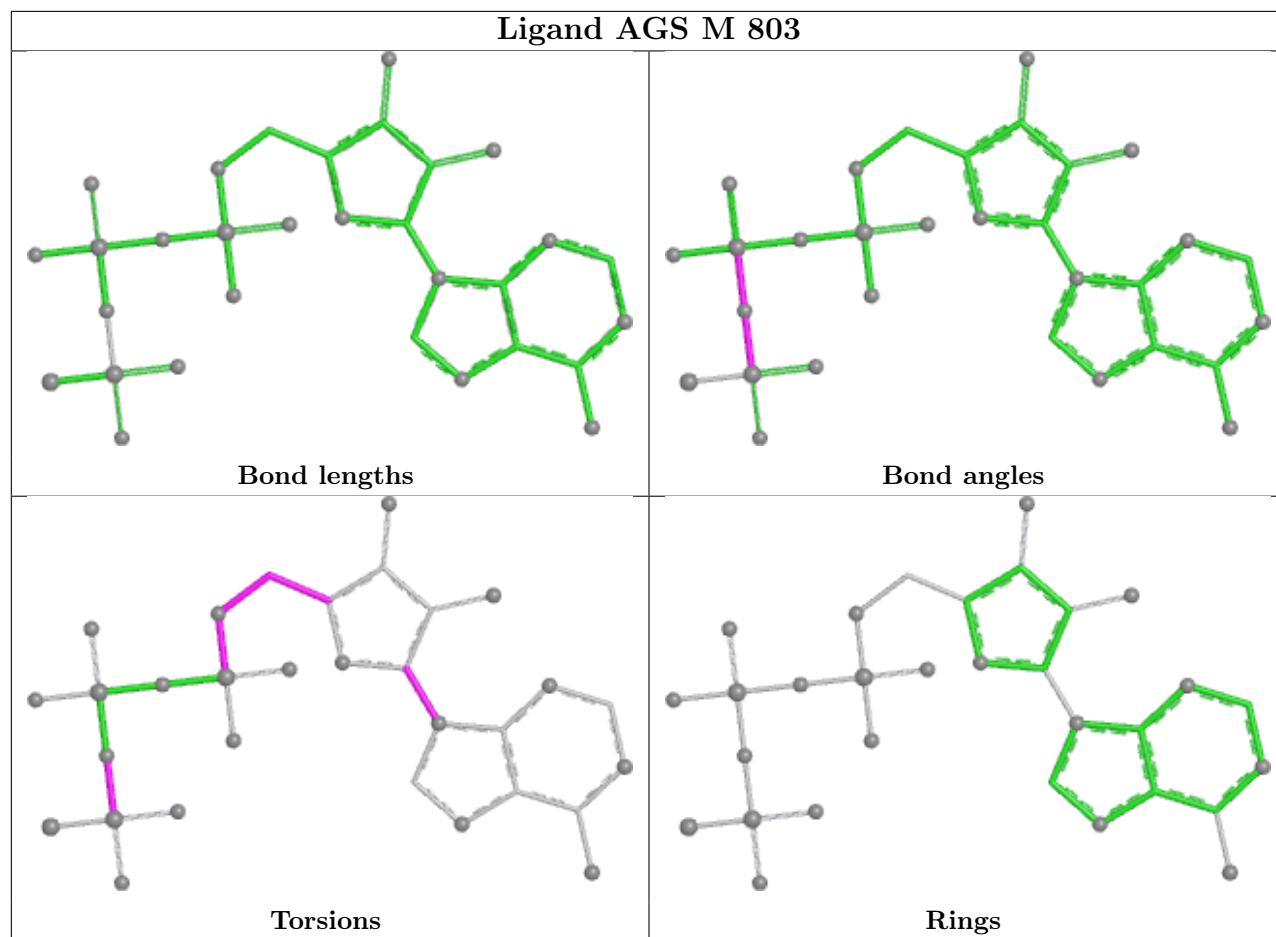


## Ligand AGS J 802

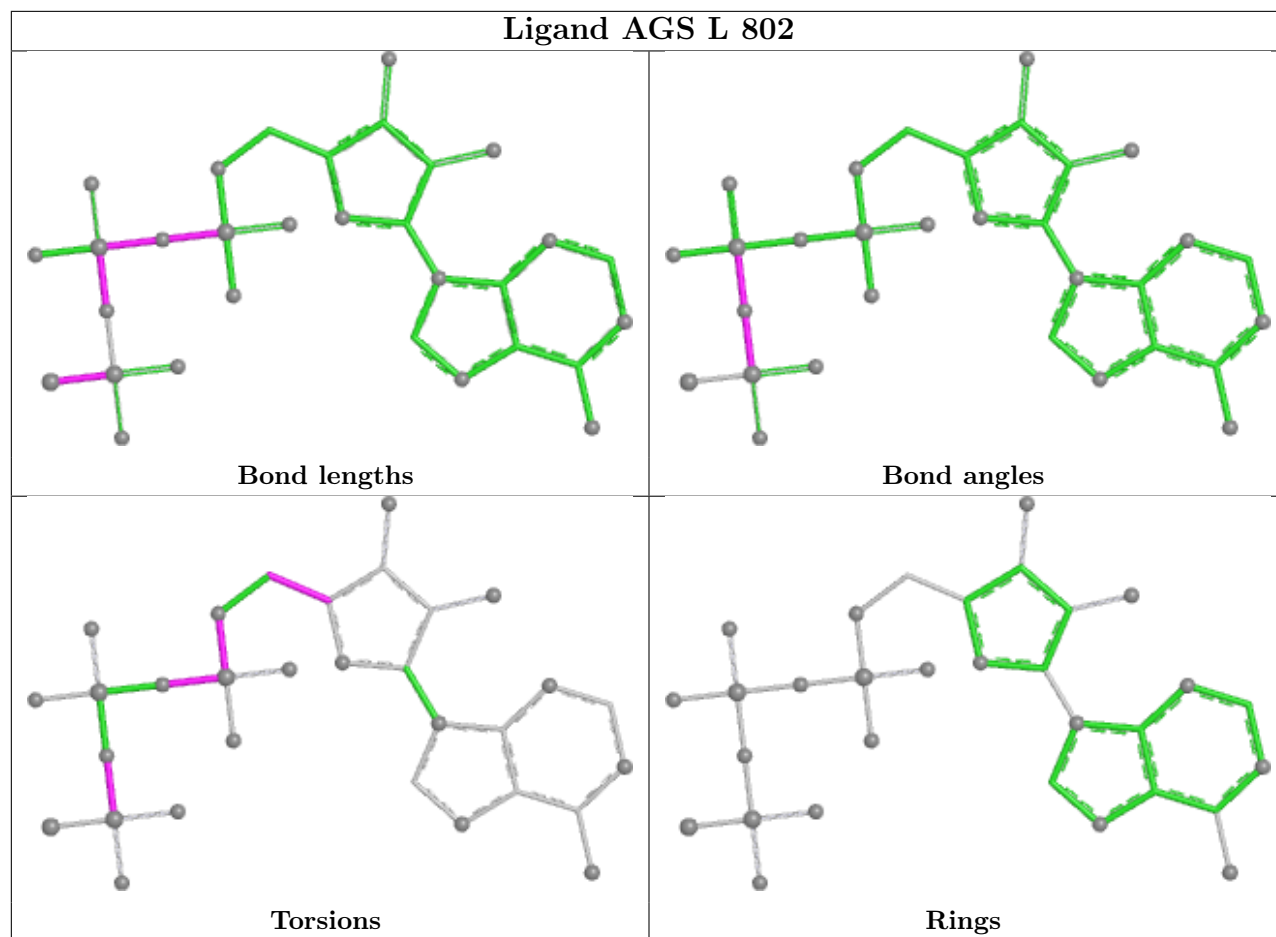


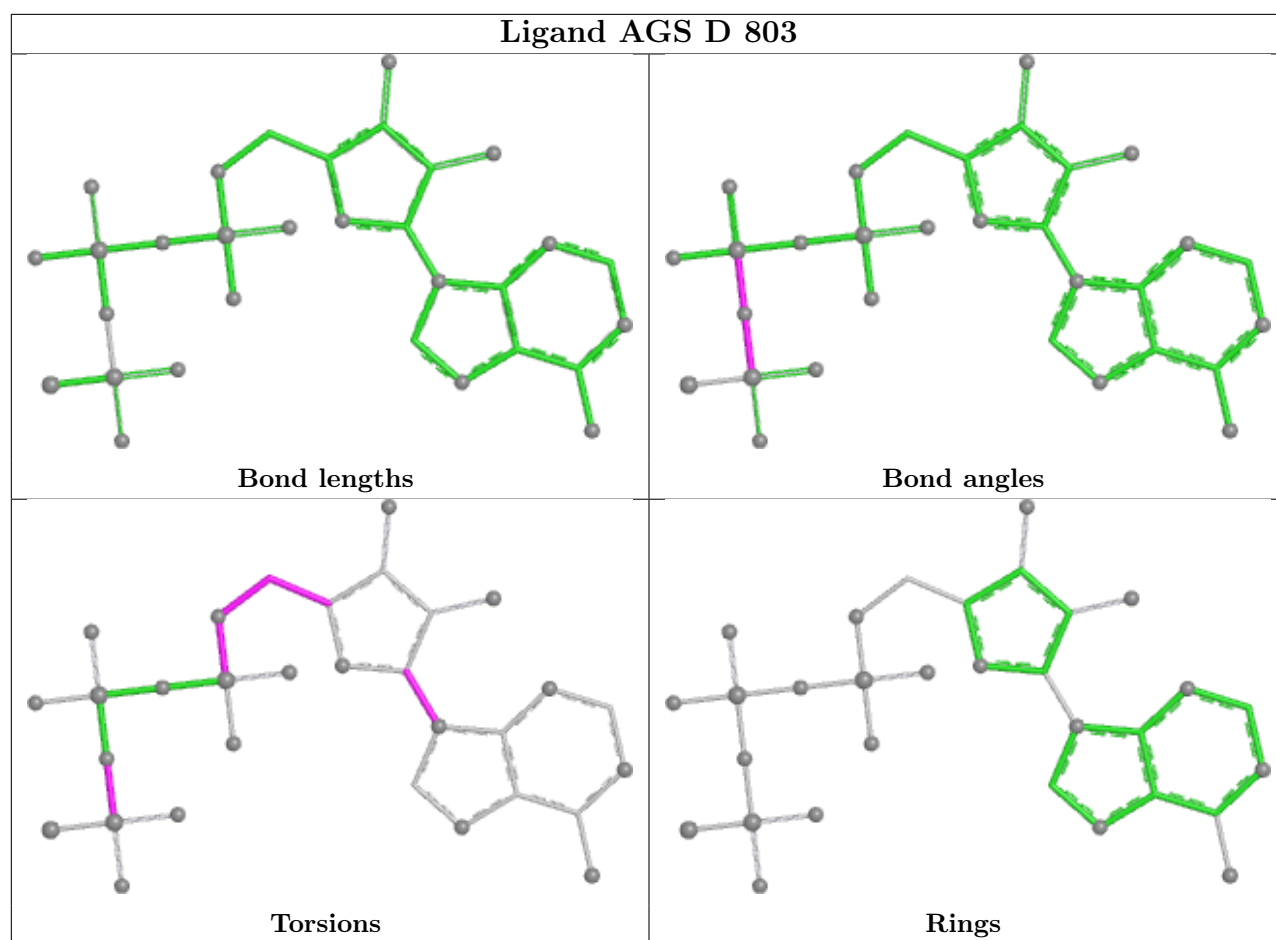




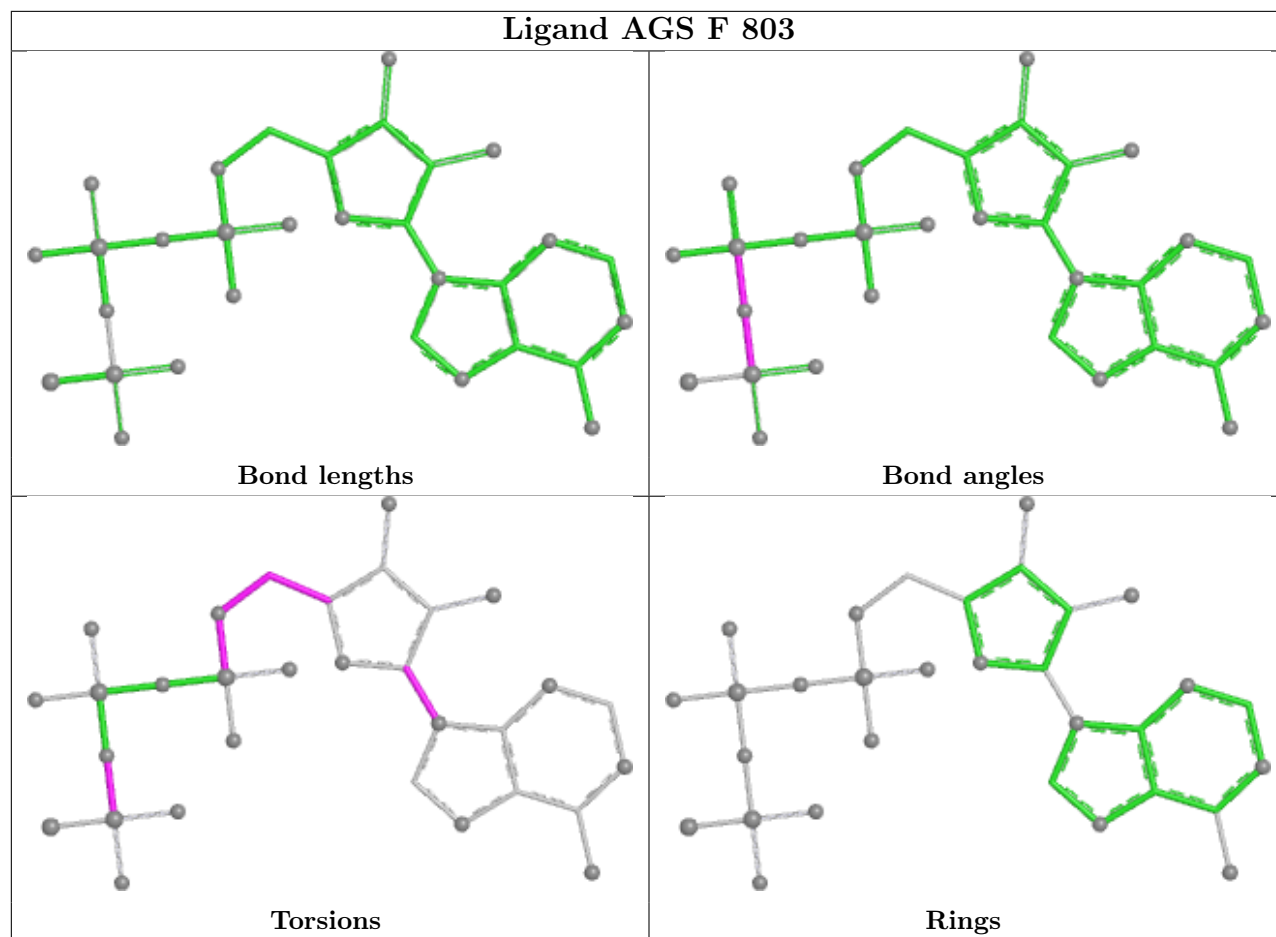


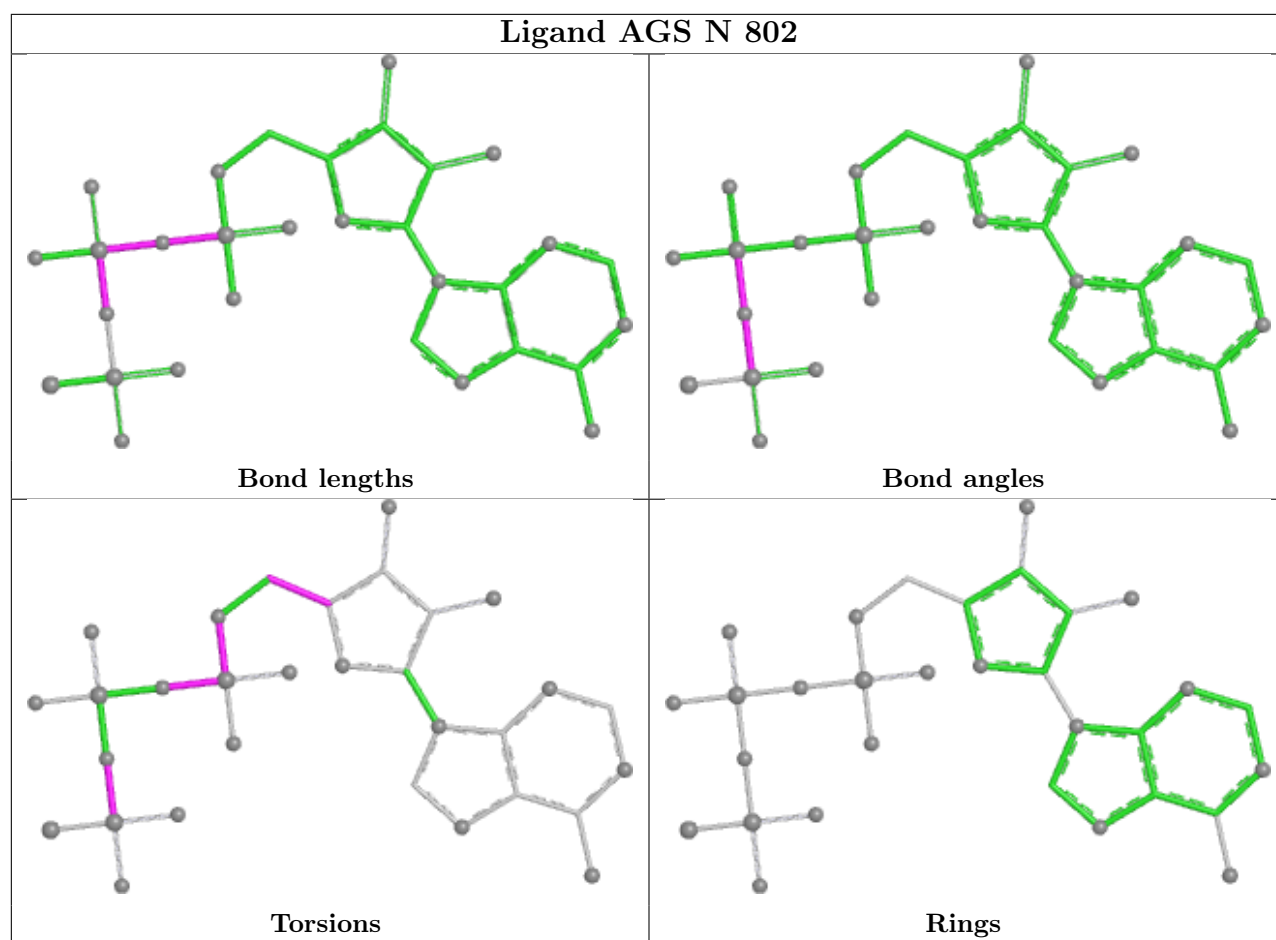
## Ligand AGS L 802



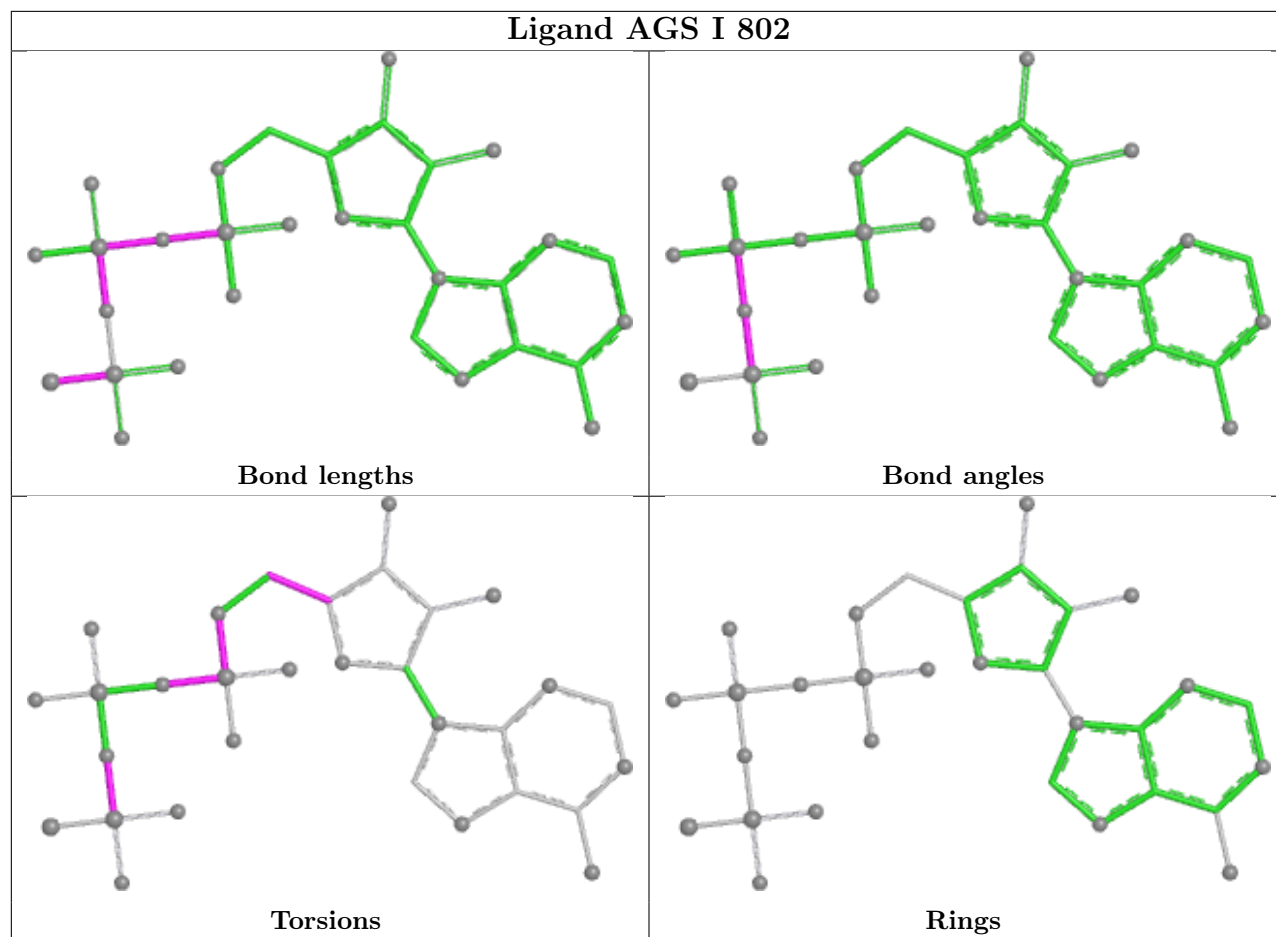


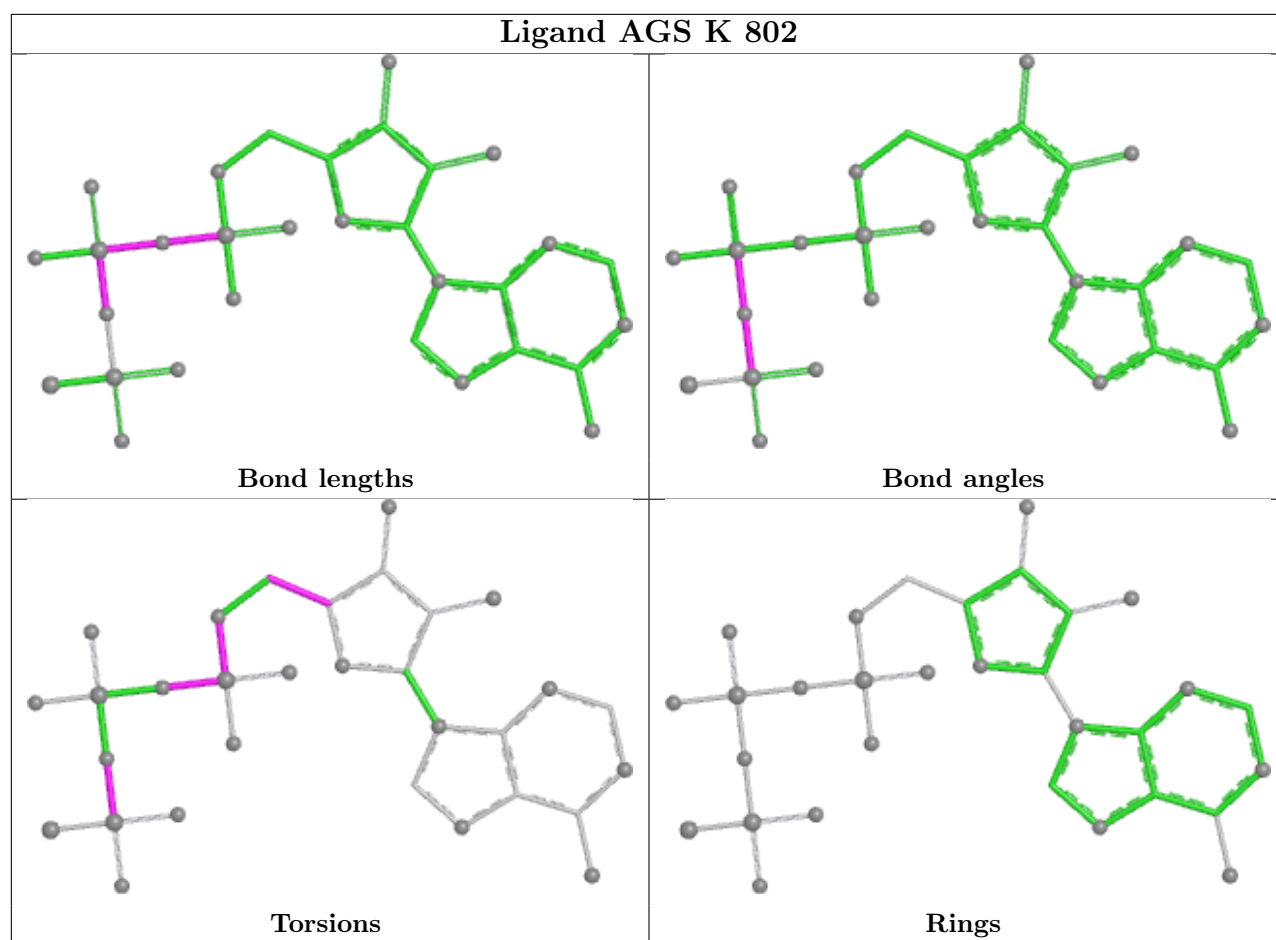
## Ligand AGS F 803



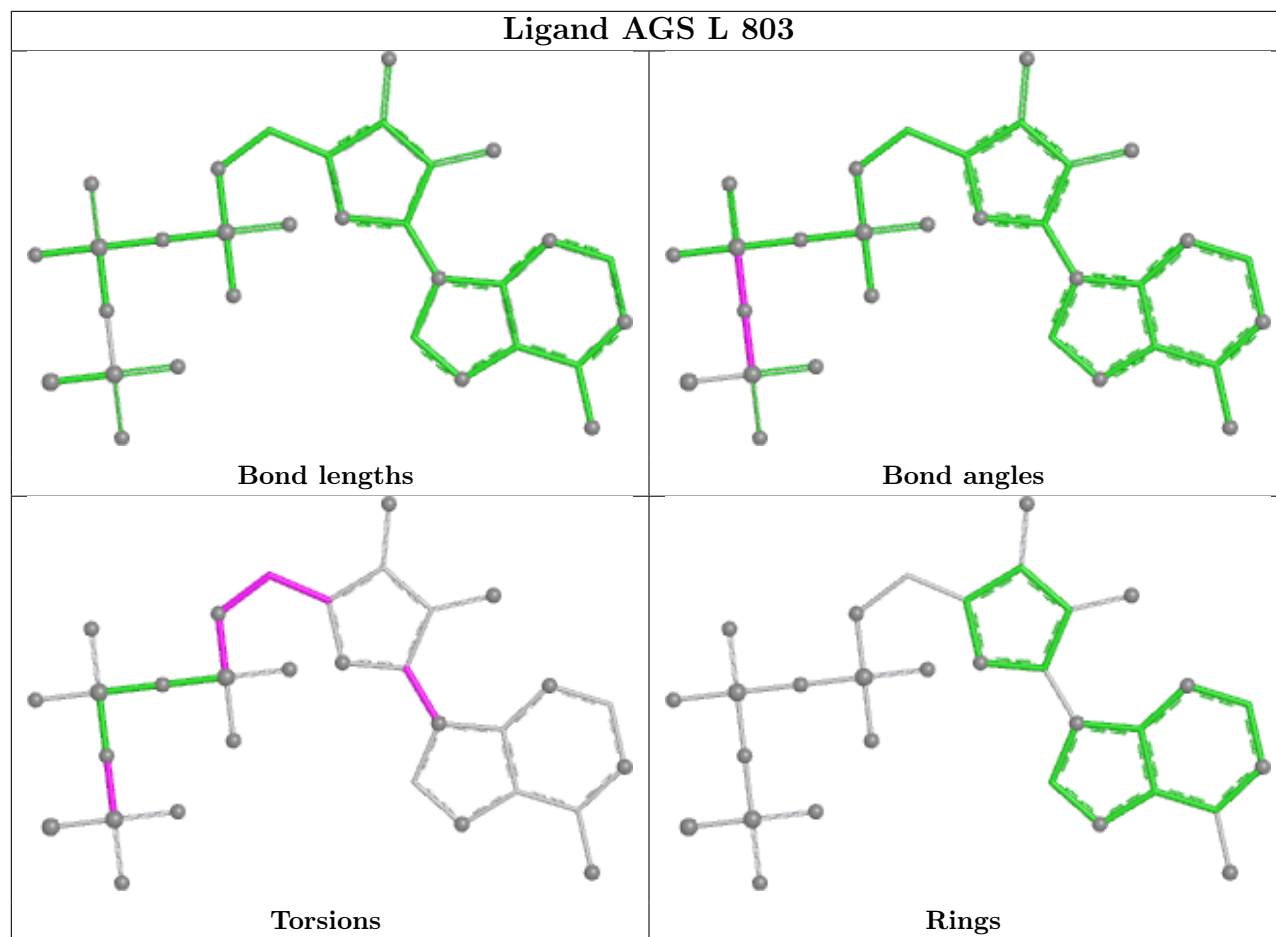


## Ligand AGS I 802

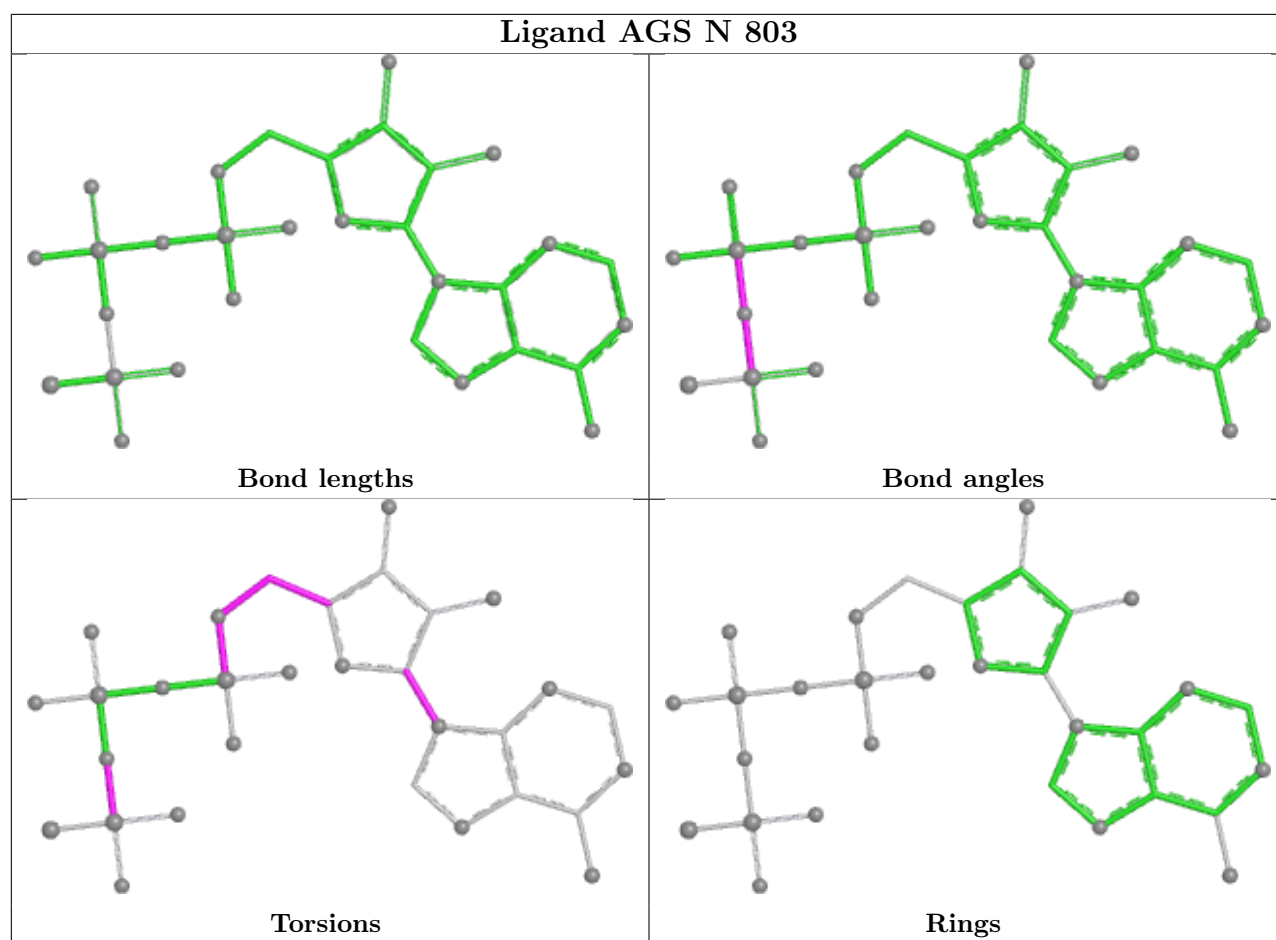


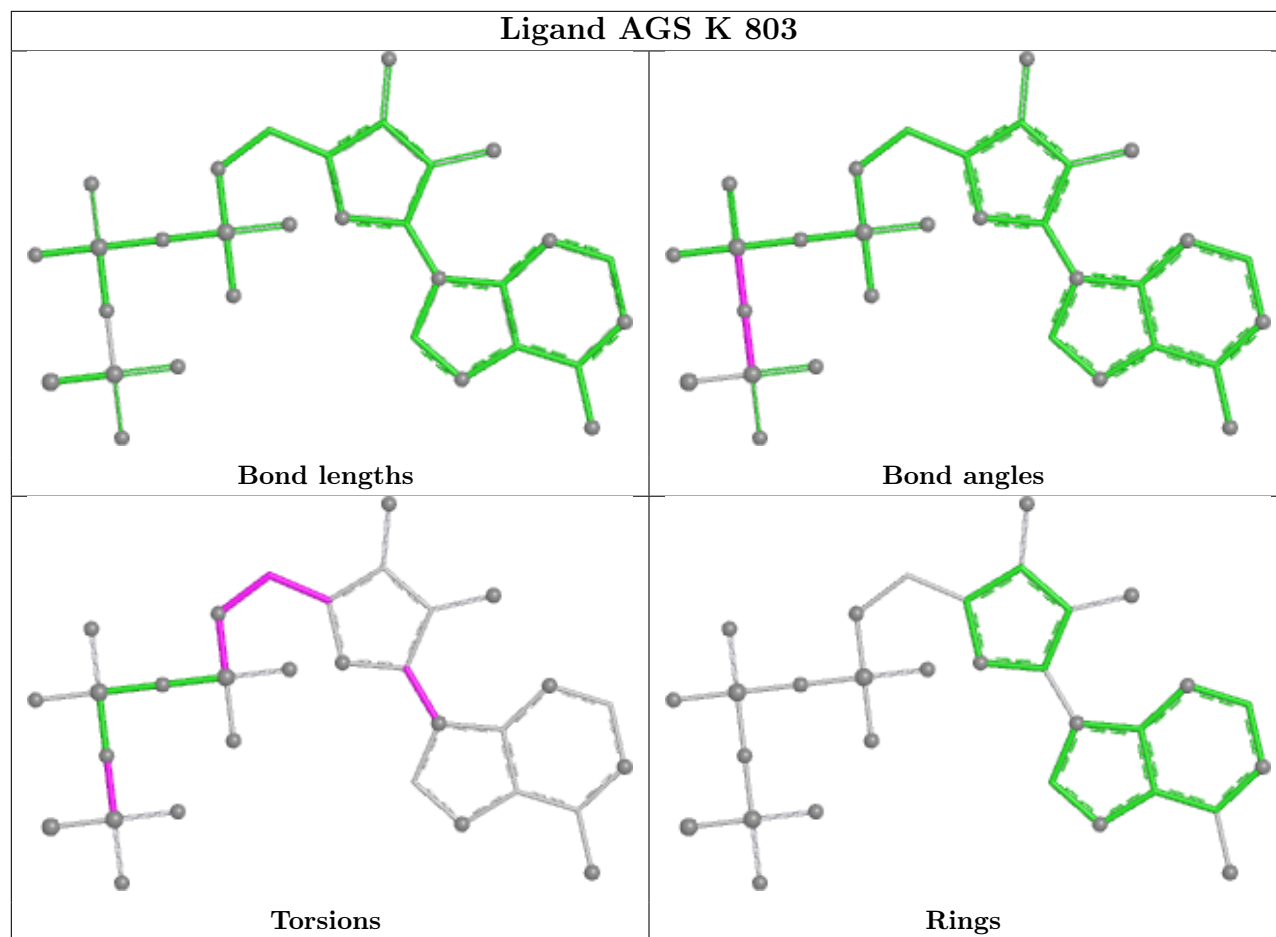


## Ligand AGS L 803

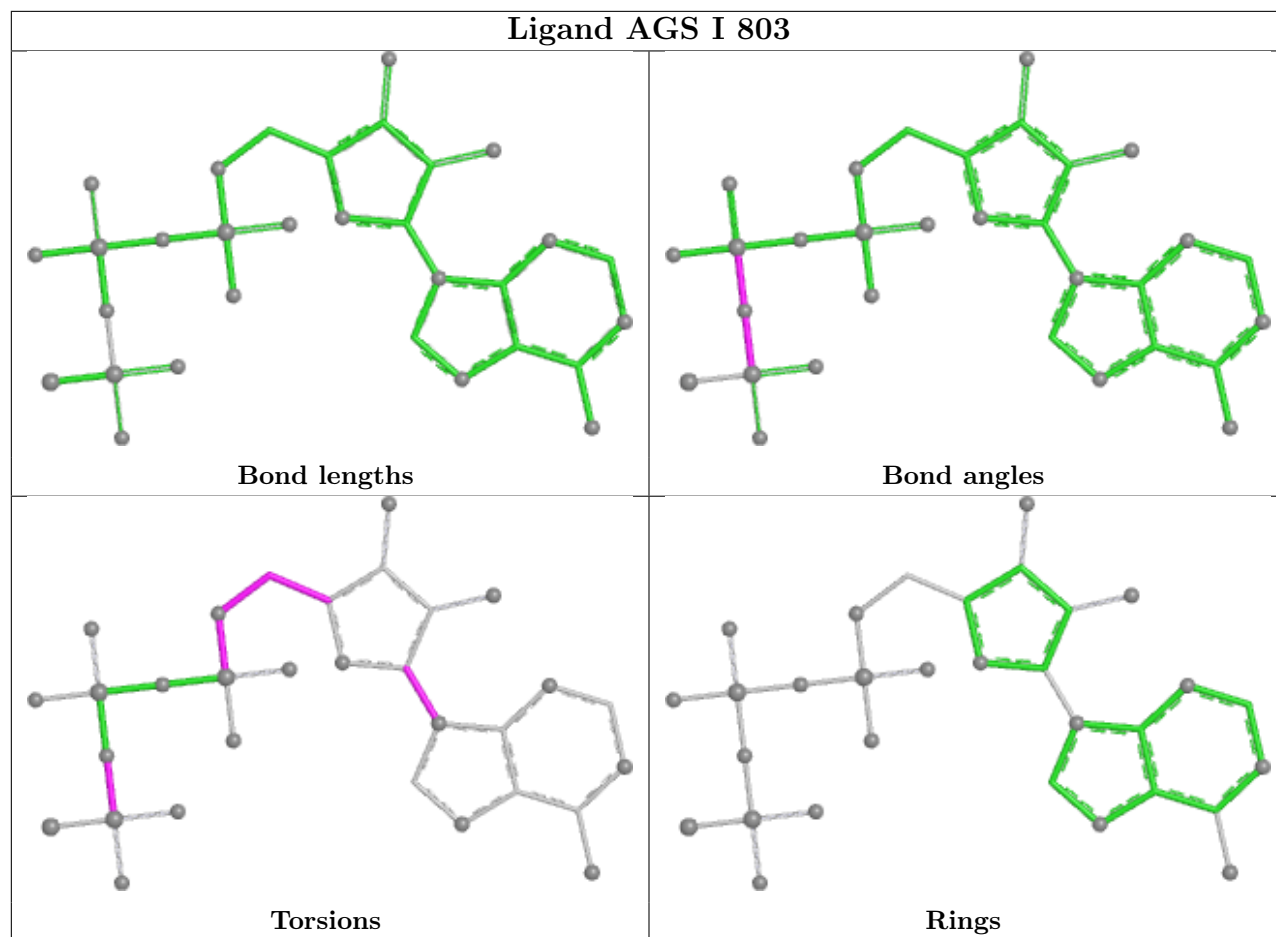




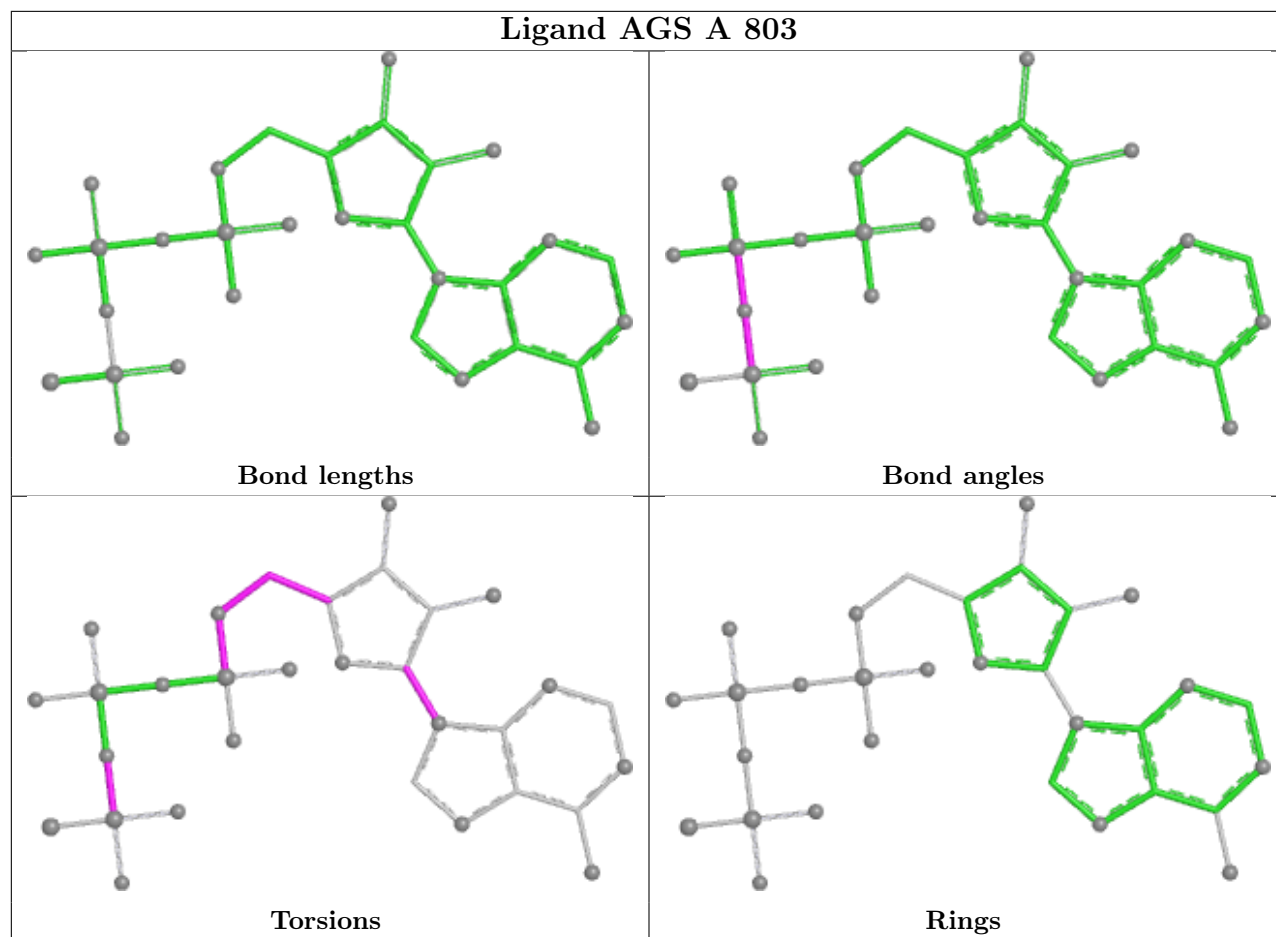




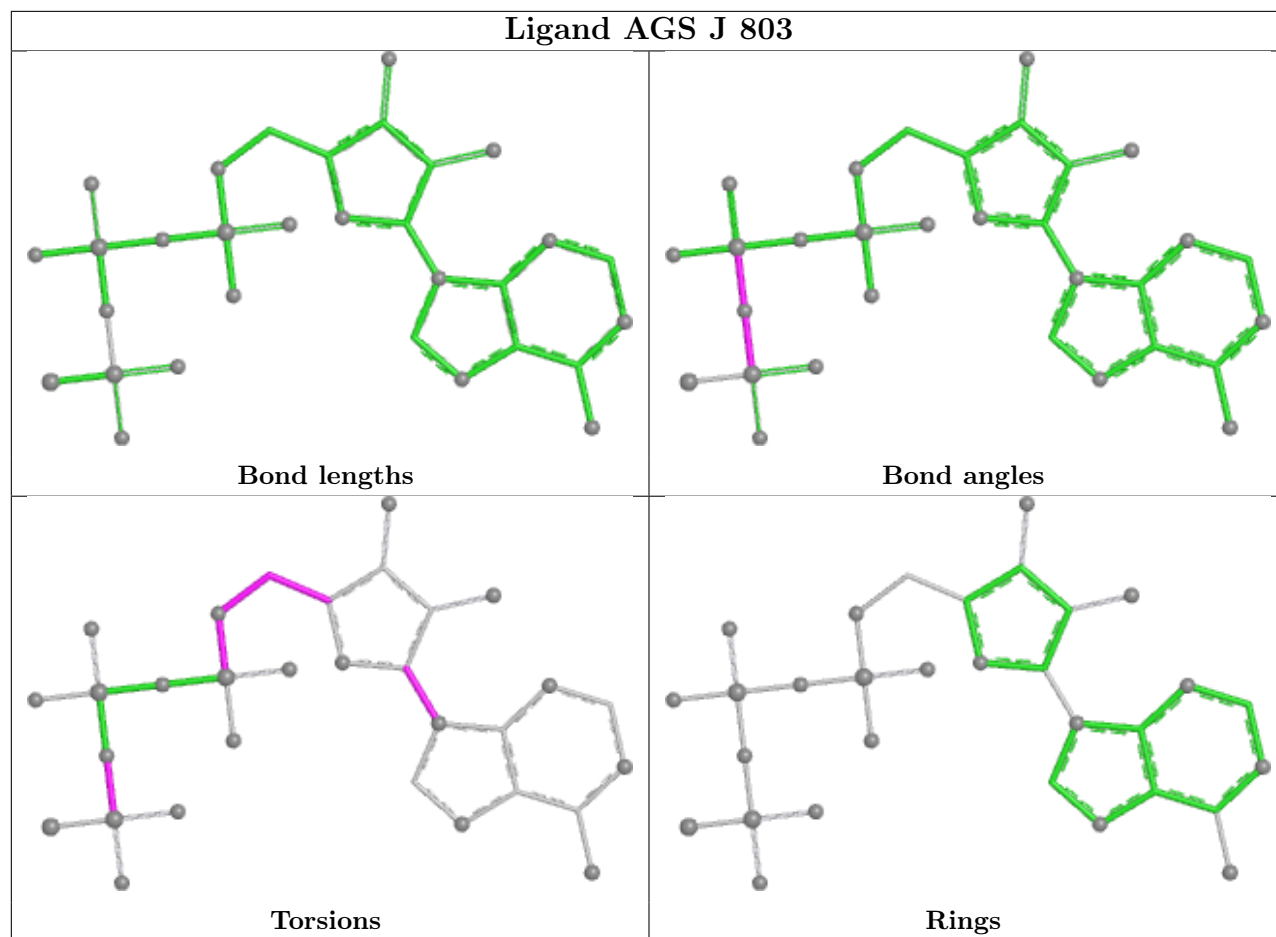
## Ligand AGS I 803



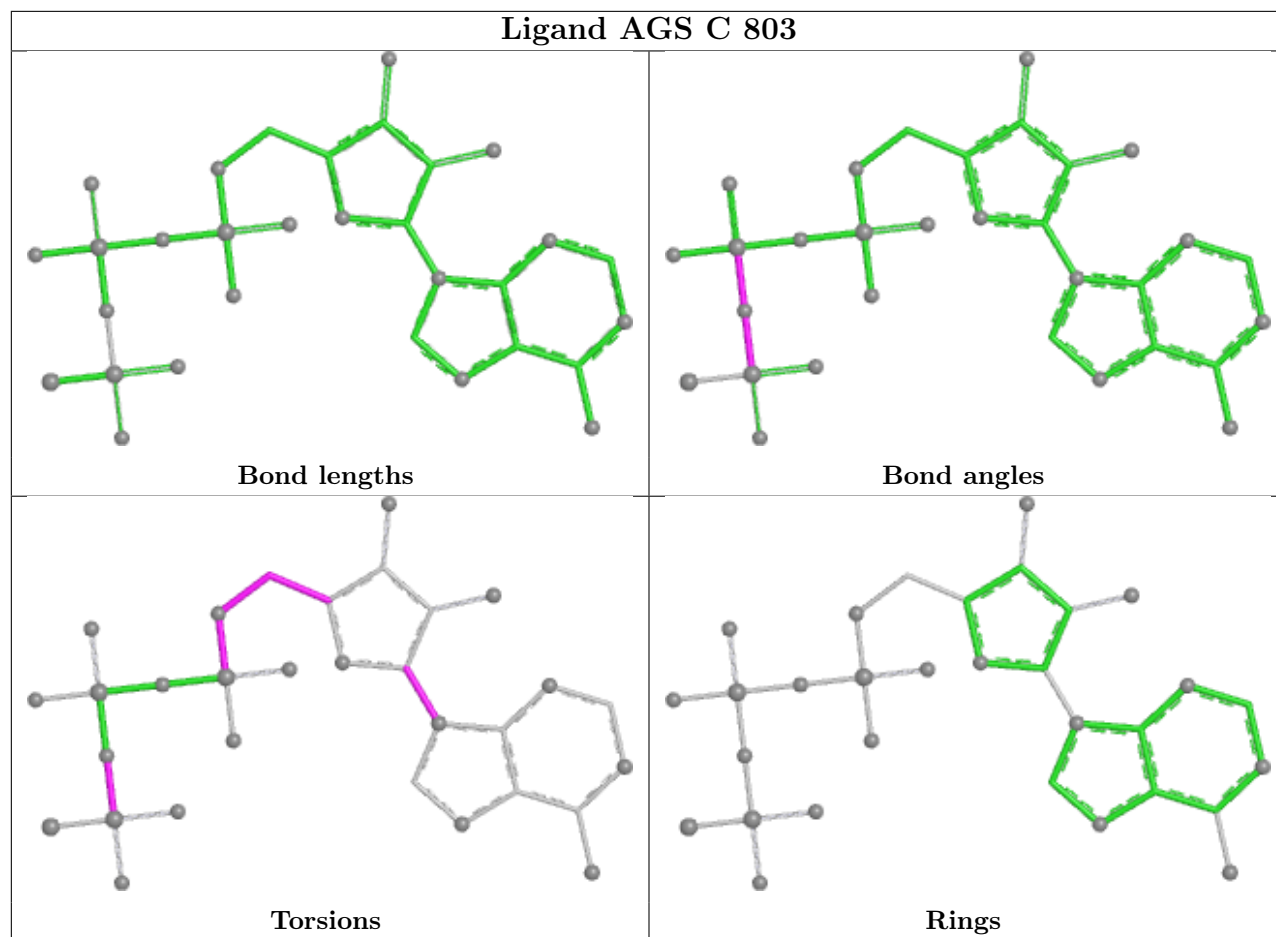
## Ligand AGS A 803



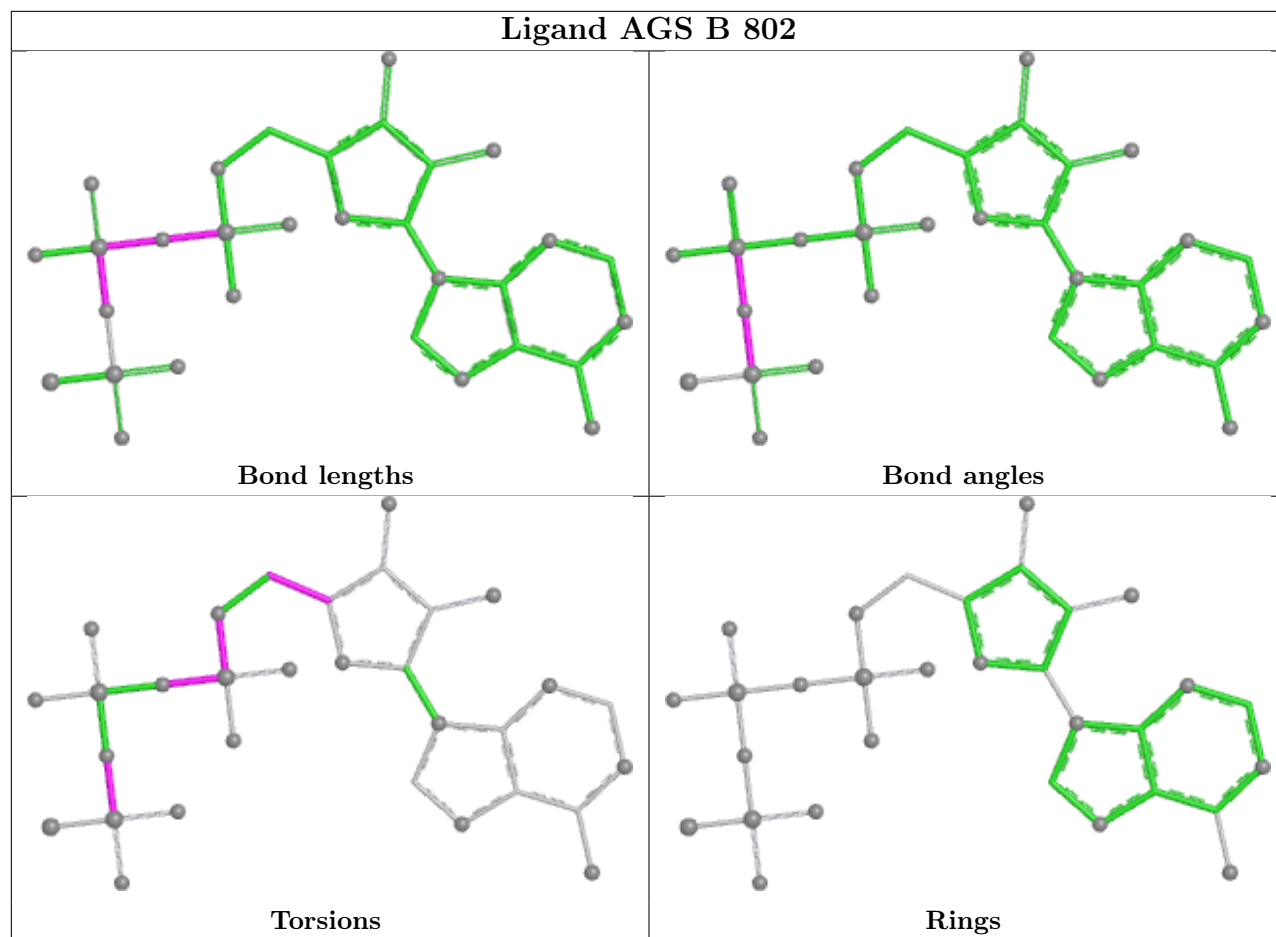
## Ligand AGS J 803

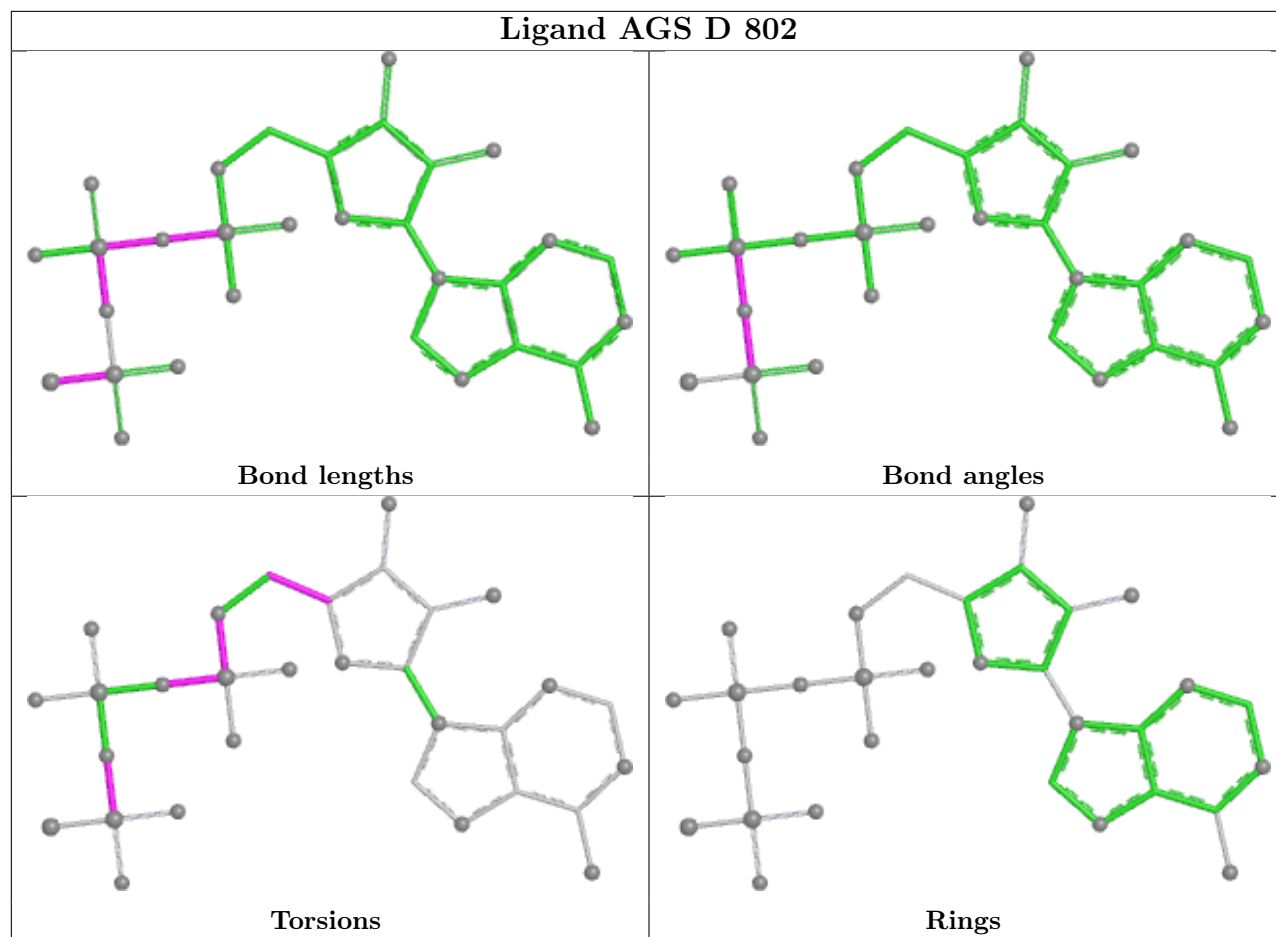


## Ligand AGS C 803



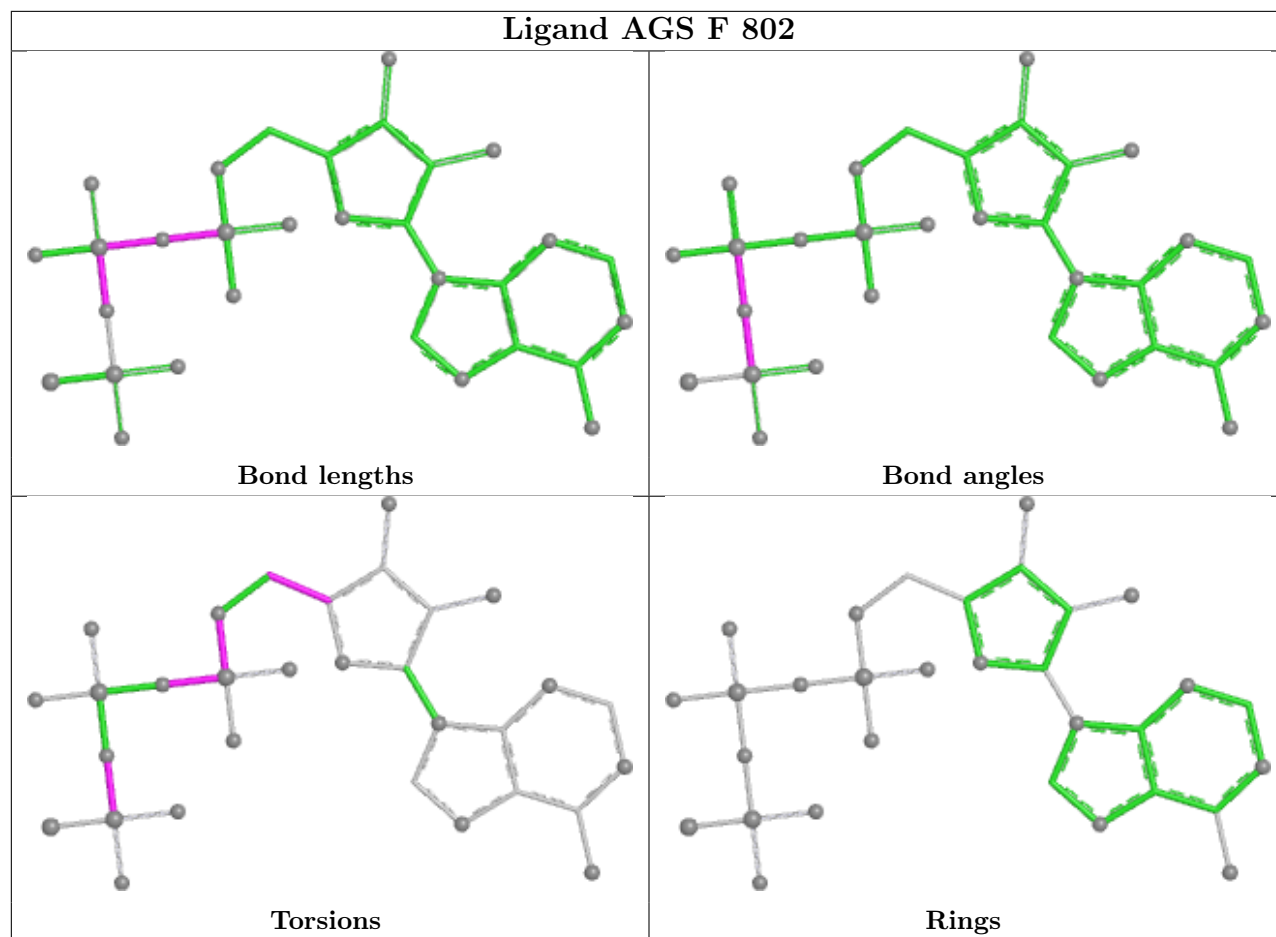
## Ligand AGS B 802



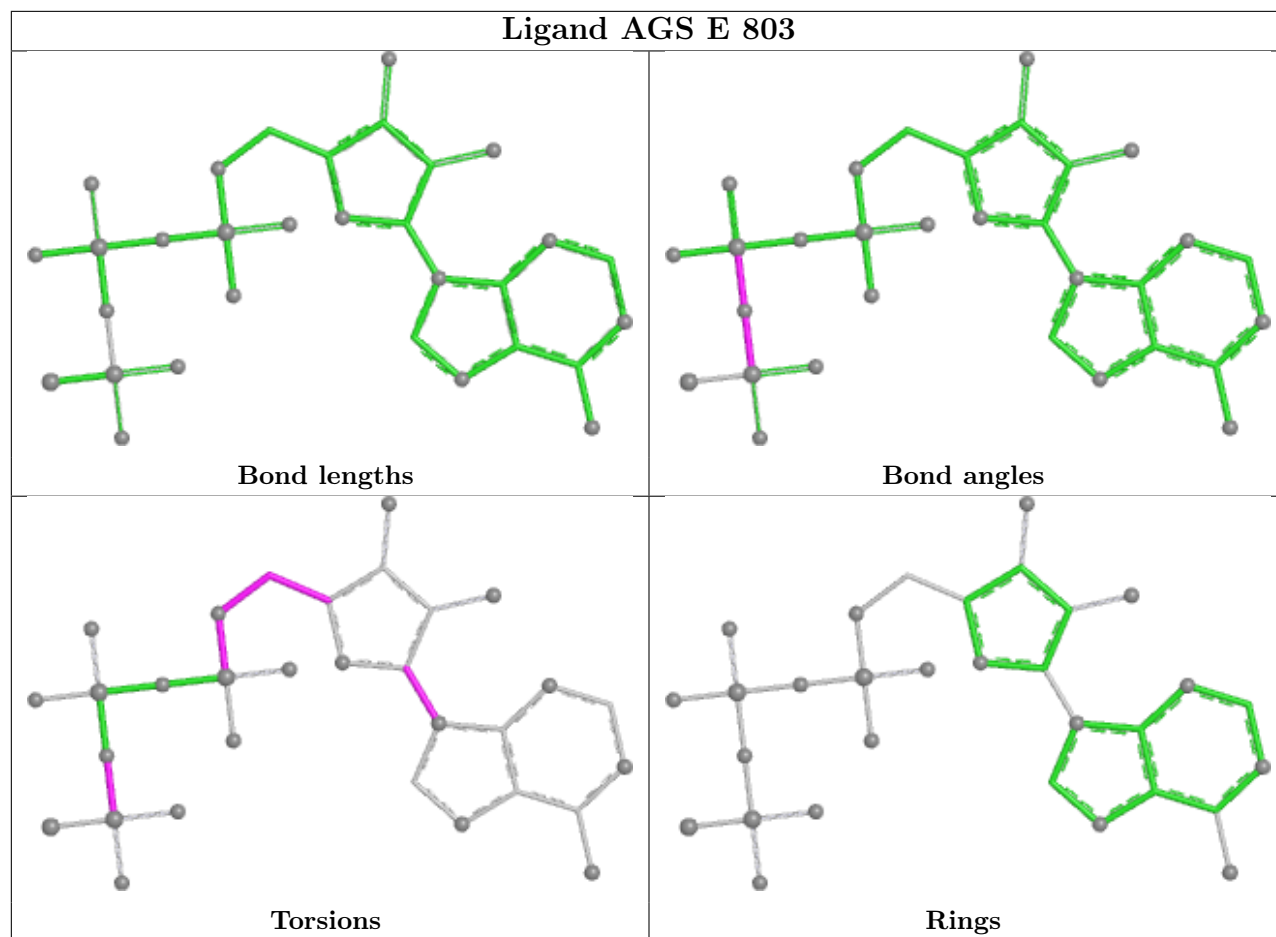


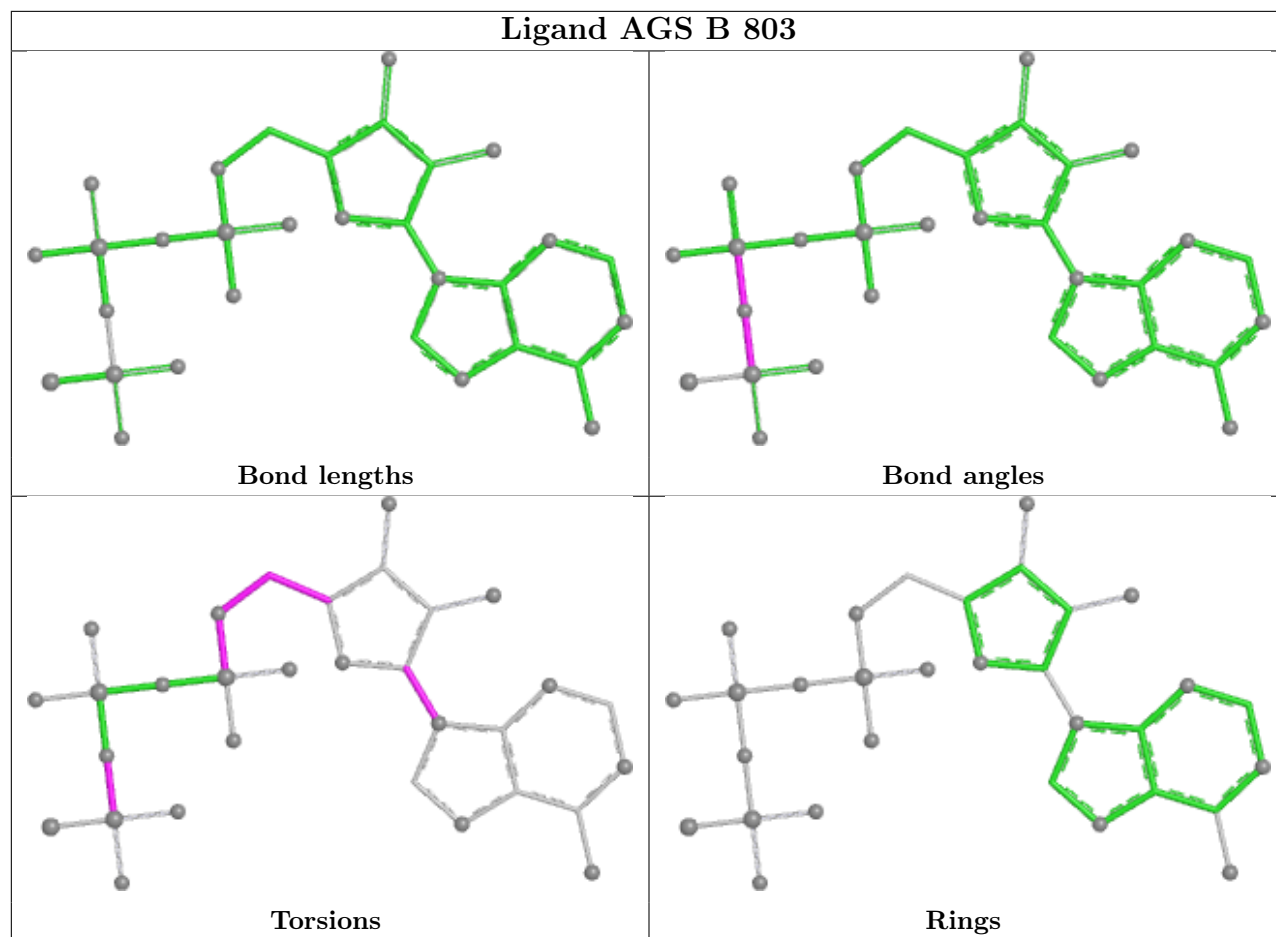


## Ligand AGS F 802

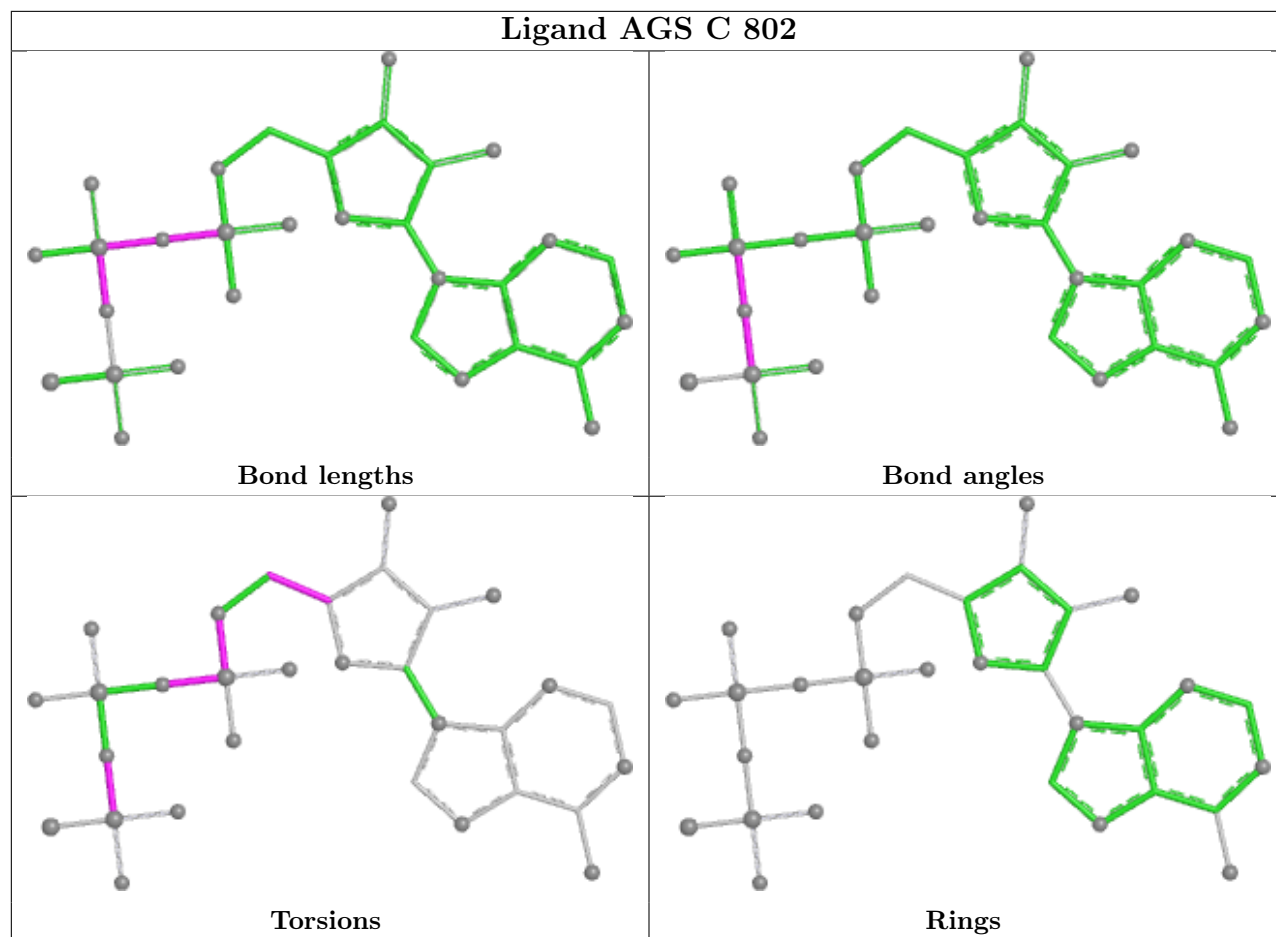


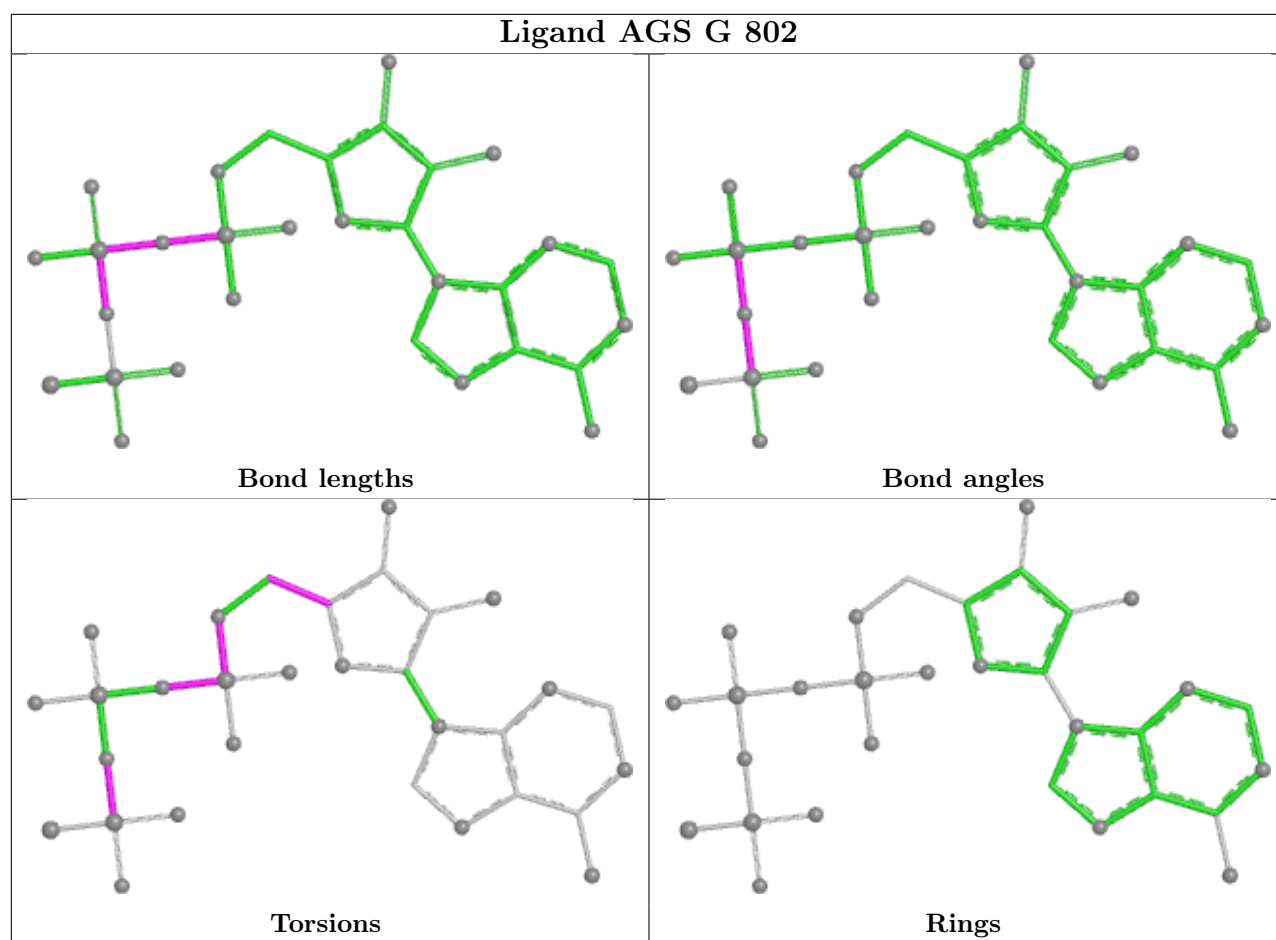
## Ligand AGS E 803





## Ligand AGS C 802





## 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.

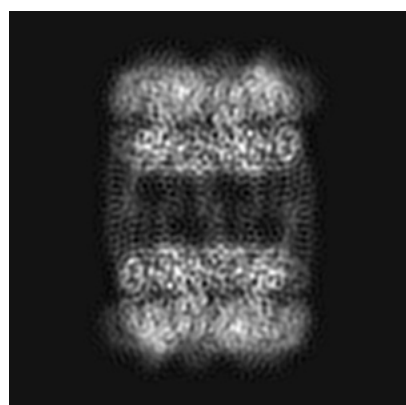
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0967. These allow visual inspection of the internal detail of the map and identification of artifacts.

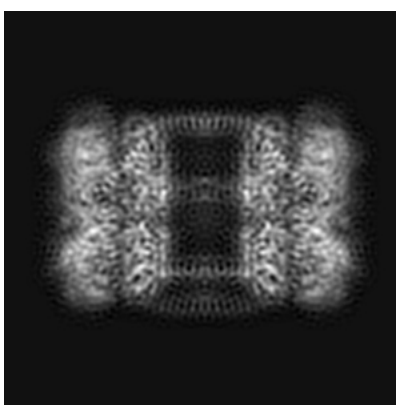
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

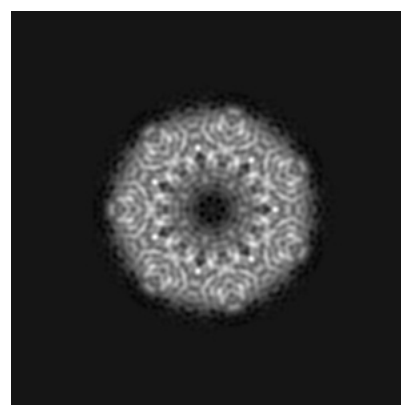
#### 6.1.1 Primary map



X



Y

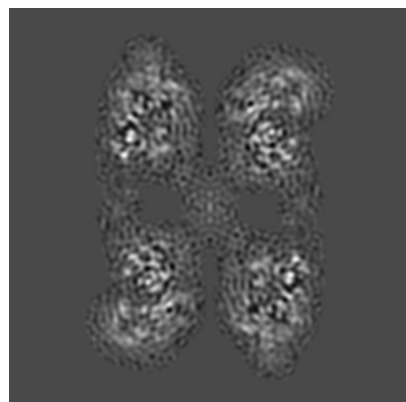


Z

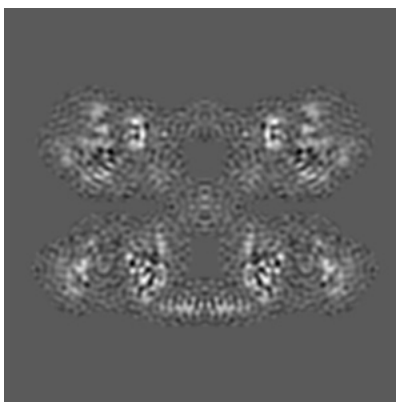
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

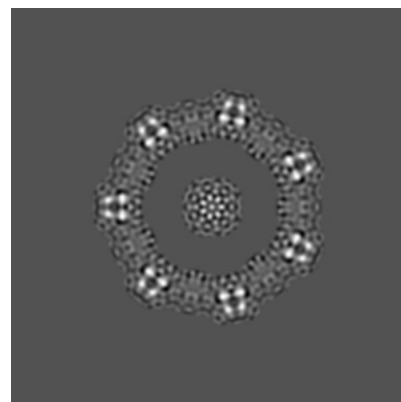
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

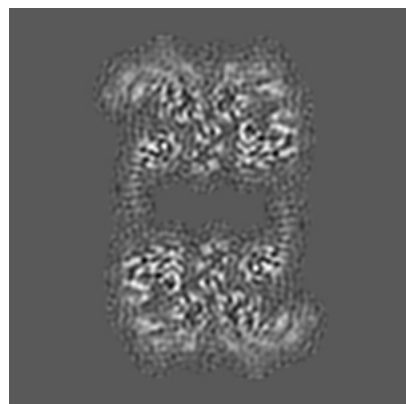


Z Index: 100

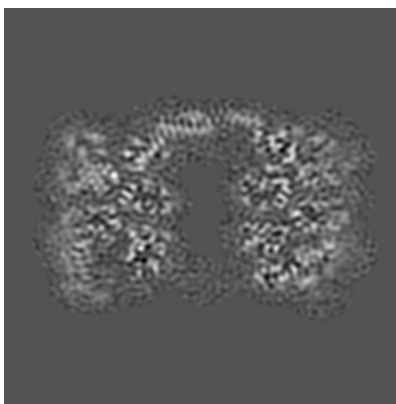
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 78



Y Index: 76

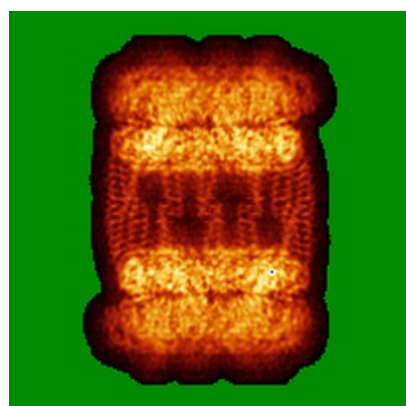


Z Index: 69

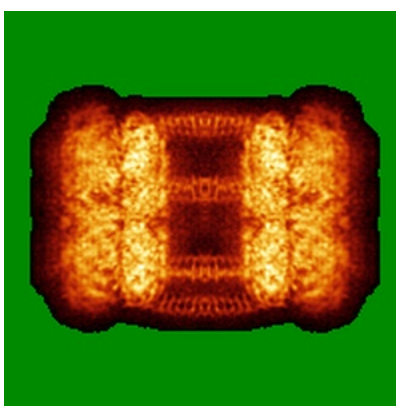
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

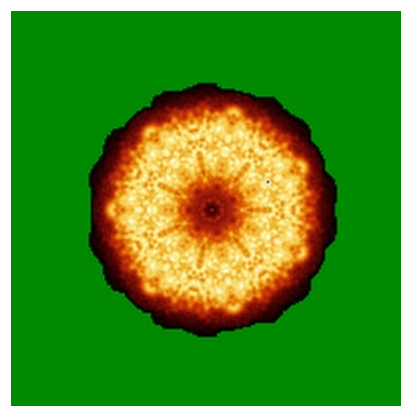
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views

This section was not generated.

## 6.6 Mask visualisation

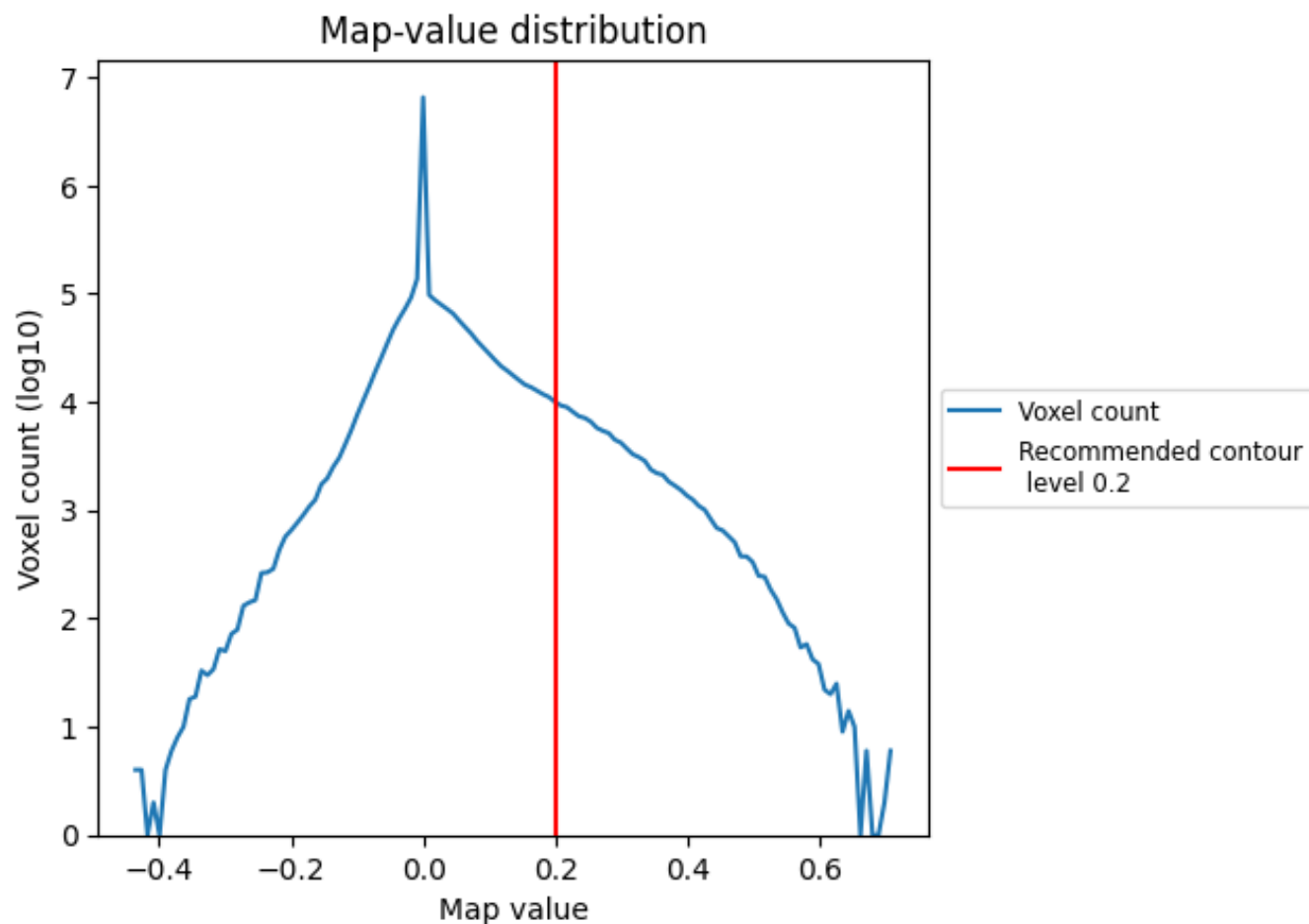
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

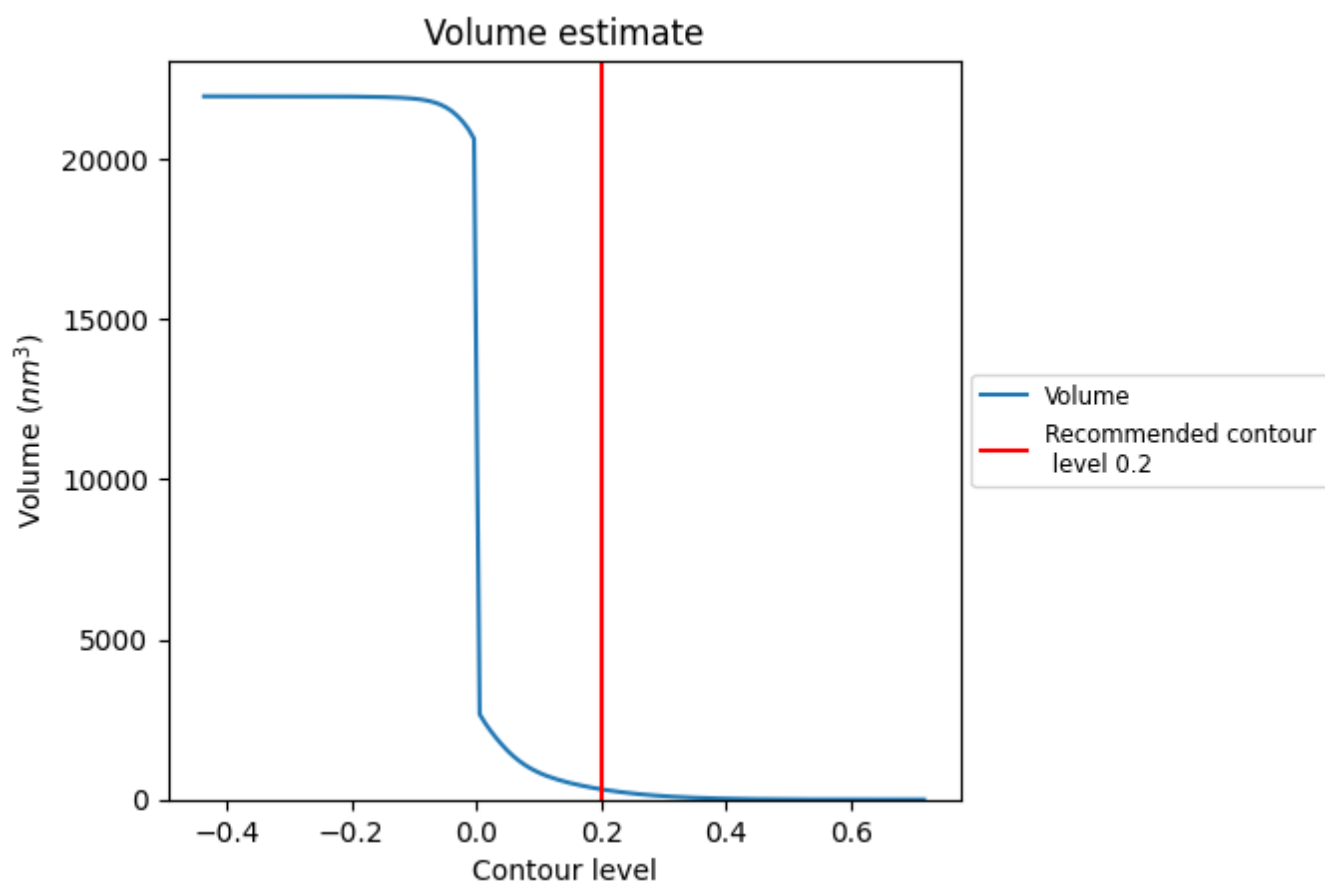
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

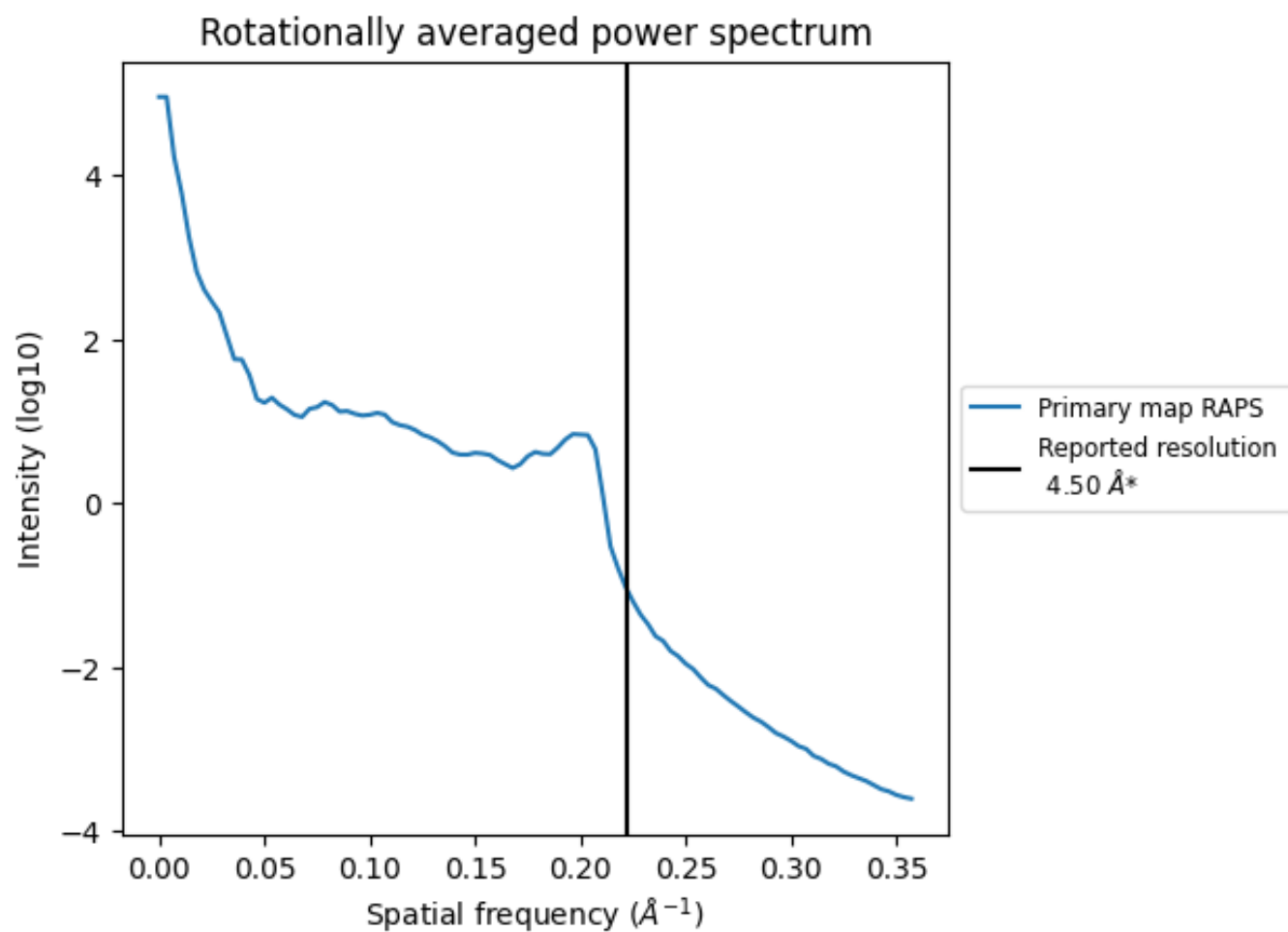
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 322 nm<sup>3</sup>; this corresponds to an approximate mass of 291 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.222 Å<sup>-1</sup>

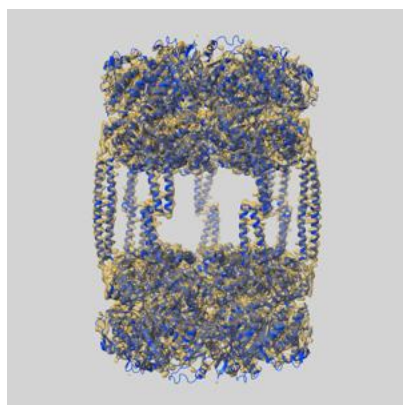
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

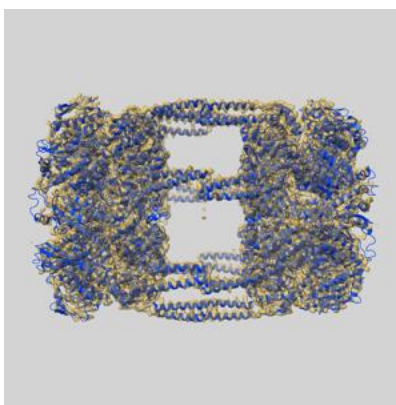
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0967 and PDB model 6LT4. Per-residue inclusion information can be found in section [3](#) on page [9](#).

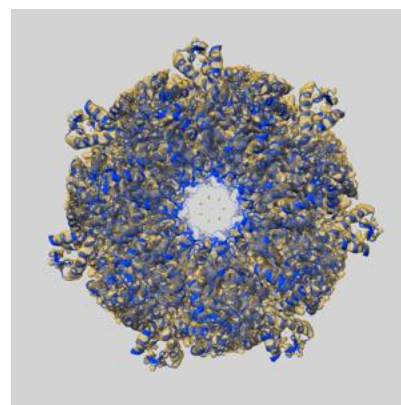
### 9.1 Map-model overlay [i](#)



X



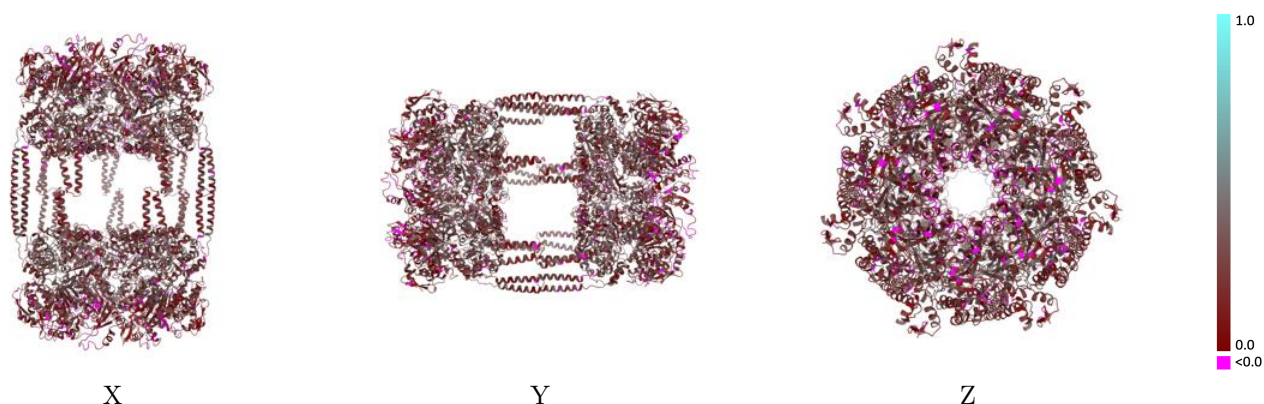
Y



Z

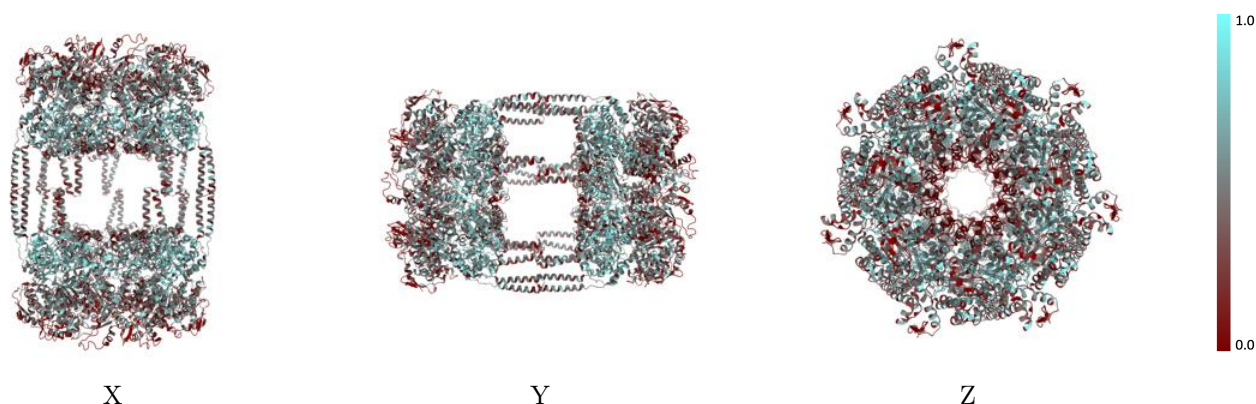
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



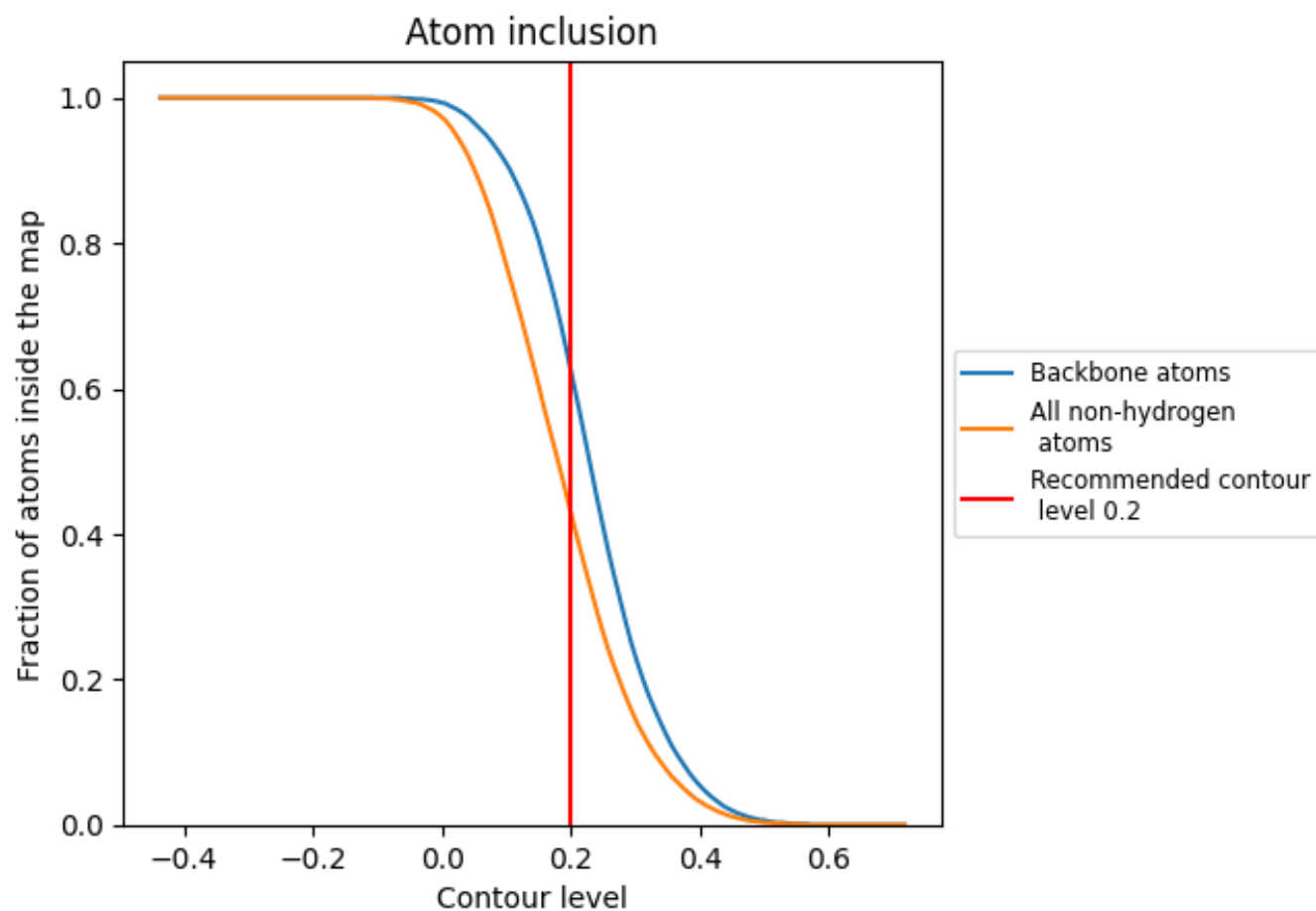
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.4290 | <div></div> 0.2270 |
| A     | <div></div> 0.4310 | <div></div> 0.2300 |
| B     | <div></div> 0.4260 | <div></div> 0.2310 |
| C     | <div></div> 0.4260 | <div></div> 0.2310 |
| D     | <div></div> 0.4350 | <div></div> 0.2300 |
| E     | <div></div> 0.4370 | <div></div> 0.2310 |
| F     | <div></div> 0.4290 | <div></div> 0.2230 |
| G     | <div></div> 0.4300 | <div></div> 0.2260 |
| H     | <div></div> 0.4250 | <div></div> 0.2260 |
| I     | <div></div> 0.4210 | <div></div> 0.2160 |
| J     | <div></div> 0.4250 | <div></div> 0.2240 |
| K     | <div></div> 0.4320 | <div></div> 0.2320 |
| L     | <div></div> 0.4340 | <div></div> 0.2330 |
| M     | <div></div> 0.4240 | <div></div> 0.2240 |
| N     | <div></div> 0.4280 | <div></div> 0.2240 |

1.0

0.0

<0.0