



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:37 AM UTC

PDB ID : 9NMQ / pdb\_00009nmq  
EMDB ID : EMD-49537  
Title : Structure of mouse RyR1 with simvastatin (Ca<sup>2+</sup>/CFF/ATP dataset; closed pore)  
Authors : Weninger, G.; Marks, A.R.  
Deposited on : 2025-03-04  
Resolution : 2.60 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:

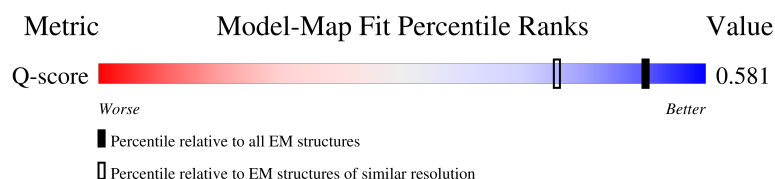
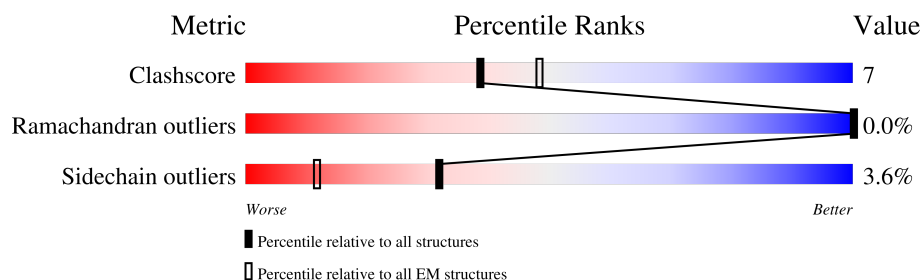
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 2.60 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                       | 8728 ( 2.10 - 3.10 )                                     |

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     | 5035   | <div> <div>8%</div> <div>75%</div> <div>10%</div> <div>13%</div> </div> |
| 1   | B     | 5035   | <div> <div>8%</div> <div>75%</div> <div>11%</div> <div>13%</div> </div> |
| 1   | C     | 5035   | <div> <div>8%</div> <div>75%</div> <div>10%</div> <div>13%</div> </div> |
| 1   | D     | 5035   | <div> <div>8%</div> <div>75%</div> <div>10%</div> <div>13%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                            |
|-----|-------|--------|---------------------------------------------------------------------------------------------|
| 2   | E     | 108    |  92% 7% . |
| 2   | F     | 108    |  92% 7% . |
| 2   | G     | 108    |  92% 7% . |
| 2   | H     | 108    |  92% 7% . |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4   | CFF  | A     | 8002 | -         | X        | -       | -                |
| 4   | CFF  | B     | 8002 | -         | X        | -       | -                |
| 4   | CFF  | C     | 8002 | -         | X        | -       | -                |
| 4   | CFF  | D     | 8002 | -         | X        | -       | -                |

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 143492 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 Ryanodine receptor 1.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 1   | A     | 4373     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 34797 | 22132 | 5983 | 6445 | 237 |         |       |
| 1   | B     | 4373     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 34797 | 22132 | 5983 | 6445 | 237 |         |       |
| 1   | C     | 4373     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 34797 | 22132 | 5983 | 6445 | 237 |         |       |
| 1   | D     | 4373     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 34797 | 22132 | 5983 | 6445 | 237 |         |       |

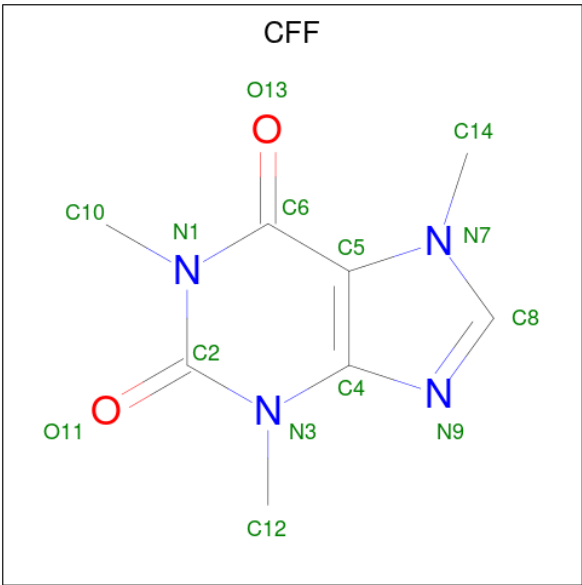
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | E     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 830   | 526 | 146 | 155 | 3 |         |       |
| 2   | F     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 830   | 526 | 146 | 155 | 3 |         |       |
| 2   | G     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 830   | 526 | 146 | 155 | 3 |         |       |
| 2   | H     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 830   | 526 | 146 | 155 | 3 |         |       |

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

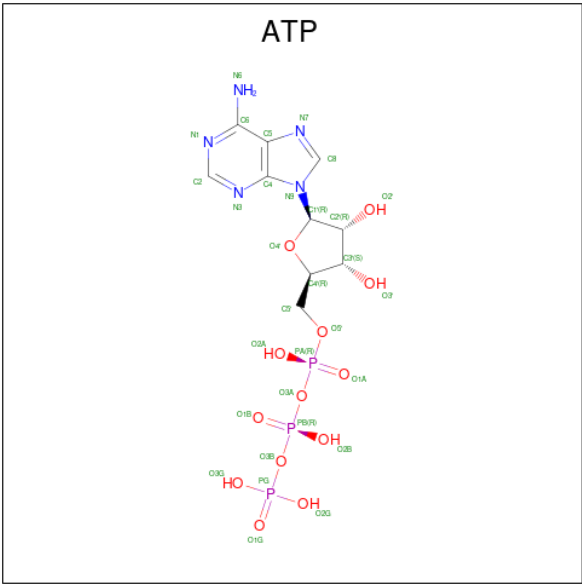
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 3   | A     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | C     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | D     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 4 | 2 |         |
| 4   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 4 | 2 |         |
| 4   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 4 | 2 |         |
| 4   | D     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 4 | 2 |         |

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

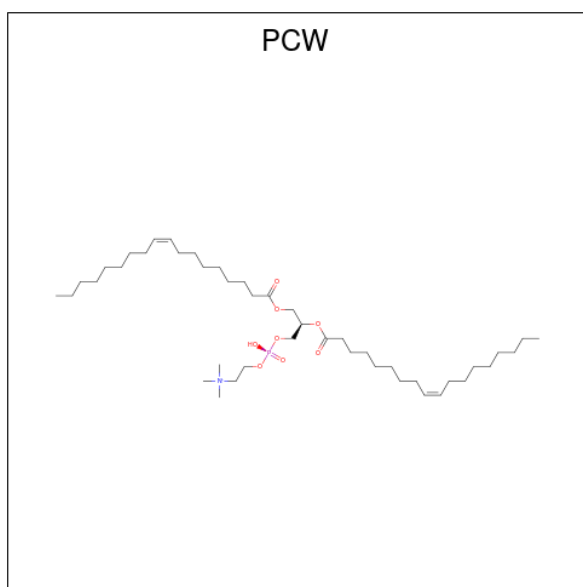


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 5   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 5   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 5   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 5   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 5   | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 5   | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 5   | D     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 5   | D     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

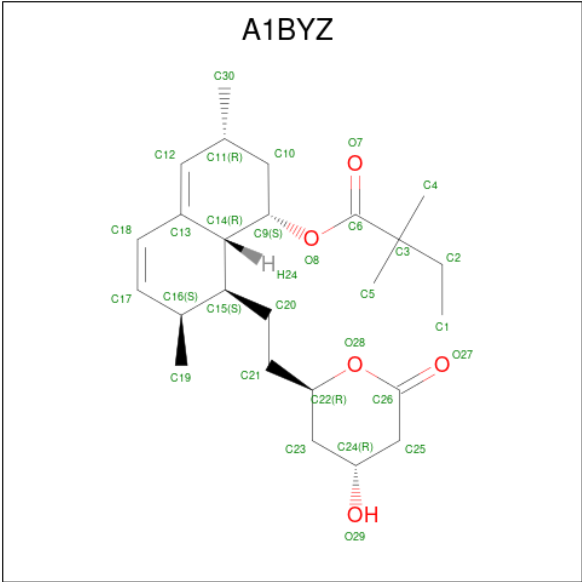
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 6   | A     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 6   | B     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 6   | C     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 6   | D     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 7   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 7   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 7   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 7   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 7   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 7   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 7   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 7   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |

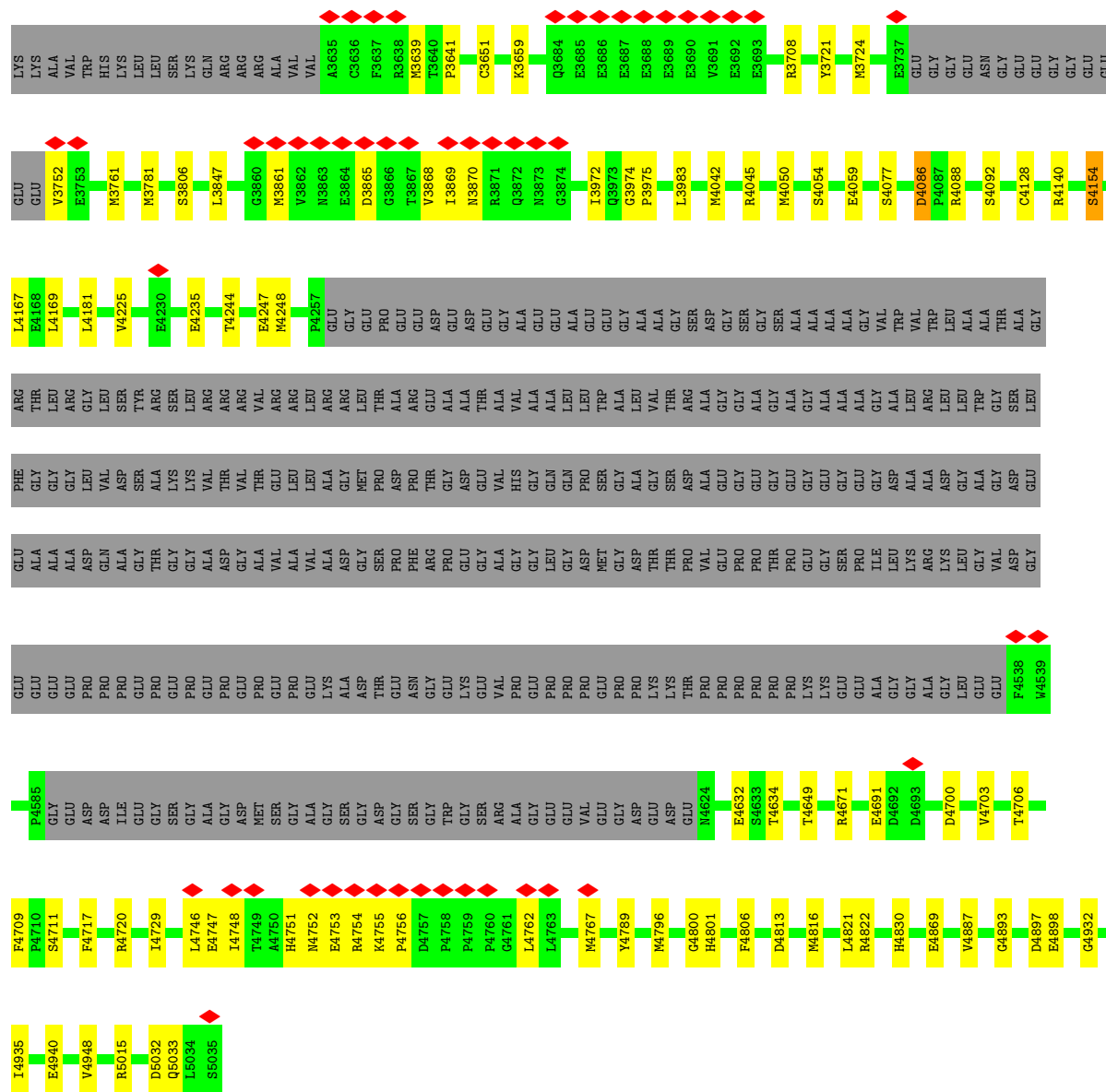
- Molecule 8 is Simvastatin (CCD ID: A1BYZ) (formula:  $C_{25}H_{38}O_5$ ) (labeled as "Ligand of Interest" by depositor).



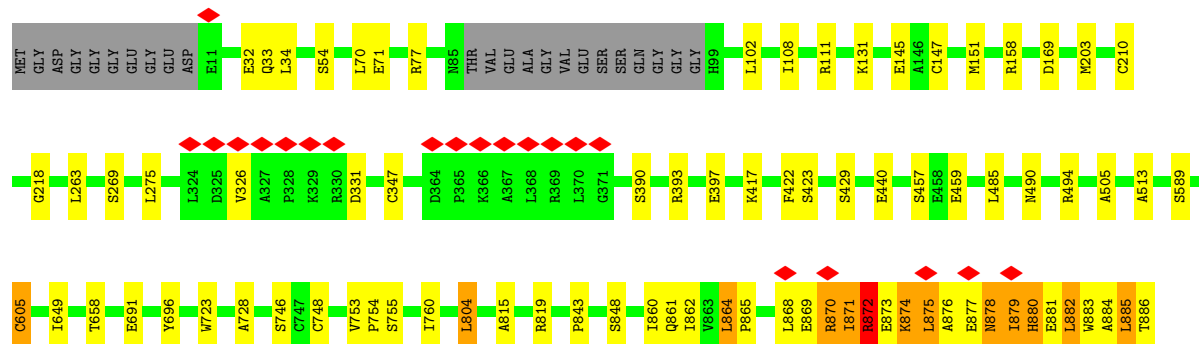
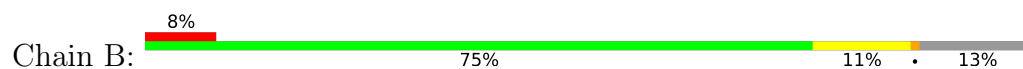
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 8   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 30    | 25 | 5 |         |
| 8   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 30    | 25 | 5 |         |
| 8   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 30    | 25 | 5 |         |
| 8   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 30    | 25 | 5 |         |
| 8   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 30    | 25 | 5 |         |
| 8   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 30    | 25 | 5 |         |
| 8   | D     | 1        | Total | C  | O | 0       |
|     |       |          | 30    | 25 | 5 |         |
| 8   | D     | 1        | Total | C  | O | 0       |
|     |       |          | 30    | 25 | 5 |         |





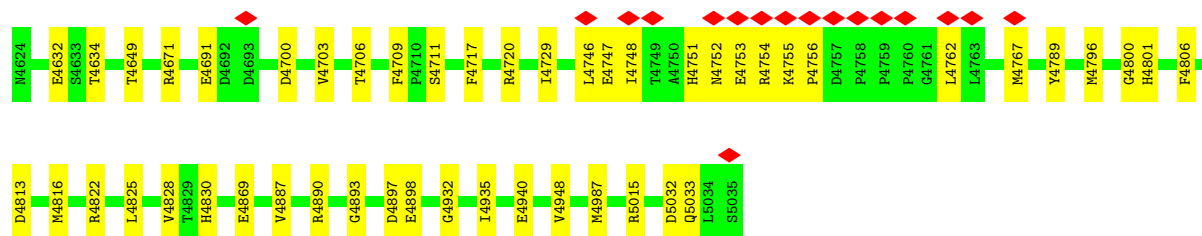


### • Molecule 1: Ryanodine receptor 1

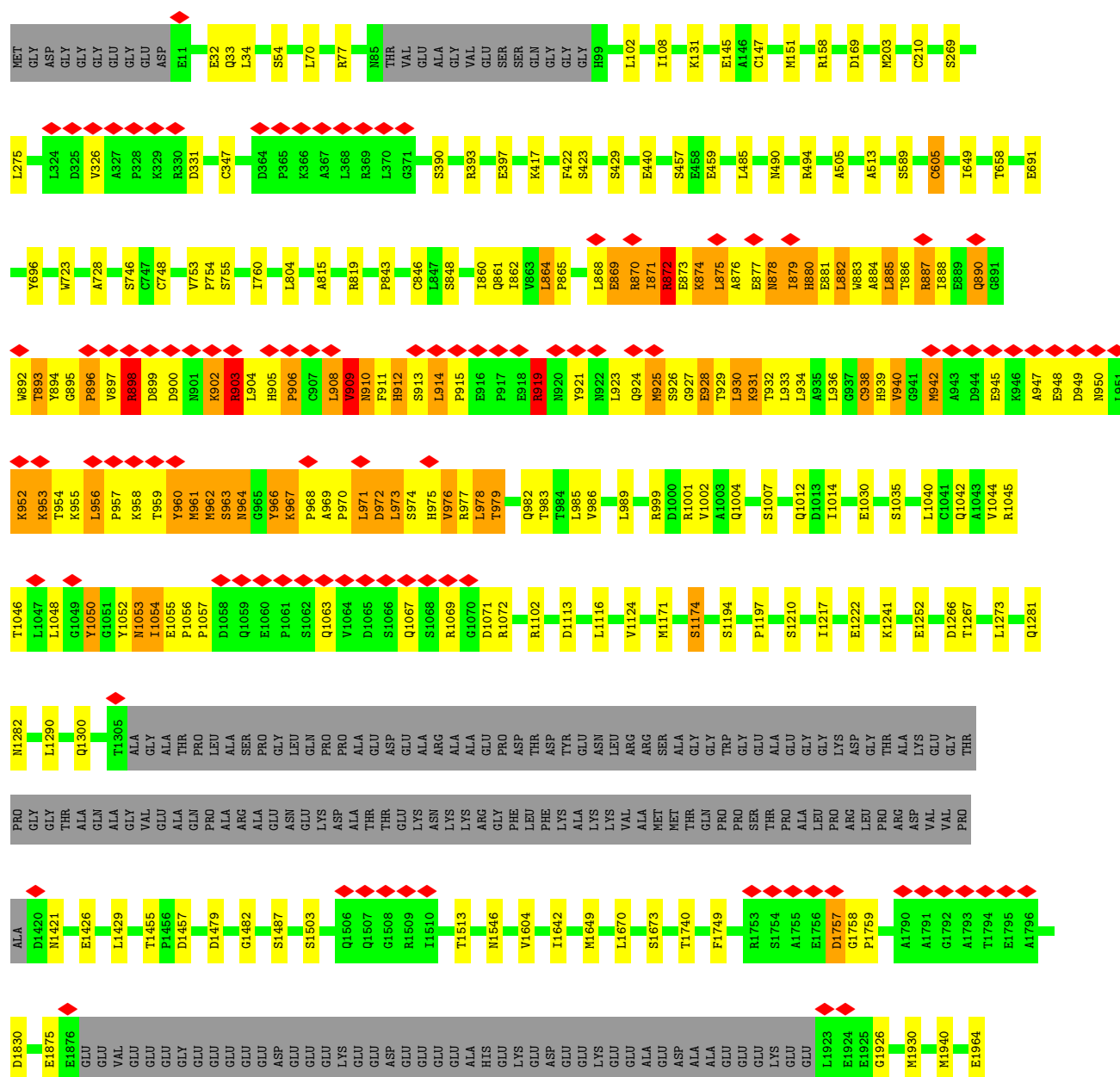
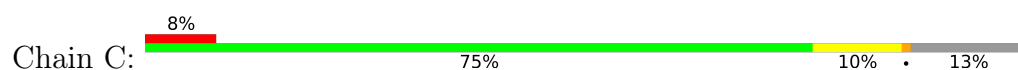






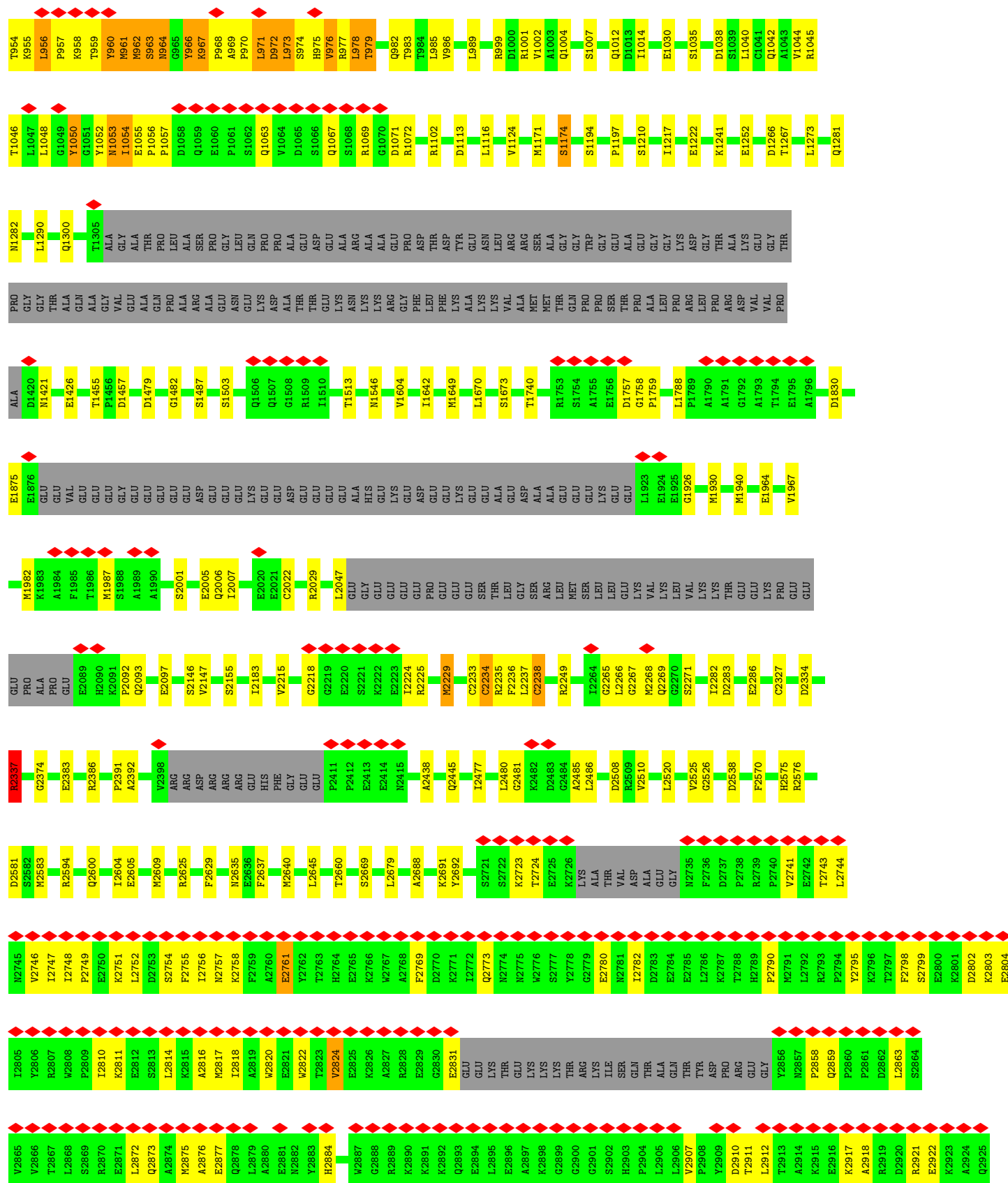


• Molecule 1: Ryanodine receptor 1













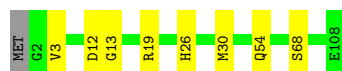
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E: 92% 7% .



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 92% 7% .



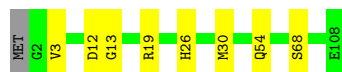
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G: 92% 7% .



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H: 92% 7% .



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 65309                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 58                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 1200                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.747                                   | Depositor |
| Minimum map value                    | 0.000                                   | Depositor |
| Average map value                    | 0.004                                   | Depositor |
| Map value standard deviation         | 0.027                                   | Depositor |
| Recommended contour level            | 0.1                                     | Depositor |
| Map size (Å)                         | 424.448, 424.448, 424.448               | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.829, 0.829, 0.829                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, PCW, CA, ZN, ATP, A1BYZ

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     | 0.28         | 1/35586 (0.0%)  | 0.43        | 10/48203 (0.0%)  |
| 1   | B     | 0.28         | 1/35586 (0.0%)  | 0.44        | 10/48203 (0.0%)  |
| 1   | C     | 0.28         | 1/35586 (0.0%)  | 0.44        | 10/48203 (0.0%)  |
| 1   | D     | 0.28         | 1/35586 (0.0%)  | 0.44        | 10/48203 (0.0%)  |
| 2   | E     | 0.20         | 0/848           | 0.32        | 0/1143           |
| 2   | F     | 0.20         | 0/848           | 0.33        | 0/1143           |
| 2   | G     | 0.20         | 0/848           | 0.32        | 0/1143           |
| 2   | H     | 0.20         | 0/848           | 0.33        | 0/1143           |
| All | All   | 0.28         | 4/145736 (0.0%) | 0.43        | 40/197384 (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                   | 7                   |
| 1   | B     | 0                   | 7                   |
| 1   | C     | 0                   | 7                   |
| 1   | D     | 0                   | 7                   |
| All | All   | 0                   | 28                  |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | A     | 2238 | CYS  | CB-SG | 5.43 | 1.99        | 1.81     |
| 1   | C     | 2238 | CYS  | CB-SG | 5.43 | 1.99        | 1.81     |
| 1   | D     | 2238 | CYS  | CB-SG | 5.43 | 1.99        | 1.81     |
| 1   | B     | 2238 | CYS  | CB-SG | 5.42 | 1.99        | 1.81     |

All (40) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | C     | 896  | PRO  | N-CA-C   | -8.38 | 101.88      | 113.53   |
| 1   | A     | 896  | PRO  | N-CA-C   | -8.37 | 101.89      | 113.53   |
| 1   | B     | 896  | PRO  | N-CA-C   | -8.37 | 101.89      | 113.53   |
| 1   | D     | 896  | PRO  | N-CA-C   | -8.37 | 101.89      | 113.53   |
| 1   | B     | 1050 | TYR  | N-CA-C   | -6.62 | 104.06      | 111.28   |
| 1   | D     | 2234 | CYS  | N-CA-CB  | 6.60  | 121.64      | 110.49   |
| 1   | B     | 2234 | CYS  | N-CA-CB  | 6.60  | 121.64      | 110.49   |
| 1   | A     | 2234 | CYS  | N-CA-CB  | 6.60  | 121.64      | 110.49   |
| 1   | A     | 1050 | TYR  | N-CA-C   | -6.59 | 104.09      | 111.28   |
| 1   | C     | 1050 | TYR  | N-CA-C   | -6.58 | 104.10      | 111.28   |
| 1   | C     | 2234 | CYS  | N-CA-CB  | 6.58  | 121.61      | 110.49   |
| 1   | D     | 1050 | TYR  | N-CA-C   | -6.57 | 104.12      | 111.28   |
| 1   | B     | 2233 | CYS  | CA-C-N   | -6.37 | 109.38      | 121.54   |
| 1   | B     | 2233 | CYS  | C-N-CA   | -6.37 | 109.38      | 121.54   |
| 1   | C     | 2233 | CYS  | CA-C-N   | -6.37 | 109.38      | 121.54   |
| 1   | C     | 2233 | CYS  | C-N-CA   | -6.37 | 109.38      | 121.54   |
| 1   | A     | 2233 | CYS  | CA-C-N   | -6.36 | 109.40      | 121.54   |
| 1   | A     | 2233 | CYS  | C-N-CA   | -6.36 | 109.40      | 121.54   |
| 1   | D     | 2233 | CYS  | CA-C-N   | -6.36 | 109.40      | 121.54   |
| 1   | D     | 2233 | CYS  | C-N-CA   | -6.36 | 109.40      | 121.54   |
| 1   | D     | 3540 | ARG  | CG-CD-NE | 6.33  | 125.94      | 112.00   |
| 1   | C     | 3540 | ARG  | CG-CD-NE | 6.33  | 125.92      | 112.00   |
| 1   | A     | 3540 | ARG  | CG-CD-NE | 6.32  | 125.90      | 112.00   |
| 1   | B     | 3540 | ARG  | CG-CD-NE | 6.30  | 125.87      | 112.00   |
| 1   | D     | 903  | ARG  | N-CA-C   | -6.24 | 104.26      | 112.24   |
| 1   | C     | 903  | ARG  | N-CA-C   | -6.21 | 104.29      | 112.24   |
| 1   | A     | 903  | ARG  | N-CA-C   | -6.20 | 104.31      | 112.24   |
| 1   | B     | 903  | ARG  | N-CA-C   | -6.19 | 104.32      | 112.24   |
| 1   | B     | 906  | PRO  | N-CA-C   | -5.58 | 105.77      | 113.53   |
| 1   | D     | 906  | PRO  | N-CA-C   | -5.58 | 105.77      | 113.53   |
| 1   | C     | 2234 | CYS  | CA-CB-SG | 5.57  | 127.21      | 114.40   |
| 1   | A     | 906  | PRO  | N-CA-C   | -5.57 | 105.79      | 113.53   |
| 1   | A     | 2234 | CYS  | CA-CB-SG | 5.56  | 127.20      | 114.40   |
| 1   | D     | 2234 | CYS  | CA-CB-SG | 5.56  | 127.19      | 114.40   |
| 1   | B     | 2234 | CYS  | CA-CB-SG | 5.55  | 127.16      | 114.40   |
| 1   | C     | 906  | PRO  | N-CA-C   | -5.54 | 105.82      | 113.53   |
| 1   | C     | 890  | GLN  | N-CA-C   | -5.40 | 106.65      | 113.18   |
| 1   | D     | 890  | GLN  | N-CA-C   | -5.40 | 106.65      | 113.18   |
| 1   | A     | 890  | GLN  | N-CA-C   | -5.38 | 106.67      | 113.18   |
| 1   | B     | 890  | GLN  | N-CA-C   | -5.35 | 106.70      | 113.18   |

There are no chirality outliers.

All (28) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 2337 | ARG  | Sidechain |
| 1   | A     | 605  | CYS  | Peptide   |
| 1   | A     | 872  | ARG  | Sidechain |
| 1   | A     | 887  | ARG  | Sidechain |
| 1   | A     | 898  | ARG  | Sidechain |
| 1   | A     | 903  | ARG  | Sidechain |
| 1   | A     | 919  | ARG  | Sidechain |
| 1   | B     | 2337 | ARG  | Sidechain |
| 1   | B     | 605  | CYS  | Peptide   |
| 1   | B     | 872  | ARG  | Sidechain |
| 1   | B     | 887  | ARG  | Sidechain |
| 1   | B     | 898  | ARG  | Sidechain |
| 1   | B     | 903  | ARG  | Sidechain |
| 1   | B     | 919  | ARG  | Sidechain |
| 1   | C     | 2337 | ARG  | Sidechain |
| 1   | C     | 605  | CYS  | Peptide   |
| 1   | C     | 872  | ARG  | Sidechain |
| 1   | C     | 887  | ARG  | Sidechain |
| 1   | C     | 898  | ARG  | Sidechain |
| 1   | C     | 903  | ARG  | Sidechain |
| 1   | C     | 919  | ARG  | Sidechain |
| 1   | D     | 2337 | ARG  | Sidechain |
| 1   | D     | 605  | CYS  | Peptide   |
| 1   | D     | 872  | ARG  | Sidechain |
| 1   | D     | 887  | ARG  | Sidechain |
| 1   | D     | 898  | ARG  | Sidechain |
| 1   | D     | 903  | ARG  | Sidechain |
| 1   | D     | 919  | ARG  | Sidechain |

## 5.2 Too-close contacts [i](#)

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     | 34797 | 0        | 34382    | 513     | 0            |
| 1   | B     | 34797 | 0        | 34382    | 529     | 0            |
| 1   | C     | 34797 | 0        | 34382    | 518     | 0            |
| 1   | D     | 34797 | 0        | 34382    | 521     | 0            |
| 2   | E     | 830   | 0        | 828      | 5       | 0            |
| 2   | F     | 830   | 0        | 828      | 5       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 2   | G     | 830    | 0        | 828      | 5       | 0            |
| 2   | H     | 830    | 0        | 828      | 5       | 0            |
| 3   | A     | 1      | 0        | 0        | 0       | 0            |
| 3   | B     | 1      | 0        | 0        | 0       | 0            |
| 3   | C     | 1      | 0        | 0        | 0       | 0            |
| 3   | D     | 1      | 0        | 0        | 0       | 0            |
| 4   | A     | 14     | 0        | 10       | 0       | 0            |
| 4   | B     | 14     | 0        | 10       | 0       | 0            |
| 4   | C     | 14     | 0        | 10       | 0       | 0            |
| 4   | D     | 14     | 0        | 10       | 0       | 0            |
| 5   | A     | 62     | 0        | 24       | 0       | 0            |
| 5   | B     | 62     | 0        | 24       | 0       | 0            |
| 5   | C     | 62     | 0        | 24       | 0       | 0            |
| 5   | D     | 62     | 0        | 24       | 0       | 0            |
| 6   | A     | 1      | 0        | 0        | 0       | 0            |
| 6   | B     | 1      | 0        | 0        | 0       | 0            |
| 6   | C     | 1      | 0        | 0        | 0       | 0            |
| 6   | D     | 1      | 0        | 0        | 0       | 0            |
| 7   | A     | 108    | 0        | 168      | 5       | 0            |
| 7   | B     | 108    | 0        | 168      | 7       | 0            |
| 7   | C     | 108    | 0        | 168      | 6       | 0            |
| 7   | D     | 108    | 0        | 168      | 6       | 0            |
| 8   | A     | 60     | 0        | 0        | 2       | 0            |
| 8   | B     | 60     | 0        | 0        | 2       | 0            |
| 8   | C     | 60     | 0        | 0        | 2       | 0            |
| 8   | D     | 60     | 0        | 0        | 2       | 0            |
| All | All   | 143492 | 0        | 141648   | 2082    | 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 7.

All (2082) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:888:ILE:HG12 | 1:D:960:TYR:HA  | 1.14                     | 1.14              |
| 1:C:888:ILE:HG12 | 1:C:960:TYR:HA  | 1.14                     | 1.12              |
| 1:B:888:ILE:HG12 | 1:B:960:TYR:HA  | 1.14                     | 1.10              |
| 1:A:884:ALA:HB3  | 1:A:968:PRO:HB3 | 1.34                     | 1.10              |
| 1:A:888:ILE:HG12 | 1:A:960:TYR:HA  | 1.14                     | 1.09              |
| 1:B:884:ALA:HB3  | 1:B:968:PRO:HB3 | 1.34                     | 1.09              |
| 1:C:884:ALA:HB3  | 1:C:968:PRO:HB3 | 1.34                     | 1.08              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:884:ALA:HB3  | 1:D:968:PRO:HB3   | 1.34                     | 1.07              |
| 1:B:953:LYS:HE3  | 1:B:969:ALA:HB1   | 1.42                     | 1.01              |
| 1:B:605:CYS:SG   | 1:B:1673:SER:OG   | 2.20                     | 1.00              |
| 1:A:953:LYS:HE3  | 1:A:969:ALA:HB1   | 1.42                     | 1.00              |
| 1:A:605:CYS:SG   | 1:A:1673:SER:OG   | 2.20                     | 1.00              |
| 1:C:953:LYS:HE3  | 1:C:969:ALA:HB1   | 1.42                     | 0.98              |
| 1:C:605:CYS:SG   | 1:C:1673:SER:OG   | 2.20                     | 0.98              |
| 1:D:605:CYS:SG   | 1:D:1673:SER:OG   | 2.20                     | 0.98              |
| 1:D:953:LYS:HE3  | 1:D:969:ALA:HB1   | 1.42                     | 0.97              |
| 1:D:899:ASP:HB3  | 1:D:902:LYS:HB2   | 1.47                     | 0.96              |
| 1:B:899:ASP:HB3  | 1:B:902:LYS:HB2   | 1.47                     | 0.94              |
| 1:A:899:ASP:HB3  | 1:A:902:LYS:HB2   | 1.47                     | 0.94              |
| 1:C:899:ASP:HB3  | 1:C:902:LYS:HB2   | 1.47                     | 0.94              |
| 1:C:986:VAL:HG22 | 1:C:1044:VAL:HG21 | 1.52                     | 0.92              |
| 1:B:986:VAL:HG22 | 1:B:1044:VAL:HG21 | 1.52                     | 0.91              |
| 1:D:986:VAL:HG22 | 1:D:1044:VAL:HG21 | 1.52                     | 0.91              |
| 1:A:986:VAL:HG22 | 1:A:1044:VAL:HG21 | 1.52                     | 0.90              |
| 1:C:868:LEU:HD13 | 1:C:930:LEU:HB3   | 1.55                     | 0.89              |
| 1:B:1281:GLN:O   | 1:B:1282:ASN:ND2  | 2.06                     | 0.89              |
| 1:B:868:LEU:HD13 | 1:B:930:LEU:HB3   | 1.55                     | 0.89              |
| 1:A:868:LEU:HD13 | 1:A:930:LEU:HB3   | 1.55                     | 0.88              |
| 1:A:1281:GLN:O   | 1:A:1282:ASN:ND2  | 2.06                     | 0.88              |
| 1:C:871:ILE:HA   | 1:C:874:LYS:HD3   | 1.55                     | 0.88              |
| 1:A:871:ILE:HA   | 1:A:874:LYS:HD3   | 1.55                     | 0.88              |
| 1:D:1281:GLN:O   | 1:D:1282:ASN:ND2  | 2.06                     | 0.88              |
| 1:C:1281:GLN:O   | 1:C:1282:ASN:ND2  | 2.06                     | 0.88              |
| 1:D:868:LEU:HD22 | 1:D:930:LEU:HG    | 1.56                     | 0.88              |
| 1:D:871:ILE:HA   | 1:D:874:LYS:HD3   | 1.55                     | 0.87              |
| 1:D:868:LEU:HD13 | 1:D:930:LEU:HB3   | 1.55                     | 0.87              |
| 1:B:871:ILE:HA   | 1:B:874:LYS:HD3   | 1.55                     | 0.87              |
| 1:C:864:LEU:HD11 | 1:C:930:LEU:HB2   | 1.57                     | 0.86              |
| 1:A:868:LEU:HD22 | 1:A:930:LEU:HG    | 1.56                     | 0.86              |
| 1:C:868:LEU:HD22 | 1:C:930:LEU:HG    | 1.56                     | 0.86              |
| 1:B:868:LEU:HD22 | 1:B:930:LEU:HG    | 1.56                     | 0.85              |
| 1:D:864:LEU:HD11 | 1:D:930:LEU:HB2   | 1.57                     | 0.85              |
| 1:B:864:LEU:HD11 | 1:B:930:LEU:HB2   | 1.57                     | 0.85              |
| 1:C:956:LEU:HD22 | 1:C:957:PRO:HD2   | 1.59                     | 0.84              |
| 1:A:2234:CYS:O   | 1:A:2235:ARG:C    | 2.20                     | 0.84              |
| 1:B:956:LEU:HD22 | 1:B:957:PRO:HD2   | 1.59                     | 0.84              |
| 1:A:864:LEU:HD11 | 1:A:930:LEU:HB2   | 1.57                     | 0.83              |
| 1:D:2234:CYS:O   | 1:D:2235:ARG:C    | 2.20                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:879:ILE:HD12 | 1:B:882:LEU:HD11 | 1.61                     | 0.83              |
| 1:B:956:LEU:HD21 | 1:B:968:PRO:HG2  | 1.60                     | 0.83              |
| 1:D:956:LEU:HD22 | 1:D:957:PRO:HD2  | 1.59                     | 0.82              |
| 1:D:879:ILE:HD12 | 1:D:882:LEU:HD11 | 1.61                     | 0.82              |
| 1:C:108:ILE:HG23 | 1:C:151:MET:HE2  | 1.62                     | 0.82              |
| 1:A:956:LEU:HD22 | 1:A:957:PRO:HD2  | 1.59                     | 0.82              |
| 1:A:1067:GLN:OE1 | 1:A:1069:ARG:NH2 | 2.13                     | 0.82              |
| 1:C:1067:GLN:OE1 | 1:C:1069:ARG:NH2 | 2.13                     | 0.82              |
| 1:A:956:LEU:HD21 | 1:A:968:PRO:HG2  | 1.60                     | 0.82              |
| 1:B:108:ILE:HG23 | 1:B:151:MET:HE2  | 1.62                     | 0.82              |
| 1:C:4816:MET:O   | 1:C:4822:ARG:NH1 | 2.13                     | 0.82              |
| 1:D:4816:MET:O   | 1:D:4822:ARG:NH1 | 2.13                     | 0.82              |
| 1:D:1067:GLN:OE1 | 1:D:1069:ARG:NH2 | 2.13                     | 0.82              |
| 1:C:879:ILE:HD12 | 1:C:882:LEU:HD11 | 1.61                     | 0.82              |
| 1:A:108:ILE:HG23 | 1:A:151:MET:HE2  | 1.62                     | 0.81              |
| 1:A:879:ILE:HD12 | 1:A:882:LEU:HD11 | 1.61                     | 0.81              |
| 1:C:956:LEU:HD21 | 1:C:968:PRO:HG2  | 1.60                     | 0.81              |
| 1:C:2234:CYS:O   | 1:C:2235:ARG:C   | 2.20                     | 0.81              |
| 1:A:4816:MET:O   | 1:A:4822:ARG:NH1 | 2.13                     | 0.81              |
| 1:B:4816:MET:O   | 1:B:4822:ARG:NH1 | 2.13                     | 0.81              |
| 1:D:956:LEU:HD21 | 1:D:968:PRO:HG2  | 1.60                     | 0.81              |
| 1:B:2234:CYS:O   | 1:B:2235:ARG:C   | 2.20                     | 0.81              |
| 1:D:108:ILE:HG23 | 1:D:151:MET:HE2  | 1.62                     | 0.81              |
| 1:B:888:ILE:HG12 | 1:B:960:TYR:CA   | 2.06                     | 0.81              |
| 1:A:2383:GLU:OE1 | 1:A:2386:ARG:NH1 | 2.14                     | 0.81              |
| 1:B:2383:GLU:OE1 | 1:B:2386:ARG:NH1 | 2.14                     | 0.80              |
| 1:C:3540:ARG:O   | 1:C:3543:LEU:N   | 2.15                     | 0.80              |
| 1:A:3540:ARG:O   | 1:A:3543:LEU:N   | 2.15                     | 0.80              |
| 1:C:2383:GLU:OE1 | 1:C:2386:ARG:NH1 | 2.14                     | 0.80              |
| 1:B:1067:GLN:OE1 | 1:B:1069:ARG:NH2 | 2.13                     | 0.80              |
| 1:B:3540:ARG:O   | 1:B:3543:LEU:N   | 2.15                     | 0.80              |
| 1:D:2268:MET:HA  | 1:D:2268:MET:HE2 | 1.64                     | 0.80              |
| 1:D:3540:ARG:O   | 1:D:3543:LEU:N   | 2.15                     | 0.80              |
| 1:D:2383:GLU:OE1 | 1:D:2386:ARG:NH1 | 2.14                     | 0.80              |
| 1:C:2268:MET:HE2 | 1:C:2268:MET:HA  | 1.64                     | 0.79              |
| 2:F:12:ASP:OD2   | 2:F:13:GLY:N     | 2.15                     | 0.79              |
| 1:A:2268:MET:HE2 | 1:A:2268:MET:HA  | 1.64                     | 0.79              |
| 2:G:12:ASP:OD2   | 2:G:13:GLY:N     | 2.15                     | 0.79              |
| 2:H:12:ASP:OD2   | 2:H:13:GLY:N     | 2.15                     | 0.79              |
| 1:B:2268:MET:HE2 | 1:B:2268:MET:HA  | 1.64                     | 0.79              |
| 1:A:888:ILE:HG12 | 1:A:960:TYR:CA   | 2.06                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:884:ALA:CB    | 1:D:968:PRO:HB3   | 2.13                     | 0.79              |
| 2:E:12:ASP:OD2    | 2:E:13:GLY:N      | 2.15                     | 0.78              |
| 1:C:884:ALA:CB    | 1:C:968:PRO:HB3   | 2.13                     | 0.78              |
| 1:A:884:ALA:CB    | 1:A:968:PRO:HB3   | 2.13                     | 0.77              |
| 1:B:1982:MET:HE2  | 1:B:1982:MET:HA   | 1.66                     | 0.77              |
| 1:D:888:ILE:HG12  | 1:D:960:TYR:CA    | 2.06                     | 0.77              |
| 1:B:2538:ASP:O    | 1:B:2594:ARG:NH1  | 2.19                     | 0.77              |
| 1:C:1982:MET:HE2  | 1:C:1982:MET:HA   | 1.66                     | 0.77              |
| 1:A:2973:GLU:OE2  | 1:A:2973:GLU:N    | 2.19                     | 0.76              |
| 1:B:2973:GLU:N    | 1:B:2973:GLU:OE2  | 2.19                     | 0.76              |
| 1:C:2538:ASP:O    | 1:C:2594:ARG:NH1  | 2.18                     | 0.76              |
| 1:A:1982:MET:HE2  | 1:A:1982:MET:HA   | 1.66                     | 0.76              |
| 1:D:2973:GLU:N    | 1:D:2973:GLU:OE2  | 2.19                     | 0.76              |
| 1:A:2538:ASP:O    | 1:A:2594:ARG:NH1  | 2.19                     | 0.76              |
| 1:C:888:ILE:HG12  | 1:C:960:TYR:CA    | 2.06                     | 0.76              |
| 1:C:2973:GLU:N    | 1:C:2973:GLU:OE2  | 2.19                     | 0.76              |
| 1:C:2982:VAL:O    | 1:C:2986:ARG:NH1  | 2.19                     | 0.76              |
| 1:A:3176:LEU:O    | 1:A:3176:LEU:HD23 | 1.87                     | 0.75              |
| 1:D:1982:MET:HA   | 1:D:1982:MET:HE2  | 1.66                     | 0.75              |
| 1:B:3176:LEU:O    | 1:B:3176:LEU:HD23 | 1.87                     | 0.75              |
| 1:D:4755:LYS:NZ   | 1:D:4756:PRO:O    | 2.19                     | 0.75              |
| 1:A:2234:CYS:O    | 1:A:2236:PHE:N    | 2.20                     | 0.75              |
| 1:D:883:TRP:HH2   | 1:D:908:LEU:HA    | 1.51                     | 0.75              |
| 1:D:2538:ASP:O    | 1:D:2594:ARG:NH1  | 2.19                     | 0.75              |
| 1:D:2982:VAL:O    | 1:D:2986:ARG:NH1  | 2.19                     | 0.75              |
| 1:D:940:VAL:HG23  | 1:D:1052:TYR:HB3  | 1.69                     | 0.75              |
| 1:A:883:TRP:HH2   | 1:A:908:LEU:HA    | 1.51                     | 0.75              |
| 1:A:2982:VAL:O    | 1:A:2986:ARG:NH1  | 2.19                     | 0.75              |
| 1:C:940:VAL:HG23  | 1:C:1052:TYR:HB3  | 1.68                     | 0.75              |
| 1:C:3176:LEU:HD23 | 1:C:3176:LEU:O    | 1.87                     | 0.75              |
| 1:B:884:ALA:CB    | 1:B:968:PRO:HB3   | 2.13                     | 0.74              |
| 1:B:2982:VAL:O    | 1:B:2986:ARG:NH1  | 2.19                     | 0.74              |
| 1:C:2234:CYS:O    | 1:C:2236:PHE:N    | 2.20                     | 0.74              |
| 1:D:2234:CYS:O    | 1:D:2236:PHE:N    | 2.20                     | 0.74              |
| 1:B:2234:CYS:O    | 1:B:2236:PHE:N    | 2.20                     | 0.74              |
| 1:D:3176:LEU:O    | 1:D:3176:LEU:HD23 | 1.87                     | 0.74              |
| 2:F:54:GLN:N      | 2:F:54:GLN:OE1    | 2.20                     | 0.74              |
| 1:B:940:VAL:HG23  | 1:B:1052:TYR:HB3  | 1.69                     | 0.74              |
| 1:B:3181:ASN:OD1  | 1:B:3183:TYR:N    | 2.20                     | 0.74              |
| 2:G:54:GLN:OE1    | 2:G:54:GLN:N      | 2.21                     | 0.74              |
| 1:A:2858:PRO:O    | 1:A:2859:GLN:NE2  | 2.21                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:54:GLN:OE1    | 2:H:54:GLN:N      | 2.20                     | 0.73              |
| 1:C:2858:PRO:O    | 1:C:2859:GLN:NE2  | 2.21                     | 0.73              |
| 1:D:2858:PRO:O    | 1:D:2859:GLN:NE2  | 2.21                     | 0.73              |
| 1:C:883:TRP:HH2   | 1:C:908:LEU:HA    | 1.51                     | 0.73              |
| 1:A:3181:ASN:OD1  | 1:A:3183:TYR:N    | 2.20                     | 0.73              |
| 1:A:4755:LYS:NZ   | 1:A:4756:PRO:O    | 2.19                     | 0.73              |
| 1:A:940:VAL:HG23  | 1:A:1052:TYR:HB3  | 1.69                     | 0.73              |
| 1:B:883:TRP:HH2   | 1:B:908:LEU:HA    | 1.51                     | 0.73              |
| 1:B:2858:PRO:O    | 1:B:2859:GLN:NE2  | 2.21                     | 0.73              |
| 1:D:3861:MET:SD   | 1:D:3868:VAL:HG21 | 2.29                     | 0.73              |
| 1:D:3181:ASN:OD1  | 1:D:3183:TYR:N    | 2.21                     | 0.73              |
| 1:D:957:PRO:HG2   | 1:D:960:TYR:HB2   | 1.71                     | 0.73              |
| 1:C:3181:ASN:OD1  | 1:C:3183:TYR:N    | 2.20                     | 0.72              |
| 1:C:3861:MET:SD   | 1:C:3868:VAL:HG21 | 2.29                     | 0.72              |
| 1:D:3540:ARG:NH2  | 1:D:3549:GLU:O    | 2.23                     | 0.72              |
| 1:B:885:LEU:HD22  | 1:B:970:PRO:HG3   | 1.72                     | 0.72              |
| 1:B:3540:ARG:NH2  | 1:B:3549:GLU:O    | 2.23                     | 0.72              |
| 1:A:957:PRO:HG2   | 1:A:960:TYR:HB2   | 1.71                     | 0.72              |
| 1:B:3861:MET:SD   | 1:B:3868:VAL:HG21 | 2.29                     | 0.72              |
| 1:C:957:PRO:HG2   | 1:C:960:TYR:HB2   | 1.71                     | 0.72              |
| 1:C:3540:ARG:NH2  | 1:C:3549:GLU:O    | 2.23                     | 0.72              |
| 1:A:885:LEU:HD22  | 1:A:970:PRO:HG3   | 1.72                     | 0.72              |
| 1:A:985:LEU:HD22  | 1:A:1056:PRO:HA   | 1.72                     | 0.71              |
| 1:D:985:LEU:HD22  | 1:D:1056:PRO:HA   | 1.72                     | 0.71              |
| 1:D:942:MET:HA    | 1:D:1052:TYR:HA   | 1.72                     | 0.71              |
| 1:B:942:MET:HA    | 1:B:1052:TYR:HA   | 1.72                     | 0.71              |
| 1:A:3861:MET:SD   | 1:A:3868:VAL:HG21 | 2.29                     | 0.71              |
| 1:D:2817:MET:SD   | 1:D:2938:VAL:HG21 | 2.31                     | 0.71              |
| 1:A:2752:LEU:HD21 | 1:A:2824:VAL:HG11 | 1.73                     | 0.71              |
| 1:B:2817:MET:SD   | 1:B:2938:VAL:HG21 | 2.31                     | 0.71              |
| 1:C:885:LEU:HD22  | 1:C:970:PRO:HG3   | 1.72                     | 0.71              |
| 1:D:973:LEU:HD21  | 1:D:1046:THR:HG22 | 1.71                     | 0.71              |
| 1:B:957:PRO:HG2   | 1:B:960:TYR:HB2   | 1.71                     | 0.71              |
| 1:B:2752:LEU:HD21 | 1:B:2824:VAL:HG11 | 1.73                     | 0.71              |
| 1:C:942:MET:HA    | 1:C:1052:TYR:HA   | 1.72                     | 0.71              |
| 1:C:973:LEU:HD21  | 1:C:1046:THR:HG22 | 1.71                     | 0.71              |
| 1:A:3540:ARG:NH2  | 1:A:3549:GLU:O    | 2.23                     | 0.71              |
| 1:B:976:VAL:HB    | 1:B:1045:ARG:HD2  | 1.72                     | 0.71              |
| 1:A:976:VAL:HB    | 1:A:1045:ARG:HD2  | 1.72                     | 0.70              |
| 1:B:3249:ARG:NH2  | 1:B:3253:GLU:OE2  | 2.24                     | 0.70              |
| 1:C:967:LYS:HE2   | 1:C:969:ALA:HB2   | 1.74                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2752:LEU:HD21 | 1:C:2824:VAL:HG11 | 1.73                     | 0.70              |
| 1:A:2817:MET:SD   | 1:A:2938:VAL:HG21 | 2.31                     | 0.70              |
| 1:B:985:LEU:HD22  | 1:B:1056:PRO:HA   | 1.72                     | 0.70              |
| 1:C:940:VAL:HA    | 1:C:1053:ASN:O    | 1.92                     | 0.70              |
| 1:C:2817:MET:SD   | 1:C:2938:VAL:HG21 | 2.31                     | 0.70              |
| 1:B:940:VAL:HA    | 1:B:1053:ASN:O    | 1.92                     | 0.70              |
| 1:D:3249:ARG:NH2  | 1:D:3253:GLU:OE2  | 2.24                     | 0.70              |
| 1:A:973:LEU:HD21  | 1:A:1046:THR:HG22 | 1.71                     | 0.70              |
| 1:A:3249:ARG:NH2  | 1:A:3253:GLU:OE2  | 2.24                     | 0.70              |
| 1:A:888:ILE:HB    | 1:A:962:MET:HE1   | 1.74                     | 0.70              |
| 1:A:942:MET:HA    | 1:A:1052:TYR:HA   | 1.72                     | 0.70              |
| 1:B:973:LEU:HD21  | 1:B:1046:THR:HG22 | 1.71                     | 0.70              |
| 1:C:3249:ARG:NH2  | 1:C:3253:GLU:OE2  | 2.24                     | 0.70              |
| 1:D:885:LEU:HD22  | 1:D:970:PRO:HG3   | 1.72                     | 0.70              |
| 1:D:940:VAL:HA    | 1:D:1053:ASN:O    | 1.92                     | 0.70              |
| 1:A:940:VAL:HA    | 1:A:1053:ASN:O    | 1.92                     | 0.70              |
| 1:C:985:LEU:HD22  | 1:C:1056:PRO:HA   | 1.72                     | 0.70              |
| 1:D:2752:LEU:HD21 | 1:D:2824:VAL:HG11 | 1.73                     | 0.70              |
| 1:B:967:LYS:HE2   | 1:B:969:ALA:HB2   | 1.73                     | 0.69              |
| 1:B:4755:LYS:NZ   | 1:B:4756:PRO:O    | 2.19                     | 0.69              |
| 1:C:888:ILE:HB    | 1:C:962:MET:HE1   | 1.74                     | 0.69              |
| 1:D:967:LYS:HE2   | 1:D:969:ALA:HB2   | 1.74                     | 0.69              |
| 1:C:976:VAL:HB    | 1:C:1045:ARG:HD2  | 1.72                     | 0.69              |
| 1:D:860:ILE:HD12  | 1:D:861:GLN:N     | 2.08                     | 0.69              |
| 1:D:976:VAL:HB    | 1:D:1045:ARG:HD2  | 1.72                     | 0.69              |
| 1:A:865:PRO:HD2   | 1:A:868:LEU:HB2   | 1.75                     | 0.69              |
| 2:E:54:GLN:OE1    | 2:E:54:GLN:N      | 2.26                     | 0.69              |
| 1:B:865:PRO:HD2   | 1:B:868:LEU:HB2   | 1.75                     | 0.69              |
| 1:C:4748:ILE:HG22 | 1:C:4754:ARG:NH2  | 2.08                     | 0.69              |
| 1:D:888:ILE:HB    | 1:D:962:MET:HE1   | 1.74                     | 0.69              |
| 1:D:2755:PHE:HD2  | 1:D:2814:LEU:HD11 | 1.58                     | 0.69              |
| 1:C:2755:PHE:HD2  | 1:C:2814:LEU:HD11 | 1.58                     | 0.69              |
| 1:A:967:LYS:HE2   | 1:A:969:ALA:HB2   | 1.74                     | 0.69              |
| 1:B:888:ILE:HB    | 1:B:962:MET:HE1   | 1.74                     | 0.69              |
| 1:C:953:LYS:HB3   | 1:C:971:LEU:HA    | 1.75                     | 0.69              |
| 1:C:956:LEU:CD1   | 1:C:960:TYR:HB3   | 2.23                     | 0.69              |
| 1:A:956:LEU:CD1   | 1:A:960:TYR:HB3   | 2.23                     | 0.68              |
| 1:A:2743:THR:OG1  | 1:A:2816:ALA:N    | 2.27                     | 0.68              |
| 1:B:956:LEU:CD1   | 1:B:960:TYR:HB3   | 2.23                     | 0.68              |
| 1:C:4755:LYS:NZ   | 1:C:4756:PRO:O    | 2.19                     | 0.68              |
| 1:A:4748:ILE:HG22 | 1:A:4754:ARG:NH2  | 2.08                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:4086:ASP:OD2  | 1:B:4088:ARG:N    | 2.26                     | 0.68              |
| 1:C:860:ILE:HD12  | 1:C:861:GLN:N     | 2.08                     | 0.68              |
| 1:D:4086:ASP:OD2  | 1:D:4088:ARG:N    | 2.26                     | 0.68              |
| 1:A:881:GLU:HB3   | 1:A:969:ALA:C     | 2.18                     | 0.68              |
| 1:B:881:GLU:HB3   | 1:B:969:ALA:C     | 2.18                     | 0.68              |
| 1:B:2743:THR:OG1  | 1:B:2816:ALA:N    | 2.27                     | 0.68              |
| 1:B:2755:PHE:HD2  | 1:B:2814:LEU:HD11 | 1.58                     | 0.68              |
| 1:B:860:ILE:HD12  | 1:B:861:GLN:N     | 2.08                     | 0.68              |
| 1:D:953:LYS:HB3   | 1:D:971:LEU:HA    | 1.75                     | 0.68              |
| 1:D:4748:ILE:HG22 | 1:D:4754:ARG:NH2  | 2.08                     | 0.68              |
| 1:A:860:ILE:HD12  | 1:A:861:GLN:N     | 2.08                     | 0.68              |
| 1:A:2755:PHE:HD2  | 1:A:2814:LEU:HD11 | 1.58                     | 0.68              |
| 1:C:4086:ASP:OD2  | 1:C:4088:ARG:N    | 2.26                     | 0.68              |
| 1:A:967:LYS:CE    | 1:A:969:ALA:HB2   | 2.24                     | 0.68              |
| 1:B:4748:ILE:HG22 | 1:B:4754:ARG:NH2  | 2.08                     | 0.68              |
| 1:D:956:LEU:CD1   | 1:D:960:TYR:HB3   | 2.23                     | 0.68              |
| 1:A:4086:ASP:OD2  | 1:A:4088:ARG:N    | 2.26                     | 0.67              |
| 1:D:2743:THR:OG1  | 1:D:2816:ALA:N    | 2.27                     | 0.67              |
| 1:B:953:LYS:HB3   | 1:B:971:LEU:HA    | 1.75                     | 0.67              |
| 1:C:2234:CYS:O    | 1:C:2237:LEU:N    | 2.28                     | 0.67              |
| 1:A:953:LYS:HB3   | 1:A:971:LEU:HA    | 1.75                     | 0.67              |
| 1:C:865:PRO:HD2   | 1:C:868:LEU:HB2   | 1.75                     | 0.67              |
| 1:D:865:PRO:HD2   | 1:D:868:LEU:HB2   | 1.75                     | 0.67              |
| 1:D:868:LEU:HD23  | 1:D:871:ILE:HD12  | 1.75                     | 0.67              |
| 1:B:2234:CYS:O    | 1:B:2237:LEU:N    | 2.28                     | 0.67              |
| 1:B:864:LEU:HD11  | 1:B:930:LEU:CB    | 2.25                     | 0.67              |
| 1:C:881:GLU:HB3   | 1:C:969:ALA:C     | 2.18                     | 0.67              |
| 1:D:930:LEU:HA    | 1:D:933:LEU:HD12  | 1.76                     | 0.67              |
| 1:A:864:LEU:HD11  | 1:A:930:LEU:CB    | 2.25                     | 0.67              |
| 1:C:2743:THR:OG1  | 1:C:2816:ALA:N    | 2.27                     | 0.67              |
| 1:D:881:GLU:HB3   | 1:D:969:ALA:C     | 2.19                     | 0.67              |
| 1:A:868:LEU:HD23  | 1:A:871:ILE:HD12  | 1.75                     | 0.67              |
| 1:D:967:LYS:CE    | 1:D:969:ALA:HB2   | 2.25                     | 0.67              |
| 1:B:868:LEU:HD23  | 1:B:871:ILE:HD12  | 1.75                     | 0.67              |
| 1:B:967:LYS:CE    | 1:B:969:ALA:HB2   | 2.25                     | 0.67              |
| 1:D:3541:TYR:HB3  | 1:D:3605:TYR:CD2  | 2.30                     | 0.67              |
| 1:C:903:ARG:HH21  | 1:C:903:ARG:HA    | 1.61                     | 0.66              |
| 1:C:930:LEU:HA    | 1:C:933:LEU:HD12  | 1.76                     | 0.66              |
| 1:B:903:ARG:HA    | 1:B:903:ARG:HH21  | 1.60                     | 0.66              |
| 1:B:3565:GLU:N    | 1:B:3565:GLU:OE1  | 2.29                     | 0.66              |
| 1:D:903:ARG:HA    | 1:D:903:ARG:HH21  | 1.61                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:2234:CYS:O    | 1:D:2237:LEU:N    | 2.28                     | 0.66              |
| 1:A:2234:CYS:O    | 1:A:2237:LEU:N    | 2.28                     | 0.66              |
| 1:A:3541:TYR:HB3  | 1:A:3605:TYR:CD2  | 2.30                     | 0.66              |
| 1:B:3541:TYR:HB3  | 1:B:3605:TYR:CD2  | 2.31                     | 0.66              |
| 1:C:868:LEU:HD23  | 1:C:871:ILE:HD12  | 1.75                     | 0.66              |
| 1:C:3565:GLU:OE1  | 1:C:3565:GLU:N    | 2.29                     | 0.66              |
| 1:B:3531:GLN:O    | 1:B:3535:VAL:HG23 | 1.96                     | 0.66              |
| 1:C:1048:LEU:HD21 | 1:C:1054:ILE:HG13 | 1.78                     | 0.66              |
| 1:B:3972:ILE:HG21 | 1:B:3983:LEU:HD12 | 1.78                     | 0.66              |
| 1:C:864:LEU:HD11  | 1:C:930:LEU:CB    | 2.25                     | 0.66              |
| 1:D:864:LEU:HD11  | 1:D:930:LEU:CB    | 2.25                     | 0.66              |
| 1:D:872:ARG:HG3   | 1:D:927:GLY:HA2   | 1.78                     | 0.66              |
| 1:D:3565:GLU:OE1  | 1:D:3565:GLU:N    | 2.29                     | 0.66              |
| 1:C:872:ARG:HG3   | 1:C:927:GLY:HA2   | 1.78                     | 0.66              |
| 1:C:967:LYS:CE    | 1:C:969:ALA:HB2   | 2.25                     | 0.66              |
| 1:C:102:LEU:HB3   | 1:C:151:MET:HE1   | 1.78                     | 0.65              |
| 1:C:3972:ILE:HG21 | 1:C:3983:LEU:HD12 | 1.78                     | 0.65              |
| 1:A:3531:GLN:O    | 1:A:3535:VAL:HG23 | 1.96                     | 0.65              |
| 1:C:3541:TYR:HB3  | 1:C:3605:TYR:CD2  | 2.30                     | 0.65              |
| 1:D:1048:LEU:HD21 | 1:D:1054:ILE:HG13 | 1.78                     | 0.65              |
| 1:A:872:ARG:HG3   | 1:A:927:GLY:HA2   | 1.78                     | 0.65              |
| 1:A:930:LEU:HA    | 1:A:933:LEU:HD12  | 1.76                     | 0.65              |
| 1:A:3972:ILE:HG21 | 1:A:3983:LEU:HD12 | 1.78                     | 0.65              |
| 1:B:1048:LEU:HD21 | 1:B:1054:ILE:HG13 | 1.78                     | 0.65              |
| 1:D:102:LEU:HB3   | 1:D:151:MET:HE1   | 1.78                     | 0.65              |
| 1:D:914:LEU:HD12  | 1:D:915:PRO:HD2   | 1.79                     | 0.65              |
| 1:D:2988:GLU:N    | 1:D:2988:GLU:OE1  | 2.30                     | 0.65              |
| 1:A:914:LEU:HD12  | 1:A:915:PRO:HD2   | 1.79                     | 0.65              |
| 1:C:914:LEU:HD12  | 1:C:915:PRO:HD2   | 1.79                     | 0.65              |
| 1:C:3531:GLN:O    | 1:C:3535:VAL:HG23 | 1.96                     | 0.65              |
| 1:A:887:ARG:HG3   | 1:A:892:TRP:CB    | 2.27                     | 0.65              |
| 1:A:3565:GLU:OE1  | 1:A:3565:GLU:N    | 2.29                     | 0.65              |
| 1:C:876:ALA:CB    | 1:C:923:LEU:HA    | 2.27                     | 0.65              |
| 1:D:887:ARG:HG3   | 1:D:892:TRP:CB    | 2.27                     | 0.65              |
| 1:B:872:ARG:HG3   | 1:B:927:GLY:HA2   | 1.78                     | 0.65              |
| 1:B:914:LEU:HD12  | 1:B:915:PRO:HD2   | 1.79                     | 0.65              |
| 1:A:903:ARG:HH21  | 1:A:903:ARG:HA    | 1.61                     | 0.65              |
| 1:A:879:ILE:HA    | 1:A:882:LEU:HD11  | 1.79                     | 0.65              |
| 1:B:102:LEU:HB3   | 1:B:151:MET:HE1   | 1.79                     | 0.65              |
| 1:B:876:ALA:CB    | 1:B:923:LEU:HA    | 2.27                     | 0.65              |
| 1:B:930:LEU:HA    | 1:B:933:LEU:HD12  | 1.76                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2988:GLU:OE1  | 1:C:2988:GLU:N    | 2.30                     | 0.65              |
| 1:A:102:LEU:HB3   | 1:A:151:MET:HE1   | 1.78                     | 0.64              |
| 1:A:2988:GLU:N    | 1:A:2988:GLU:OE1  | 2.30                     | 0.64              |
| 1:B:2988:GLU:OE1  | 1:B:2988:GLU:N    | 2.30                     | 0.64              |
| 1:C:887:ARG:HG3   | 1:C:892:TRP:HB2   | 1.79                     | 0.64              |
| 1:A:887:ARG:HG3   | 1:A:892:TRP:HB2   | 1.79                     | 0.64              |
| 1:B:2741:VAL:HG11 | 1:B:2820:TRP:NE1  | 2.12                     | 0.64              |
| 1:D:3531:GLN:O    | 1:D:3535:VAL:HG23 | 1.96                     | 0.64              |
| 1:A:1048:LEU:HD21 | 1:A:1054:ILE:HG13 | 1.78                     | 0.64              |
| 1:B:887:ARG:HG3   | 1:B:892:TRP:HB2   | 1.79                     | 0.64              |
| 1:D:872:ARG:HH21  | 1:D:873:GLU:HA    | 1.62                     | 0.64              |
| 1:D:887:ARG:HG3   | 1:D:892:TRP:HB2   | 1.79                     | 0.64              |
| 1:D:2635:ASN:OD1  | 1:D:2637:PHE:N    | 2.31                     | 0.64              |
| 1:A:876:ALA:CB    | 1:A:923:LEU:HA    | 2.27                     | 0.64              |
| 1:B:879:ILE:HA    | 1:B:882:LEU:HD11  | 1.79                     | 0.64              |
| 1:C:2741:VAL:HG11 | 1:C:2820:TRP:NE1  | 2.12                     | 0.64              |
| 1:A:2741:VAL:HG11 | 1:A:2820:TRP:NE1  | 2.12                     | 0.64              |
| 1:B:3546:THR:OG1  | 1:B:3548:GLU:OE2  | 2.15                     | 0.64              |
| 1:C:2756:ILE:HG13 | 1:C:2814:LEU:HD12 | 1.80                     | 0.64              |
| 1:D:2741:VAL:HG11 | 1:D:2820:TRP:NE1  | 2.12                     | 0.64              |
| 1:D:3972:ILE:HG21 | 1:D:3983:LEU:HD12 | 1.78                     | 0.64              |
| 1:B:887:ARG:HG3   | 1:B:892:TRP:CB    | 2.27                     | 0.64              |
| 1:C:887:ARG:HG3   | 1:C:892:TRP:CB    | 2.27                     | 0.64              |
| 1:C:902:LYS:HB3   | 1:C:904:LEU:HG    | 1.80                     | 0.64              |
| 1:A:872:ARG:HH21  | 1:A:873:GLU:HA    | 1.62                     | 0.64              |
| 1:C:868:LEU:HD23  | 1:C:871:ILE:CD1   | 2.28                     | 0.64              |
| 1:D:879:ILE:HA    | 1:D:882:LEU:HD11  | 1.79                     | 0.64              |
| 1:C:2249:ARG:NH2  | 1:C:2286:GLU:OE2  | 2.31                     | 0.64              |
| 1:C:4042:MET:SD   | 1:C:4045:ARG:NH1  | 2.71                     | 0.64              |
| 1:D:876:ALA:CB    | 1:D:923:LEU:HA    | 2.27                     | 0.64              |
| 1:A:865:PRO:HD2   | 1:A:868:LEU:CB    | 2.28                     | 0.64              |
| 1:A:2249:ARG:NH2  | 1:A:2286:GLU:OE2  | 2.31                     | 0.64              |
| 1:A:4154:SER:HB2  | 1:A:4167:LEU:HD11 | 1.79                     | 0.64              |
| 1:C:872:ARG:HH21  | 1:C:873:GLU:HA    | 1.62                     | 0.64              |
| 1:D:909:VAL:HB    | 1:D:913:SER:HB3   | 1.80                     | 0.64              |
| 1:D:902:LYS:HB3   | 1:D:904:LEU:HG    | 1.80                     | 0.64              |
| 1:D:2688:ALA:O    | 1:D:2994:GLN:NE2  | 2.31                     | 0.64              |
| 1:D:4748:ILE:O    | 1:D:4754:ARG:NH1  | 2.27                     | 0.64              |
| 1:A:868:LEU:HD23  | 1:A:871:ILE:CD1   | 2.28                     | 0.63              |
| 1:B:902:LYS:HB3   | 1:B:904:LEU:HG    | 1.79                     | 0.63              |
| 1:B:2756:ILE:HG13 | 1:B:2814:LEU:HD12 | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:865:PRO:HD2   | 1:C:868:LEU:HD12  | 1.80                     | 0.63              |
| 1:C:2688:ALA:O    | 1:C:2994:GLN:NE2  | 2.31                     | 0.63              |
| 1:C:4767:MET:HE2  | 1:C:4767:MET:HA   | 1.80                     | 0.63              |
| 1:D:865:PRO:HD2   | 1:D:868:LEU:HD12  | 1.80                     | 0.63              |
| 1:B:4154:SER:HB2  | 1:B:4167:LEU:HD11 | 1.79                     | 0.63              |
| 1:A:902:LYS:HB3   | 1:A:904:LEU:HG    | 1.80                     | 0.63              |
| 1:B:872:ARG:HH21  | 1:B:873:GLU:HA    | 1.62                     | 0.63              |
| 1:D:865:PRO:HD2   | 1:D:868:LEU:CB    | 2.28                     | 0.63              |
| 1:D:2249:ARG:NH2  | 1:D:2286:GLU:OE2  | 2.31                     | 0.63              |
| 1:D:4767:MET:HA   | 1:D:4767:MET:HE2  | 1.80                     | 0.63              |
| 1:A:865:PRO:HD2   | 1:A:868:LEU:HD12  | 1.80                     | 0.63              |
| 1:B:2799:SER:N    | 1:B:2802:ASP:OD2  | 2.32                     | 0.63              |
| 1:D:2756:ILE:HG13 | 1:D:2814:LEU:HD12 | 1.80                     | 0.63              |
| 1:D:2799:SER:N    | 1:D:2802:ASP:OD2  | 2.32                     | 0.63              |
| 1:A:875:LEU:HB3   | 1:A:926:SER:HB2   | 1.81                     | 0.63              |
| 1:B:2863:LEU:HD12 | 1:B:2926:GLU:OE1  | 1.98                     | 0.63              |
| 1:C:2635:ASN:OD1  | 1:C:2637:PHE:N    | 2.31                     | 0.63              |
| 1:C:2863:LEU:HD12 | 1:C:2926:GLU:OE1  | 1.98                     | 0.63              |
| 1:D:883:TRP:CH2   | 1:D:908:LEU:HA    | 2.33                     | 0.63              |
| 1:D:4042:MET:SD   | 1:D:4045:ARG:NH1  | 2.71                     | 0.63              |
| 1:A:875:LEU:HA    | 1:A:878:ASN:HD22  | 1.64                     | 0.63              |
| 1:A:909:VAL:HB    | 1:A:913:SER:HB3   | 1.80                     | 0.63              |
| 1:A:2756:ILE:HG13 | 1:A:2814:LEU:HD12 | 1.80                     | 0.63              |
| 1:B:865:PRO:HD2   | 1:B:868:LEU:CB    | 2.28                     | 0.63              |
| 1:B:865:PRO:HD2   | 1:B:868:LEU:HD12  | 1.80                     | 0.63              |
| 1:B:868:LEU:HD23  | 1:B:871:ILE:CD1   | 2.28                     | 0.63              |
| 1:C:909:VAL:HB    | 1:C:913:SER:HB3   | 1.80                     | 0.63              |
| 1:D:875:LEU:HA    | 1:D:878:ASN:HD22  | 1.64                     | 0.63              |
| 1:B:875:LEU:HB3   | 1:B:926:SER:HB2   | 1.81                     | 0.63              |
| 1:B:4042:MET:SD   | 1:B:4045:ARG:NH1  | 2.71                     | 0.63              |
| 1:B:4767:MET:HE2  | 1:B:4767:MET:HA   | 1.80                     | 0.63              |
| 1:C:875:LEU:HB3   | 1:C:926:SER:HB2   | 1.81                     | 0.63              |
| 1:A:2863:LEU:HD12 | 1:A:2926:GLU:OE1  | 1.98                     | 0.63              |
| 1:B:893:THR:HG22  | 1:B:904:LEU:HD22  | 1.80                     | 0.63              |
| 1:D:875:LEU:HB3   | 1:D:926:SER:HB2   | 1.81                     | 0.63              |
| 1:D:2863:LEU:HD12 | 1:D:2926:GLU:OE1  | 1.98                     | 0.63              |
| 1:A:893:THR:HG22  | 1:A:904:LEU:HD22  | 1.81                     | 0.63              |
| 1:C:883:TRP:CH2   | 1:C:908:LEU:HA    | 2.33                     | 0.63              |
| 1:A:2799:SER:N    | 1:A:2802:ASP:OD2  | 2.32                     | 0.62              |
| 1:A:4748:ILE:O    | 1:A:4754:ARG:NH1  | 2.27                     | 0.62              |
| 1:C:879:ILE:HA    | 1:C:882:LEU:HD11  | 1.79                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:4154:SER:HB2  | 1:C:4167:LEU:HD11 | 1.79                     | 0.62              |
| 1:D:4154:SER:HB2  | 1:D:4167:LEU:HD11 | 1.79                     | 0.62              |
| 1:A:1421:ASN:O    | 1:A:1421:ASN:ND2  | 2.33                     | 0.62              |
| 1:A:4042:MET:SD   | 1:A:4045:ARG:NH1  | 2.71                     | 0.62              |
| 1:B:909:VAL:HB    | 1:B:913:SER:HB3   | 1.80                     | 0.62              |
| 1:C:1421:ASN:ND2  | 1:C:1421:ASN:O    | 2.33                     | 0.62              |
| 1:A:2635:ASN:OD1  | 1:A:2637:PHE:N    | 2.31                     | 0.62              |
| 1:A:5032:ASP:OD2  | 1:A:5033:GLN:N    | 2.33                     | 0.62              |
| 1:B:883:TRP:CH2   | 1:B:908:LEU:HA    | 2.33                     | 0.62              |
| 1:B:5032:ASP:OD2  | 1:B:5033:GLN:N    | 2.33                     | 0.62              |
| 1:C:875:LEU:HA    | 1:C:878:ASN:HD22  | 1.64                     | 0.62              |
| 1:C:5032:ASP:OD2  | 1:C:5033:GLN:N    | 2.33                     | 0.62              |
| 1:B:2249:ARG:NH2  | 1:B:2286:GLU:OE2  | 2.31                     | 0.62              |
| 1:B:2635:ASN:OD1  | 1:B:2637:PHE:N    | 2.31                     | 0.62              |
| 1:B:3176:LEU:HD21 | 1:B:3184:VAL:HG13 | 1.82                     | 0.62              |
| 1:C:865:PRO:HD2   | 1:C:868:LEU:CB    | 2.28                     | 0.62              |
| 1:A:872:ARG:HH12  | 1:A:923:LEU:HB3   | 1.65                     | 0.62              |
| 1:A:883:TRP:CH2   | 1:A:908:LEU:HA    | 2.33                     | 0.62              |
| 1:B:875:LEU:HA    | 1:B:878:ASN:HD22  | 1.64                     | 0.62              |
| 1:C:956:LEU:CB    | 1:C:967:LYS:HB2   | 2.29                     | 0.62              |
| 1:C:2799:SER:N    | 1:C:2802:ASP:OD2  | 2.31                     | 0.62              |
| 1:D:956:LEU:CB    | 1:D:967:LYS:HB2   | 2.29                     | 0.62              |
| 1:D:5032:ASP:OD2  | 1:D:5033:GLN:N    | 2.33                     | 0.62              |
| 1:A:3176:LEU:HD21 | 1:A:3184:VAL:HG13 | 1.82                     | 0.62              |
| 1:B:956:LEU:CB    | 1:B:967:LYS:HB2   | 2.29                     | 0.62              |
| 1:B:2688:ALA:O    | 1:B:2994:GLN:NE2  | 2.31                     | 0.62              |
| 1:D:868:LEU:HD23  | 1:D:871:ILE:CD1   | 2.28                     | 0.62              |
| 1:A:956:LEU:CB    | 1:A:967:LYS:HB2   | 2.29                     | 0.62              |
| 1:A:4767:MET:HA   | 1:A:4767:MET:HE2  | 1.80                     | 0.61              |
| 1:A:2877:GLU:OE1  | 1:A:2921:ARG:NE   | 2.33                     | 0.61              |
| 1:B:2942:LEU:O    | 1:B:2945:MET:HE1  | 2.00                     | 0.61              |
| 1:B:4748:ILE:O    | 1:B:4754:ARG:NH1  | 2.27                     | 0.61              |
| 1:C:2877:GLU:OE1  | 1:C:2921:ARG:NE   | 2.33                     | 0.61              |
| 1:D:928:GLU:HA    | 1:D:931:LYS:HG3   | 1.83                     | 0.61              |
| 1:D:2877:GLU:OE1  | 1:D:2921:ARG:NE   | 2.33                     | 0.61              |
| 1:A:3546:THR:OG1  | 1:A:3548:GLU:OE2  | 2.15                     | 0.61              |
| 1:C:2942:LEU:O    | 1:C:2945:MET:HE1  | 2.00                     | 0.61              |
| 1:A:2688:ALA:O    | 1:A:2994:GLN:NE2  | 2.31                     | 0.61              |
| 1:D:893:THR:HG22  | 1:D:904:LEU:HD22  | 1.81                     | 0.61              |
| 1:C:864:LEU:HD21  | 1:C:930:LEU:HD23  | 1.83                     | 0.61              |
| 1:A:928:GLU:HA    | 1:A:931:LYS:HG3   | 1.83                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:864:LEU:HD21  | 1:A:930:LEU:HD23  | 1.83                     | 0.61              |
| 1:D:872:ARG:HH12  | 1:D:923:LEU:HB3   | 1.65                     | 0.61              |
| 1:D:1421:ASN:O    | 1:D:1421:ASN:ND2  | 2.33                     | 0.61              |
| 1:B:872:ARG:HH12  | 1:B:923:LEU:HB3   | 1.65                     | 0.61              |
| 1:B:1421:ASN:O    | 1:B:1421:ASN:ND2  | 2.33                     | 0.61              |
| 1:D:3176:LEU:HD21 | 1:D:3184:VAL:HG13 | 1.82                     | 0.61              |
| 1:A:2942:LEU:O    | 1:A:2945:MET:HE1  | 2.00                     | 0.61              |
| 1:B:4632:GLU:OE2  | 1:B:4634:THR:OG1  | 2.17                     | 0.61              |
| 1:D:2942:LEU:O    | 1:D:2945:MET:HE1  | 2.00                     | 0.60              |
| 1:C:1987:MET:N    | 1:C:1987:MET:SD   | 2.74                     | 0.60              |
| 1:B:892:TRP:HB3   | 1:B:908:LEU:HD11  | 1.84                     | 0.60              |
| 1:C:893:THR:HG22  | 1:C:904:LEU:HD22  | 1.81                     | 0.60              |
| 1:C:3176:LEU:HD21 | 1:C:3184:VAL:HG13 | 1.82                     | 0.60              |
| 1:B:892:TRP:HA    | 1:B:903:ARG:O     | 2.02                     | 0.60              |
| 1:B:914:LEU:HD11  | 1:B:919:ARG:N     | 2.16                     | 0.60              |
| 1:C:914:LEU:HD11  | 1:C:919:ARG:N     | 2.16                     | 0.60              |
| 1:A:3421:ARG:HG2  | 1:A:3521:ILE:HD11 | 1.84                     | 0.60              |
| 1:B:956:LEU:HD13  | 1:B:960:TYR:HB3   | 1.84                     | 0.60              |
| 1:C:928:GLU:HA    | 1:C:931:LYS:HG3   | 1.82                     | 0.60              |
| 1:C:4748:ILE:O    | 1:C:4754:ARG:NH1  | 2.27                     | 0.60              |
| 1:A:892:TRP:HA    | 1:A:903:ARG:O     | 2.02                     | 0.60              |
| 1:A:914:LEU:HD11  | 1:A:919:ARG:N     | 2.16                     | 0.60              |
| 1:B:108:ILE:CG2   | 1:B:151:MET:HE2   | 2.31                     | 0.60              |
| 1:C:108:ILE:CG2   | 1:C:151:MET:HE2   | 2.31                     | 0.60              |
| 1:C:872:ARG:HH12  | 1:C:923:LEU:HB3   | 1.65                     | 0.60              |
| 1:A:956:LEU:HD13  | 1:A:960:TYR:HB3   | 1.84                     | 0.60              |
| 1:B:864:LEU:HD21  | 1:B:930:LEU:HD23  | 1.83                     | 0.60              |
| 1:B:2877:GLU:OE1  | 1:B:2921:ARG:NE   | 2.33                     | 0.60              |
| 1:C:4720:ARG:HH21 | 1:C:4746:LEU:HD13 | 1.66                     | 0.60              |
| 1:A:2749:PRO:HD2  | 1:A:2752:LEU:HD12 | 1.84                     | 0.60              |
| 1:A:892:TRP:HB3   | 1:A:908:LEU:HD11  | 1.84                     | 0.60              |
| 1:D:914:LEU:HD11  | 1:D:919:ARG:N     | 2.16                     | 0.60              |
| 1:D:892:TRP:HB3   | 1:D:908:LEU:HD11  | 1.84                     | 0.60              |
| 1:D:892:TRP:HA    | 1:D:903:ARG:O     | 2.02                     | 0.60              |
| 1:D:1987:MET:N    | 1:D:1987:MET:SD   | 2.74                     | 0.60              |
| 1:B:956:LEU:HD21  | 1:B:960:TYR:HD2   | 1.67                     | 0.59              |
| 1:C:892:TRP:HA    | 1:C:903:ARG:O     | 2.02                     | 0.59              |
| 1:C:956:LEU:HD21  | 1:C:960:TYR:HD2   | 1.67                     | 0.59              |
| 1:D:3421:ARG:HG2  | 1:D:3521:ILE:HD11 | 1.84                     | 0.59              |
| 1:D:864:LEU:HD21  | 1:D:930:LEU:HD23  | 1.83                     | 0.59              |
| 1:D:3536:LEU:HD23 | 1:D:3553:PHE:HZ   | 1.67                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:956:LEU:HD21  | 1:A:960:TYR:HD2   | 1.67                     | 0.59              |
| 1:B:928:GLU:HA    | 1:B:931:LYS:HG3   | 1.83                     | 0.59              |
| 1:B:3421:ARG:HG2  | 1:B:3521:ILE:HD11 | 1.84                     | 0.59              |
| 1:C:1300:GLN:OE1  | 1:C:1546:ASN:ND2  | 2.35                     | 0.59              |
| 1:A:894:TYR:OH    | 1:A:896:PRO:HA    | 2.03                     | 0.59              |
| 1:A:4720:ARG:HH21 | 1:A:4746:LEU:HD13 | 1.66                     | 0.59              |
| 1:C:2477:ILE:HD12 | 1:C:2477:ILE:O    | 2.02                     | 0.59              |
| 1:A:108:ILE:CG2   | 1:A:151:MET:HE2   | 2.31                     | 0.59              |
| 1:A:2912:LEU:O    | 1:A:2917:LYS:NZ   | 2.32                     | 0.59              |
| 1:C:892:TRP:HB3   | 1:C:908:LEU:HD11  | 1.84                     | 0.59              |
| 1:C:4632:GLU:OE2  | 1:C:4634:THR:OG1  | 2.17                     | 0.59              |
| 1:D:894:TYR:OH    | 1:D:896:PRO:HA    | 2.03                     | 0.59              |
| 1:D:4747:GLU:O    | 1:D:4751:HIS:ND1  | 2.36                     | 0.59              |
| 1:B:2749:PRO:HD2  | 1:B:2752:LEU:HD12 | 1.84                     | 0.59              |
| 1:C:32:GLU:OE1    | 1:C:32:GLU:HA     | 2.03                     | 0.59              |
| 1:C:4747:GLU:O    | 1:C:4751:HIS:ND1  | 2.36                     | 0.59              |
| 1:D:2477:ILE:HD12 | 1:D:2477:ILE:O    | 2.02                     | 0.59              |
| 1:A:3536:LEU:HD23 | 1:A:3553:PHE:HZ   | 1.67                     | 0.59              |
| 1:B:459:GLU:N     | 1:B:459:GLU:OE2   | 2.36                     | 0.59              |
| 1:B:2477:ILE:O    | 1:B:2477:ILE:HD12 | 2.02                     | 0.59              |
| 1:B:3536:LEU:HD23 | 1:B:3553:PHE:HZ   | 1.67                     | 0.59              |
| 1:C:956:LEU:HD13  | 1:C:960:TYR:HB3   | 1.84                     | 0.59              |
| 1:C:1426:GLU:OE1  | 1:C:1426:GLU:N    | 2.34                     | 0.59              |
| 1:C:3421:ARG:HG2  | 1:C:3521:ILE:HD11 | 1.84                     | 0.59              |
| 1:D:956:LEU:HD21  | 1:D:960:TYR:HD2   | 1.67                     | 0.59              |
| 1:D:1300:GLN:OE1  | 1:D:1546:ASN:ND2  | 2.35                     | 0.59              |
| 1:D:3257:LEU:HD23 | 1:D:3267:MET:HE3  | 1.85                     | 0.59              |
| 1:B:1300:GLN:OE1  | 1:B:1546:ASN:ND2  | 2.35                     | 0.59              |
| 1:C:2749:PRO:HD2  | 1:C:2752:LEU:HD12 | 1.84                     | 0.59              |
| 1:C:3377:GLU:OE2  | 1:C:3451:ASN:ND2  | 2.33                     | 0.59              |
| 1:A:2477:ILE:HD12 | 1:A:2477:ILE:O    | 2.02                     | 0.58              |
| 1:D:875:LEU:HD23  | 1:D:930:LEU:HD21  | 1.85                     | 0.58              |
| 1:D:956:LEU:HD13  | 1:D:960:TYR:HB3   | 1.84                     | 0.58              |
| 1:A:875:LEU:HD23  | 1:A:930:LEU:HD21  | 1.85                     | 0.58              |
| 1:A:4747:GLU:O    | 1:A:4751:HIS:ND1  | 2.36                     | 0.58              |
| 1:B:32:GLU:OE1    | 1:B:32:GLU:HA     | 2.03                     | 0.58              |
| 1:B:4720:ARG:HH21 | 1:B:4746:LEU:HD13 | 1.66                     | 0.58              |
| 1:D:4720:ARG:HH21 | 1:D:4746:LEU:HD13 | 1.66                     | 0.58              |
| 1:C:3536:LEU:HD23 | 1:C:3553:PHE:HZ   | 1.67                     | 0.58              |
| 1:A:32:GLU:OE1    | 1:A:32:GLU:HA     | 2.03                     | 0.58              |
| 1:A:911:PHE:HA    | 1:A:914:LEU:HD23  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3257:LEU:HD23 | 1:A:3267:MET:HE3  | 1.85                     | 0.58              |
| 1:C:459:GLU:N     | 1:C:459:GLU:OE2   | 2.36                     | 0.58              |
| 1:A:2876:ALA:HB3  | 1:A:2921:ARG:NH1  | 2.19                     | 0.58              |
| 1:B:875:LEU:HD23  | 1:B:930:LEU:HD21  | 1.85                     | 0.58              |
| 1:B:1987:MET:N    | 1:B:1987:MET:SD   | 2.74                     | 0.58              |
| 1:B:3334:SER:O    | 1:B:3337:LYS:NZ   | 2.36                     | 0.58              |
| 1:C:3257:LEU:HD23 | 1:C:3267:MET:HE3  | 1.85                     | 0.58              |
| 1:B:956:LEU:CD2   | 1:B:968:PRO:HG2   | 2.33                     | 0.58              |
| 1:B:4747:GLU:O    | 1:B:4751:HIS:ND1  | 2.36                     | 0.58              |
| 1:D:32:GLU:OE1    | 1:D:32:GLU:HA     | 2.03                     | 0.58              |
| 1:D:459:GLU:N     | 1:D:459:GLU:OE2   | 2.36                     | 0.58              |
| 1:D:2749:PRO:HD2  | 1:D:2752:LEU:HD12 | 1.84                     | 0.58              |
| 1:D:2876:ALA:HB3  | 1:D:2921:ARG:NH1  | 2.19                     | 0.58              |
| 1:A:914:LEU:HD21  | 1:A:919:ARG:HB2   | 1.86                     | 0.58              |
| 1:A:1426:GLU:OE1  | 1:A:1426:GLU:N    | 2.34                     | 0.58              |
| 1:B:894:TYR:OH    | 1:B:896:PRO:HA    | 2.03                     | 0.58              |
| 1:B:2876:ALA:HB3  | 1:B:2921:ARG:NH1  | 2.19                     | 0.58              |
| 1:B:4752:ASN:O    | 1:B:4754:ARG:NH1  | 2.37                     | 0.58              |
| 1:C:876:ALA:HB1   | 1:C:923:LEU:HA    | 1.85                     | 0.58              |
| 1:B:958:LYS:HA    | 1:B:961:MET:CE    | 2.34                     | 0.58              |
| 1:C:894:TYR:OH    | 1:C:896:PRO:HA    | 2.03                     | 0.58              |
| 1:C:2876:ALA:HB3  | 1:C:2921:ARG:NH1  | 2.19                     | 0.58              |
| 1:C:4752:ASN:O    | 1:C:4754:ARG:NH1  | 2.37                     | 0.58              |
| 1:D:2822:TRP:CE3  | 1:D:2875:MET:HE2  | 2.39                     | 0.58              |
| 1:D:4752:ASN:O    | 1:D:4754:ARG:NH1  | 2.37                     | 0.58              |
| 1:C:877:GLU:HG3   | 1:C:911:PHE:CG    | 2.39                     | 0.58              |
| 1:C:911:PHE:HA    | 1:C:914:LEU:HD23  | 1.86                     | 0.58              |
| 1:D:958:LYS:HA    | 1:D:961:MET:CE    | 2.34                     | 0.58              |
| 1:B:914:LEU:HD21  | 1:B:919:ARG:HB2   | 1.86                     | 0.58              |
| 1:B:956:LEU:HD11  | 1:B:968:PRO:HD2   | 1.86                     | 0.58              |
| 1:C:875:LEU:HD23  | 1:C:930:LEU:HD21  | 1.85                     | 0.58              |
| 1:D:108:ILE:CG2   | 1:D:151:MET:HE2   | 2.31                     | 0.58              |
| 1:D:3334:SER:O    | 1:D:3337:LYS:NZ   | 2.36                     | 0.58              |
| 1:A:459:GLU:OE2   | 1:A:459:GLU:N     | 2.36                     | 0.57              |
| 1:A:1300:GLN:OE1  | 1:A:1546:ASN:ND2  | 2.35                     | 0.57              |
| 1:C:2691:LYS:NZ   | 1:C:2692:TYR:O    | 2.37                     | 0.57              |
| 1:C:3369:ARG:O    | 1:C:3373:VAL:HG23 | 2.04                     | 0.57              |
| 1:D:914:LEU:HD21  | 1:D:919:ARG:HB2   | 1.86                     | 0.57              |
| 1:D:956:LEU:CG    | 1:D:967:LYS:HB2   | 2.34                     | 0.57              |
| 1:A:876:ALA:HB1   | 1:A:923:LEU:HA    | 1.85                     | 0.57              |
| 1:A:958:LYS:HA    | 1:A:961:MET:CE    | 2.34                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:956:LEU:CG    | 1:B:967:LYS:HB2   | 2.34                     | 0.57              |
| 1:C:914:LEU:HD21  | 1:C:919:ARG:HB2   | 1.86                     | 0.57              |
| 1:C:3334:SER:O    | 1:C:3337:LYS:NZ   | 2.36                     | 0.57              |
| 1:D:3369:ARG:O    | 1:D:3373:VAL:HG23 | 2.04                     | 0.57              |
| 1:A:877:GLU:HG3   | 1:A:911:PHE:CG    | 2.39                     | 0.57              |
| 1:A:3334:SER:O    | 1:A:3337:LYS:NZ   | 2.36                     | 0.57              |
| 1:A:3369:ARG:O    | 1:A:3373:VAL:HG23 | 2.04                     | 0.57              |
| 1:A:4752:ASN:O    | 1:A:4754:ARG:NH1  | 2.37                     | 0.57              |
| 1:B:903:ARG:HA    | 1:B:903:ARG:NH2   | 2.19                     | 0.57              |
| 1:B:3257:LEU:HD23 | 1:B:3267:MET:HE3  | 1.85                     | 0.57              |
| 1:C:956:LEU:CG    | 1:C:967:LYS:HB2   | 2.34                     | 0.57              |
| 1:A:956:LEU:CD2   | 1:A:968:PRO:HG2   | 2.33                     | 0.57              |
| 1:A:2822:TRP:CE3  | 1:A:2875:MET:HE2  | 2.39                     | 0.57              |
| 1:D:921:TYR:O     | 1:D:924:GLN:HG3   | 2.04                     | 0.57              |
| 1:A:921:TYR:O     | 1:A:924:GLN:HG3   | 2.04                     | 0.57              |
| 1:A:1987:MET:N    | 1:A:1987:MET:SD   | 2.74                     | 0.57              |
| 1:A:2625:ARG:NH1  | 1:A:2907:VAL:HG21 | 2.20                     | 0.57              |
| 1:A:2691:LYS:NZ   | 1:A:2692:TYR:O    | 2.37                     | 0.57              |
| 1:B:877:GLU:HG3   | 1:B:911:PHE:CG    | 2.39                     | 0.57              |
| 1:D:1426:GLU:OE1  | 1:D:1426:GLU:N    | 2.34                     | 0.57              |
| 1:A:903:ARG:HA    | 1:A:903:ARG:NH2   | 2.19                     | 0.57              |
| 1:A:956:LEU:HD11  | 1:A:968:PRO:HD2   | 1.86                     | 0.57              |
| 1:B:2691:LYS:NZ   | 1:B:2692:TYR:O    | 2.37                     | 0.57              |
| 1:B:876:ALA:HB1   | 1:B:923:LEU:HA    | 1.85                     | 0.57              |
| 1:B:3377:GLU:OE2  | 1:B:3451:ASN:ND2  | 2.33                     | 0.57              |
| 1:A:956:LEU:CG    | 1:A:967:LYS:HB2   | 2.34                     | 0.57              |
| 1:A:3472:THR:HG23 | 1:B:1171:MET:HE3  | 1.86                     | 0.57              |
| 1:B:911:PHE:HA    | 1:B:914:LEU:HD23  | 1.85                     | 0.57              |
| 1:B:1116:LEU:HD12 | 1:B:1194:SER:HB2  | 1.86                     | 0.57              |
| 1:B:2625:ARG:NH1  | 1:B:2907:VAL:HG21 | 2.20                     | 0.57              |
| 1:C:958:LYS:HA    | 1:C:961:MET:CE    | 2.34                     | 0.57              |
| 1:D:2691:LYS:NZ   | 1:D:2692:TYR:O    | 2.37                     | 0.57              |
| 1:A:908:LEU:HD22  | 1:A:962:MET:HG3   | 1.87                     | 0.57              |
| 1:B:921:TYR:O     | 1:B:924:GLN:HG3   | 2.04                     | 0.57              |
| 1:C:908:LEU:HD22  | 1:C:962:MET:HG3   | 1.87                     | 0.57              |
| 1:C:921:TYR:O     | 1:C:924:GLN:HG3   | 2.04                     | 0.57              |
| 1:C:2001:SER:O    | 1:C:2006:GLN:NE2  | 2.37                     | 0.57              |
| 1:C:2822:TRP:CE3  | 1:C:2875:MET:HE2  | 2.39                     | 0.57              |
| 1:D:876:ALA:HB1   | 1:D:923:LEU:HA    | 1.85                     | 0.57              |
| 1:A:1116:LEU:HD12 | 1:A:1194:SER:HB2  | 1.86                     | 0.56              |
| 1:A:3570:LEU:H    | 1:A:3570:LEU:HD22 | 1.71                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2822:TRP:CE3  | 1:B:2875:MET:HE2  | 2.39                     | 0.56              |
| 1:C:1116:LEU:HD12 | 1:C:1194:SER:HB2  | 1.86                     | 0.56              |
| 1:D:877:GLU:HG3   | 1:D:911:PHE:CG    | 2.39                     | 0.56              |
| 1:A:882:LEU:CA    | 1:A:970:PRO:HB3   | 2.36                     | 0.56              |
| 1:A:3377:GLU:OE2  | 1:A:3451:ASN:ND2  | 2.33                     | 0.56              |
| 1:B:1426:GLU:OE1  | 1:B:1426:GLU:N    | 2.34                     | 0.56              |
| 1:B:3570:LEU:H    | 1:B:3570:LEU:HD22 | 1.71                     | 0.56              |
| 1:C:956:LEU:HD11  | 1:C:968:PRO:HD2   | 1.86                     | 0.56              |
| 1:D:911:PHE:HA    | 1:D:914:LEU:HD23  | 1.85                     | 0.56              |
| 1:B:3369:ARG:O    | 1:B:3373:VAL:HG23 | 2.04                     | 0.56              |
| 1:C:903:ARG:HA    | 1:C:903:ARG:NH2   | 2.19                     | 0.56              |
| 1:C:2625:ARG:NH1  | 1:C:2907:VAL:HG21 | 2.20                     | 0.56              |
| 1:C:2748:ILE:HA   | 1:C:2818:ILE:HD13 | 1.88                     | 0.56              |
| 1:C:2752:LEU:HD12 | 1:C:2818:ILE:HD11 | 1.87                     | 0.56              |
| 1:C:2755:PHE:CD2  | 1:C:2814:LEU:HD11 | 2.40                     | 0.56              |
| 1:C:4753:GLU:C    | 1:C:4754:ARG:HD2  | 2.31                     | 0.56              |
| 1:D:872:ARG:HH22  | 1:D:923:LEU:HD23  | 1.71                     | 0.56              |
| 1:D:2625:ARG:NH1  | 1:D:2907:VAL:HG21 | 2.20                     | 0.56              |
| 1:D:2752:LEU:HD12 | 1:D:2818:ILE:HD11 | 1.87                     | 0.56              |
| 1:A:2022:CYS:O    | 1:A:2029:ARG:NH2  | 2.38                     | 0.56              |
| 1:B:862:ILE:HG21  | 1:B:931:LYS:HA    | 1.88                     | 0.56              |
| 1:C:956:LEU:CD2   | 1:C:968:PRO:HG2   | 2.33                     | 0.56              |
| 1:D:956:LEU:HD11  | 1:D:968:PRO:HD2   | 1.86                     | 0.56              |
| 1:A:872:ARG:HH22  | 1:A:923:LEU:HD23  | 1.71                     | 0.56              |
| 1:A:942:MET:CE    | 1:A:945:GLU:HG3   | 2.35                     | 0.56              |
| 1:A:4753:GLU:C    | 1:A:4754:ARG:HD2  | 2.31                     | 0.56              |
| 1:C:2266:LEU:HD21 | 1:C:2327:CYS:HB2  | 1.88                     | 0.56              |
| 1:C:3570:LEU:HD22 | 1:C:3570:LEU:H    | 1.71                     | 0.56              |
| 1:A:2266:LEU:HD21 | 1:A:2327:CYS:HB2  | 1.88                     | 0.56              |
| 1:C:942:MET:CE    | 1:C:945:GLU:HG3   | 2.35                     | 0.56              |
| 8:C:8009:A1BYZ:C5 | 8:C:8009:A1BYZ:C9 | 2.84                     | 0.56              |
| 1:D:2266:LEU:HD21 | 1:D:2327:CYS:HB2  | 1.88                     | 0.56              |
| 1:D:4753:GLU:C    | 1:D:4754:ARG:HD2  | 2.31                     | 0.56              |
| 1:D:871:ILE:HA    | 1:D:874:LYS:CD    | 2.33                     | 0.56              |
| 1:D:2912:LEU:O    | 1:D:2917:LYS:NZ   | 2.32                     | 0.56              |
| 1:D:3570:LEU:H    | 1:D:3570:LEU:HD22 | 1.71                     | 0.56              |
| 1:B:2266:LEU:HD21 | 1:B:2327:CYS:HB2  | 1.88                     | 0.56              |
| 1:B:4753:GLU:C    | 1:B:4754:ARG:HD2  | 2.31                     | 0.56              |
| 8:B:8009:A1BYZ:C5 | 8:B:8009:A1BYZ:C9 | 2.84                     | 0.56              |
| 1:C:882:LEU:CA    | 1:C:970:PRO:HB3   | 2.36                     | 0.56              |
| 1:D:877:GLU:HG3   | 1:D:911:PHE:CB    | 2.36                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:882:LEU:CA    | 1:D:970:PRO:HB3   | 2.36                     | 0.56              |
| 1:D:908:LEU:HD22  | 1:D:962:MET:HG3   | 1.87                     | 0.56              |
| 1:D:1116:LEU:HD12 | 1:D:1194:SER:HB2  | 1.86                     | 0.56              |
| 1:A:2743:THR:HG23 | 1:A:2744:LEU:N    | 2.21                     | 0.56              |
| 1:A:2748:ILE:HA   | 1:A:2818:ILE:HD13 | 1.88                     | 0.56              |
| 1:A:3422:ALA:HB1  | 1:B:1217:ILE:HD13 | 1.88                     | 0.56              |
| 1:B:882:LEU:CA    | 1:B:970:PRO:HB3   | 2.36                     | 0.56              |
| 1:B:908:LEU:HD22  | 1:B:962:MET:HG3   | 1.86                     | 0.56              |
| 1:C:2743:THR:HG23 | 1:C:2744:LEU:N    | 2.21                     | 0.56              |
| 1:D:903:ARG:HA    | 1:D:903:ARG:NH2   | 2.19                     | 0.56              |
| 1:D:2022:CYS:O    | 1:D:2029:ARG:NH2  | 2.38                     | 0.56              |
| 1:B:2755:PHE:CD2  | 1:B:2814:LEU:HD11 | 2.40                     | 0.56              |
| 1:C:862:ILE:HG21  | 1:C:931:LYS:HA    | 1.88                     | 0.56              |
| 1:C:871:ILE:HA    | 1:C:874:LYS:CD    | 2.33                     | 0.56              |
| 1:D:942:MET:CE    | 1:D:945:GLU:HG3   | 2.35                     | 0.56              |
| 1:A:877:GLU:HG3   | 1:A:911:PHE:CB    | 2.36                     | 0.55              |
| 1:B:942:MET:CE    | 1:B:945:GLU:HG3   | 2.35                     | 0.55              |
| 1:D:2743:THR:HG23 | 1:D:2744:LEU:N    | 2.21                     | 0.55              |
| 1:A:4632:GLU:OE2  | 1:A:4634:THR:OG1  | 2.17                     | 0.55              |
| 1:A:2752:LEU:HD12 | 1:A:2818:ILE:HD11 | 1.87                     | 0.55              |
| 1:B:2748:ILE:HA   | 1:B:2818:ILE:HD13 | 1.88                     | 0.55              |
| 1:D:2755:PHE:CD2  | 1:D:2814:LEU:HD11 | 2.40                     | 0.55              |
| 1:A:2873:GLN:O    | 1:A:2877:GLU:HG2  | 2.07                     | 0.55              |
| 1:B:1014:ILE:H    | 1:B:1014:ILE:HD12 | 1.72                     | 0.55              |
| 1:D:862:ILE:HG21  | 1:D:931:LYS:HA    | 1.88                     | 0.55              |
| 1:B:2743:THR:HG23 | 1:B:2744:LEU:N    | 2.21                     | 0.55              |
| 1:D:908:LEU:HD22  | 1:D:962:MET:CG    | 2.37                     | 0.55              |
| 1:D:3344:GLN:O    | 1:D:3347:VAL:HG12 | 2.07                     | 0.55              |
| 1:D:4887:VAL:HG12 | 1:D:4898:GLU:HG3  | 1.89                     | 0.55              |
| 1:A:3576:LEU:O    | 1:A:3580:VAL:HG23 | 2.07                     | 0.55              |
| 1:A:4887:VAL:HG12 | 1:A:4898:GLU:HG3  | 1.89                     | 0.55              |
| 1:B:2752:LEU:HD12 | 1:B:2818:ILE:HD11 | 1.87                     | 0.55              |
| 1:C:908:LEU:HD22  | 1:C:962:MET:CG    | 2.37                     | 0.55              |
| 1:C:2022:CYS:O    | 1:C:2029:ARG:NH2  | 2.38                     | 0.55              |
| 1:D:2748:ILE:HA   | 1:D:2818:ILE:HD13 | 1.88                     | 0.55              |
| 1:D:3576:LEU:O    | 1:D:3580:VAL:HG23 | 2.07                     | 0.55              |
| 1:A:1014:ILE:H    | 1:A:1014:ILE:HD12 | 1.72                     | 0.55              |
| 1:A:3847:LEU:HD13 | 1:B:77:ARG:NH1    | 2.22                     | 0.55              |
| 1:B:2022:CYS:O    | 1:B:2029:ARG:NH2  | 2.38                     | 0.55              |
| 8:D:8009:A1BYZ:C5 | 8:D:8009:A1BYZ:C9 | 2.84                     | 0.55              |
| 8:A:8009:A1BYZ:C5 | 8:A:8009:A1BYZ:C9 | 2.84                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3576:LEU:O    | 1:B:3580:VAL:HG23 | 2.07                     | 0.55              |
| 1:B:4887:VAL:HG12 | 1:B:4898:GLU:HG3  | 1.89                     | 0.55              |
| 1:C:2873:GLN:O    | 1:C:2877:GLU:HG2  | 2.07                     | 0.55              |
| 1:D:2520:LEU:HD13 | 1:D:2576:ARG:HG3  | 1.89                     | 0.55              |
| 1:D:3450:HIS:O    | 1:D:3450:HIS:ND1  | 2.35                     | 0.55              |
| 1:B:2873:GLN:O    | 1:B:2877:GLU:HG2  | 2.07                     | 0.55              |
| 1:C:2520:LEU:HD13 | 1:C:2576:ARG:HG3  | 1.89                     | 0.55              |
| 1:D:1014:ILE:H    | 1:D:1014:ILE:HD12 | 1.72                     | 0.55              |
| 1:D:2873:GLN:O    | 1:D:2877:GLU:HG2  | 2.07                     | 0.55              |
| 1:A:2755:PHE:CD2  | 1:A:2814:LEU:HD11 | 2.40                     | 0.54              |
| 1:B:605:CYS:SG    | 1:B:1670:LEU:HD12 | 2.47                     | 0.54              |
| 1:B:3536:LEU:HD23 | 1:B:3553:PHE:CZ   | 2.42                     | 0.54              |
| 1:B:3861:MET:HE1  | 1:B:3870:ASN:HA   | 1.89                     | 0.54              |
| 1:A:862:ILE:HG21  | 1:A:931:LYS:HA    | 1.88                     | 0.54              |
| 1:B:908:LEU:HD22  | 1:B:962:MET:CG    | 2.37                     | 0.54              |
| 1:C:877:GLU:HG3   | 1:C:911:PHE:CB    | 2.36                     | 0.54              |
| 1:D:885:LEU:CD2   | 1:D:970:PRO:HG3   | 2.37                     | 0.54              |
| 1:B:877:GLU:HG3   | 1:B:911:PHE:CB    | 2.36                     | 0.54              |
| 1:C:872:ARG:HH22  | 1:C:923:LEU:HD23  | 1.71                     | 0.54              |
| 1:C:1014:ILE:H    | 1:C:1014:ILE:HD12 | 1.72                     | 0.54              |
| 1:D:605:CYS:SG    | 1:D:1670:LEU:HD12 | 2.47                     | 0.54              |
| 1:A:3344:GLN:O    | 1:A:3347:VAL:HG12 | 2.07                     | 0.54              |
| 1:B:872:ARG:HH22  | 1:B:923:LEU:HD23  | 1.71                     | 0.54              |
| 1:B:2570:PHE:CE1  | 1:B:2583:MET:HE1  | 2.43                     | 0.54              |
| 1:C:605:CYS:SG    | 1:C:1670:LEU:HD12 | 2.47                     | 0.54              |
| 1:C:3344:GLN:O    | 1:C:3347:VAL:HG12 | 2.07                     | 0.54              |
| 1:D:976:VAL:HG11  | 1:D:1045:ARG:O    | 2.08                     | 0.54              |
| 1:D:2001:SER:O    | 1:D:2006:GLN:NE2  | 2.37                     | 0.54              |
| 1:A:605:CYS:SG    | 1:A:1670:LEU:HD12 | 2.47                     | 0.54              |
| 1:A:908:LEU:HD22  | 1:A:962:MET:CG    | 2.37                     | 0.54              |
| 1:A:976:VAL:HG11  | 1:A:1045:ARG:O    | 2.08                     | 0.54              |
| 1:B:2758:LYS:NZ   | 1:B:2831:GLU:O    | 2.24                     | 0.54              |
| 1:B:3344:GLN:O    | 1:B:3347:VAL:HG12 | 2.07                     | 0.54              |
| 1:C:2912:LEU:O    | 1:C:2917:LYS:NZ   | 2.32                     | 0.54              |
| 1:A:2570:PHE:CE1  | 1:A:2583:MET:HE1  | 2.43                     | 0.54              |
| 1:A:3456:GLU:OE2  | 1:A:3457:GLN:N    | 2.41                     | 0.54              |
| 1:A:3536:LEU:HD23 | 1:A:3553:PHE:CZ   | 2.42                     | 0.54              |
| 1:A:3861:MET:HE1  | 1:A:3870:ASN:HA   | 1.89                     | 0.54              |
| 1:D:865:PRO:CD    | 1:D:868:LEU:HD12  | 2.38                     | 0.54              |
| 1:B:942:MET:SD    | 1:B:945:GLU:HA    | 2.48                     | 0.54              |
| 1:C:3576:LEU:O    | 1:C:3580:VAL:HG23 | 2.07                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:4887:VAL:HG12 | 1:C:4898:GLU:HG3  | 1.89                     | 0.54              |
| 8:C:8009:A1BYZ:C9 | 8:C:8009:A1BYZ:C4 | 2.86                     | 0.54              |
| 8:B:8009:A1BYZ:C9 | 8:B:8009:A1BYZ:C4 | 2.86                     | 0.54              |
| 1:C:976:VAL:HG11  | 1:C:1045:ARG:O    | 2.08                     | 0.54              |
| 1:C:2570:PHE:CE1  | 1:C:2583:MET:HE1  | 2.43                     | 0.54              |
| 1:C:3861:MET:HE1  | 1:C:3870:ASN:HA   | 1.89                     | 0.54              |
| 1:B:976:VAL:HG11  | 1:B:1045:ARG:O    | 2.08                     | 0.54              |
| 1:B:3456:GLU:OE2  | 1:B:3457:GLN:N    | 2.41                     | 0.54              |
| 1:C:961:MET:HG3   | 1:C:967:LYS:HB3   | 1.90                     | 0.54              |
| 1:D:2570:PHE:CE1  | 1:D:2583:MET:HE1  | 2.43                     | 0.54              |
| 1:A:942:MET:SD    | 1:A:945:GLU:HA    | 2.48                     | 0.54              |
| 1:B:894:TYR:H     | 1:B:962:MET:HB3   | 1.72                     | 0.54              |
| 1:B:2520:LEU:HD13 | 1:B:2576:ARG:HG3  | 1.89                     | 0.54              |
| 1:C:942:MET:SD    | 1:C:945:GLU:HA    | 2.48                     | 0.54              |
| 1:D:875:LEU:HA    | 1:D:878:ASN:ND2   | 2.23                     | 0.54              |
| 1:A:875:LEU:HA    | 1:A:878:ASN:ND2   | 2.23                     | 0.53              |
| 1:B:2005:GLU:OE2  | 1:B:2005:GLU:HA   | 2.08                     | 0.53              |
| 1:C:865:PRO:CD    | 1:C:868:LEU:HD12  | 2.38                     | 0.53              |
| 1:C:894:TYR:H     | 1:C:962:MET:HB3   | 1.72                     | 0.53              |
| 1:C:3536:LEU:HD23 | 1:C:3553:PHE:CZ   | 2.43                     | 0.53              |
| 1:D:2758:LYS:NZ   | 1:D:2831:GLU:O    | 2.24                     | 0.53              |
| 1:D:3536:LEU:HD23 | 1:D:3553:PHE:CZ   | 2.42                     | 0.53              |
| 8:D:8009:A1BYZ:C9 | 8:D:8009:A1BYZ:C4 | 2.86                     | 0.53              |
| 1:D:956:LEU:CD2   | 1:D:968:PRO:HG2   | 2.33                     | 0.53              |
| 1:D:2005:GLU:HA   | 1:D:2005:GLU:OE2  | 2.08                     | 0.53              |
| 1:D:3456:GLU:OE2  | 1:D:3457:GLN:N    | 2.41                     | 0.53              |
| 1:A:914:LEU:HD21  | 1:A:919:ARG:HA    | 1.90                     | 0.53              |
| 1:A:2005:GLU:HA   | 1:A:2005:GLU:OE2  | 2.08                     | 0.53              |
| 1:C:658:THR:HG22  | 1:C:1002:VAL:CG2  | 2.39                     | 0.53              |
| 1:C:3208:GLU:OE2  | 1:C:3306:THR:OG1  | 2.15                     | 0.53              |
| 1:A:2520:LEU:HD13 | 1:A:2576:ARG:HG3  | 1.89                     | 0.53              |
| 1:B:885:LEU:CD2   | 1:B:970:PRO:HG3   | 2.38                     | 0.53              |
| 1:B:957:PRO:CG    | 1:B:960:TYR:HB2   | 2.38                     | 0.53              |
| 1:C:2758:LYS:NZ   | 1:C:2831:GLU:O    | 2.24                     | 0.53              |
| 1:A:908:LEU:O     | 1:A:909:VAL:HG13  | 2.09                     | 0.53              |
| 1:A:956:LEU:HD11  | 1:A:960:TYR:HB3   | 1.90                     | 0.53              |
| 1:A:961:MET:HG3   | 1:A:967:LYS:HB3   | 1.90                     | 0.53              |
| 1:B:4935:ILE:HG12 | 1:C:4932:GLY:HA2  | 1.91                     | 0.53              |
| 1:C:898:ARG:HB2   | 1:C:906:PRO:CD    | 2.39                     | 0.53              |
| 1:C:908:LEU:O     | 1:C:909:VAL:HG13  | 2.09                     | 0.53              |
| 1:D:894:TYR:H     | 1:D:962:MET:HB3   | 1.72                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:914:LEU:HD21  | 1:D:919:ARG:HA    | 1.90                     | 0.53              |
| 1:D:961:MET:HG3   | 1:D:967:LYS:HB3   | 1.90                     | 0.53              |
| 1:B:882:LEU:HA    | 1:B:885:LEU:HD23  | 1.91                     | 0.53              |
| 1:B:961:MET:HG3   | 1:B:967:LYS:HB3   | 1.90                     | 0.53              |
| 1:D:658:THR:HG22  | 1:D:1002:VAL:CG2  | 2.39                     | 0.53              |
| 1:D:3861:MET:HE1  | 1:D:3870:ASN:HA   | 1.89                     | 0.53              |
| 1:A:865:PRO:CD    | 1:A:868:LEU:HD12  | 2.38                     | 0.53              |
| 8:A:8009:A1BYZ:C9 | 8:A:8009:A1BYZ:C4 | 2.86                     | 0.53              |
| 1:B:871:ILE:HA    | 1:B:874:LYS:CD    | 2.33                     | 0.53              |
| 1:C:2480:LEU:HD13 | 1:C:2486:LEU:HD12 | 1.91                     | 0.53              |
| 1:C:3546:THR:OG1  | 1:C:3548:GLU:OE2  | 2.15                     | 0.53              |
| 1:D:898:ARG:HB2   | 1:D:906:PRO:CD    | 2.39                     | 0.53              |
| 1:D:942:MET:SD    | 1:D:945:GLU:HA    | 2.48                     | 0.53              |
| 1:A:894:TYR:H     | 1:A:962:MET:HB3   | 1.72                     | 0.53              |
| 1:A:2756:ILE:CG1  | 1:A:2814:LEU:HD12 | 2.39                     | 0.53              |
| 1:B:914:LEU:HD21  | 1:B:919:ARG:HA    | 1.90                     | 0.53              |
| 1:C:956:LEU:CD2   | 1:C:960:TYR:HD2   | 2.22                     | 0.53              |
| 1:A:885:LEU:CD2   | 1:A:970:PRO:HG3   | 2.37                     | 0.53              |
| 1:A:956:LEU:HB2   | 1:A:967:LYS:HD2   | 1.91                     | 0.53              |
| 1:B:956:LEU:HD11  | 1:B:960:TYR:HB3   | 1.90                     | 0.53              |
| 1:C:914:LEU:HD21  | 1:C:919:ARG:HA    | 1.90                     | 0.53              |
| 1:C:3847:LEU:HD13 | 1:D:77:ARG:NH1    | 2.24                     | 0.53              |
| 1:A:882:LEU:HA    | 1:A:885:LEU:HD23  | 1.91                     | 0.53              |
| 1:A:1171:MET:HE3  | 1:D:3472:THR:HG23 | 1.91                     | 0.53              |
| 1:A:2758:LYS:NZ   | 1:A:2831:GLU:O    | 2.24                     | 0.53              |
| 1:C:3456:GLU:OE2  | 1:C:3457:GLN:N    | 2.41                     | 0.53              |
| 1:C:4935:ILE:HG12 | 1:D:4932:GLY:HA2  | 1.91                     | 0.53              |
| 1:D:3377:GLU:OE2  | 1:D:3451:ASN:ND2  | 2.33                     | 0.53              |
| 1:A:2265:GLY:O    | 1:A:2267:GLY:N    | 2.42                     | 0.52              |
| 1:B:2822:TRP:CZ3  | 1:B:2875:MET:HE2  | 2.45                     | 0.52              |
| 1:C:911:PHE:CE2   | 1:C:923:LEU:HG    | 2.44                     | 0.52              |
| 1:C:2822:TRP:CZ3  | 1:C:2875:MET:HE2  | 2.45                     | 0.52              |
| 1:D:908:LEU:O     | 1:D:909:VAL:HG13  | 2.09                     | 0.52              |
| 1:A:871:ILE:HA    | 1:A:874:LYS:CD    | 2.33                     | 0.52              |
| 1:A:2822:TRP:CZ3  | 1:A:2875:MET:HE2  | 2.45                     | 0.52              |
| 1:A:4225:VAL:HG11 | 1:A:4948:VAL:HA   | 1.91                     | 0.52              |
| 1:B:2756:ILE:CG1  | 1:B:2814:LEU:HD12 | 2.39                     | 0.52              |
| 1:C:875:LEU:HA    | 1:C:878:ASN:ND2   | 2.23                     | 0.52              |
| 1:D:956:LEU:HD11  | 1:D:960:TYR:HB3   | 1.90                     | 0.52              |
| 1:D:2756:ILE:CG1  | 1:D:2814:LEU:HD12 | 2.39                     | 0.52              |
| 1:D:2822:TRP:CZ3  | 1:D:2875:MET:HE2  | 2.45                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:870:ARG:CZ    | 1:A:870:ARG:HB3   | 2.39                     | 0.52              |
| 1:A:892:TRP:CE2   | 1:A:903:ARG:HD3   | 2.44                     | 0.52              |
| 1:B:865:PRO:CD    | 1:B:868:LEU:HD12  | 2.38                     | 0.52              |
| 1:B:658:THR:HG22  | 1:B:1002:VAL:CG2  | 2.39                     | 0.52              |
| 1:B:875:LEU:HA    | 1:B:878:ASN:ND2   | 2.23                     | 0.52              |
| 1:C:882:LEU:HA    | 1:C:885:LEU:HD23  | 1.91                     | 0.52              |
| 1:C:956:LEU:HB2   | 1:C:967:LYS:HD2   | 1.91                     | 0.52              |
| 1:C:2005:GLU:HA   | 1:C:2005:GLU:OE2  | 2.08                     | 0.52              |
| 1:D:885:LEU:HG    | 1:D:886:THR:N     | 2.25                     | 0.52              |
| 1:B:908:LEU:O     | 1:B:909:VAL:HG13  | 2.09                     | 0.52              |
| 1:B:3472:THR:HG23 | 1:C:1171:MET:HE3  | 1.90                     | 0.52              |
| 1:B:3847:LEU:HD13 | 1:C:77:ARG:NH1    | 2.24                     | 0.52              |
| 1:D:2480:LEU:HD13 | 1:D:2486:LEU:HD12 | 1.91                     | 0.52              |
| 1:A:649:ILE:HG23  | 1:A:815:ALA:HB3   | 1.91                     | 0.52              |
| 1:A:658:THR:HG22  | 1:A:1002:VAL:CG2  | 2.39                     | 0.52              |
| 1:A:2001:SER:O    | 1:A:2006:GLN:NE2  | 2.38                     | 0.52              |
| 1:A:2884:HIS:CE1  | 1:A:2912:LEU:HD11 | 2.45                     | 0.52              |
| 1:B:956:LEU:CD2   | 1:B:960:TYR:HD2   | 2.22                     | 0.52              |
| 1:B:956:LEU:HB2   | 1:B:967:LYS:HD2   | 1.91                     | 0.52              |
| 1:B:2884:HIS:CE1  | 1:B:2912:LEU:HD11 | 2.45                     | 0.52              |
| 1:B:4225:VAL:HG11 | 1:B:4948:VAL:HA   | 1.91                     | 0.52              |
| 1:D:892:TRP:CE2   | 1:D:903:ARG:HD3   | 2.44                     | 0.52              |
| 1:D:911:PHE:CE2   | 1:D:923:LEU:HG    | 2.44                     | 0.52              |
| 1:B:892:TRP:CE2   | 1:B:903:ARG:HD3   | 2.44                     | 0.52              |
| 1:B:4649:THR:OG1  | 1:B:4801:HIS:NE2  | 2.39                     | 0.52              |
| 1:C:892:TRP:CE2   | 1:C:903:ARG:HD3   | 2.44                     | 0.52              |
| 1:C:2265:GLY:O    | 1:C:2267:GLY:N    | 2.42                     | 0.52              |
| 1:C:2884:HIS:CE1  | 1:C:2912:LEU:HD11 | 2.45                     | 0.52              |
| 1:C:3472:THR:HG23 | 1:D:1171:MET:HE3  | 1.90                     | 0.52              |
| 1:C:4244:THR:HG22 | 1:C:4248:MET:HE3  | 1.92                     | 0.52              |
| 1:D:979:THR:H     | 1:D:982:GLN:HB2   | 1.75                     | 0.52              |
| 1:D:2265:GLY:O    | 1:D:2267:GLY:N    | 2.42                     | 0.52              |
| 1:A:956:LEU:CD2   | 1:A:960:TYR:HD2   | 2.22                     | 0.52              |
| 1:A:2480:LEU:HD13 | 1:A:2486:LEU:HD12 | 1.91                     | 0.52              |
| 1:B:911:PHE:CE2   | 1:B:923:LEU:HG    | 2.44                     | 0.52              |
| 1:C:979:THR:H     | 1:C:982:GLN:HB2   | 1.75                     | 0.52              |
| 1:A:3384:ALA:N    | 1:A:3387:GLU:OE1  | 2.41                     | 0.52              |
| 1:B:898:ARG:HB2   | 1:B:906:PRO:CD    | 2.39                     | 0.52              |
| 1:B:4244:THR:HG22 | 1:B:4248:MET:HE3  | 1.92                     | 0.52              |
| 1:D:882:LEU:HA    | 1:D:885:LEU:HD23  | 1.91                     | 0.52              |
| 1:D:956:LEU:CD2   | 1:D:960:TYR:HD2   | 2.22                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1758:GLY:N    | 1:D:1759:PRO:CD   | 2.73                     | 0.52              |
| 1:A:911:PHE:CE2   | 1:A:923:LEU:HG    | 2.44                     | 0.52              |
| 1:B:331:ASP:OD1   | 1:B:331:ASP:C     | 2.53                     | 0.52              |
| 1:C:870:ARG:HB3   | 1:C:870:ARG:CZ    | 2.39                     | 0.52              |
| 1:C:1455:THR:OG1  | 1:C:1457:ASP:OD1  | 2.27                     | 0.52              |
| 1:C:1758:GLY:N    | 1:C:1759:PRO:CD   | 2.73                     | 0.52              |
| 1:B:2001:SER:O    | 1:B:2006:GLN:NE2  | 2.37                     | 0.51              |
| 1:B:2265:GLY:O    | 1:B:2267:GLY:N    | 2.42                     | 0.51              |
| 1:C:894:TYR:CB    | 1:C:962:MET:HB3   | 2.40                     | 0.51              |
| 1:D:870:ARG:CZ    | 1:D:870:ARG:HB3   | 2.39                     | 0.51              |
| 1:D:1455:THR:OG1  | 1:D:1457:ASP:OD1  | 2.28                     | 0.51              |
| 1:A:898:ARG:HB2   | 1:A:906:PRO:CD    | 2.39                     | 0.51              |
| 1:A:1455:THR:OG1  | 1:A:1457:ASP:OD1  | 2.27                     | 0.51              |
| 1:A:4244:THR:HG22 | 1:A:4248:MET:HE3  | 1.92                     | 0.51              |
| 1:B:649:ILE:HG23  | 1:B:815:ALA:HB3   | 1.92                     | 0.51              |
| 1:B:893:THR:HA    | 1:B:962:MET:SD    | 2.51                     | 0.51              |
| 1:B:942:MET:HE3   | 1:B:945:GLU:HG3   | 1.92                     | 0.51              |
| 1:D:2751:LYS:O    | 1:D:2754:SER:OG   | 2.26                     | 0.51              |
| 1:D:4086:ASP:OD1  | 1:D:4088:ARG:NH2  | 2.43                     | 0.51              |
| 1:D:4244:THR:HG22 | 1:D:4248:MET:HE3  | 1.92                     | 0.51              |
| 1:A:942:MET:HE3   | 1:A:945:GLU:HG3   | 1.92                     | 0.51              |
| 1:A:957:PRO:CG    | 1:A:960:TYR:HB2   | 2.38                     | 0.51              |
| 1:A:3541:TYR:HB3  | 1:A:3605:TYR:HD2  | 1.75                     | 0.51              |
| 1:A:4893:GLY:N    | 1:A:4897:ASP:OD1  | 2.41                     | 0.51              |
| 1:B:881:GLU:HB3   | 1:B:970:PRO:N     | 2.25                     | 0.51              |
| 1:C:2756:ILE:CG1  | 1:C:2814:LEU:HD12 | 2.39                     | 0.51              |
| 1:D:894:TYR:CB    | 1:D:962:MET:HB3   | 2.40                     | 0.51              |
| 1:B:870:ARG:HB3   | 1:B:870:ARG:CZ    | 2.39                     | 0.51              |
| 1:C:331:ASP:C     | 1:C:331:ASP:OD1   | 2.53                     | 0.51              |
| 1:D:957:PRO:CG    | 1:D:960:TYR:HB2   | 2.38                     | 0.51              |
| 1:A:894:TYR:CB    | 1:A:962:MET:HB3   | 2.40                     | 0.51              |
| 1:A:2751:LYS:O    | 1:A:2754:SER:OG   | 2.26                     | 0.51              |
| 1:B:1455:THR:OG1  | 1:B:1457:ASP:OD1  | 2.27                     | 0.51              |
| 1:B:2948:ASP:OD1  | 1:B:2948:ASP:N    | 2.44                     | 0.51              |
| 1:C:893:THR:HA    | 1:C:962:MET:SD    | 2.51                     | 0.51              |
| 1:C:956:LEU:HD11  | 1:C:960:TYR:HB3   | 1.90                     | 0.51              |
| 1:C:1222:GLU:OE1  | 1:C:1222:GLU:N    | 2.40                     | 0.51              |
| 1:D:2884:HIS:CE1  | 1:D:2912:LEU:HD11 | 2.45                     | 0.51              |
| 1:D:4225:VAL:HG11 | 1:D:4948:VAL:HA   | 1.91                     | 0.51              |
| 1:A:1222:GLU:OE1  | 1:A:1222:GLU:N    | 2.40                     | 0.51              |
| 1:A:1758:GLY:N    | 1:A:1759:PRO:CD   | 2.73                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:881:GLU:HB3   | 1:C:970:PRO:N     | 2.25                     | 0.51              |
| 1:C:885:LEU:CD2   | 1:C:970:PRO:HG3   | 2.37                     | 0.51              |
| 1:C:1113:ASP:OD1  | 1:C:1113:ASP:N    | 2.41                     | 0.51              |
| 1:C:3447:SER:O    | 1:C:3453:LYS:NZ   | 2.40                     | 0.51              |
| 1:D:956:LEU:HB2   | 1:D:967:LYS:HD2   | 1.91                     | 0.51              |
| 1:D:4649:THR:OG1  | 1:D:4801:HIS:NE2  | 2.39                     | 0.51              |
| 1:A:876:ALA:HB2   | 1:A:923:LEU:HA    | 1.92                     | 0.51              |
| 1:A:885:LEU:HG    | 1:A:886:THR:N     | 2.25                     | 0.51              |
| 1:A:911:PHE:CZ    | 1:A:923:LEU:HG    | 2.46                     | 0.51              |
| 1:A:3105:GLU:O    | 1:A:3108:VAL:HG12 | 2.11                     | 0.51              |
| 1:B:1758:GLY:N    | 1:B:1759:PRO:CD   | 2.73                     | 0.51              |
| 1:B:4086:ASP:OD1  | 1:B:4088:ARG:NH2  | 2.43                     | 0.51              |
| 1:C:2215:VAL:HG11 | 1:C:2229:MET:HE2  | 1.93                     | 0.51              |
| 1:D:2215:VAL:HG11 | 1:D:2229:MET:HE2  | 1.93                     | 0.51              |
| 1:D:3388:ALA:O    | 1:D:3392:GLU:N    | 2.39                     | 0.51              |
| 1:A:4649:THR:OG1  | 1:A:4801:HIS:NE2  | 2.39                     | 0.51              |
| 1:B:894:TYR:CB    | 1:B:962:MET:HB3   | 2.40                     | 0.51              |
| 1:B:952:LYS:O     | 1:B:972:ASP:HB3   | 2.11                     | 0.51              |
| 1:B:2215:VAL:HG11 | 1:B:2229:MET:HE2  | 1.93                     | 0.51              |
| 1:B:4893:GLY:N    | 1:B:4897:ASP:OD1  | 2.41                     | 0.51              |
| 1:A:2215:VAL:HG11 | 1:A:2229:MET:HE2  | 1.93                     | 0.51              |
| 1:A:4800:GLY:HA2  | 1:A:4806:PHE:HB2  | 1.93                     | 0.51              |
| 1:B:885:LEU:HG    | 1:B:886:THR:N     | 2.25                     | 0.51              |
| 1:B:979:THR:H     | 1:B:982:GLN:HB2   | 1.75                     | 0.51              |
| 1:B:1222:GLU:OE1  | 1:B:1222:GLU:N    | 2.40                     | 0.51              |
| 1:C:912:HIS:HA    | 1:C:919:ARG:NH1   | 2.26                     | 0.51              |
| 1:D:3347:VAL:HG11 | 1:D:3415:ARG:HB2  | 1.93                     | 0.51              |
| 1:D:4800:GLY:HA2  | 1:D:4806:PHE:HB2  | 1.93                     | 0.51              |
| 1:A:331:ASP:C     | 1:A:331:ASP:OD1   | 2.53                     | 0.51              |
| 1:A:893:THR:HA    | 1:A:962:MET:SD    | 2.51                     | 0.51              |
| 1:B:911:PHE:CZ    | 1:B:923:LEU:HG    | 2.46                     | 0.51              |
| 1:C:862:ILE:HB    | 1:C:931:LYS:HE2   | 1.93                     | 0.51              |
| 1:D:876:ALA:HB2   | 1:D:923:LEU:HA    | 1.92                     | 0.51              |
| 1:D:3384:ALA:N    | 1:D:3387:GLU:OE1  | 2.41                     | 0.51              |
| 1:A:952:LYS:O     | 1:A:972:ASP:HB3   | 2.11                     | 0.50              |
| 1:A:3472:THR:HG23 | 1:B:1171:MET:CE   | 2.42                     | 0.50              |
| 1:B:2480:LEU:HD13 | 1:B:2486:LEU:HD12 | 1.91                     | 0.50              |
| 1:C:876:ALA:HB2   | 1:C:923:LEU:HA    | 1.92                     | 0.50              |
| 1:C:952:LYS:O     | 1:C:972:ASP:HB3   | 2.11                     | 0.50              |
| 1:D:649:ILE:HG23  | 1:D:815:ALA:HB3   | 1.92                     | 0.50              |
| 1:D:881:GLU:HB3   | 1:D:970:PRO:N     | 2.25                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:952:LYS:O     | 1:D:972:ASP:HB3   | 2.11                     | 0.50              |
| 1:A:1048:LEU:HD21 | 1:A:1054:ILE:CG1  | 2.42                     | 0.50              |
| 1:A:1300:GLN:O    | 1:A:1300:GLN:NE2  | 2.41                     | 0.50              |
| 1:B:876:ALA:HB2   | 1:B:923:LEU:HA    | 1.92                     | 0.50              |
| 1:C:4086:ASP:OD1  | 1:C:4088:ARG:NH2  | 2.43                     | 0.50              |
| 1:C:4225:VAL:HG11 | 1:C:4948:VAL:HA   | 1.91                     | 0.50              |
| 1:D:942:MET:HE3   | 1:D:945:GLU:HG3   | 1.92                     | 0.50              |
| 1:B:658:THR:HG22  | 1:B:1002:VAL:HG21 | 1.94                     | 0.50              |
| 1:B:912:HIS:HA    | 1:B:919:ARG:NH1   | 2.26                     | 0.50              |
| 1:B:2912:LEU:O    | 1:B:2917:LYS:NZ   | 2.32                     | 0.50              |
| 1:C:649:ILE:HG23  | 1:C:815:ALA:HB3   | 1.92                     | 0.50              |
| 1:C:911:PHE:CZ    | 1:C:923:LEU:HG    | 2.46                     | 0.50              |
| 1:A:979:THR:H     | 1:A:982:GLN:HB2   | 1.75                     | 0.50              |
| 1:B:964:ASN:OD1   | 1:B:966:TYR:HB3   | 2.11                     | 0.50              |
| 1:B:2234:CYS:C    | 1:B:2236:PHE:N    | 2.70                     | 0.50              |
| 1:B:3105:GLU:O    | 1:B:3108:VAL:HG12 | 2.11                     | 0.50              |
| 1:C:3541:TYR:HB3  | 1:C:3605:TYR:HD2  | 1.75                     | 0.50              |
| 1:C:3542:ALA:O    | 1:C:3544:LYS:HE3  | 2.11                     | 0.50              |
| 1:A:862:ILE:HB    | 1:A:931:LYS:HE2   | 1.93                     | 0.50              |
| 1:A:2218:GLY:O    | 1:A:2225:ARG:NH1  | 2.38                     | 0.50              |
| 1:A:3542:ALA:O    | 1:A:3544:LYS:HE3  | 2.11                     | 0.50              |
| 1:C:942:MET:HE3   | 1:C:945:GLU:HG3   | 1.91                     | 0.50              |
| 1:D:331:ASP:C     | 1:D:331:ASP:OD1   | 2.53                     | 0.50              |
| 1:D:893:THR:HA    | 1:D:962:MET:SD    | 2.51                     | 0.50              |
| 1:D:1300:GLN:O    | 1:D:1300:GLN:NE2  | 2.41                     | 0.50              |
| 1:D:2218:GLY:O    | 1:D:2225:ARG:NH1  | 2.38                     | 0.50              |
| 1:A:912:HIS:HA    | 1:A:919:ARG:NH1   | 2.26                     | 0.50              |
| 1:A:2948:ASP:N    | 1:A:2948:ASP:OD1  | 2.44                     | 0.50              |
| 1:A:3347:VAL:HG11 | 1:A:3415:ARG:HB2  | 1.93                     | 0.50              |
| 1:C:4800:GLY:HA2  | 1:C:4806:PHE:HB2  | 1.93                     | 0.50              |
| 1:D:911:PHE:CZ    | 1:D:923:LEU:HG    | 2.46                     | 0.50              |
| 1:D:3105:GLU:O    | 1:D:3108:VAL:HG12 | 2.11                     | 0.50              |
| 1:A:658:THR:HG22  | 1:A:1002:VAL:HG21 | 1.94                     | 0.50              |
| 1:A:3584:GLU:OE1  | 1:A:3584:GLU:N    | 2.42                     | 0.50              |
| 1:B:3459:PHE:C    | 1:B:3459:PHE:CD2  | 2.90                     | 0.50              |
| 1:B:3541:TYR:HB3  | 1:B:3605:TYR:HD2  | 1.75                     | 0.50              |
| 1:B:3542:ALA:O    | 1:B:3544:LYS:HE3  | 2.11                     | 0.50              |
| 1:C:964:ASN:OD1   | 1:C:966:TYR:HB3   | 2.11                     | 0.50              |
| 1:D:2971:SER:HA   | 1:D:2974:PHE:CE2  | 2.47                     | 0.50              |
| 1:D:3584:GLU:OE1  | 1:D:3584:GLU:N    | 2.42                     | 0.50              |
| 1:B:862:ILE:HB    | 1:B:931:LYS:HE2   | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2948:ASP:OD1  | 1:C:2948:ASP:N    | 2.44                     | 0.50              |
| 1:C:3105:GLU:O    | 1:C:3108:VAL:HG12 | 2.11                     | 0.50              |
| 1:C:957:PRO:CG    | 1:C:960:TYR:HB2   | 2.38                     | 0.50              |
| 1:C:2910:ASP:OD1  | 1:C:2911:THR:N    | 2.45                     | 0.50              |
| 1:A:881:GLU:HB3   | 1:A:970:PRO:N     | 2.25                     | 0.49              |
| 1:A:2872:LEU:O    | 1:A:2875:MET:HB3  | 2.12                     | 0.49              |
| 1:A:2971:SER:HA   | 1:A:2974:PHE:CE2  | 2.47                     | 0.49              |
| 1:B:4800:GLY:HA2  | 1:B:4806:PHE:HB2  | 1.93                     | 0.49              |
| 1:C:1048:LEU:HD21 | 1:C:1054:ILE:CG1  | 2.42                     | 0.49              |
| 1:C:2971:SER:HA   | 1:C:2974:PHE:CE2  | 2.47                     | 0.49              |
| 1:D:912:HIS:HA    | 1:D:919:ARG:NH1   | 2.26                     | 0.49              |
| 1:D:2949:THR:OG1  | 1:D:2950:SER:N    | 2.46                     | 0.49              |
| 1:D:3347:VAL:HG11 | 1:D:3415:ARG:CB   | 2.42                     | 0.49              |
| 1:D:3459:PHE:C    | 1:D:3459:PHE:CD2  | 2.90                     | 0.49              |
| 1:A:3347:VAL:HG11 | 1:A:3415:ARG:CB   | 2.42                     | 0.49              |
| 1:C:658:THR:HG22  | 1:C:1002:VAL:HG21 | 1.94                     | 0.49              |
| 1:D:3541:TYR:HB3  | 1:D:3605:TYR:HD2  | 1.75                     | 0.49              |
| 1:B:953:LYS:HA    | 1:B:971:LEU:HA    | 1.94                     | 0.49              |
| 1:B:3347:VAL:HG11 | 1:B:3415:ARG:HB2  | 1.93                     | 0.49              |
| 1:C:953:LYS:HA    | 1:C:971:LEU:HA    | 1.94                     | 0.49              |
| 1:D:2234:CYS:C    | 1:D:2236:PHE:N    | 2.70                     | 0.49              |
| 1:D:2948:ASP:N    | 1:D:2948:ASP:OD1  | 2.44                     | 0.49              |
| 1:A:3459:PHE:C    | 1:A:3459:PHE:CD2  | 2.90                     | 0.49              |
| 1:B:2438:ALA:HB2  | 1:B:2510:VAL:HG22 | 1.95                     | 0.49              |
| 1:B:3347:VAL:HG11 | 1:B:3415:ARG:CB   | 2.42                     | 0.49              |
| 1:B:3422:ALA:HB1  | 1:C:1217:ILE:HD13 | 1.94                     | 0.49              |
| 1:C:885:LEU:HG    | 1:C:886:THR:N     | 2.25                     | 0.49              |
| 1:C:956:LEU:HD22  | 1:C:957:PRO:CD    | 2.39                     | 0.49              |
| 1:D:658:THR:HG22  | 1:D:1002:VAL:HG21 | 1.94                     | 0.49              |
| 1:D:953:LYS:HA    | 1:D:971:LEU:HA    | 1.94                     | 0.49              |
| 1:D:956:LEU:HB2   | 1:D:967:LYS:NZ    | 2.28                     | 0.49              |
| 1:A:926:SER:O     | 1:A:930:LEU:HD22  | 2.13                     | 0.49              |
| 1:A:982:GLN:HG2   | 1:A:1054:ILE:HD11 | 1.95                     | 0.49              |
| 1:B:2872:LEU:O    | 1:B:2875:MET:HB3  | 2.12                     | 0.49              |
| 1:C:2928:LEU:O    | 1:C:2928:LEU:HD13 | 2.13                     | 0.49              |
| 1:D:964:ASN:OD1   | 1:D:966:TYR:HB3   | 2.11                     | 0.49              |
| 1:D:4632:GLU:OE2  | 1:D:4634:THR:OG1  | 2.17                     | 0.49              |
| 1:B:884:ALA:O     | 1:B:888:ILE:HG22  | 2.13                     | 0.49              |
| 1:B:3384:ALA:N    | 1:B:3387:GLU:OE1  | 2.41                     | 0.49              |
| 1:C:3347:VAL:HG11 | 1:C:3415:ARG:CB   | 2.42                     | 0.49              |
| 1:C:3347:VAL:HG11 | 1:C:3415:ARG:HB2  | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:910:ASN:H     | 1:D:913:SER:HB3   | 1.78                     | 0.49              |
| 1:D:2928:LEU:O    | 1:D:2928:LEU:HD13 | 2.13                     | 0.49              |
| 1:A:884:ALA:O     | 1:A:888:ILE:HG22  | 2.13                     | 0.49              |
| 1:A:910:ASN:H     | 1:A:913:SER:HB3   | 1.78                     | 0.49              |
| 1:A:2438:ALA:HB2  | 1:A:2510:VAL:HG22 | 1.95                     | 0.49              |
| 1:B:870:ARG:HH21  | 1:B:871:ILE:HG23  | 1.78                     | 0.49              |
| 1:C:926:SER:O     | 1:C:930:LEU:HD22  | 2.13                     | 0.49              |
| 1:C:956:LEU:HB2   | 1:C:967:LYS:NZ    | 2.28                     | 0.49              |
| 1:C:3388:ALA:O    | 1:C:3392:GLU:N    | 2.39                     | 0.49              |
| 1:D:870:ARG:HH21  | 1:D:871:ILE:HG23  | 1.78                     | 0.49              |
| 1:D:2872:LEU:O    | 1:D:2875:MET:HB3  | 2.12                     | 0.49              |
| 1:D:3208:GLU:OE2  | 1:D:3306:THR:OG1  | 2.15                     | 0.49              |
| 1:A:890:GLN:HB2   | 1:A:892:TRP:HD1   | 1.78                     | 0.49              |
| 1:A:953:LYS:HA    | 1:A:971:LEU:HA    | 1.94                     | 0.49              |
| 1:C:903:ARG:C     | 1:C:904:LEU:HD23  | 2.38                     | 0.49              |
| 1:D:862:ILE:HB    | 1:D:931:LYS:HE2   | 1.93                     | 0.49              |
| 1:D:1048:LEU:HD21 | 1:D:1054:ILE:CG1  | 2.42                     | 0.49              |
| 1:A:964:ASN:OD1   | 1:A:966:TYR:HB3   | 2.11                     | 0.49              |
| 1:A:3447:SER:O    | 1:A:3453:LYS:NZ   | 2.40                     | 0.49              |
| 1:A:4935:ILE:HG12 | 1:B:4932:GLY:HA2  | 1.95                     | 0.49              |
| 1:C:878:ASN:O     | 1:C:881:GLU:HB2   | 2.13                     | 0.49              |
| 1:C:890:GLN:HB2   | 1:C:892:TRP:HD1   | 1.78                     | 0.49              |
| 1:D:890:GLN:HB2   | 1:D:892:TRP:HD1   | 1.78                     | 0.49              |
| 1:D:899:ASP:CB    | 1:D:902:LYS:HB2   | 2.33                     | 0.49              |
| 1:D:3542:ALA:O    | 1:D:3544:LYS:HE3  | 2.11                     | 0.49              |
| 1:B:956:LEU:HD22  | 1:B:957:PRO:CD    | 2.39                     | 0.49              |
| 1:C:2949:THR:OG1  | 1:C:2950:SER:N    | 2.46                     | 0.49              |
| 1:C:3422:ALA:HB1  | 1:D:1217:ILE:HD13 | 1.94                     | 0.49              |
| 1:C:3459:PHE:C    | 1:C:3459:PHE:CD2  | 2.90                     | 0.49              |
| 1:D:903:ARG:C     | 1:D:904:LEU:HD23  | 2.38                     | 0.49              |
| 1:D:956:LEU:HB3   | 1:D:967:LYS:HB2   | 1.94                     | 0.49              |
| 1:D:1758:GLY:N    | 1:D:1759:PRO:HD2  | 2.28                     | 0.49              |
| 1:A:956:LEU:HB3   | 1:A:967:LYS:HB2   | 1.94                     | 0.48              |
| 1:A:2234:CYS:C    | 1:A:2236:PHE:N    | 2.70                     | 0.48              |
| 1:A:2910:ASP:OD1  | 1:A:2911:THR:N    | 2.45                     | 0.48              |
| 1:A:2949:THR:OG1  | 1:A:2950:SER:N    | 2.45                     | 0.48              |
| 1:A:4086:ASP:OD1  | 1:A:4088:ARG:NH2  | 2.43                     | 0.48              |
| 1:B:870:ARG:NH2   | 1:B:871:ILE:HG23  | 2.28                     | 0.48              |
| 1:B:895:GLY:O     | 1:B:906:PRO:HA    | 2.13                     | 0.48              |
| 1:B:910:ASN:H     | 1:B:913:SER:HB3   | 1.78                     | 0.48              |
| 1:B:926:SER:O     | 1:B:930:LEU:HD22  | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2910:ASP:OD1  | 1:B:2911:THR:N    | 2.45                     | 0.48              |
| 1:B:2928:LEU:HD13 | 1:B:2928:LEU:O    | 2.13                     | 0.48              |
| 1:B:2969:ASP:O    | 1:B:2973:GLU:OE2  | 2.31                     | 0.48              |
| 1:C:1758:GLY:N    | 1:C:1759:PRO:HD2  | 2.28                     | 0.48              |
| 1:C:2872:LEU:O    | 1:C:2875:MET:HB3  | 2.12                     | 0.48              |
| 1:D:884:ALA:O     | 1:D:888:ILE:HG22  | 2.13                     | 0.48              |
| 1:D:926:SER:O     | 1:D:930:LEU:HD22  | 2.13                     | 0.48              |
| 1:A:3243:ASP:N    | 1:A:3243:ASP:OD1  | 2.46                     | 0.48              |
| 1:B:1048:LEU:HD21 | 1:B:1054:ILE:CG1  | 2.42                     | 0.48              |
| 1:B:1758:GLY:N    | 1:B:1759:PRO:HD2  | 2.28                     | 0.48              |
| 1:B:3450:HIS:O    | 1:B:3450:HIS:ND1  | 2.35                     | 0.48              |
| 1:C:884:ALA:O     | 1:C:888:ILE:HG22  | 2.13                     | 0.48              |
| 1:C:956:LEU:HB3   | 1:C:967:LYS:HB2   | 1.94                     | 0.48              |
| 1:C:2761:GLU:OE2  | 1:C:2795:TYR:CG   | 2.66                     | 0.48              |
| 1:B:890:GLN:HB2   | 1:B:892:TRP:HD1   | 1.78                     | 0.48              |
| 1:C:2751:LYS:O    | 1:C:2754:SER:OG   | 2.26                     | 0.48              |
| 1:D:982:GLN:HG2   | 1:D:1054:ILE:HD11 | 1.95                     | 0.48              |
| 1:D:2438:ALA:HB2  | 1:D:2510:VAL:HG22 | 1.95                     | 0.48              |
| 1:D:2761:GLU:OE2  | 1:D:2795:TYR:CG   | 2.67                     | 0.48              |
| 1:D:2802:ASP:OD1  | 1:D:2803:LYS:N    | 2.46                     | 0.48              |
| 1:A:895:GLY:O     | 1:A:906:PRO:HA    | 2.13                     | 0.48              |
| 1:A:956:LEU:HB2   | 1:A:967:LYS:NZ    | 2.27                     | 0.48              |
| 1:A:2928:LEU:O    | 1:A:2928:LEU:HD13 | 2.13                     | 0.48              |
| 1:B:2971:SER:HA   | 1:B:2974:PHE:CE2  | 2.47                     | 0.48              |
| 1:D:1222:GLU:OE1  | 1:D:1222:GLU:N    | 2.40                     | 0.48              |
| 1:D:2969:ASP:O    | 1:D:2973:GLU:OE2  | 2.31                     | 0.48              |
| 1:A:870:ARG:NH2   | 1:A:871:ILE:HG23  | 2.28                     | 0.48              |
| 1:A:870:ARG:HH21  | 1:A:871:ILE:HG23  | 1.78                     | 0.48              |
| 1:A:888:ILE:HG21  | 1:A:960:TYR:CG    | 2.49                     | 0.48              |
| 1:A:1102:ARG:NH1  | 1:A:1116:LEU:O    | 2.44                     | 0.48              |
| 1:A:1758:GLY:N    | 1:A:1759:PRO:HD2  | 2.28                     | 0.48              |
| 1:A:2743:THR:HG23 | 1:A:2744:LEU:H    | 1.77                     | 0.48              |
| 1:B:878:ASN:O     | 1:B:881:GLU:HB2   | 2.13                     | 0.48              |
| 1:B:888:ILE:HG21  | 1:B:960:TYR:CG    | 2.49                     | 0.48              |
| 1:C:870:ARG:HH21  | 1:C:871:ILE:HG23  | 1.78                     | 0.48              |
| 1:C:895:GLY:O     | 1:C:906:PRO:HA    | 2.13                     | 0.48              |
| 1:C:989:LEU:HB3   | 1:C:1040:LEU:HD12 | 1.95                     | 0.48              |
| 1:D:956:LEU:HD22  | 1:D:957:PRO:CD    | 2.39                     | 0.48              |
| 1:A:2761:GLU:OE2  | 1:A:2795:TYR:CG   | 2.66                     | 0.48              |
| 1:B:903:ARG:C     | 1:B:904:LEU:HD23  | 2.38                     | 0.48              |
| 1:B:956:LEU:HB2   | 1:B:967:LYS:NZ    | 2.28                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:2761:GLU:OE2 | 1:B:2795:TYR:CG   | 2.67                     | 0.48              |
| 1:C:942:MET:HE2  | 1:C:1052:TYR:CE2  | 2.49                     | 0.48              |
| 1:C:1102:ARG:NH1 | 1:C:1116:LEU:O    | 2.45                     | 0.48              |
| 1:C:2802:ASP:OD1 | 1:C:2803:LYS:N    | 2.46                     | 0.48              |
| 1:C:2969:ASP:O   | 1:C:2973:GLU:OE2  | 2.31                     | 0.48              |
| 1:C:4235:GLU:OE2 | 1:C:5015:ARG:NH2  | 2.47                     | 0.48              |
| 1:D:1266:ASP:OD1 | 1:D:1266:ASP:N    | 2.47                     | 0.48              |
| 1:D:2910:ASP:OD1 | 1:D:2911:THR:N    | 2.45                     | 0.48              |
| 1:B:2751:LYS:O   | 1:B:2754:SER:OG   | 2.26                     | 0.48              |
| 1:B:3540:ARG:HD2 | 1:B:3545:ASP:OD2  | 2.14                     | 0.48              |
| 1:C:888:ILE:HG21 | 1:C:960:TYR:CG    | 2.49                     | 0.48              |
| 1:D:868:LEU:HA   | 1:D:871:ILE:CD1   | 2.44                     | 0.48              |
| 1:D:878:ASN:O    | 1:D:881:GLU:HB2   | 2.13                     | 0.48              |
| 1:D:932:THR:O    | 1:D:936:LEU:HG    | 2.14                     | 0.48              |
| 1:A:868:LEU:HA   | 1:A:871:ILE:CD1   | 2.44                     | 0.48              |
| 1:A:932:THR:O    | 1:A:936:LEU:HG    | 2.14                     | 0.48              |
| 1:A:989:LEU:HB3  | 1:A:1040:LEU:HD12 | 1.95                     | 0.48              |
| 1:B:2802:ASP:OD1 | 1:B:2803:LYS:N    | 2.46                     | 0.48              |
| 1:C:870:ARG:NH2  | 1:C:871:ILE:HG23  | 2.28                     | 0.48              |
| 1:C:902:LYS:HD2  | 1:C:902:LYS:HA    | 1.41                     | 0.48              |
| 1:C:2438:ALA:HB2 | 1:C:2510:VAL:HG22 | 1.95                     | 0.48              |
| 1:D:3243:ASP:N   | 1:D:3243:ASP:OD1  | 2.46                     | 0.48              |
| 1:D:3540:ARG:HD2 | 1:D:3545:ASP:OD2  | 2.14                     | 0.48              |
| 1:A:942:MET:HE2  | 1:A:1052:TYR:CE2  | 2.49                     | 0.48              |
| 1:A:3540:ARG:O   | 1:A:3541:TYR:C    | 2.57                     | 0.48              |
| 1:A:3540:ARG:HD2 | 1:A:3545:ASP:OD2  | 2.14                     | 0.48              |
| 1:B:3388:ALA:O   | 1:B:3392:GLU:N    | 2.39                     | 0.48              |
| 1:C:3243:ASP:OD1 | 1:C:3243:ASP:N    | 2.46                     | 0.48              |
| 1:D:875:LEU:CB   | 1:D:926:SER:HB2   | 2.43                     | 0.48              |
| 1:D:888:ILE:HG21 | 1:D:960:TYR:CG    | 2.49                     | 0.48              |
| 1:D:895:GLY:O    | 1:D:906:PRO:HA    | 2.13                     | 0.48              |
| 1:A:2969:ASP:O   | 1:A:2973:GLU:OE2  | 2.31                     | 0.48              |
| 1:B:932:THR:O    | 1:B:936:LEU:HG    | 2.14                     | 0.48              |
| 1:B:3584:GLU:OE1 | 1:B:3584:GLU:N    | 2.43                     | 0.48              |
| 1:C:868:LEU:HA   | 1:C:871:ILE:CD1   | 2.44                     | 0.48              |
| 1:C:914:LEU:CD2  | 1:C:919:ARG:HB2   | 2.44                     | 0.48              |
| 1:C:932:THR:O    | 1:C:936:LEU:HG    | 2.14                     | 0.48              |
| 1:D:871:ILE:H    | 1:D:871:ILE:HG13  | 1.40                     | 0.48              |
| 1:D:2947:LEU:O   | 1:D:2950:SER:OG   | 2.26                     | 0.48              |
| 1:D:4893:GLY:N   | 1:D:4897:ASP:OD1  | 2.41                     | 0.48              |
| 1:B:868:LEU:HA   | 1:B:871:ILE:CD1   | 2.44                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:942:MET:HE2  | 1:B:1052:TYR:CE2  | 2.49                     | 0.47              |
| 1:B:989:LEU:HB3  | 1:B:1040:LEU:HD12 | 1.95                     | 0.47              |
| 1:C:885:LEU:HD12 | 1:C:960:TYR:HE2   | 1.79                     | 0.47              |
| 1:C:910:ASN:H    | 1:C:913:SER:HB3   | 1.78                     | 0.47              |
| 1:C:911:PHE:O    | 1:C:914:LEU:HD23  | 2.14                     | 0.47              |
| 1:C:919:ARG:HG3  | 1:C:923:LEU:CD1   | 2.44                     | 0.47              |
| 1:C:1300:GLN:O   | 1:C:1300:GLN:NE2  | 2.41                     | 0.47              |
| 1:C:2234:CYS:C   | 1:C:2236:PHE:N    | 2.70                     | 0.47              |
| 1:D:898:ARG:HB2  | 1:D:906:PRO:HD3   | 1.96                     | 0.47              |
| 1:D:911:PHE:O    | 1:D:914:LEU:HD23  | 2.14                     | 0.47              |
| 1:D:942:MET:HE2  | 1:D:1052:TYR:CE2  | 2.49                     | 0.47              |
| 1:A:903:ARG:HA   | 1:A:903:ARG:NE    | 2.29                     | 0.47              |
| 1:A:911:PHE:O    | 1:A:914:LEU:HD23  | 2.14                     | 0.47              |
| 1:A:1072:ARG:HA  | 1:A:1072:ARG:HE   | 1.79                     | 0.47              |
| 1:A:2802:ASP:OD1 | 1:A:2803:LYS:N    | 2.46                     | 0.47              |
| 2:H:12:ASP:OD2   | 2:H:12:ASP:C      | 2.57                     | 0.47              |
| 1:B:911:PHE:O    | 1:B:914:LEU:HD23  | 2.14                     | 0.47              |
| 1:B:914:LEU:CD2  | 1:B:919:ARG:HB2   | 2.44                     | 0.47              |
| 1:B:919:ARG:HG3  | 1:B:923:LEU:CD1   | 2.44                     | 0.47              |
| 1:B:4235:GLU:OE2 | 1:B:5015:ARG:NH2  | 2.47                     | 0.47              |
| 1:D:870:ARG:NH2  | 1:D:871:ILE:HG23  | 2.28                     | 0.47              |
| 1:D:903:ARG:HA   | 1:D:903:ARG:NE    | 2.29                     | 0.47              |
| 1:D:4235:GLU:OE2 | 1:D:5015:ARG:NH2  | 2.47                     | 0.47              |
| 1:A:985:LEU:HD13 | 1:A:1057:PRO:HD2  | 1.96                     | 0.47              |
| 1:B:956:LEU:HB3  | 1:B:967:LYS:HB2   | 1.94                     | 0.47              |
| 1:B:2391:PRO:O   | 1:B:2392:ALA:HB3  | 2.15                     | 0.47              |
| 1:B:2949:THR:OG1 | 1:B:2950:SER:N    | 2.45                     | 0.47              |
| 1:C:898:ARG:HB2  | 1:C:906:PRO:HD3   | 1.96                     | 0.47              |
| 1:D:914:LEU:CD2  | 1:D:919:ARG:HB2   | 2.44                     | 0.47              |
| 1:A:875:LEU:CB   | 1:A:926:SER:HB2   | 2.44                     | 0.47              |
| 1:B:885:LEU:HD12 | 1:B:960:TYR:HE2   | 1.79                     | 0.47              |
| 1:C:982:GLN:HG2  | 1:C:1054:ILE:HD11 | 1.95                     | 0.47              |
| 1:C:4830:HIS:NE2 | 1:C:4940:GLU:OE1  | 2.48                     | 0.47              |
| 1:D:985:LEU:HD13 | 1:D:1057:PRO:HD2  | 1.96                     | 0.47              |
| 1:A:878:ASN:O    | 1:A:881:GLU:HB2   | 2.13                     | 0.47              |
| 1:A:914:LEU:CD2  | 1:A:919:ARG:HB2   | 2.44                     | 0.47              |
| 1:A:3468:MET:SD  | 1:B:1174:SER:O    | 2.72                     | 0.47              |
| 1:A:4235:GLU:OE2 | 1:A:5015:ARG:NH2  | 2.47                     | 0.47              |
| 2:G:12:ASP:OD2   | 2:G:12:ASP:C      | 2.57                     | 0.47              |
| 1:B:982:GLN:HG2  | 1:B:1054:ILE:HD11 | 1.95                     | 0.47              |
| 1:B:3389:GLU:O   | 1:B:3393:LEU:HD23 | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:4830:HIS:NE2  | 1:B:4940:GLU:OE1  | 2.48                     | 0.47              |
| 1:C:2234:CYS:O    | 1:C:2236:PHE:C    | 2.58                     | 0.47              |
| 1:C:2743:THR:HG23 | 1:C:2744:LEU:H    | 1.77                     | 0.47              |
| 1:D:885:LEU:HD12  | 1:D:960:TYR:HE2   | 1.79                     | 0.47              |
| 1:D:905:HIS:O     | 1:D:908:LEU:HB2   | 2.15                     | 0.47              |
| 1:D:1072:ARG:HA   | 1:D:1072:ARG:HE   | 1.79                     | 0.47              |
| 1:A:903:ARG:C     | 1:A:904:LEU:HD23  | 2.38                     | 0.47              |
| 1:A:1266:ASP:N    | 1:A:1266:ASP:OD1  | 2.47                     | 0.47              |
| 1:A:2391:PRO:O    | 1:A:2392:ALA:HB3  | 2.15                     | 0.47              |
| 2:F:12:ASP:OD2    | 2:F:12:ASP:C      | 2.57                     | 0.47              |
| 1:B:877:GLU:HA    | 1:B:911:PHE:CD1   | 2.49                     | 0.47              |
| 1:B:903:ARG:HA    | 1:B:903:ARG:NE    | 2.29                     | 0.47              |
| 1:B:1300:GLN:O    | 1:B:1300:GLN:NE2  | 2.41                     | 0.47              |
| 1:A:877:GLU:HA    | 1:A:911:PHE:CD1   | 2.49                     | 0.47              |
| 1:A:885:LEU:HD12  | 1:A:960:TYR:HE2   | 1.79                     | 0.47              |
| 1:A:956:LEU:HD22  | 1:A:957:PRO:CD    | 2.39                     | 0.47              |
| 2:E:12:ASP:OD2    | 2:E:12:ASP:C      | 2.57                     | 0.47              |
| 1:B:440:GLU:CD    | 1:B:440:GLU:H     | 2.22                     | 0.47              |
| 1:B:905:HIS:O     | 1:B:908:LEU:HB2   | 2.15                     | 0.47              |
| 1:B:978:LEU:HD22  | 1:B:982:GLN:OE1   | 2.15                     | 0.47              |
| 1:B:986:VAL:HA    | 1:B:989:LEU:HD12  | 1.97                     | 0.47              |
| 1:B:1102:ARG:NH1  | 1:B:1116:LEU:O    | 2.45                     | 0.47              |
| 1:B:2218:GLY:O    | 1:B:2225:ARG:NH1  | 2.38                     | 0.47              |
| 1:B:2234:CYS:O    | 1:B:2236:PHE:C    | 2.58                     | 0.47              |
| 1:B:2743:THR:HG23 | 1:B:2744:LEU:H    | 1.77                     | 0.47              |
| 1:B:4789:TYR:OH   | 1:B:4813:ASP:OD1  | 2.28                     | 0.47              |
| 1:C:877:GLU:HA    | 1:C:911:PHE:CD1   | 2.49                     | 0.47              |
| 1:C:899:ASP:CB    | 1:C:902:LYS:HB2   | 2.33                     | 0.47              |
| 1:C:903:ARG:HA    | 1:C:903:ARG:NE    | 2.29                     | 0.47              |
| 1:C:905:HIS:O     | 1:C:908:LEU:HB2   | 2.15                     | 0.47              |
| 1:C:1266:ASP:OD1  | 1:C:1266:ASP:N    | 2.47                     | 0.47              |
| 1:C:2926:GLU:OE1  | 1:C:2926:GLU:HA   | 2.15                     | 0.47              |
| 1:C:2947:LEU:O    | 1:C:2950:SER:OG   | 2.26                     | 0.47              |
| 1:C:3389:GLU:O    | 1:C:3393:LEU:HD23 | 2.15                     | 0.47              |
| 1:D:440:GLU:H     | 1:D:440:GLU:CD    | 2.22                     | 0.47              |
| 1:D:989:LEU:HB3   | 1:D:1040:LEU:HD12 | 1.95                     | 0.47              |
| 1:A:77:ARG:NH1    | 1:D:3847:LEU:HD13 | 2.29                     | 0.47              |
| 1:A:894:TYR:HB3   | 1:A:964:ASN:H     | 1.80                     | 0.47              |
| 1:A:905:HIS:O     | 1:A:908:LEU:HB2   | 2.15                     | 0.47              |
| 1:A:2876:ALA:HB3  | 1:A:2921:ARG:HH12 | 1.79                     | 0.47              |
| 1:A:3389:GLU:O    | 1:A:3393:LEU:HD23 | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:19:ARG:HB3    | 2:E:19:ARG:NH1    | 2.30                     | 0.47              |
| 1:C:875:LEU:CB    | 1:C:926:SER:HB2   | 2.44                     | 0.47              |
| 1:C:978:LEU:HD22  | 1:C:982:GLN:OE1   | 2.15                     | 0.47              |
| 1:C:2391:PRO:O    | 1:C:2392:ALA:HB3  | 2.15                     | 0.47              |
| 1:D:1102:ARG:NH1  | 1:D:1116:LEU:O    | 2.45                     | 0.47              |
| 1:D:2746:VAL:HG22 | 1:D:2747:ILE:N    | 2.30                     | 0.47              |
| 1:D:2926:GLU:OE1  | 1:D:2926:GLU:HA   | 2.15                     | 0.47              |
| 1:A:898:ARG:HB2   | 1:A:906:PRO:HD3   | 1.97                     | 0.47              |
| 1:B:893:THR:O     | 1:B:904:LEU:HA    | 2.15                     | 0.47              |
| 1:C:985:LEU:HD13  | 1:C:1057:PRO:HD2  | 1.96                     | 0.47              |
| 1:D:2234:CYS:O    | 1:D:2236:PHE:C    | 2.58                     | 0.47              |
| 1:A:440:GLU:H     | 1:A:440:GLU:CD    | 2.22                     | 0.47              |
| 1:B:1072:ARG:HA   | 1:B:1072:ARG:HE   | 1.79                     | 0.47              |
| 1:B:4796:MET:HE1  | 7:B:8006:PCW:H212 | 1.97                     | 0.47              |
| 1:C:605:CYS:CB    | 1:C:1673:SER:OG   | 2.63                     | 0.47              |
| 1:C:986:VAL:HA    | 1:C:989:LEU:HD12  | 1.97                     | 0.47              |
| 1:C:2746:VAL:HG22 | 1:C:2747:ILE:N    | 2.30                     | 0.47              |
| 1:C:4796:MET:HE1  | 7:C:8006:PCW:H212 | 1.97                     | 0.47              |
| 1:D:877:GLU:HA    | 1:D:911:PHE:CD1   | 2.49                     | 0.47              |
| 1:D:919:ARG:HG3   | 1:D:923:LEU:CD1   | 2.44                     | 0.47              |
| 1:D:3389:GLU:O    | 1:D:3393:LEU:HD23 | 2.15                     | 0.47              |
| 1:D:4709:PHE:CD1  | 1:D:4709:PHE:C    | 2.93                     | 0.47              |
| 1:A:2481:GLY:O    | 1:A:2485:ALA:HB3  | 2.16                     | 0.46              |
| 1:B:605:CYS:CB    | 1:B:1673:SER:OG   | 2.63                     | 0.46              |
| 1:B:872:ARG:NH2   | 1:B:873:GLU:HA    | 2.30                     | 0.46              |
| 1:B:898:ARG:HB2   | 1:B:906:PRO:HD3   | 1.97                     | 0.46              |
| 1:B:902:LYS:HA    | 1:B:902:LYS:HD2   | 1.42                     | 0.46              |
| 1:B:985:LEU:HD13  | 1:B:1057:PRO:HD2  | 1.96                     | 0.46              |
| 1:B:2481:GLY:O    | 1:B:2485:ALA:HB3  | 2.15                     | 0.46              |
| 1:B:3472:THR:HG23 | 1:C:1171:MET:CE   | 2.45                     | 0.46              |
| 1:C:3024:LYS:NZ   | 1:C:3024:LYS:HB3  | 2.30                     | 0.46              |
| 1:C:3384:ALA:N    | 1:C:3387:GLU:OE1  | 2.41                     | 0.46              |
| 1:C:3540:ARG:HD2  | 1:C:3545:ASP:OD2  | 2.14                     | 0.46              |
| 1:D:887:ARG:HG3   | 1:D:908:LEU:HD11  | 1.98                     | 0.46              |
| 1:D:3605:TYR:CD1  | 1:D:3605:TYR:C    | 2.92                     | 0.46              |
| 1:A:887:ARG:HG3   | 1:A:908:LEU:HD11  | 1.98                     | 0.46              |
| 1:A:893:THR:O     | 1:A:904:LEU:HA    | 2.15                     | 0.46              |
| 1:A:919:ARG:HG3   | 1:A:923:LEU:CD1   | 2.44                     | 0.46              |
| 1:A:986:VAL:HA    | 1:A:989:LEU:HD12  | 1.97                     | 0.46              |
| 1:A:3605:TYR:CD1  | 1:A:3605:TYR:C    | 2.92                     | 0.46              |
| 1:B:875:LEU:CB    | 1:B:926:SER:HB2   | 2.43                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2481:GLY:O    | 1:C:2485:ALA:HB3  | 2.15                     | 0.46              |
| 1:A:899:ASP:CB    | 1:A:902:LYS:HB2   | 2.33                     | 0.46              |
| 1:A:978:LEU:HD22  | 1:A:982:GLN:OE1   | 2.15                     | 0.46              |
| 1:A:2374:GLY:O    | 1:B:131:LYS:NZ    | 2.48                     | 0.46              |
| 1:B:819:ARG:NH2   | 1:B:1030:GLU:OE1  | 2.49                     | 0.46              |
| 1:B:879:ILE:HA    | 1:B:882:LEU:CD1   | 2.45                     | 0.46              |
| 1:B:2974:PHE:C    | 1:B:2974:PHE:CD1  | 2.93                     | 0.46              |
| 1:C:1072:ARG:HA   | 1:C:1072:ARG:HE   | 1.80                     | 0.46              |
| 1:C:4709:PHE:CD1  | 1:C:4709:PHE:C    | 2.93                     | 0.46              |
| 1:D:978:LEU:HD12  | 1:D:983:THR:HG22  | 1.98                     | 0.46              |
| 1:A:819:ARG:NH2   | 1:A:1030:GLU:OE1  | 2.49                     | 0.46              |
| 1:A:3024:LYS:HB3  | 1:A:3024:LYS:NZ   | 2.30                     | 0.46              |
| 1:A:4709:PHE:CD1  | 1:A:4709:PHE:C    | 2.93                     | 0.46              |
| 1:B:887:ARG:HG3   | 1:B:908:LEU:HD11  | 1.98                     | 0.46              |
| 1:B:2215:VAL:HG21 | 1:B:2229:MET:CE   | 2.46                     | 0.46              |
| 1:B:2374:GLY:O    | 1:C:131:LYS:NZ    | 2.49                     | 0.46              |
| 1:B:4703:VAL:O    | 1:B:4706:THR:OG1  | 2.34                     | 0.46              |
| 1:C:894:TYR:HB3   | 1:C:962:MET:HB3   | 1.98                     | 0.46              |
| 1:C:961:MET:CG    | 1:C:967:LYS:HB3   | 2.45                     | 0.46              |
| 1:D:961:MET:CG    | 1:D:967:LYS:HB3   | 2.45                     | 0.46              |
| 1:D:1113:ASP:OD1  | 1:D:1113:ASP:N    | 2.41                     | 0.46              |
| 1:D:2747:ILE:N    | 1:D:2747:ILE:HD12 | 2.31                     | 0.46              |
| 1:D:3024:LYS:HB3  | 1:D:3024:LYS:NZ   | 2.30                     | 0.46              |
| 1:A:4729:ILE:HD12 | 1:A:4729:ILE:N    | 2.30                     | 0.46              |
| 2:H:19:ARG:HB3    | 2:H:19:ARG:NH1    | 2.30                     | 0.46              |
| 1:B:2746:VAL:HG22 | 1:B:2747:ILE:N    | 2.30                     | 0.46              |
| 1:C:819:ARG:NH2   | 1:C:1030:GLU:OE1  | 2.49                     | 0.46              |
| 1:C:978:LEU:HD12  | 1:C:983:THR:HG22  | 1.98                     | 0.46              |
| 1:C:2215:VAL:HG21 | 1:C:2229:MET:CE   | 2.46                     | 0.46              |
| 1:C:2876:ALA:HB3  | 1:C:2921:ARG:HH12 | 1.79                     | 0.46              |
| 1:C:4703:VAL:O    | 1:C:4706:THR:OG1  | 2.34                     | 0.46              |
| 1:D:893:THR:HG22  | 1:D:904:LEU:HD13  | 1.98                     | 0.46              |
| 1:D:3540:ARG:O    | 1:D:3541:TYR:C    | 2.57                     | 0.46              |
| 1:A:605:CYS:CB    | 1:A:1673:SER:OG   | 2.63                     | 0.46              |
| 1:A:872:ARG:NH2   | 1:A:873:GLU:HA    | 2.30                     | 0.46              |
| 1:A:961:MET:CG    | 1:A:967:LYS:HB3   | 2.46                     | 0.46              |
| 1:A:2747:ILE:HD12 | 1:A:2747:ILE:N    | 2.31                     | 0.46              |
| 2:G:19:ARG:NH1    | 2:G:19:ARG:HB3    | 2.30                     | 0.46              |
| 1:B:2926:GLU:OE1  | 1:B:2926:GLU:HA   | 2.15                     | 0.46              |
| 1:B:3024:LYS:NZ   | 1:B:3024:LYS:HB3  | 2.30                     | 0.46              |
| 1:B:3243:ASP:OD1  | 1:B:3243:ASP:N    | 2.46                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1252:GLU:N    | 1:C:1252:GLU:OE2  | 2.48                     | 0.46              |
| 1:C:2374:GLY:O    | 1:D:131:LYS:NZ    | 2.49                     | 0.46              |
| 1:D:819:ARG:NH2   | 1:D:1030:GLU:OE1  | 2.49                     | 0.46              |
| 1:D:2974:PHE:CD1  | 1:D:2974:PHE:C    | 2.93                     | 0.46              |
| 1:A:723:TRP:CZ2   | 1:A:728:ALA:HB2   | 2.51                     | 0.46              |
| 1:A:2215:VAL:HG21 | 1:A:2229:MET:CE   | 2.46                     | 0.46              |
| 1:A:2746:VAL:HG22 | 1:A:2747:ILE:N    | 2.30                     | 0.46              |
| 1:A:4796:MET:HE1  | 7:A:8006:PCW:H20  | 1.98                     | 0.46              |
| 1:A:4830:HIS:NE2  | 1:A:4940:GLU:OE1  | 2.48                     | 0.46              |
| 1:B:1266:ASP:OD1  | 1:B:1266:ASP:N    | 2.46                     | 0.46              |
| 1:B:3447:SER:O    | 1:B:3453:LYS:NZ   | 2.40                     | 0.46              |
| 1:B:4796:MET:HE1  | 7:B:8006:PCW:H20  | 1.98                     | 0.46              |
| 1:C:440:GLU:H     | 1:C:440:GLU:CD    | 2.22                     | 0.46              |
| 1:C:3605:TYR:CD1  | 1:C:3605:TYR:C    | 2.92                     | 0.46              |
| 1:D:1252:GLU:N    | 1:D:1252:GLU:OE2  | 2.48                     | 0.46              |
| 1:D:2391:PRO:O    | 1:D:2392:ALA:HB3  | 2.15                     | 0.46              |
| 1:D:2481:GLY:O    | 1:D:2485:ALA:HB3  | 2.16                     | 0.46              |
| 1:B:961:MET:CG    | 1:B:967:LYS:HB3   | 2.45                     | 0.46              |
| 1:C:887:ARG:HG3   | 1:C:908:LEU:HD11  | 1.98                     | 0.46              |
| 1:C:2974:PHE:CD1  | 1:C:2974:PHE:C    | 2.93                     | 0.46              |
| 1:C:4729:ILE:HD12 | 1:C:4729:ILE:N    | 2.30                     | 0.46              |
| 1:D:893:THR:O     | 1:D:904:LEU:HA    | 2.15                     | 0.46              |
| 1:D:2743:THR:HG23 | 1:D:2744:LEU:H    | 1.77                     | 0.46              |
| 1:A:883:TRP:HE1   | 1:A:887:ARG:HH11  | 1.64                     | 0.46              |
| 1:A:2926:GLU:OE1  | 1:A:2926:GLU:HA   | 2.15                     | 0.46              |
| 1:A:2974:PHE:CD1  | 1:A:2974:PHE:C    | 2.93                     | 0.46              |
| 2:F:19:ARG:HB3    | 2:F:19:ARG:NH1    | 2.30                     | 0.46              |
| 1:B:3384:ALA:O    | 1:B:3388:ALA:HB2  | 2.16                     | 0.46              |
| 1:C:723:TRP:CZ2   | 1:C:728:ALA:HB2   | 2.51                     | 0.46              |
| 1:C:3472:THR:HG23 | 1:D:1171:MET:CE   | 2.46                     | 0.46              |
| 1:D:605:CYS:CB    | 1:D:1673:SER:OG   | 2.63                     | 0.46              |
| 1:D:978:LEU:HD22  | 1:D:982:GLN:OE1   | 2.15                     | 0.46              |
| 1:D:986:VAL:HA    | 1:D:989:LEU:HD12  | 1.97                     | 0.46              |
| 1:D:3546:THR:OG1  | 1:D:3548:GLU:OE2  | 2.15                     | 0.46              |
| 1:A:893:THR:HG22  | 1:A:904:LEU:HD13  | 1.98                     | 0.46              |
| 1:B:894:TYR:HB3   | 1:B:962:MET:HB3   | 1.98                     | 0.46              |
| 1:B:894:TYR:HB3   | 1:B:964:ASN:H     | 1.80                     | 0.46              |
| 1:B:957:PRO:HG2   | 1:B:960:TYR:CB    | 2.44                     | 0.46              |
| 1:B:3108:VAL:HG23 | 1:B:3176:LEU:CD1  | 2.47                     | 0.46              |
| 1:B:3282:LEU:HD12 | 1:B:3316:LEU:HD22 | 1.98                     | 0.46              |
| 1:C:953:LYS:CB    | 1:C:971:LEU:HA    | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1001:ARG:NH2  | 1:C:1004:GLN:OE1  | 2.49                     | 0.46              |
| 1:C:3600:VAL:HG12 | 1:C:3604:LEU:CD1  | 2.46                     | 0.46              |
| 1:D:894:TYR:HB3   | 1:D:964:ASN:H     | 1.80                     | 0.46              |
| 1:D:957:PRO:HG2   | 1:D:960:TYR:CB    | 2.44                     | 0.46              |
| 1:D:1001:ARG:NH2  | 1:D:1004:GLN:OE1  | 2.49                     | 0.46              |
| 1:D:2215:VAL:HG21 | 1:D:2229:MET:CE   | 2.46                     | 0.46              |
| 1:A:894:TYR:HB3   | 1:A:962:MET:HB3   | 1.98                     | 0.45              |
| 1:A:978:LEU:HD12  | 1:A:983:THR:HG22  | 1.98                     | 0.45              |
| 1:A:2234:CYS:O    | 1:A:2236:PHE:C    | 2.58                     | 0.45              |
| 1:B:899:ASP:CB    | 1:B:902:LYS:HB2   | 2.33                     | 0.45              |
| 1:B:978:LEU:HD12  | 1:B:983:THR:HG22  | 1.98                     | 0.45              |
| 1:B:2795:TYR:CZ   | 1:B:2803:LYS:HG2  | 2.52                     | 0.45              |
| 7:B:8005:PCW:H231 | 7:B:8005:PCW:H20  | 1.72                     | 0.45              |
| 1:C:872:ARG:CG    | 1:C:927:GLY:HA2   | 2.46                     | 0.45              |
| 1:C:880:HIS:CE1   | 1:C:914:LEU:HD22  | 2.52                     | 0.45              |
| 1:C:892:TRP:HB3   | 1:C:908:LEU:CD1   | 2.46                     | 0.45              |
| 1:C:2746:VAL:HG22 | 1:C:2747:ILE:H    | 1.81                     | 0.45              |
| 1:C:3540:ARG:O    | 1:C:3541:TYR:C    | 2.57                     | 0.45              |
| 1:D:723:TRP:CZ2   | 1:D:728:ALA:HB2   | 2.51                     | 0.45              |
| 1:A:892:TRP:HB3   | 1:A:908:LEU:CD1   | 2.46                     | 0.45              |
| 1:A:3108:VAL:HG23 | 1:A:3176:LEU:CD1  | 2.46                     | 0.45              |
| 1:A:4703:VAL:O    | 1:A:4706:THR:OG1  | 2.34                     | 0.45              |
| 1:B:723:TRP:CZ2   | 1:B:728:ALA:HB2   | 2.51                     | 0.45              |
| 1:B:872:ARG:CG    | 1:B:927:GLY:HA2   | 2.46                     | 0.45              |
| 1:B:883:TRP:HE1   | 1:B:887:ARG:HH11  | 1.64                     | 0.45              |
| 1:B:1875:GLU:HA   | 1:B:1875:GLU:OE2  | 2.17                     | 0.45              |
| 1:B:4729:ILE:N    | 1:B:4729:ILE:HD12 | 2.30                     | 0.45              |
| 1:C:3384:ALA:O    | 1:C:3388:ALA:HB2  | 2.16                     | 0.45              |
| 1:D:879:ILE:HA    | 1:D:882:LEU:CD1   | 2.45                     | 0.45              |
| 1:D:931:LYS:HE2   | 1:D:931:LYS:HB3   | 1.69                     | 0.45              |
| 1:D:2234:CYS:HB3  | 1:D:2238:CYS:HB2  | 1.63                     | 0.45              |
| 1:D:2876:ALA:HB3  | 1:D:2921:ARG:HH12 | 1.79                     | 0.45              |
| 1:D:4796:MET:HE1  | 7:D:8006:PCW:H212 | 1.98                     | 0.45              |
| 1:A:971:LEU:H     | 1:A:971:LEU:HG    | 1.52                     | 0.45              |
| 1:A:1001:ARG:NH2  | 1:A:1004:GLN:OE1  | 2.49                     | 0.45              |
| 1:A:1252:GLU:N    | 1:A:1252:GLU:OE2  | 2.48                     | 0.45              |
| 1:A:1273:LEU:HD22 | 1:A:1290:LEU:HD11 | 1.98                     | 0.45              |
| 1:A:3282:LEU:HD12 | 1:A:3316:LEU:HD22 | 1.98                     | 0.45              |
| 1:A:4796:MET:HE1  | 7:A:8006:PCW:H212 | 1.97                     | 0.45              |
| 1:B:892:TRP:HB3   | 1:B:908:LEU:CD1   | 2.46                     | 0.45              |
| 1:B:2876:ALA:HB3  | 1:B:2921:ARG:HH12 | 1.79                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:879:ILE:HA    | 1:C:882:LEU:CD1   | 2.44                     | 0.45              |
| 1:C:893:THR:O     | 1:C:904:LEU:HA    | 2.15                     | 0.45              |
| 1:C:2218:GLY:O    | 1:C:2225:ARG:NH1  | 2.38                     | 0.45              |
| 1:C:2795:TYR:CZ   | 1:C:2803:LYS:HG2  | 2.51                     | 0.45              |
| 1:D:4729:ILE:N    | 1:D:4729:ILE:HD12 | 2.30                     | 0.45              |
| 1:A:2234:CYS:HB2  | 1:A:2271:SER:HB3  | 1.99                     | 0.45              |
| 1:B:158:ARG:HG2   | 1:B:158:ARG:HH11  | 1.81                     | 0.45              |
| 1:B:871:ILE:H     | 1:B:871:ILE:HG13  | 1.40                     | 0.45              |
| 1:B:956:LEU:CD1   | 1:B:968:PRO:HD2   | 2.47                     | 0.45              |
| 1:C:1116:LEU:HD13 | 1:C:1124:VAL:HG11 | 1.98                     | 0.45              |
| 1:C:3282:LEU:HD12 | 1:C:3316:LEU:HD22 | 1.98                     | 0.45              |
| 1:C:4893:GLY:N    | 1:C:4897:ASP:OD1  | 2.41                     | 0.45              |
| 1:D:978:LEU:HB3   | 1:D:983:THR:HG23  | 1.98                     | 0.45              |
| 1:D:3282:LEU:HD12 | 1:D:3316:LEU:HD22 | 1.98                     | 0.45              |
| 1:D:3686:GLU:OE1  | 1:D:3686:GLU:N    | 2.46                     | 0.45              |
| 1:A:892:TRP:CE3   | 1:A:905:HIS:HB2   | 2.52                     | 0.45              |
| 1:A:3600:VAL:HG12 | 1:A:3604:LEU:CD1  | 2.46                     | 0.45              |
| 1:B:880:HIS:CE1   | 1:B:914:LEU:HD22  | 2.52                     | 0.45              |
| 1:B:2746:VAL:HG22 | 1:B:2747:ILE:H    | 1.81                     | 0.45              |
| 1:C:894:TYR:HB3   | 1:C:964:ASN:H     | 1.80                     | 0.45              |
| 1:C:978:LEU:HB3   | 1:C:983:THR:HG23  | 1.98                     | 0.45              |
| 1:C:4796:MET:HE1  | 7:C:8006:PCW:H20  | 1.98                     | 0.45              |
| 1:D:880:HIS:CE1   | 1:D:914:LEU:HD22  | 2.52                     | 0.45              |
| 1:D:2795:TYR:CZ   | 1:D:2803:LYS:HG2  | 2.51                     | 0.45              |
| 1:A:871:ILE:H     | 1:A:871:ILE:HG13  | 1.40                     | 0.45              |
| 1:A:902:LYS:CB    | 1:A:904:LEU:HG    | 2.47                     | 0.45              |
| 1:A:3384:ALA:O    | 1:A:3388:ALA:HB2  | 2.16                     | 0.45              |
| 1:B:1740:THR:HG22 | 1:B:2147:VAL:HG22 | 1.98                     | 0.45              |
| 1:B:2747:ILE:N    | 1:B:2747:ILE:HD12 | 2.31                     | 0.45              |
| 1:B:2947:LEU:O    | 1:B:2950:SER:OG   | 2.26                     | 0.45              |
| 1:C:872:ARG:NH2   | 1:C:873:GLU:HA    | 2.30                     | 0.45              |
| 1:C:883:TRP:HE1   | 1:C:887:ARG:HH11  | 1.64                     | 0.45              |
| 1:C:893:THR:HG22  | 1:C:904:LEU:HD13  | 1.98                     | 0.45              |
| 7:C:8006:PCW:H411 | 1:D:4848:LEU:HD22 | 1.99                     | 0.45              |
| 1:D:158:ARG:HG2   | 1:D:158:ARG:HH11  | 1.81                     | 0.45              |
| 1:D:3108:VAL:HG23 | 1:D:3176:LEU:CD1  | 2.47                     | 0.45              |
| 1:A:882:LEU:HD23  | 1:A:970:PRO:CB    | 2.47                     | 0.45              |
| 1:A:882:LEU:HD23  | 1:A:970:PRO:HB3   | 1.99                     | 0.45              |
| 1:B:3540:ARG:O    | 1:B:3541:TYR:C    | 2.57                     | 0.45              |
| 7:B:8006:PCW:H411 | 1:C:4848:LEU:HD22 | 1.99                     | 0.45              |
| 1:C:893:THR:HG23  | 1:C:963:SER:HB3   | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:892:TRP:CE3   | 1:D:905:HIS:HB2   | 2.52                     | 0.45              |
| 1:D:1273:LEU:HD22 | 1:D:1290:LEU:HD11 | 1.98                     | 0.45              |
| 1:D:3384:ALA:O    | 1:D:3388:ALA:HB2  | 2.16                     | 0.45              |
| 1:D:4796:MET:HE1  | 7:D:8006:PCW:H2O  | 1.98                     | 0.45              |
| 1:A:158:ARG:HH11  | 1:A:158:ARG:HG2   | 1.81                     | 0.45              |
| 1:A:2795:TYR:CZ   | 1:A:2803:LYS:HG2  | 2.51                     | 0.45              |
| 1:A:3421:ARG:CG   | 1:A:3521:ILE:HD11 | 2.47                     | 0.45              |
| 1:B:882:LEU:HD23  | 1:B:970:PRO:HB3   | 1.99                     | 0.45              |
| 1:B:931:LYS:HE2   | 1:B:931:LYS:HB3   | 1.69                     | 0.45              |
| 1:B:978:LEU:HB3   | 1:B:983:THR:HG23  | 1.98                     | 0.45              |
| 1:B:1252:GLU:N    | 1:B:1252:GLU:OE2  | 2.48                     | 0.45              |
| 1:C:892:TRP:CE3   | 1:C:905:HIS:HB2   | 2.52                     | 0.45              |
| 1:C:2747:ILE:N    | 1:C:2747:ILE:HD12 | 2.31                     | 0.45              |
| 1:C:3108:VAL:HG23 | 1:C:3176:LEU:CD1  | 2.47                     | 0.45              |
| 1:D:894:TYR:HB3   | 1:D:962:MET:HB3   | 1.98                     | 0.45              |
| 1:A:1740:THR:HG22 | 1:A:2147:VAL:HG22 | 1.98                     | 0.45              |
| 1:B:892:TRP:CE3   | 1:B:905:HIS:HB2   | 2.52                     | 0.45              |
| 1:C:843:PRO:O     | 1:C:1197:PRO:HA   | 2.17                     | 0.45              |
| 1:D:1012:GLN:OE1  | 1:D:1014:ILE:HD11 | 2.17                     | 0.45              |
| 1:A:879:ILE:HA    | 1:A:882:LEU:CD1   | 2.44                     | 0.45              |
| 1:B:956:LEU:CB    | 1:B:967:LYS:HD2   | 2.47                     | 0.45              |
| 1:B:1001:ARG:NH2  | 1:B:1004:GLN:OE1  | 2.49                     | 0.45              |
| 1:B:1113:ASP:OD1  | 1:B:1113:ASP:N    | 2.41                     | 0.45              |
| 1:B:2234:CYS:HB2  | 1:B:2271:SER:HB3  | 1.99                     | 0.45              |
| 1:B:3421:ARG:CG   | 1:B:3521:ILE:HD11 | 2.47                     | 0.45              |
| 1:B:3600:VAL:HG12 | 1:B:3604:LEU:CD1  | 2.46                     | 0.45              |
| 1:C:882:LEU:HD23  | 1:C:970:PRO:HB3   | 1.99                     | 0.45              |
| 1:C:1740:THR:HG22 | 1:C:2147:VAL:HG22 | 1.98                     | 0.45              |
| 1:D:882:LEU:HD23  | 1:D:970:PRO:HB3   | 1.99                     | 0.45              |
| 1:D:2234:CYS:HB2  | 1:D:2271:SER:HB3  | 1.99                     | 0.45              |
| 1:A:978:LEU:HB3   | 1:A:983:THR:HG23  | 1.98                     | 0.44              |
| 1:B:2755:PHE:CZ   | 1:B:2931:LEU:HG   | 2.52                     | 0.44              |
| 1:C:957:PRO:HG2   | 1:C:960:TYR:CB    | 2.44                     | 0.44              |
| 1:C:2755:PHE:CZ   | 1:C:2931:LEU:HG   | 2.52                     | 0.44              |
| 1:D:865:PRO:HD2   | 1:D:868:LEU:CD1   | 2.47                     | 0.44              |
| 1:D:882:LEU:HD23  | 1:D:970:PRO:CB    | 2.47                     | 0.44              |
| 1:D:883:TRP:HE1   | 1:D:887:ARG:HH11  | 1.64                     | 0.44              |
| 1:D:1875:GLU:OE2  | 1:D:1875:GLU:HA   | 2.17                     | 0.44              |
| 1:A:843:PRO:O     | 1:A:1197:PRO:HA   | 2.17                     | 0.44              |
| 1:A:872:ARG:CG    | 1:A:927:GLY:HA2   | 2.46                     | 0.44              |
| 1:A:1042:GLN:O    | 1:A:1046:THR:HG23 | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2755:PHE:CZ   | 1:A:2931:LEU:HG   | 2.52                     | 0.44              |
| 1:A:3283:PRO:HG3  | 1:A:3346:ILE:HG22 | 2.00                     | 0.44              |
| 1:B:865:PRO:HD2   | 1:B:868:LEU:CD1   | 2.47                     | 0.44              |
| 1:B:1012:GLN:OE1  | 1:B:1014:ILE:HD11 | 2.17                     | 0.44              |
| 1:C:865:PRO:HD2   | 1:C:868:LEU:CD1   | 2.47                     | 0.44              |
| 1:C:1273:LEU:HD22 | 1:C:1290:LEU:HD11 | 1.98                     | 0.44              |
| 1:C:1940:MET:HA   | 1:C:1940:MET:HE3  | 2.00                     | 0.44              |
| 1:C:3004:LEU:HB2  | 1:C:3005:PRO:HD3  | 1.99                     | 0.44              |
| 1:D:1116:LEU:HD13 | 1:D:1124:VAL:HG11 | 1.98                     | 0.44              |
| 1:D:2746:VAL:HG22 | 1:D:2747:ILE:H    | 1.81                     | 0.44              |
| 1:D:2780:GLU:OE1  | 1:D:2780:GLU:N    | 2.44                     | 0.44              |
| 1:D:3600:VAL:HG12 | 1:D:3604:LEU:CD1  | 2.46                     | 0.44              |
| 1:D:4703:VAL:O    | 1:D:4706:THR:OG1  | 2.34                     | 0.44              |
| 1:A:893:THR:HG23  | 1:A:963:SER:HB3   | 1.99                     | 0.44              |
| 1:A:925:MET:O     | 1:A:929:THR:HG23  | 2.18                     | 0.44              |
| 1:A:1217:ILE:HD13 | 1:D:3422:ALA:HB1  | 2.00                     | 0.44              |
| 1:A:2234:CYS:SG   | 1:A:2271:SER:HB3  | 2.57                     | 0.44              |
| 1:A:2746:VAL:HG22 | 1:A:2747:ILE:H    | 1.81                     | 0.44              |
| 1:B:879:ILE:HD12  | 1:B:879:ILE:HA    | 1.78                     | 0.44              |
| 1:B:893:THR:HG22  | 1:B:904:LEU:HD13  | 1.98                     | 0.44              |
| 1:B:3423:HIS:ND1  | 1:B:3423:HIS:C    | 2.76                     | 0.44              |
| 1:B:3605:TYR:C    | 1:B:3605:TYR:CD1  | 2.92                     | 0.44              |
| 1:C:158:ARG:HG2   | 1:C:158:ARG:HH11  | 1.81                     | 0.44              |
| 1:C:868:LEU:HD23  | 1:C:868:LEU:HA    | 1.77                     | 0.44              |
| 1:C:2757:ASN:O    | 1:C:2761:GLU:OE1  | 2.35                     | 0.44              |
| 1:C:3450:HIS:O    | 1:C:3450:HIS:ND1  | 2.35                     | 0.44              |
| 1:D:872:ARG:NH2   | 1:D:873:GLU:HA    | 2.30                     | 0.44              |
| 1:D:3548:GLU:CD   | 1:D:3548:GLU:H    | 2.25                     | 0.44              |
| 1:A:880:HIS:CE1   | 1:A:914:LEU:HD22  | 2.52                     | 0.44              |
| 1:A:956:LEU:CD1   | 1:A:968:PRO:HD2   | 2.47                     | 0.44              |
| 1:A:1116:LEU:HD13 | 1:A:1124:VAL:HG11 | 1.98                     | 0.44              |
| 1:B:843:PRO:O     | 1:B:1197:PRO:HA   | 2.17                     | 0.44              |
| 1:B:902:LYS:CB    | 1:B:904:LEU:HG    | 2.47                     | 0.44              |
| 1:B:925:MET:O     | 1:B:929:THR:HG23  | 2.18                     | 0.44              |
| 1:B:1940:MET:HA   | 1:B:1940:MET:HE3  | 2.00                     | 0.44              |
| 1:C:925:MET:O     | 1:C:929:THR:HG23  | 2.18                     | 0.44              |
| 1:C:3105:GLU:OE2  | 1:C:3168:ARG:NE   | 2.51                     | 0.44              |
| 1:D:925:MET:O     | 1:D:929:THR:HG23  | 2.18                     | 0.44              |
| 1:D:2747:ILE:HG22 | 1:D:2748:ILE:N    | 2.33                     | 0.44              |
| 1:D:2755:PHE:CZ   | 1:D:2931:LEU:HG   | 2.52                     | 0.44              |
| 1:D:2757:ASN:O    | 1:D:2761:GLU:OE1  | 2.35                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:957:PRO:HG2   | 1:A:960:TYR:CB    | 2.44                     | 0.44              |
| 1:A:1113:ASP:OD1  | 1:A:1113:ASP:N    | 2.41                     | 0.44              |
| 1:A:3592:LYS:O    | 1:A:3596:ARG:HG2  | 2.18                     | 0.44              |
| 1:B:882:LEU:HD23  | 1:B:970:PRO:CB    | 2.47                     | 0.44              |
| 1:B:1116:LEU:HD13 | 1:B:1124:VAL:HG11 | 1.98                     | 0.44              |
| 1:B:3004:LEU:HB2  | 1:B:3005:PRO:HD3  | 1.99                     | 0.44              |
| 1:B:3283:PRO:HG3  | 1:B:3346:ILE:HG22 | 2.00                     | 0.44              |
| 1:C:882:LEU:HD23  | 1:C:970:PRO:CB    | 2.47                     | 0.44              |
| 1:C:1875:GLU:HA   | 1:C:1875:GLU:OE2  | 2.17                     | 0.44              |
| 1:C:2234:CYS:HB2  | 1:C:2271:SER:HB3  | 1.99                     | 0.44              |
| 1:C:2761:GLU:OE2  | 1:C:2795:TYR:CD1  | 2.71                     | 0.44              |
| 1:D:892:TRP:HB3   | 1:D:908:LEU:CD1   | 2.46                     | 0.44              |
| 1:D:1940:MET:HA   | 1:D:1940:MET:HE3  | 2.00                     | 0.44              |
| 1:D:3224:SER:OG   | 1:D:3227:GLU:OE2  | 2.31                     | 0.44              |
| 1:A:1012:GLN:OE1  | 1:A:1014:ILE:HD11 | 2.17                     | 0.44              |
| 1:B:1042:GLN:O    | 1:B:1046:THR:HG23 | 2.17                     | 0.44              |
| 1:B:3548:GLU:H    | 1:B:3548:GLU:CD   | 2.25                     | 0.44              |
| 1:C:902:LYS:CB    | 1:C:904:LEU:HG    | 2.47                     | 0.44              |
| 1:C:2234:CYS:SG   | 1:C:2271:SER:HB3  | 2.57                     | 0.44              |
| 1:D:843:PRO:O     | 1:D:1197:PRO:HA   | 2.17                     | 0.44              |
| 1:D:902:LYS:HD2   | 1:D:902:LYS:HA    | 1.42                     | 0.44              |
| 1:D:956:LEU:CB    | 1:D:967:LYS:HD2   | 2.47                     | 0.44              |
| 1:D:1740:THR:HG22 | 1:D:2147:VAL:HG22 | 1.98                     | 0.44              |
| 1:D:2234:CYS:SG   | 1:D:2271:SER:HB3  | 2.57                     | 0.44              |
| 1:D:2782:ILE:HG23 | 1:D:2790:PRO:CD   | 2.48                     | 0.44              |
| 1:D:3240:MET:HE2  | 1:D:3240:MET:HA   | 2.00                     | 0.44              |
| 1:A:956:LEU:CB    | 1:A:967:LYS:HD2   | 2.47                     | 0.44              |
| 1:C:1012:GLN:OE1  | 1:C:1014:ILE:HD11 | 2.17                     | 0.44              |
| 1:C:2747:ILE:HG22 | 1:C:2748:ILE:N    | 2.33                     | 0.44              |
| 1:C:2755:PHE:HB2  | 1:C:2936:TYR:CZ   | 2.53                     | 0.44              |
| 1:C:2782:ILE:HG23 | 1:C:2790:PRO:CD   | 2.48                     | 0.44              |
| 1:D:893:THR:HG23  | 1:D:963:SER:HB3   | 1.99                     | 0.44              |
| 1:D:956:LEU:CD1   | 1:D:968:PRO:HD2   | 2.47                     | 0.44              |
| 1:D:2755:PHE:HB2  | 1:D:2936:TYR:CZ   | 2.53                     | 0.44              |
| 1:D:4830:HIS:NE2  | 1:D:4940:GLU:OE1  | 2.48                     | 0.44              |
| 1:A:70:LEU:HD21   | 1:A:203:MET:HE1   | 2.00                     | 0.44              |
| 1:A:3450:HIS:O    | 1:A:3450:HIS:ND1  | 2.35                     | 0.44              |
| 2:F:30:MET:HE3    | 2:F:30:MET:HB2    | 1.95                     | 0.44              |
| 2:H:30:MET:HE3    | 2:H:30:MET:HB2    | 1.95                     | 0.44              |
| 1:B:956:LEU:HD22  | 1:B:956:LEU:HA    | 1.75                     | 0.44              |
| 1:B:1273:LEU:HD22 | 1:B:1290:LEU:HD11 | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:4059:GLU:HG2  | 1:B:4169:LEU:HD13 | 2.00                     | 0.44              |
| 1:C:956:LEU:CD1   | 1:C:968:PRO:HD2   | 2.47                     | 0.44              |
| 1:C:4825:LEU:HD21 | 1:D:4841:LEU:HD21 | 2.00                     | 0.44              |
| 1:D:3283:PRO:HG3  | 1:D:3346:ILE:HG22 | 2.00                     | 0.44              |
| 1:A:1875:GLU:HA   | 1:A:1875:GLU:OE2  | 2.17                     | 0.44              |
| 1:A:2747:ILE:HG22 | 1:A:2748:ILE:N    | 2.33                     | 0.44              |
| 1:A:2761:GLU:OE2  | 1:A:2795:TYR:CD1  | 2.71                     | 0.44              |
| 1:A:2782:ILE:HG23 | 1:A:2790:PRO:CD   | 2.48                     | 0.44              |
| 1:A:3548:GLU:CD   | 1:A:3548:GLU:H    | 2.25                     | 0.44              |
| 1:B:2600:GLN:O    | 1:B:2604:ILE:HG13 | 2.18                     | 0.44              |
| 1:B:2761:GLU:OE2  | 1:B:2795:TYR:CD1  | 2.71                     | 0.44              |
| 1:C:1054:ILE:C    | 1:C:1054:ILE:HD12 | 2.43                     | 0.44              |
| 1:C:3584:GLU:OE1  | 1:C:3584:GLU:N    | 2.43                     | 0.44              |
| 1:D:909:VAL:HB    | 1:D:910:ASN:H     | 1.72                     | 0.44              |
| 1:D:1042:GLN:O    | 1:D:1046:THR:HG23 | 2.17                     | 0.44              |
| 1:D:3547:ASP:N    | 1:D:3547:ASP:OD1  | 2.51                     | 0.44              |
| 1:A:892:TRP:NE1   | 1:A:903:ARG:HD3   | 2.33                     | 0.43              |
| 1:A:1940:MET:HA   | 1:A:1940:MET:HE3  | 2.00                     | 0.43              |
| 1:B:70:LEU:HD21   | 1:B:203:MET:HE1   | 2.00                     | 0.43              |
| 1:B:2782:ILE:HG23 | 1:B:2790:PRO:CD   | 2.48                     | 0.43              |
| 1:B:3291:GLU:CG   | 1:B:3291:GLU:O    | 2.66                     | 0.43              |
| 1:C:70:LEU:HD21   | 1:C:203:MET:HE1   | 2.00                     | 0.43              |
| 1:C:1042:GLN:O    | 1:C:1046:THR:HG23 | 2.17                     | 0.43              |
| 1:C:2600:GLN:O    | 1:C:2604:ILE:HG13 | 2.18                     | 0.43              |
| 1:C:3283:PRO:HG3  | 1:C:3346:ILE:HG22 | 2.00                     | 0.43              |
| 1:D:70:LEU:HD21   | 1:D:203:MET:HE1   | 2.00                     | 0.43              |
| 1:D:3592:LYS:O    | 1:D:3596:ARG:HG2  | 2.18                     | 0.43              |
| 1:A:1054:ILE:C    | 1:A:1054:ILE:HD12 | 2.43                     | 0.43              |
| 1:A:4789:TYR:OH   | 1:A:4813:ASP:OD1  | 2.28                     | 0.43              |
| 1:B:1055:GLU:O    | 1:B:1056:PRO:C    | 2.61                     | 0.43              |
| 1:B:2605:GLU:O    | 1:B:2609:MET:HG2  | 2.18                     | 0.43              |
| 1:B:2747:ILE:HG22 | 1:B:2748:ILE:N    | 2.33                     | 0.43              |
| 1:B:2757:ASN:O    | 1:B:2761:GLU:OE1  | 2.35                     | 0.43              |
| 1:B:3592:LYS:O    | 1:B:3596:ARG:HG2  | 2.18                     | 0.43              |
| 1:C:956:LEU:CB    | 1:C:967:LYS:HD2   | 2.47                     | 0.43              |
| 1:C:2581:ASP:OD1  | 1:C:2581:ASP:C    | 2.61                     | 0.43              |
| 1:C:3006:LEU:O    | 1:C:3007:ILE:C    | 2.62                     | 0.43              |
| 1:C:3548:GLU:CD   | 1:C:3548:GLU:H    | 2.25                     | 0.43              |
| 1:D:1054:ILE:C    | 1:D:1054:ILE:HD12 | 2.43                     | 0.43              |
| 1:D:2225:ARG:N    | 1:D:2225:ARG:HD3  | 2.33                     | 0.43              |
| 1:D:2600:GLN:O    | 1:D:2604:ILE:HG13 | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:2761:GLU:OE2  | 1:D:2795:TYR:CD1  | 2.71                     | 0.43              |
| 1:D:3176:LEU:HD22 | 1:D:3191:LEU:HD13 | 2.00                     | 0.43              |
| 1:D:3291:GLU:CG   | 1:D:3291:GLU:O    | 2.66                     | 0.43              |
| 1:D:3421:ARG:CG   | 1:D:3521:ILE:HD11 | 2.47                     | 0.43              |
| 1:D:4869:GLU:HA   | 1:D:4869:GLU:OE2  | 2.18                     | 0.43              |
| 1:A:931:LYS:HE2   | 1:A:931:LYS:HB3   | 1.69                     | 0.43              |
| 1:A:2225:ARG:HD3  | 1:A:2225:ARG:N    | 2.33                     | 0.43              |
| 1:A:3291:GLU:O    | 1:A:3291:GLU:CG   | 2.66                     | 0.43              |
| 1:A:4932:GLY:HA2  | 1:D:4935:ILE:HG12 | 1.99                     | 0.43              |
| 1:B:921:TYR:CE2   | 1:B:925:MET:HE2   | 2.54                     | 0.43              |
| 1:C:3423:HIS:ND1  | 1:C:3423:HIS:C    | 2.76                     | 0.43              |
| 1:C:4789:TYR:OH   | 1:C:4813:ASP:OD1  | 2.28                     | 0.43              |
| 1:D:921:TYR:CE2   | 1:D:925:MET:HE2   | 2.53                     | 0.43              |
| 1:D:975:HIS:CD2   | 1:D:975:HIS:H     | 2.36                     | 0.43              |
| 1:D:3105:GLU:OE2  | 1:D:3168:ARG:NE   | 2.51                     | 0.43              |
| 1:A:919:ARG:HG3   | 1:A:923:LEU:HD11  | 2.01                     | 0.43              |
| 1:A:1055:GLU:O    | 1:A:1056:PRO:C    | 2.61                     | 0.43              |
| 1:A:2804:GLU:O    | 1:A:2811:LYS:NZ   | 2.51                     | 0.43              |
| 1:A:3006:LEU:O    | 1:A:3007:ILE:C    | 2.62                     | 0.43              |
| 1:B:2234:CYS:SG   | 1:B:2271:SER:HB3  | 2.57                     | 0.43              |
| 1:B:3176:LEU:HD22 | 1:B:3191:LEU:HD13 | 2.00                     | 0.43              |
| 1:B:4825:LEU:HD21 | 1:C:4841:LEU:HD21 | 2.00                     | 0.43              |
| 1:C:948:GLU:HA    | 1:C:1050:TYR:HA   | 2.01                     | 0.43              |
| 1:D:2804:GLU:O    | 1:D:2811:LYS:NZ   | 2.51                     | 0.43              |
| 1:D:3004:LEU:HB2  | 1:D:3005:PRO:HD3  | 1.99                     | 0.43              |
| 1:A:882:LEU:CB    | 1:A:970:PRO:HB3   | 2.49                     | 0.43              |
| 1:A:2761:GLU:OE2  | 1:A:2761:GLU:CA   | 2.67                     | 0.43              |
| 1:A:3176:LEU:HD22 | 1:A:3191:LEU:HD13 | 2.00                     | 0.43              |
| 1:A:3761:MET:HE2  | 1:A:3761:MET:HA   | 2.00                     | 0.43              |
| 1:B:893:THR:HG23  | 1:B:963:SER:HB3   | 1.99                     | 0.43              |
| 1:B:1054:ILE:C    | 1:B:1054:ILE:HD12 | 2.43                     | 0.43              |
| 1:B:2225:ARG:HD3  | 1:B:2225:ARG:N    | 2.33                     | 0.43              |
| 1:B:2755:PHE:HB2  | 1:B:2936:TYR:CZ   | 2.53                     | 0.43              |
| 1:B:3761:MET:HE2  | 1:B:3761:MET:HA   | 2.01                     | 0.43              |
| 1:B:4709:PHE:CD1  | 1:B:4709:PHE:C    | 2.93                     | 0.43              |
| 7:B:8006:PCW:C41  | 1:C:4848:LEU:HD22 | 2.48                     | 0.43              |
| 1:C:947:ALA:HA    | 1:C:950:ASN:ND2   | 2.34                     | 0.43              |
| 1:C:3421:ARG:CG   | 1:C:3521:ILE:HD11 | 2.47                     | 0.43              |
| 1:C:3592:LYS:O    | 1:C:3596:ARG:HG2  | 2.18                     | 0.43              |
| 1:D:948:GLU:HA    | 1:D:1050:TYR:HA   | 2.01                     | 0.43              |
| 1:D:3447:SER:O    | 1:D:3453:LYS:NZ   | 2.40                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:131:LYS:NZ    | 1:D:2374:GLY:O    | 2.52                     | 0.43              |
| 1:A:921:TYR:CE2   | 1:A:925:MET:HE2   | 2.53                     | 0.43              |
| 1:A:2092:PRO:O    | 1:A:2097:GLU:OE1  | 2.37                     | 0.43              |
| 1:A:2266:LEU:O    | 1:A:2269:GLN:NE2  | 2.52                     | 0.43              |
| 1:A:3004:LEU:HB2  | 1:A:3005:PRO:HD3  | 1.99                     | 0.43              |
| 1:A:3423:HIS:ND1  | 1:A:3423:HIS:C    | 2.76                     | 0.43              |
| 1:B:892:TRP:NE1   | 1:B:903:ARG:HD3   | 2.33                     | 0.43              |
| 1:B:4828:VAL:CG2  | 1:C:4929:ILE:HD11 | 2.49                     | 0.43              |
| 1:C:2605:GLU:O    | 1:C:2609:MET:HG2  | 2.18                     | 0.43              |
| 1:C:2804:GLU:O    | 1:C:2811:LYS:NZ   | 2.51                     | 0.43              |
| 1:D:919:ARG:HG3   | 1:D:923:LEU:HD11  | 2.01                     | 0.43              |
| 1:D:2047:LEU:HD22 | 1:D:2047:LEU:N    | 2.34                     | 0.43              |
| 1:D:3541:TYR:OH   | 1:D:3598:GLN:NE2  | 2.48                     | 0.43              |
| 1:A:2605:GLU:O    | 1:A:2609:MET:HG2  | 2.18                     | 0.43              |
| 1:A:3847:LEU:HD13 | 1:B:77:ARG:HH11   | 1.82                     | 0.43              |
| 1:A:4869:GLU:HA   | 1:A:4869:GLU:OE2  | 2.18                     | 0.43              |
| 1:B:947:ALA:HA    | 1:B:950:ASN:ND2   | 2.34                     | 0.43              |
| 1:C:892:TRP:NE1   | 1:C:903:ARG:HD3   | 2.33                     | 0.43              |
| 1:C:919:ARG:HG3   | 1:C:923:LEU:HD11  | 2.01                     | 0.43              |
| 1:C:3761:MET:HE2  | 1:C:3761:MET:HA   | 2.00                     | 0.43              |
| 1:D:892:TRP:NE1   | 1:D:903:ARG:HD3   | 2.33                     | 0.43              |
| 1:D:947:ALA:HA    | 1:D:950:ASN:ND2   | 2.34                     | 0.43              |
| 1:D:2605:GLU:O    | 1:D:2609:MET:HG2  | 2.18                     | 0.43              |
| 1:D:3041:THR:HA   | 1:D:3076:LEU:HD21 | 2.01                     | 0.43              |
| 1:A:34:LEU:HD12   | 1:A:54:SER:HB2    | 2.01                     | 0.43              |
| 1:A:947:ALA:HA    | 1:A:950:ASN:ND2   | 2.34                     | 0.43              |
| 1:A:979:THR:HG23  | 1:A:982:GLN:CD    | 2.44                     | 0.43              |
| 1:A:2600:GLN:O    | 1:A:2604:ILE:HG13 | 2.18                     | 0.43              |
| 1:A:3041:THR:HA   | 1:A:3076:LEU:HD21 | 2.01                     | 0.43              |
| 1:A:3227:GLU:O    | 1:A:3228:ARG:HB2  | 2.19                     | 0.43              |
| 1:B:2581:ASP:C    | 1:B:2581:ASP:OD1  | 2.62                     | 0.43              |
| 1:B:3450:HIS:HD1  | 1:B:3450:HIS:C    | 2.25                     | 0.43              |
| 1:C:985:LEU:HD23  | 1:C:1054:ILE:HD13 | 2.01                     | 0.43              |
| 1:C:2266:LEU:O    | 1:C:2269:GLN:NE2  | 2.52                     | 0.43              |
| 1:C:2795:TYR:HA   | 1:C:2798:PHE:HB3  | 2.01                     | 0.43              |
| 1:C:3176:LEU:HD22 | 1:C:3191:LEU:HD13 | 2.00                     | 0.43              |
| 1:C:3291:GLU:CG   | 1:C:3291:GLU:O    | 2.66                     | 0.43              |
| 1:C:4050:MET:HE3  | 1:C:4050:MET:HB3  | 1.96                     | 0.43              |
| 1:C:4869:GLU:HA   | 1:C:4869:GLU:OE2  | 2.18                     | 0.43              |
| 1:A:691:GLU:OE2   | 1:A:691:GLU:HA    | 2.19                     | 0.43              |
| 1:A:865:PRO:HD2   | 1:A:868:LEU:CD1   | 2.47                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2047:LEU:HD22 | 1:A:2047:LEU:N    | 2.34                     | 0.43              |
| 1:A:2757:ASN:O    | 1:A:2761:GLU:OE1  | 2.35                     | 0.43              |
| 1:B:691:GLU:HA    | 1:B:691:GLU:OE2   | 2.19                     | 0.43              |
| 1:B:2761:GLU:OE2  | 1:B:2761:GLU:CA   | 2.67                     | 0.43              |
| 1:B:4869:GLU:HA   | 1:B:4869:GLU:OE2  | 2.19                     | 0.43              |
| 1:C:2225:ARG:HD3  | 1:C:2225:ARG:N    | 2.33                     | 0.43              |
| 1:D:902:LYS:CB    | 1:D:904:LEU:HG    | 2.47                     | 0.43              |
| 1:D:2761:GLU:OE2  | 1:D:2761:GLU:CA   | 2.67                     | 0.43              |
| 1:D:3006:LEU:O    | 1:D:3007:ILE:C    | 2.62                     | 0.43              |
| 1:A:422:PHE:O     | 1:A:423:SER:C     | 2.62                     | 0.43              |
| 1:A:1171:MET:CE   | 1:D:3472:THR:HG23 | 2.49                     | 0.43              |
| 1:A:2755:PHE:HB2  | 1:A:2936:TYR:CZ   | 2.53                     | 0.43              |
| 1:B:2092:PRO:O    | 1:B:2097:GLU:OE1  | 2.37                     | 0.43              |
| 1:B:3240:MET:HE2  | 1:B:3240:MET:HA   | 2.00                     | 0.43              |
| 1:C:691:GLU:HA    | 1:C:691:GLU:OE2   | 2.19                     | 0.43              |
| 1:C:1479:ASP:N    | 1:C:1482:GLY:O    | 2.47                     | 0.43              |
| 1:C:2761:GLU:OE2  | 1:C:2761:GLU:CA   | 2.67                     | 0.43              |
| 1:C:3240:MET:HA   | 1:C:3240:MET:HE2  | 2.00                     | 0.43              |
| 1:C:3591:GLU:HA   | 1:C:3594:VAL:HG22 | 2.01                     | 0.43              |
| 1:C:4059:GLU:HG2  | 1:C:4169:LEU:HD13 | 2.00                     | 0.43              |
| 1:C:4649:THR:OG1  | 1:C:4801:HIS:NE2  | 2.39                     | 0.43              |
| 1:D:882:LEU:H     | 1:D:882:LEU:HG    | 1.55                     | 0.43              |
| 1:D:985:LEU:HD23  | 1:D:1054:ILE:HD13 | 2.01                     | 0.43              |
| 1:D:2795:TYR:HA   | 1:D:2798:PHE:HB3  | 2.01                     | 0.43              |
| 1:D:4671:ARG:NH1  | 1:D:4700:ASP:OD1  | 2.52                     | 0.43              |
| 1:A:894:TYR:CZ    | 1:A:896:PRO:HA    | 2.54                     | 0.42              |
| 1:A:2780:GLU:OE1  | 1:A:2780:GLU:N    | 2.44                     | 0.42              |
| 1:A:2863:LEU:HA   | 1:A:2933:MET:HE1  | 2.01                     | 0.42              |
| 1:A:4059:GLU:HG2  | 1:A:4169:LEU:HD13 | 2.00                     | 0.42              |
| 2:E:30:MET:HE3    | 2:E:30:MET:HB2    | 1.95                     | 0.42              |
| 1:B:887:ARG:O     | 1:B:892:TRP:HB2   | 2.19                     | 0.42              |
| 1:B:979:THR:HG23  | 1:B:982:GLN:CD    | 2.44                     | 0.42              |
| 1:B:3106:LYS:O    | 1:B:3109:GLU:HG3  | 2.19                     | 0.42              |
| 1:B:4050:MET:HE3  | 1:B:4050:MET:HB3  | 1.96                     | 0.42              |
| 1:B:4752:ASN:HB3  | 1:B:4754:ARG:CZ   | 2.49                     | 0.42              |
| 1:C:921:TYR:CE2   | 1:C:925:MET:HE2   | 2.53                     | 0.42              |
| 1:C:979:THR:HG23  | 1:C:982:GLN:CD    | 2.44                     | 0.42              |
| 1:C:3761:MET:HE3  | 1:C:4717:PHE:HE1  | 1.84                     | 0.42              |
| 1:D:953:LYS:HE2   | 1:D:953:LYS:HB2   | 1.47                     | 0.42              |
| 1:D:2575:HIS:CD2  | 1:D:2575:HIS:H    | 2.37                     | 0.42              |
| 1:D:2581:ASP:OD1  | 1:D:2581:ASP:C    | 2.61                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:3423:HIS:C    | 1:D:3423:HIS:ND1 | 2.76                     | 0.42              |
| 1:A:948:GLU:HA    | 1:A:1050:TYR:HA  | 2.01                     | 0.42              |
| 1:A:3240:MET:HE2  | 1:A:3240:MET:HA  | 2.00                     | 0.42              |
| 1:A:4050:MET:HE3  | 1:A:4050:MET:HB3 | 1.96                     | 0.42              |
| 1:B:33:GLN:OE1    | 1:B:33:GLN:HA    | 2.19                     | 0.42              |
| 1:B:882:LEU:CB    | 1:B:970:PRO:HB3  | 2.48                     | 0.42              |
| 1:B:948:GLU:HA    | 1:B:1050:TYR:HA  | 2.01                     | 0.42              |
| 1:C:33:GLN:OE1    | 1:C:33:GLN:HA    | 2.19                     | 0.42              |
| 1:D:872:ARG:CG    | 1:D:927:GLY:HA2  | 2.46                     | 0.42              |
| 1:D:882:LEU:CB    | 1:D:970:PRO:HB3  | 2.49                     | 0.42              |
| 1:D:1479:ASP:N    | 1:D:1482:GLY:O   | 2.47                     | 0.42              |
| 1:D:2922:GLU:O    | 1:D:2926:GLU:HG2 | 2.20                     | 0.42              |
| 1:D:3761:MET:HE3  | 1:D:4717:PHE:HE1 | 1.84                     | 0.42              |
| 1:A:2795:TYR:HA   | 1:A:2798:PHE:HB3 | 2.01                     | 0.42              |
| 1:B:34:LEU:HD12   | 1:B:54:SER:HB2   | 2.01                     | 0.42              |
| 1:B:919:ARG:HG3   | 1:B:923:LEU:HD11 | 2.01                     | 0.42              |
| 1:B:2804:GLU:O    | 1:B:2811:LYS:NZ  | 2.51                     | 0.42              |
| 1:B:3227:GLU:O    | 1:B:3228:ARG:HB2 | 2.19                     | 0.42              |
| 1:B:3410:TYR:N    | 1:B:3411:PRO:HD2 | 2.34                     | 0.42              |
| 1:C:422:PHE:O     | 1:C:423:SER:C    | 2.62                     | 0.42              |
| 1:C:3227:GLU:O    | 1:C:3228:ARG:HB2 | 2.19                     | 0.42              |
| 1:C:3410:TYR:N    | 1:C:3411:PRO:HD2 | 2.34                     | 0.42              |
| 1:D:1830:ASP:OD1  | 1:D:1830:ASP:N   | 2.52                     | 0.42              |
| 1:A:879:ILE:HD12  | 1:A:879:ILE:HA   | 1.79                     | 0.42              |
| 1:A:942:MET:HE3   | 1:A:945:GLU:OE2  | 2.20                     | 0.42              |
| 1:A:2575:HIS:H    | 1:A:2575:HIS:CD2 | 2.37                     | 0.42              |
| 1:B:1642:ILE:HD11 | 1:B:1649:MET:HE3 | 2.02                     | 0.42              |
| 1:B:2922:GLU:O    | 1:B:2926:GLU:HG2 | 2.20                     | 0.42              |
| 1:B:2978:LEU:HD23 | 1:B:2978:LEU:O   | 2.19                     | 0.42              |
| 1:B:3006:LEU:O    | 1:B:3007:ILE:C   | 2.62                     | 0.42              |
| 1:B:3570:LEU:HD22 | 1:B:3570:LEU:N   | 2.35                     | 0.42              |
| 1:C:2334:ASP:HA   | 1:C:2337:ARG:HD3 | 2.01                     | 0.42              |
| 1:D:979:THR:HG23  | 1:D:982:GLN:CD   | 2.44                     | 0.42              |
| 1:D:2266:LEU:O    | 1:D:2269:GLN:NE2 | 2.52                     | 0.42              |
| 1:D:2334:ASP:HA   | 1:D:2337:ARG:HD3 | 2.01                     | 0.42              |
| 1:D:3410:TYR:N    | 1:D:3411:PRO:HD2 | 2.34                     | 0.42              |
| 1:A:3570:LEU:HD22 | 1:A:3570:LEU:N   | 2.35                     | 0.42              |
| 1:A:3974:GLY:N    | 1:A:3975:PRO:HA  | 2.35                     | 0.42              |
| 1:B:942:MET:HE3   | 1:B:945:GLU:OE2  | 2.20                     | 0.42              |
| 1:B:2183:ILE:HG23 | 1:B:2236:PHE:HB2 | 2.02                     | 0.42              |
| 1:B:2266:LEU:O    | 1:B:2269:GLN:NE2 | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2795:TYR:HA   | 1:B:2798:PHE:HB3  | 2.01                     | 0.42              |
| 1:C:2629:PHE:CD1  | 1:C:2629:PHE:C    | 2.98                     | 0.42              |
| 1:C:2863:LEU:HA   | 1:C:2933:MET:HE1  | 2.01                     | 0.42              |
| 1:C:2978:LEU:HD23 | 1:C:2978:LEU:O    | 2.19                     | 0.42              |
| 1:D:422:PHE:O     | 1:D:423:SER:C     | 2.62                     | 0.42              |
| 1:D:2183:ILE:HG23 | 1:D:2236:PHE:HB2  | 2.02                     | 0.42              |
| 1:D:2863:LEU:HA   | 1:D:2933:MET:HE1  | 2.02                     | 0.42              |
| 1:D:3974:GLY:N    | 1:D:3975:PRO:HA   | 2.35                     | 0.42              |
| 1:A:1830:ASP:OD1  | 1:A:1830:ASP:N    | 2.52                     | 0.42              |
| 1:A:3761:MET:HE3  | 1:A:4717:PHE:HE1  | 1.84                     | 0.42              |
| 1:B:894:TYR:CZ    | 1:B:896:PRO:HA    | 2.54                     | 0.42              |
| 1:B:2863:LEU:CD2  | 1:B:2933:MET:SD   | 3.08                     | 0.42              |
| 1:B:3686:GLU:OE1  | 1:B:3686:GLU:N    | 2.46                     | 0.42              |
| 1:C:887:ARG:O     | 1:C:892:TRP:HB2   | 2.19                     | 0.42              |
| 1:C:1926:GLY:O    | 1:C:1930:MET:HG3  | 2.20                     | 0.42              |
| 1:C:3106:LYS:O    | 1:C:3109:GLU:HG3  | 2.19                     | 0.42              |
| 1:C:3847:LEU:HD13 | 1:D:77:ARG:HH11   | 1.84                     | 0.42              |
| 7:C:8006:PCW:C41  | 1:D:4848:LEU:HD22 | 2.49                     | 0.42              |
| 1:D:894:TYR:CZ    | 1:D:896:PRO:HA    | 2.54                     | 0.42              |
| 1:D:2863:LEU:CD2  | 1:D:2933:MET:SD   | 3.08                     | 0.42              |
| 1:D:3227:GLU:O    | 1:D:3228:ARG:HB2  | 2.19                     | 0.42              |
| 1:A:956:LEU:HD12  | 1:A:967:LYS:HB2   | 2.01                     | 0.42              |
| 1:A:2183:ILE:HG23 | 1:A:2236:PHE:HB2  | 2.02                     | 0.42              |
| 1:A:2817:MET:SD   | 1:A:2822:TRP:HE3  | 2.42                     | 0.42              |
| 1:A:3105:GLU:OE2  | 1:A:3168:ARG:NE   | 2.51                     | 0.42              |
| 1:A:3639:MET:HE3  | 1:A:3639:MET:HB2  | 1.98                     | 0.42              |
| 1:A:4671:ARG:NH1  | 1:A:4700:ASP:OD1  | 2.52                     | 0.42              |
| 1:B:1926:GLY:O    | 1:B:1930:MET:HG3  | 2.19                     | 0.42              |
| 1:B:2234:CYS:HB3  | 1:B:2238:CYS:HB2  | 1.62                     | 0.42              |
| 1:B:4247:GLU:OE2  | 1:B:4247:GLU:HA   | 2.20                     | 0.42              |
| 1:B:4671:ARG:NH1  | 1:B:4700:ASP:OD1  | 2.52                     | 0.42              |
| 1:C:2047:LEU:HD22 | 1:C:2047:LEU:N    | 2.34                     | 0.42              |
| 1:C:2817:MET:SD   | 1:C:2822:TRP:HE3  | 2.42                     | 0.42              |
| 1:C:4828:VAL:CG2  | 1:D:4929:ILE:HD11 | 2.49                     | 0.42              |
| 1:D:2092:PRO:O    | 1:D:2097:GLU:OE1  | 2.37                     | 0.42              |
| 1:D:2224:ILE:HD11 | 1:D:2268:MET:HE1  | 2.02                     | 0.42              |
| 1:D:3591:GLU:HA   | 1:D:3594:VAL:HG22 | 2.01                     | 0.42              |
| 1:D:4753:GLU:OE1  | 1:D:4753:GLU:N    | 2.53                     | 0.42              |
| 1:A:1044:VAL:HG12 | 1:A:1048:LEU:HD12 | 2.02                     | 0.42              |
| 1:A:2229:MET:HE3  | 1:A:2229:MET:HB3  | 1.99                     | 0.42              |
| 1:A:2922:GLU:O    | 1:A:2926:GLU:HG2  | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:985:LEU:HD23  | 1:B:1054:ILE:HD13 | 2.01                     | 0.42              |
| 1:C:490:ASN:O     | 1:C:494:ARG:HG2   | 2.20                     | 0.42              |
| 1:C:879:ILE:HD12  | 1:C:879:ILE:HA    | 1.79                     | 0.42              |
| 1:C:942:MET:HE3   | 1:C:945:GLU:OE2   | 2.20                     | 0.42              |
| 1:C:2009:MET:HE3  | 1:C:2009:MET:HB3  | 1.94                     | 0.42              |
| 1:C:2092:PRO:O    | 1:C:2097:GLU:OE1  | 2.37                     | 0.42              |
| 1:C:2224:ILE:HD11 | 1:C:2268:MET:HE1  | 2.02                     | 0.42              |
| 1:C:2756:ILE:HG23 | 1:C:2810:ILE:HB   | 2.02                     | 0.42              |
| 1:C:3468:MET:SD   | 1:D:1174:SER:O    | 2.78                     | 0.42              |
| 1:C:4649:THR:HG1  | 1:C:4801:HIS:CD2  | 2.33                     | 0.42              |
| 1:C:4752:ASN:HB3  | 1:C:4754:ARG:CZ   | 2.49                     | 0.42              |
| 7:C:8006:PCW:H272 | 7:C:8006:PCW:H483 | 2.02                     | 0.42              |
| 1:D:169:ASP:OD1   | 1:D:169:ASP:N     | 2.53                     | 0.42              |
| 1:D:942:MET:HE3   | 1:D:945:GLU:OE2   | 2.20                     | 0.42              |
| 1:D:1044:VAL:HG12 | 1:D:1048:LEU:HD12 | 2.02                     | 0.42              |
| 1:D:2817:MET:SD   | 1:D:2822:TRP:HE3  | 2.42                     | 0.42              |
| 1:A:985:LEU:HD23  | 1:A:1054:ILE:HD13 | 2.01                     | 0.42              |
| 1:A:2863:LEU:CD2  | 1:A:2933:MET:SD   | 3.08                     | 0.42              |
| 1:A:3106:LYS:O    | 1:A:3109:GLU:HG3  | 2.19                     | 0.42              |
| 1:A:3721:TYR:HA   | 1:A:3724:MET:HE3  | 2.02                     | 0.42              |
| 1:A:4247:GLU:HA   | 1:A:4247:GLU:OE2  | 2.20                     | 0.42              |
| 1:A:4752:ASN:HB3  | 1:A:4754:ARG:CZ   | 2.49                     | 0.42              |
| 2:G:30:MET:HE3    | 2:G:30:MET:HB2    | 1.95                     | 0.42              |
| 1:B:956:LEU:HD12  | 1:B:967:LYS:HB2   | 2.01                     | 0.42              |
| 1:C:34:LEU:HD12   | 1:C:54:SER:HB2    | 2.01                     | 0.42              |
| 1:C:894:TYR:CZ    | 1:C:896:PRO:HA    | 2.54                     | 0.42              |
| 1:C:1642:ILE:HD11 | 1:C:1649:MET:HE3  | 2.02                     | 0.42              |
| 1:C:2183:ILE:HG23 | 1:C:2236:PHE:HB2  | 2.02                     | 0.42              |
| 1:C:2863:LEU:CD2  | 1:C:2933:MET:SD   | 3.08                     | 0.42              |
| 1:D:3293:PRO:O    | 1:D:3295:PRO:CD   | 2.68                     | 0.42              |
| 1:D:3761:MET:HE2  | 1:D:3761:MET:HA   | 2.00                     | 0.42              |
| 1:A:957:PRO:HG2   | 1:A:960:TYR:CG    | 2.55                     | 0.42              |
| 1:A:2629:PHE:CD1  | 1:A:2629:PHE:C    | 2.98                     | 0.42              |
| 1:A:3547:ASP:N    | 1:A:3547:ASP:OD1  | 2.51                     | 0.42              |
| 1:A:3591:GLU:HA   | 1:A:3594:VAL:HG22 | 2.01                     | 0.42              |
| 1:B:2445:GLN:OE1  | 1:B:2445:GLN:HA   | 2.20                     | 0.42              |
| 1:B:2863:LEU:HA   | 1:B:2933:MET:HE1  | 2.02                     | 0.42              |
| 1:B:3105:GLU:OE2  | 1:B:3168:ARG:NE   | 2.51                     | 0.42              |
| 1:B:3721:TYR:HA   | 1:B:3724:MET:HE3  | 2.02                     | 0.42              |
| 1:C:882:LEU:CB    | 1:C:970:PRO:HB3   | 2.49                     | 0.42              |
| 1:C:1044:VAL:HG12 | 1:C:1048:LEU:HD12 | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1055:GLU:O    | 1:C:1056:PRO:C    | 2.61                     | 0.42              |
| 1:C:3570:LEU:HD22 | 1:C:3570:LEU:N    | 2.35                     | 0.42              |
| 1:D:490:ASN:O     | 1:D:494:ARG:HG2   | 2.20                     | 0.42              |
| 1:D:956:LEU:HD22  | 1:D:956:LEU:HA    | 1.75                     | 0.42              |
| 1:D:2445:GLN:OE1  | 1:D:2445:GLN:HA   | 2.20                     | 0.42              |
| 1:D:3106:LYS:O    | 1:D:3109:GLU:HG3  | 2.19                     | 0.42              |
| 1:D:4059:GLU:HG2  | 1:D:4169:LEU:HD13 | 2.00                     | 0.42              |
| 1:D:4752:ASN:HB3  | 1:D:4754:ARG:CZ   | 2.49                     | 0.42              |
| 1:A:4821:LEU:HD23 | 1:A:4821:LEU:HA   | 1.92                     | 0.41              |
| 7:A:8006:PCW:H341 | 7:A:8006:PCW:O31  | 2.20                     | 0.41              |
| 1:B:957:PRO:HG2   | 1:B:960:TYR:CG    | 2.55                     | 0.41              |
| 1:B:2817:MET:SD   | 1:B:2822:TRP:HE3  | 2.42                     | 0.41              |
| 1:B:3041:THR:HA   | 1:B:3076:LEU:HD21 | 2.01                     | 0.41              |
| 1:B:3108:VAL:CG2  | 1:B:3176:LEU:HB2  | 2.50                     | 0.41              |
| 1:B:3974:GLY:N    | 1:B:3975:PRO:HA   | 2.35                     | 0.41              |
| 1:C:956:LEU:HD12  | 1:C:967:LYS:HB2   | 2.01                     | 0.41              |
| 1:C:1830:ASP:N    | 1:C:1830:ASP:OD1  | 2.52                     | 0.41              |
| 1:C:3041:THR:HA   | 1:C:3076:LEU:HD21 | 2.01                     | 0.41              |
| 1:C:3865:ASP:HA   | 1:C:3868:VAL:HG22 | 2.02                     | 0.41              |
| 1:C:4247:GLU:OE2  | 1:C:4247:GLU:HA   | 2.20                     | 0.41              |
| 1:D:34:LEU:HD12   | 1:D:54:SER:HB2    | 2.01                     | 0.41              |
| 1:D:887:ARG:O     | 1:D:892:TRP:HB2   | 2.19                     | 0.41              |
| 1:D:956:LEU:HD12  | 1:D:967:LYS:HB2   | 2.01                     | 0.41              |
| 1:D:1926:GLY:O    | 1:D:1930:MET:HG3  | 2.20                     | 0.41              |
| 1:D:2215:VAL:HG11 | 1:D:2229:MET:CE   | 2.50                     | 0.41              |
| 1:D:4050:MET:HE3  | 1:D:4050:MET:HB3  | 1.96                     | 0.41              |
| 1:A:902:LYS:HA    | 1:A:902:LYS:HD2   | 1.41                     | 0.41              |
| 1:A:953:LYS:CB    | 1:A:971:LEU:HA    | 2.45                     | 0.41              |
| 1:A:1642:ILE:HD11 | 1:A:1649:MET:HE3  | 2.02                     | 0.41              |
| 1:A:3410:TYR:N    | 1:A:3411:PRO:HD2  | 2.34                     | 0.41              |
| 1:B:882:LEU:H     | 1:B:882:LEU:HG    | 1.55                     | 0.41              |
| 1:B:4890:ARG:NH1  | 1:C:4897:ASP:OD2  | 2.53                     | 0.41              |
| 7:B:8006:PCW:O31  | 7:B:8006:PCW:H341 | 2.20                     | 0.41              |
| 1:D:696:TYR:CD2   | 1:D:1241:LYS:HD2  | 2.55                     | 0.41              |
| 1:D:2978:LEU:O    | 1:D:2978:LEU:HD23 | 2.19                     | 0.41              |
| 1:D:3721:TYR:HA   | 1:D:3724:MET:HE3  | 2.02                     | 0.41              |
| 7:D:8006:PCW:H341 | 7:D:8006:PCW:O31  | 2.20                     | 0.41              |
| 1:A:887:ARG:O     | 1:A:892:TRP:HB2   | 2.19                     | 0.41              |
| 1:A:938:CYS:HB3   | 1:A:1057:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:3108:VAL:CG2  | 1:A:3176:LEU:HB2  | 2.50                     | 0.41              |
| 1:A:3781:MET:HE2  | 1:A:3781:MET:HB3  | 1.96                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2645:LEU:HD13 | 1:B:2679:LEU:HD21 | 2.03                     | 0.41              |
| 1:B:3293:PRO:O    | 1:B:3295:PRO:CD   | 2.68                     | 0.41              |
| 1:C:169:ASP:OD1   | 1:C:169:ASP:N     | 2.53                     | 0.41              |
| 1:C:760:ILE:HG23  | 1:C:760:ILE:O     | 2.20                     | 0.41              |
| 1:C:931:LYS:HE2   | 1:C:931:LYS:HB3   | 1.69                     | 0.41              |
| 1:D:999:ARG:HH11  | 1:D:999:ARG:HG2   | 1.86                     | 0.41              |
| 1:D:4227:GLU:O    | 1:D:4227:GLU:CG   | 2.69                     | 0.41              |
| 1:A:1964:GLU:HA   | 1:A:3651:CYS:SG   | 2.61                     | 0.41              |
| 1:A:2525:VAL:HG23 | 1:A:2526:GLY:N    | 2.36                     | 0.41              |
| 1:A:2747:ILE:HD12 | 1:A:2747:ILE:H    | 1.86                     | 0.41              |
| 1:A:4753:GLU:OE1  | 1:A:4753:GLU:N    | 2.53                     | 0.41              |
| 1:B:953:LYS:HB2   | 1:B:953:LYS:HE2   | 1.46                     | 0.41              |
| 1:B:1044:VAL:HG12 | 1:B:1048:LEU:HD12 | 2.02                     | 0.41              |
| 1:B:2334:ASP:HA   | 1:B:2337:ARG:HD3  | 2.01                     | 0.41              |
| 1:B:3108:VAL:HG23 | 1:B:3176:LEU:HD12 | 2.02                     | 0.41              |
| 1:B:3458:ASN:O    | 1:B:3459:PHE:C    | 2.63                     | 0.41              |
| 1:B:3468:MET:SD   | 1:C:1174:SER:O    | 2.78                     | 0.41              |
| 1:B:3761:MET:HE3  | 1:B:4717:PHE:HE1  | 1.84                     | 0.41              |
| 1:C:3108:VAL:CG2  | 1:C:3176:LEU:HB2  | 2.50                     | 0.41              |
| 1:C:3721:TYR:HA   | 1:C:3724:MET:HE3  | 2.02                     | 0.41              |
| 1:D:33:GLN:HA     | 1:D:33:GLN:OE1    | 2.19                     | 0.41              |
| 1:D:691:GLU:HA    | 1:D:691:GLU:OE2   | 2.19                     | 0.41              |
| 1:D:1116:LEU:HD23 | 1:D:1116:LEU:HA   | 1.95                     | 0.41              |
| 1:D:2525:VAL:HG23 | 1:D:2526:GLY:N    | 2.36                     | 0.41              |
| 1:A:1926:GLY:O    | 1:A:1930:MET:HG3  | 2.20                     | 0.41              |
| 1:A:2224:ILE:HD11 | 1:A:2268:MET:HE1  | 2.02                     | 0.41              |
| 1:A:2445:GLN:OE1  | 1:A:2445:GLN:HA   | 2.20                     | 0.41              |
| 1:A:2581:ASP:OD1  | 1:A:2581:ASP:C    | 2.62                     | 0.41              |
| 1:A:2645:LEU:HD13 | 1:A:2679:LEU:HD21 | 2.02                     | 0.41              |
| 1:A:3108:VAL:HG23 | 1:A:3176:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:3293:PRO:O    | 1:A:3295:PRO:CD   | 2.68                     | 0.41              |
| 1:B:804:LEU:HD22  | 1:B:804:LEU:HA    | 1.96                     | 0.41              |
| 1:B:938:CYS:HB3   | 1:B:1057:PRO:HD3  | 2.02                     | 0.41              |
| 1:B:1749:PHE:HB2  | 1:B:1757:ASP:HA   | 2.03                     | 0.41              |
| 1:B:2047:LEU:HD22 | 1:B:2047:LEU:N    | 2.34                     | 0.41              |
| 1:B:4753:GLU:OE1  | 1:B:4753:GLU:N    | 2.53                     | 0.41              |
| 7:B:8006:PCW:H272 | 7:B:8006:PCW:H483 | 2.02                     | 0.41              |
| 1:C:2922:GLU:O    | 1:C:2926:GLU:HG2  | 2.20                     | 0.41              |
| 1:C:3108:VAL:HG23 | 1:C:3176:LEU:HD12 | 2.02                     | 0.41              |
| 1:C:4227:GLU:O    | 1:C:4227:GLU:CG   | 2.69                     | 0.41              |
| 1:C:4753:GLU:OE1  | 1:C:4753:GLU:N    | 2.53                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:885:LEU:HD12  | 1:D:960:TYR:CE2   | 2.55                     | 0.41              |
| 1:D:2629:PHE:CD1  | 1:D:2629:PHE:C    | 2.98                     | 0.41              |
| 1:D:3108:VAL:CG2  | 1:D:3176:LEU:HB2  | 2.50                     | 0.41              |
| 1:D:3600:VAL:HG12 | 1:D:3604:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:33:GLN:OE1    | 1:A:33:GLN:HA     | 2.19                     | 0.41              |
| 1:A:3521:ILE:N    | 1:A:3521:ILE:HD12 | 2.36                     | 0.41              |
| 1:B:169:ASP:N     | 1:B:169:ASP:OD1   | 2.53                     | 0.41              |
| 1:B:760:ILE:HG23  | 1:B:760:ILE:O     | 2.20                     | 0.41              |
| 1:B:999:ARG:HG2   | 1:B:999:ARG:HH11  | 1.86                     | 0.41              |
| 1:B:4691:GLU:CD   | 1:B:4691:GLU:N    | 2.79                     | 0.41              |
| 1:C:871:ILE:H     | 1:C:871:ILE:HG13  | 1.40                     | 0.41              |
| 1:C:938:CYS:HB3   | 1:C:1057:PRO:HD3  | 2.02                     | 0.41              |
| 1:C:2575:HIS:CD2  | 1:C:2575:HIS:H    | 2.37                     | 0.41              |
| 1:C:3541:TYR:OH   | 1:C:3598:GLN:NE2  | 2.48                     | 0.41              |
| 1:C:3607:LEU:HD23 | 1:C:3607:LEU:HA   | 1.93                     | 0.41              |
| 1:D:2640:MET:HE3  | 1:D:2640:MET:HB3  | 2.00                     | 0.41              |
| 1:D:3291:GLU:O    | 1:D:3291:GLU:HG2  | 2.21                     | 0.41              |
| 1:D:3570:LEU:HD22 | 1:D:3570:LEU:N    | 2.35                     | 0.41              |
| 1:A:999:ARG:HG2   | 1:A:999:ARG:HH11  | 1.86                     | 0.41              |
| 1:A:2215:VAL:HG11 | 1:A:2229:MET:CE   | 2.50                     | 0.41              |
| 1:A:2942:LEU:H    | 1:A:2942:LEU:HD12 | 1.86                     | 0.41              |
| 1:A:3231:LEU:HD12 | 1:A:3231:LEU:H    | 1.86                     | 0.41              |
| 1:B:490:ASN:O     | 1:B:494:ARG:HG2   | 2.20                     | 0.41              |
| 1:B:696:TYR:CD2   | 1:B:1241:LYS:HD2  | 2.55                     | 0.41              |
| 1:B:753:VAL:HB    | 1:B:754:PRO:C     | 2.46                     | 0.41              |
| 1:B:971:LEU:H     | 1:B:971:LEU:HG    | 1.52                     | 0.41              |
| 1:B:1830:ASP:N    | 1:B:1830:ASP:OD1  | 2.52                     | 0.41              |
| 1:B:3591:GLU:HA   | 1:B:3594:VAL:HG22 | 2.01                     | 0.41              |
| 1:C:999:ARG:HH11  | 1:C:999:ARG:HG2   | 1.86                     | 0.41              |
| 1:C:2799:SER:O    | 1:C:2802:ASP:OD1  | 2.39                     | 0.41              |
| 1:C:3293:PRO:O    | 1:C:3295:PRO:CD   | 2.68                     | 0.41              |
| 1:C:3600:VAL:HG12 | 1:C:3604:LEU:HD12 | 2.02                     | 0.41              |
| 1:C:4691:GLU:CD   | 1:C:4691:GLU:N    | 2.79                     | 0.41              |
| 1:D:760:ILE:O     | 1:D:760:ILE:HG23  | 2.20                     | 0.41              |
| 1:D:914:LEU:HD21  | 1:D:919:ARG:CB    | 2.51                     | 0.41              |
| 1:D:953:LYS:H     | 1:D:953:LYS:HG3   | 1.64                     | 0.41              |
| 1:D:982:GLN:CG    | 1:D:1054:ILE:HD11 | 2.51                     | 0.41              |
| 1:D:2645:LEU:HD13 | 1:D:2679:LEU:HD21 | 2.03                     | 0.41              |
| 1:D:2756:ILE:HG23 | 1:D:2810:ILE:HB   | 2.02                     | 0.41              |
| 1:D:3458:ASN:O    | 1:D:3459:PHE:C    | 2.63                     | 0.41              |
| 1:D:3865:ASP:HA   | 1:D:3868:VAL:HG22 | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:753:VAL:HB    | 1:A:754:PRO:C     | 2.46                     | 0.41              |
| 1:A:760:ILE:HG23  | 1:A:760:ILE:O     | 2.20                     | 0.41              |
| 1:A:2978:LEU:O    | 1:A:2978:LEU:HD23 | 2.19                     | 0.41              |
| 7:A:8006:PCW:H272 | 7:A:8006:PCW:H483 | 2.02                     | 0.41              |
| 1:B:218:GLY:N     | 1:B:263:LEU:O     | 2.48                     | 0.41              |
| 1:B:422:PHE:O     | 1:B:423:SER:C     | 2.62                     | 0.41              |
| 1:B:982:GLN:CG    | 1:B:1054:ILE:HD11 | 2.51                     | 0.41              |
| 1:B:2756:ILE:HG23 | 1:B:2810:ILE:HB   | 2.02                     | 0.41              |
| 1:B:2799:SER:O    | 1:B:2802:ASP:OD1  | 2.39                     | 0.41              |
| 1:C:753:VAL:HB    | 1:C:754:PRO:C     | 2.46                     | 0.41              |
| 1:C:3521:ILE:N    | 1:C:3521:ILE:HD12 | 2.36                     | 0.41              |
| 1:C:3974:GLY:N    | 1:C:3975:PRO:HA   | 2.35                     | 0.41              |
| 1:D:938:CYS:HB3   | 1:D:1057:PRO:HD3  | 2.02                     | 0.41              |
| 1:D:1055:GLU:O    | 1:D:1056:PRO:C    | 2.61                     | 0.41              |
| 1:D:4691:GLU:N    | 1:D:4691:GLU:CD   | 2.79                     | 0.41              |
| 1:A:696:TYR:CD2   | 1:A:1241:LYS:HD2  | 2.55                     | 0.41              |
| 1:A:885:LEU:HD12  | 1:A:960:TYR:CE2   | 2.56                     | 0.41              |
| 1:A:2769:PHE:O    | 1:A:2773:GLN:HG2  | 2.21                     | 0.41              |
| 1:A:2800:GLU:HA   | 1:A:2803:LYS:HD3  | 2.03                     | 0.41              |
| 1:A:3388:ALA:O    | 1:A:3392:GLU:N    | 2.39                     | 0.41              |
| 1:A:3458:ASN:O    | 1:A:3459:PHE:C    | 2.63                     | 0.41              |
| 1:A:3865:ASP:HA   | 1:A:3868:VAL:HG22 | 2.02                     | 0.41              |
| 1:B:885:LEU:HD12  | 1:B:960:TYR:CE2   | 2.56                     | 0.41              |
| 1:B:1964:GLU:HA   | 1:B:3651:CYS:SG   | 2.61                     | 0.41              |
| 1:B:2224:ILE:HD11 | 1:B:2268:MET:HE1  | 2.02                     | 0.41              |
| 1:B:2413:GLU:HB2  | 1:B:2416:ARG:HE   | 1.86                     | 0.41              |
| 1:B:2575:HIS:CD2  | 1:B:2575:HIS:H    | 2.37                     | 0.41              |
| 1:B:2701:MET:HB3  | 1:B:2702:PRO:HD3  | 2.03                     | 0.41              |
| 1:B:3639:MET:HE3  | 1:B:3639:MET:HB2  | 1.98                     | 0.41              |
| 1:B:3639:MET:O    | 1:B:3641:PRO:HD3  | 2.21                     | 0.41              |
| 1:B:3865:ASP:HA   | 1:B:3868:VAL:HG22 | 2.03                     | 0.41              |
| 1:C:696:TYR:CD2   | 1:C:1241:LYS:HD2  | 2.55                     | 0.41              |
| 1:C:885:LEU:HD12  | 1:C:960:TYR:CE2   | 2.56                     | 0.41              |
| 1:C:1964:GLU:HA   | 1:C:3651:CYS:SG   | 2.60                     | 0.41              |
| 1:C:2215:VAL:HG11 | 1:C:2229:MET:CE   | 2.50                     | 0.41              |
| 1:C:2445:GLN:OE1  | 1:C:2445:GLN:HA   | 2.20                     | 0.41              |
| 1:C:2863:LEU:CD1  | 1:C:2926:GLU:OE1  | 2.68                     | 0.41              |
| 1:C:3291:GLU:O    | 1:C:3291:GLU:HG2  | 2.21                     | 0.41              |
| 1:C:3547:ASP:N    | 1:C:3547:ASP:OD1  | 2.51                     | 0.41              |
| 1:C:4890:ARG:NH1  | 1:D:4897:ASP:OD2  | 2.54                     | 0.41              |
| 1:D:1642:ILE:HD11 | 1:D:1649:MET:HE3  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:2747:ILE:HD12 | 1:D:2747:ILE:H    | 1.86                     | 0.41              |
| 1:D:2918:ALA:HA   | 1:D:2921:ARG:HB3  | 2.03                     | 0.41              |
| 1:D:2942:LEU:HD12 | 1:D:2942:LEU:H    | 1.86                     | 0.41              |
| 1:D:3639:MET:HE3  | 1:D:3639:MET:HB2  | 1.98                     | 0.41              |
| 1:D:3639:MET:O    | 1:D:3641:PRO:HD3  | 2.21                     | 0.41              |
| 7:D:8006:PCW:H272 | 7:D:8006:PCW:H483 | 2.02                     | 0.41              |
| 1:A:490:ASN:O     | 1:A:494:ARG:HG2   | 2.20                     | 0.41              |
| 1:A:822:LEU:HD23  | 1:A:823:HIS:N     | 2.36                     | 0.41              |
| 1:A:2334:ASP:HA   | 1:A:2337:ARG:HD3  | 2.01                     | 0.41              |
| 1:A:3639:MET:O    | 1:A:3641:PRO:HD3  | 2.21                     | 0.41              |
| 1:B:3224:SER:OG   | 1:B:3227:GLU:OE2  | 2.31                     | 0.41              |
| 1:C:957:PRO:HG2   | 1:C:960:TYR:CG    | 2.55                     | 0.41              |
| 1:C:2480:LEU:HD11 | 1:C:2484:GLY:HA2  | 2.03                     | 0.41              |
| 1:D:1788:LEU:HD12 | 1:D:1788:LEU:HA   | 1.95                     | 0.41              |
| 1:A:1063:GLN:OE1  | 1:A:1063:GLN:N    | 2.55                     | 0.40              |
| 1:A:3540:ARG:NH2  | 1:A:3549:GLU:C    | 2.80                     | 0.40              |
| 1:A:3540:ARG:NH1  | 1:A:3545:ASP:OD2  | 2.54                     | 0.40              |
| 1:B:2629:PHE:CD1  | 1:B:2629:PHE:C    | 2.98                     | 0.40              |
| 1:B:3547:ASP:N    | 1:B:3547:ASP:OD1  | 2.51                     | 0.40              |
| 1:B:3600:VAL:HG12 | 1:B:3604:LEU:HD12 | 2.02                     | 0.40              |
| 1:C:1063:GLN:N    | 1:C:1063:GLN:OE1  | 2.54                     | 0.40              |
| 1:C:2701:MET:HB3  | 1:C:2702:PRO:HD3  | 2.03                     | 0.40              |
| 1:C:3330:ILE:O    | 1:C:3404:ARG:NH2  | 2.53                     | 0.40              |
| 1:D:908:LEU:C     | 1:D:909:VAL:HG22  | 2.46                     | 0.40              |
| 1:D:1063:GLN:OE1  | 1:D:1063:GLN:N    | 2.55                     | 0.40              |
| 1:D:2635:ASN:OD1  | 1:D:2635:ASN:C    | 2.65                     | 0.40              |
| 1:D:3108:VAL:HG23 | 1:D:3176:LEU:HD12 | 2.03                     | 0.40              |
| 1:D:4796:MET:HE1  | 7:D:8006:PCW:C21  | 2.51                     | 0.40              |
| 1:A:1788:LEU:HD12 | 1:A:1788:LEU:HA   | 1.95                     | 0.40              |
| 1:A:2635:ASN:OD1  | 1:A:2635:ASN:C    | 2.65                     | 0.40              |
| 1:A:3600:VAL:HG12 | 1:A:3604:LEU:HD12 | 2.02                     | 0.40              |
| 1:A:4796:MET:HE1  | 7:A:8006:PCW:C21  | 2.51                     | 0.40              |
| 1:B:2009:MET:HE3  | 1:B:2009:MET:HB3  | 1.94                     | 0.40              |
| 1:B:2769:PHE:O    | 1:B:2773:GLN:HG2  | 2.21                     | 0.40              |
| 1:B:2942:LEU:H    | 1:B:2942:LEU:HD12 | 1.86                     | 0.40              |
| 1:B:3351:ARG:HH11 | 1:B:3351:ARG:HG2  | 1.87                     | 0.40              |
| 1:B:3521:ILE:HD12 | 1:B:3521:ILE:N    | 2.36                     | 0.40              |
| 1:C:908:LEU:C     | 1:C:909:VAL:HG22  | 2.46                     | 0.40              |
| 1:C:975:HIS:CD2   | 1:C:975:HIS:H     | 2.36                     | 0.40              |
| 1:C:2215:VAL:HG21 | 1:C:2229:MET:HE3  | 2.04                     | 0.40              |
| 1:C:3589:ASP:OD1  | 1:C:3590:PRO:CD   | 2.70                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:957:PRO:HG2   | 1:D:960:TYR:CG    | 2.55                     | 0.40              |
| 1:D:1964:GLU:HA   | 1:D:3651:CYS:SG   | 2.60                     | 0.40              |
| 1:D:3540:ARG:NH2  | 1:D:3549:GLU:C    | 2.80                     | 0.40              |
| 1:A:323:LYS:O     | 1:A:323:LYS:HG3   | 2.21                     | 0.40              |
| 1:A:2723:LYS:O    | 1:A:2724:THR:C    | 2.65                     | 0.40              |
| 1:A:2918:ALA:HA   | 1:A:2921:ARG:HB3  | 2.03                     | 0.40              |
| 1:A:3589:ASP:OD1  | 1:A:3590:PRO:CD   | 2.70                     | 0.40              |
| 1:A:4754:ARG:HD2  | 1:A:4754:ARG:N    | 2.37                     | 0.40              |
| 1:B:71:GLU:OE1    | 1:B:111:ARG:NE    | 2.38                     | 0.40              |
| 1:B:2215:VAL:HG21 | 1:B:2229:MET:HE3  | 2.04                     | 0.40              |
| 1:B:2514:GLU:C    | 1:B:2514:GLU:OE2  | 2.65                     | 0.40              |
| 1:B:2525:VAL:HG23 | 1:B:2526:GLY:N    | 2.36                     | 0.40              |
| 1:B:2747:ILE:H    | 1:B:2747:ILE:HD12 | 1.86                     | 0.40              |
| 1:B:2863:LEU:CD1  | 1:B:2926:GLU:OE1  | 2.68                     | 0.40              |
| 1:B:2863:LEU:HD22 | 1:B:2933:MET:SD   | 2.61                     | 0.40              |
| 1:B:3589:ASP:OD1  | 1:B:3590:PRO:CD   | 2.70                     | 0.40              |
| 1:B:4140:ARG:HH11 | 1:B:4140:ARG:HG2  | 1.86                     | 0.40              |
| 1:B:4754:ARG:HD2  | 1:B:4754:ARG:N    | 2.37                     | 0.40              |
| 1:C:505:ALA:HB2   | 1:C:513:ALA:CB    | 2.51                     | 0.40              |
| 1:C:864:LEU:HB3   | 1:C:869:GLU:HG2   | 2.04                     | 0.40              |
| 1:C:953:LYS:HB2   | 1:C:953:LYS:HE2   | 1.47                     | 0.40              |
| 1:C:2863:LEU:HD22 | 1:C:2933:MET:SD   | 2.61                     | 0.40              |
| 1:C:2928:LEU:O    | 1:C:2932:GLN:HG2  | 2.21                     | 0.40              |
| 1:C:3540:ARG:NH1  | 1:C:3545:ASP:OD2  | 2.54                     | 0.40              |
| 1:C:4796:MET:HE1  | 7:C:8006:PCW:C21  | 2.51                     | 0.40              |
| 1:D:505:ALA:HB2   | 1:D:513:ALA:CB    | 2.51                     | 0.40              |
| 1:D:753:VAL:HB    | 1:D:754:PRO:C     | 2.46                     | 0.40              |
| 1:A:975:HIS:CD2   | 1:A:975:HIS:H     | 2.36                     | 0.40              |
| 1:A:978:LEU:HD22  | 1:A:978:LEU:HA    | 1.89                     | 0.40              |
| 1:A:982:GLN:CG    | 1:A:1054:ILE:HD11 | 2.51                     | 0.40              |
| 1:A:2413:GLU:HB2  | 1:A:2416:ARG:HE   | 1.86                     | 0.40              |
| 1:A:2514:GLU:OE2  | 1:A:2514:GLU:C    | 2.65                     | 0.40              |
| 1:A:4140:ARG:HH11 | 1:A:4140:ARG:HG2  | 1.87                     | 0.40              |
| 1:A:4691:GLU:CD   | 1:A:4691:GLU:N    | 2.79                     | 0.40              |
| 1:B:505:ALA:HB2   | 1:B:513:ALA:CB    | 2.51                     | 0.40              |
| 1:B:882:LEU:HA    | 1:B:970:PRO:HG3   | 2.03                     | 0.40              |
| 1:B:2800:GLU:HA   | 1:B:2803:LYS:HD3  | 2.03                     | 0.40              |
| 1:B:2975:ILE:HD13 | 1:B:2975:ILE:HA   | 1.93                     | 0.40              |
| 1:B:3540:ARG:NH1  | 1:B:3545:ASP:OD2  | 2.54                     | 0.40              |
| 1:B:3847:LEU:HD13 | 1:C:77:ARG:HH11   | 1.84                     | 0.40              |
| 1:C:2514:GLU:C    | 1:C:2514:GLU:OE2  | 2.65                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:868:LEU:HD23  | 1:D:868:LEU:HA    | 1.77                     | 0.40              |
| 1:D:2799:SER:O    | 1:D:2802:ASP:OD1  | 2.39                     | 0.40              |
| 1:D:2928:LEU:O    | 1:D:2932:GLN:HG2  | 2.21                     | 0.40              |
| 1:D:3008:ASN:OD1  | 1:D:3008:ASN:C    | 2.65                     | 0.40              |
| 1:A:914:LEU:HD21  | 1:A:919:ARG:CB    | 2.51                     | 0.40              |
| 1:A:2640:MET:HE3  | 1:A:2640:MET:HB3  | 2.00                     | 0.40              |
| 1:A:2947:LEU:O    | 1:A:2950:SER:OG   | 2.26                     | 0.40              |
| 1:A:3541:TYR:OH   | 1:A:3598:GLN:NE2  | 2.48                     | 0.40              |
| 1:B:874:LYS:H     | 1:B:874:LYS:HG3   | 1.63                     | 0.40              |
| 1:B:1063:GLN:OE1  | 1:B:1063:GLN:N    | 2.54                     | 0.40              |
| 1:B:1116:LEU:HD23 | 1:B:1116:LEU:HA   | 1.95                     | 0.40              |
| 1:B:1479:ASP:N    | 1:B:1482:GLY:O    | 2.47                     | 0.40              |
| 1:B:2215:VAL:HG11 | 1:B:2229:MET:CE   | 2.50                     | 0.40              |
| 1:B:2928:LEU:O    | 1:B:2932:GLN:HG2  | 2.21                     | 0.40              |
| 1:B:2971:SER:HA   | 1:B:2974:PHE:CD2  | 2.57                     | 0.40              |
| 1:B:4227:GLU:CG   | 1:B:4227:GLU:O    | 2.69                     | 0.40              |
| 1:B:4248:MET:HE1  | 1:B:4987:MET:HE1  | 2.04                     | 0.40              |
| 1:C:1749:PHE:HB2  | 1:C:1757:ASP:HA   | 2.03                     | 0.40              |
| 1:C:2747:ILE:H    | 1:C:2747:ILE:HD12 | 1.86                     | 0.40              |
| 1:C:4754:ARG:HD2  | 1:C:4754:ARG:N    | 2.37                     | 0.40              |
| 1:D:2723:LYS:O    | 1:D:2724:THR:C    | 2.65                     | 0.40              |
| 1:D:2769:PHE:O    | 1:D:2773:GLN:HG2  | 2.21                     | 0.40              |
| 1:D:3521:ILE:HD12 | 1:D:3521:ILE:N    | 2.36                     | 0.40              |
| 1:D:4140:ARG:HG2  | 1:D:4140:ARG:HH11 | 1.86                     | 0.40              |
| 7:D:8005:PCW:H231 | 7:D:8005:PCW:H20  | 1.72                     | 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     | 4345/5035 (86%) | 4217 (97%) | 126 (3%) | 2 (0%)   | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1   | B     | 4345/5035 (86%)   | 4218 (97%)  | 125 (3%) | 2 (0%)   | 100         | 100 |
| 1   | C     | 4345/5035 (86%)   | 4217 (97%)  | 126 (3%) | 2 (0%)   | 100         | 100 |
| 1   | D     | 4345/5035 (86%)   | 4216 (97%)  | 127 (3%) | 2 (0%)   | 100         | 100 |
| 2   | E     | 105/108 (97%)     | 102 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 2   | F     | 105/108 (97%)     | 102 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 2   | G     | 105/108 (97%)     | 102 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 2   | H     | 105/108 (97%)     | 102 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| All | All   | 17800/20572 (86%) | 17276 (97%) | 516 (3%) | 8 (0%)   | 100         | 100 |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 909  | VAL  |
| 1   | B     | 909  | VAL  |
| 1   | C     | 909  | VAL  |
| 1   | D     | 909  | VAL  |
| 1   | A     | 2283 | ASP  |
| 1   | B     | 2283 | ASP  |
| 1   | C     | 2283 | ASP  |
| 1   | D     | 2283 | ASP  |

### 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     | 3806/4296 (89%) | 3670 (96%) | 136 (4%) | 31          | 58 |
| 1   | B     | 3806/4296 (89%) | 3668 (96%) | 138 (4%) | 31          | 58 |
| 1   | C     | 3806/4296 (89%) | 3665 (96%) | 141 (4%) | 30          | 57 |
| 1   | D     | 3806/4296 (89%) | 3669 (96%) | 137 (4%) | 31          | 58 |
| 2   | E     | 89/90 (99%)     | 86 (97%)   | 3 (3%)   | 32          | 60 |
| 2   | F     | 89/90 (99%)     | 86 (97%)   | 3 (3%)   | 32          | 60 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|-------------|----|
| 2   | G     | 89/90 (99%)       | 86 (97%)    | 3 (3%)   | 32          | 60 |
| 2   | H     | 89/90 (99%)       | 86 (97%)    | 3 (3%)   | 32          | 60 |
| All | All   | 15580/17544 (89%) | 15016 (96%) | 564 (4%) | 32          | 58 |

All (564) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 145 | GLU  |
| 1   | A     | 147 | CYS  |
| 1   | A     | 210 | CYS  |
| 1   | A     | 269 | SER  |
| 1   | A     | 275 | LEU  |
| 1   | A     | 326 | VAL  |
| 1   | A     | 347 | CYS  |
| 1   | A     | 390 | SER  |
| 1   | A     | 393 | ARG  |
| 1   | A     | 397 | GLU  |
| 1   | A     | 417 | LYS  |
| 1   | A     | 429 | SER  |
| 1   | A     | 457 | SER  |
| 1   | A     | 485 | LEU  |
| 1   | A     | 589 | SER  |
| 1   | A     | 746 | SER  |
| 1   | A     | 748 | CYS  |
| 1   | A     | 755 | SER  |
| 1   | A     | 804 | LEU  |
| 1   | A     | 848 | SER  |
| 1   | A     | 864 | LEU  |
| 1   | A     | 869 | GLU  |
| 1   | A     | 870 | ARG  |
| 1   | A     | 871 | ILE  |
| 1   | A     | 872 | ARG  |
| 1   | A     | 874 | LYS  |
| 1   | A     | 875 | LEU  |
| 1   | A     | 878 | ASN  |
| 1   | A     | 879 | ILE  |
| 1   | A     | 880 | HIS  |
| 1   | A     | 882 | LEU  |
| 1   | A     | 885 | LEU  |
| 1   | A     | 893 | THR  |
| 1   | A     | 897 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 898  | ARG  |
| 1   | A     | 900  | ASP  |
| 1   | A     | 902  | LYS  |
| 1   | A     | 903  | ARG  |
| 1   | A     | 908  | LEU  |
| 1   | A     | 909  | VAL  |
| 1   | A     | 910  | ASN  |
| 1   | A     | 912  | HIS  |
| 1   | A     | 914  | LEU  |
| 1   | A     | 919  | ARG  |
| 1   | A     | 925  | MET  |
| 1   | A     | 928  | GLU  |
| 1   | A     | 930  | LEU  |
| 1   | A     | 931  | LYS  |
| 1   | A     | 934  | LEU  |
| 1   | A     | 938  | CYS  |
| 1   | A     | 939  | HIS  |
| 1   | A     | 940  | VAL  |
| 1   | A     | 942  | MET  |
| 1   | A     | 949  | ASP  |
| 1   | A     | 952  | LYS  |
| 1   | A     | 953  | LYS  |
| 1   | A     | 954  | THR  |
| 1   | A     | 955  | LYS  |
| 1   | A     | 956  | LEU  |
| 1   | A     | 959  | THR  |
| 1   | A     | 960  | TYR  |
| 1   | A     | 961  | MET  |
| 1   | A     | 962  | MET  |
| 1   | A     | 963  | SER  |
| 1   | A     | 964  | ASN  |
| 1   | A     | 966  | TYR  |
| 1   | A     | 967  | LYS  |
| 1   | A     | 971  | LEU  |
| 1   | A     | 972  | ASP  |
| 1   | A     | 973  | LEU  |
| 1   | A     | 974  | SER  |
| 1   | A     | 976  | VAL  |
| 1   | A     | 977  | ARG  |
| 1   | A     | 978  | LEU  |
| 1   | A     | 979  | THR  |
| 1   | A     | 1007 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1035 | SER  |
| 1   | A     | 1053 | ASN  |
| 1   | A     | 1054 | ILE  |
| 1   | A     | 1071 | ASP  |
| 1   | A     | 1174 | SER  |
| 1   | A     | 1210 | SER  |
| 1   | A     | 1267 | THR  |
| 1   | A     | 1487 | SER  |
| 1   | A     | 1503 | SER  |
| 1   | A     | 1513 | THR  |
| 1   | A     | 1604 | VAL  |
| 1   | A     | 1757 | ASP  |
| 1   | A     | 1788 | LEU  |
| 1   | A     | 1967 | VAL  |
| 1   | A     | 2007 | ILE  |
| 1   | A     | 2093 | GLN  |
| 1   | A     | 2146 | SER  |
| 1   | A     | 2155 | SER  |
| 1   | A     | 2229 | MET  |
| 1   | A     | 2282 | ILE  |
| 1   | A     | 2337 | ARG  |
| 1   | A     | 2508 | ASP  |
| 1   | A     | 2660 | THR  |
| 1   | A     | 2669 | SER  |
| 1   | A     | 2761 | GLU  |
| 1   | A     | 2824 | VAL  |
| 1   | A     | 2973 | GLU  |
| 1   | A     | 2975 | ILE  |
| 1   | A     | 2990 | SER  |
| 1   | A     | 3035 | LYS  |
| 1   | A     | 3040 | ILE  |
| 1   | A     | 3156 | ASP  |
| 1   | A     | 3233 | LEU  |
| 1   | A     | 3236 | SER  |
| 1   | A     | 3273 | ILE  |
| 1   | A     | 3297 | LEU  |
| 1   | A     | 3324 | ILE  |
| 1   | A     | 3374 | VAL  |
| 1   | A     | 3400 | SER  |
| 1   | A     | 3447 | SER  |
| 1   | A     | 3449 | SER  |
| 1   | A     | 3509 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3529 | THR  |
| 1   | A     | 3557 | ASN  |
| 1   | A     | 3564 | VAL  |
| 1   | A     | 3612 | HIS  |
| 1   | A     | 3659 | LYS  |
| 1   | A     | 3708 | ARG  |
| 1   | A     | 3752 | VAL  |
| 1   | A     | 3806 | SER  |
| 1   | A     | 3869 | ILE  |
| 1   | A     | 4054 | SER  |
| 1   | A     | 4077 | SER  |
| 1   | A     | 4086 | ASP  |
| 1   | A     | 4092 | SER  |
| 1   | A     | 4128 | CYS  |
| 1   | A     | 4154 | SER  |
| 1   | A     | 4181 | LEU  |
| 1   | A     | 4711 | SER  |
| 1   | A     | 4762 | LEU  |
| 2   | E     | 3    | VAL  |
| 2   | E     | 26   | HIS  |
| 2   | E     | 68   | SER  |
| 2   | F     | 3    | VAL  |
| 2   | F     | 26   | HIS  |
| 2   | F     | 68   | SER  |
| 2   | G     | 3    | VAL  |
| 2   | G     | 26   | HIS  |
| 2   | G     | 68   | SER  |
| 2   | H     | 3    | VAL  |
| 2   | H     | 26   | HIS  |
| 2   | H     | 68   | SER  |
| 1   | B     | 145  | GLU  |
| 1   | B     | 147  | CYS  |
| 1   | B     | 210  | CYS  |
| 1   | B     | 269  | SER  |
| 1   | B     | 275  | LEU  |
| 1   | B     | 326  | VAL  |
| 1   | B     | 347  | CYS  |
| 1   | B     | 390  | SER  |
| 1   | B     | 393  | ARG  |
| 1   | B     | 397  | GLU  |
| 1   | B     | 417  | LYS  |
| 1   | B     | 429  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 457 | SER  |
| 1   | B     | 485 | LEU  |
| 1   | B     | 589 | SER  |
| 1   | B     | 746 | SER  |
| 1   | B     | 748 | CYS  |
| 1   | B     | 755 | SER  |
| 1   | B     | 804 | LEU  |
| 1   | B     | 848 | SER  |
| 1   | B     | 864 | LEU  |
| 1   | B     | 869 | GLU  |
| 1   | B     | 870 | ARG  |
| 1   | B     | 871 | ILE  |
| 1   | B     | 872 | ARG  |
| 1   | B     | 874 | LYS  |
| 1   | B     | 875 | LEU  |
| 1   | B     | 878 | ASN  |
| 1   | B     | 879 | ILE  |
| 1   | B     | 880 | HIS  |
| 1   | B     | 882 | LEU  |
| 1   | B     | 885 | LEU  |
| 1   | B     | 893 | THR  |
| 1   | B     | 897 | VAL  |
| 1   | B     | 898 | ARG  |
| 1   | B     | 900 | ASP  |
| 1   | B     | 902 | LYS  |
| 1   | B     | 903 | ARG  |
| 1   | B     | 908 | LEU  |
| 1   | B     | 909 | VAL  |
| 1   | B     | 910 | ASN  |
| 1   | B     | 912 | HIS  |
| 1   | B     | 914 | LEU  |
| 1   | B     | 919 | ARG  |
| 1   | B     | 925 | MET  |
| 1   | B     | 928 | GLU  |
| 1   | B     | 930 | LEU  |
| 1   | B     | 931 | LYS  |
| 1   | B     | 934 | LEU  |
| 1   | B     | 938 | CYS  |
| 1   | B     | 939 | HIS  |
| 1   | B     | 940 | VAL  |
| 1   | B     | 942 | MET  |
| 1   | B     | 949 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 952  | LYS  |
| 1   | B     | 953  | LYS  |
| 1   | B     | 954  | THR  |
| 1   | B     | 955  | LYS  |
| 1   | B     | 956  | LEU  |
| 1   | B     | 959  | THR  |
| 1   | B     | 960  | TYR  |
| 1   | B     | 961  | MET  |
| 1   | B     | 962  | MET  |
| 1   | B     | 963  | SER  |
| 1   | B     | 964  | ASN  |
| 1   | B     | 966  | TYR  |
| 1   | B     | 967  | LYS  |
| 1   | B     | 971  | LEU  |
| 1   | B     | 972  | ASP  |
| 1   | B     | 973  | LEU  |
| 1   | B     | 974  | SER  |
| 1   | B     | 976  | VAL  |
| 1   | B     | 977  | ARG  |
| 1   | B     | 978  | LEU  |
| 1   | B     | 979  | THR  |
| 1   | B     | 1007 | SER  |
| 1   | B     | 1035 | SER  |
| 1   | B     | 1038 | ASP  |
| 1   | B     | 1053 | ASN  |
| 1   | B     | 1054 | ILE  |
| 1   | B     | 1071 | ASP  |
| 1   | B     | 1174 | SER  |
| 1   | B     | 1210 | SER  |
| 1   | B     | 1267 | THR  |
| 1   | B     | 1487 | SER  |
| 1   | B     | 1503 | SER  |
| 1   | B     | 1513 | THR  |
| 1   | B     | 1604 | VAL  |
| 1   | B     | 1757 | ASP  |
| 1   | B     | 1788 | LEU  |
| 1   | B     | 1967 | VAL  |
| 1   | B     | 2007 | ILE  |
| 1   | B     | 2093 | GLN  |
| 1   | B     | 2146 | SER  |
| 1   | B     | 2155 | SER  |
| 1   | B     | 2229 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 2282 | ILE  |
| 1   | B     | 2337 | ARG  |
| 1   | B     | 2508 | ASP  |
| 1   | B     | 2660 | THR  |
| 1   | B     | 2669 | SER  |
| 1   | B     | 2761 | GLU  |
| 1   | B     | 2824 | VAL  |
| 1   | B     | 2973 | GLU  |
| 1   | B     | 2975 | ILE  |
| 1   | B     | 2990 | SER  |
| 1   | B     | 2996 | ILE  |
| 1   | B     | 3035 | LYS  |
| 1   | B     | 3040 | ILE  |
| 1   | B     | 3156 | ASP  |
| 1   | B     | 3233 | LEU  |
| 1   | B     | 3236 | SER  |
| 1   | B     | 3273 | ILE  |
| 1   | B     | 3297 | LEU  |
| 1   | B     | 3324 | ILE  |
| 1   | B     | 3374 | VAL  |
| 1   | B     | 3400 | SER  |
| 1   | B     | 3447 | SER  |
| 1   | B     | 3449 | SER  |
| 1   | B     | 3509 | SER  |
| 1   | B     | 3529 | THR  |
| 1   | B     | 3557 | ASN  |
| 1   | B     | 3564 | VAL  |
| 1   | B     | 3612 | HIS  |
| 1   | B     | 3659 | LYS  |
| 1   | B     | 3708 | ARG  |
| 1   | B     | 3752 | VAL  |
| 1   | B     | 3806 | SER  |
| 1   | B     | 3869 | ILE  |
| 1   | B     | 4054 | SER  |
| 1   | B     | 4077 | SER  |
| 1   | B     | 4086 | ASP  |
| 1   | B     | 4092 | SER  |
| 1   | B     | 4128 | CYS  |
| 1   | B     | 4154 | SER  |
| 1   | B     | 4181 | LEU  |
| 1   | B     | 4711 | SER  |
| 1   | B     | 4762 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 145 | GLU  |
| 1   | C     | 147 | CYS  |
| 1   | C     | 210 | CYS  |
| 1   | C     | 269 | SER  |
| 1   | C     | 275 | LEU  |
| 1   | C     | 326 | VAL  |
| 1   | C     | 347 | CYS  |
| 1   | C     | 390 | SER  |
| 1   | C     | 393 | ARG  |
| 1   | C     | 397 | GLU  |
| 1   | C     | 417 | LYS  |
| 1   | C     | 429 | SER  |
| 1   | C     | 457 | SER  |
| 1   | C     | 485 | LEU  |
| 1   | C     | 589 | SER  |
| 1   | C     | 746 | SER  |
| 1   | C     | 748 | CYS  |
| 1   | C     | 755 | SER  |
| 1   | C     | 804 | LEU  |
| 1   | C     | 846 | CYS  |
| 1   | C     | 848 | SER  |
| 1   | C     | 864 | LEU  |
| 1   | C     | 869 | GLU  |
| 1   | C     | 870 | ARG  |
| 1   | C     | 871 | ILE  |
| 1   | C     | 872 | ARG  |
| 1   | C     | 874 | LYS  |
| 1   | C     | 875 | LEU  |
| 1   | C     | 878 | ASN  |
| 1   | C     | 879 | ILE  |
| 1   | C     | 880 | HIS  |
| 1   | C     | 882 | LEU  |
| 1   | C     | 885 | LEU  |
| 1   | C     | 893 | THR  |
| 1   | C     | 897 | VAL  |
| 1   | C     | 898 | ARG  |
| 1   | C     | 900 | ASP  |
| 1   | C     | 902 | LYS  |
| 1   | C     | 903 | ARG  |
| 1   | C     | 908 | LEU  |
| 1   | C     | 909 | VAL  |
| 1   | C     | 910 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 912  | HIS  |
| 1   | C     | 914  | LEU  |
| 1   | C     | 919  | ARG  |
| 1   | C     | 925  | MET  |
| 1   | C     | 928  | GLU  |
| 1   | C     | 930  | LEU  |
| 1   | C     | 931  | LYS  |
| 1   | C     | 934  | LEU  |
| 1   | C     | 938  | CYS  |
| 1   | C     | 939  | HIS  |
| 1   | C     | 940  | VAL  |
| 1   | C     | 942  | MET  |
| 1   | C     | 949  | ASP  |
| 1   | C     | 952  | LYS  |
| 1   | C     | 953  | LYS  |
| 1   | C     | 954  | THR  |
| 1   | C     | 955  | LYS  |
| 1   | C     | 956  | LEU  |
| 1   | C     | 959  | THR  |
| 1   | C     | 960  | TYR  |
| 1   | C     | 961  | MET  |
| 1   | C     | 962  | MET  |
| 1   | C     | 963  | SER  |
| 1   | C     | 964  | ASN  |
| 1   | C     | 966  | TYR  |
| 1   | C     | 967  | LYS  |
| 1   | C     | 971  | LEU  |
| 1   | C     | 972  | ASP  |
| 1   | C     | 973  | LEU  |
| 1   | C     | 974  | SER  |
| 1   | C     | 976  | VAL  |
| 1   | C     | 977  | ARG  |
| 1   | C     | 978  | LEU  |
| 1   | C     | 979  | THR  |
| 1   | C     | 1007 | SER  |
| 1   | C     | 1035 | SER  |
| 1   | C     | 1053 | ASN  |
| 1   | C     | 1054 | ILE  |
| 1   | C     | 1071 | ASP  |
| 1   | C     | 1174 | SER  |
| 1   | C     | 1210 | SER  |
| 1   | C     | 1267 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1429 | LEU  |
| 1   | C     | 1487 | SER  |
| 1   | C     | 1503 | SER  |
| 1   | C     | 1513 | THR  |
| 1   | C     | 1604 | VAL  |
| 1   | C     | 1757 | ASP  |
| 1   | C     | 1967 | VAL  |
| 1   | C     | 2007 | ILE  |
| 1   | C     | 2093 | GLN  |
| 1   | C     | 2146 | SER  |
| 1   | C     | 2155 | SER  |
| 1   | C     | 2181 | GLN  |
| 1   | C     | 2229 | MET  |
| 1   | C     | 2282 | ILE  |
| 1   | C     | 2337 | ARG  |
| 1   | C     | 2508 | ASP  |
| 1   | C     | 2660 | THR  |
| 1   | C     | 2669 | SER  |
| 1   | C     | 2761 | GLU  |
| 1   | C     | 2824 | VAL  |
| 1   | C     | 2973 | GLU  |
| 1   | C     | 2975 | ILE  |
| 1   | C     | 2990 | SER  |
| 1   | C     | 2996 | ILE  |
| 1   | C     | 3035 | LYS  |
| 1   | C     | 3040 | ILE  |
| 1   | C     | 3156 | ASP  |
| 1   | C     | 3233 | LEU  |
| 1   | C     | 3236 | SER  |
| 1   | C     | 3273 | ILE  |
| 1   | C     | 3297 | LEU  |
| 1   | C     | 3324 | ILE  |
| 1   | C     | 3374 | VAL  |
| 1   | C     | 3400 | SER  |
| 1   | C     | 3447 | SER  |
| 1   | C     | 3449 | SER  |
| 1   | C     | 3509 | SER  |
| 1   | C     | 3529 | THR  |
| 1   | C     | 3557 | ASN  |
| 1   | C     | 3564 | VAL  |
| 1   | C     | 3612 | HIS  |
| 1   | C     | 3659 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 3708 | ARG  |
| 1   | C     | 3752 | VAL  |
| 1   | C     | 3806 | SER  |
| 1   | C     | 3828 | GLU  |
| 1   | C     | 3869 | ILE  |
| 1   | C     | 4054 | SER  |
| 1   | C     | 4077 | SER  |
| 1   | C     | 4086 | ASP  |
| 1   | C     | 4092 | SER  |
| 1   | C     | 4128 | CYS  |
| 1   | C     | 4154 | SER  |
| 1   | C     | 4181 | LEU  |
| 1   | C     | 4711 | SER  |
| 1   | C     | 4762 | LEU  |
| 1   | C     | 4979 | GLU  |
| 1   | D     | 145  | GLU  |
| 1   | D     | 147  | CYS  |
| 1   | D     | 210  | CYS  |
| 1   | D     | 269  | SER  |
| 1   | D     | 275  | LEU  |
| 1   | D     | 326  | VAL  |
| 1   | D     | 347  | CYS  |
| 1   | D     | 390  | SER  |
| 1   | D     | 393  | ARG  |
| 1   | D     | 397  | GLU  |
| 1   | D     | 417  | LYS  |
| 1   | D     | 429  | SER  |
| 1   | D     | 457  | SER  |
| 1   | D     | 485  | LEU  |
| 1   | D     | 589  | SER  |
| 1   | D     | 746  | SER  |
| 1   | D     | 748  | CYS  |
| 1   | D     | 755  | SER  |
| 1   | D     | 804  | LEU  |
| 1   | D     | 848  | SER  |
| 1   | D     | 864  | LEU  |
| 1   | D     | 869  | GLU  |
| 1   | D     | 870  | ARG  |
| 1   | D     | 871  | ILE  |
| 1   | D     | 872  | ARG  |
| 1   | D     | 874  | LYS  |
| 1   | D     | 875  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 878 | ASN  |
| 1   | D     | 879 | ILE  |
| 1   | D     | 880 | HIS  |
| 1   | D     | 882 | LEU  |
| 1   | D     | 885 | LEU  |
| 1   | D     | 893 | THR  |
| 1   | D     | 897 | VAL  |
| 1   | D     | 898 | ARG  |
| 1   | D     | 900 | ASP  |
| 1   | D     | 902 | LYS  |
| 1   | D     | 903 | ARG  |
| 1   | D     | 908 | LEU  |
| 1   | D     | 909 | VAL  |
| 1   | D     | 910 | ASN  |
| 1   | D     | 912 | HIS  |
| 1   | D     | 914 | LEU  |
| 1   | D     | 919 | ARG  |
| 1   | D     | 925 | MET  |
| 1   | D     | 928 | GLU  |
| 1   | D     | 930 | LEU  |
| 1   | D     | 931 | LYS  |
| 1   | D     | 934 | LEU  |
| 1   | D     | 938 | CYS  |
| 1   | D     | 939 | HIS  |
| 1   | D     | 940 | VAL  |
| 1   | D     | 942 | MET  |
| 1   | D     | 949 | ASP  |
| 1   | D     | 952 | LYS  |
| 1   | D     | 953 | LYS  |
| 1   | D     | 954 | THR  |
| 1   | D     | 955 | LYS  |
| 1   | D     | 956 | LEU  |
| 1   | D     | 959 | THR  |
| 1   | D     | 960 | TYR  |
| 1   | D     | 961 | MET  |
| 1   | D     | 962 | MET  |
| 1   | D     | 963 | SER  |
| 1   | D     | 964 | ASN  |
| 1   | D     | 966 | TYR  |
| 1   | D     | 967 | LYS  |
| 1   | D     | 971 | LEU  |
| 1   | D     | 972 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 973  | LEU  |
| 1   | D     | 974  | SER  |
| 1   | D     | 976  | VAL  |
| 1   | D     | 977  | ARG  |
| 1   | D     | 978  | LEU  |
| 1   | D     | 979  | THR  |
| 1   | D     | 1007 | SER  |
| 1   | D     | 1035 | SER  |
| 1   | D     | 1038 | ASP  |
| 1   | D     | 1053 | ASN  |
| 1   | D     | 1054 | ILE  |
| 1   | D     | 1071 | ASP  |
| 1   | D     | 1174 | SER  |
| 1   | D     | 1210 | SER  |
| 1   | D     | 1267 | THR  |
| 1   | D     | 1487 | SER  |
| 1   | D     | 1503 | SER  |
| 1   | D     | 1513 | THR  |
| 1   | D     | 1604 | VAL  |
| 1   | D     | 1757 | ASP  |
| 1   | D     | 1967 | VAL  |
| 1   | D     | 2007 | ILE  |
| 1   | D     | 2093 | GLN  |
| 1   | D     | 2146 | SER  |
| 1   | D     | 2155 | SER  |
| 1   | D     | 2229 | MET  |
| 1   | D     | 2282 | ILE  |
| 1   | D     | 2337 | ARG  |
| 1   | D     | 2508 | ASP  |
| 1   | D     | 2660 | THR  |
| 1   | D     | 2669 | SER  |
| 1   | D     | 2761 | GLU  |
| 1   | D     | 2824 | VAL  |
| 1   | D     | 2973 | GLU  |
| 1   | D     | 2975 | ILE  |
| 1   | D     | 2990 | SER  |
| 1   | D     | 2996 | ILE  |
| 1   | D     | 3035 | LYS  |
| 1   | D     | 3040 | ILE  |
| 1   | D     | 3156 | ASP  |
| 1   | D     | 3233 | LEU  |
| 1   | D     | 3236 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 3273 | ILE  |
| 1   | D     | 3297 | LEU  |
| 1   | D     | 3324 | ILE  |
| 1   | D     | 3374 | VAL  |
| 1   | D     | 3400 | SER  |
| 1   | D     | 3447 | SER  |
| 1   | D     | 3449 | SER  |
| 1   | D     | 3509 | SER  |
| 1   | D     | 3529 | THR  |
| 1   | D     | 3557 | ASN  |
| 1   | D     | 3564 | VAL  |
| 1   | D     | 3612 | HIS  |
| 1   | D     | 3659 | LYS  |
| 1   | D     | 3708 | ARG  |
| 1   | D     | 3752 | VAL  |
| 1   | D     | 3806 | SER  |
| 1   | D     | 3869 | ILE  |
| 1   | D     | 4054 | SER  |
| 1   | D     | 4077 | SER  |
| 1   | D     | 4086 | ASP  |
| 1   | D     | 4092 | SER  |
| 1   | D     | 4128 | CYS  |
| 1   | D     | 4154 | SER  |
| 1   | D     | 4181 | LEU  |
| 1   | D     | 4711 | SER  |
| 1   | D     | 4762 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 182  | HIS  |
| 1   | A     | 350  | GLN  |
| 1   | A     | 395  | GLN  |
| 1   | A     | 400  | GLN  |
| 1   | A     | 462  | HIS  |
| 1   | A     | 766  | GLN  |
| 1   | A     | 878  | ASN  |
| 1   | A     | 880  | HIS  |
| 1   | A     | 922  | ASN  |
| 1   | A     | 950  | ASN  |
| 1   | A     | 1485 | HIS  |
| 1   | A     | 1564 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1570 | GLN  |
| 1   | A     | 1939 | GLN  |
| 1   | A     | 2030 | GLN  |
| 1   | A     | 2757 | ASN  |
| 1   | A     | 2932 | GLN  |
| 1   | A     | 2977 | HIS  |
| 1   | A     | 3031 | HIS  |
| 1   | A     | 3326 | ASN  |
| 1   | A     | 3419 | ASN  |
| 1   | A     | 3463 | ASN  |
| 1   | A     | 3609 | GLN  |
| 1   | A     | 3809 | ASN  |
| 1   | A     | 3917 | ASN  |
| 1   | A     | 3963 | GLN  |
| 1   | A     | 3981 | GLN  |
| 1   | A     | 4097 | GLN  |
| 1   | A     | 4112 | GLN  |
| 1   | A     | 4212 | GLN  |
| 1   | A     | 4219 | GLN  |
| 1   | A     | 4226 | ASN  |
| 1   | A     | 4660 | ASN  |
| 2   | E     | 44   | ASN  |
| 2   | E     | 66   | GLN  |
| 2   | E     | 88   | HIS  |
| 2   | F     | 44   | ASN  |
| 2   | F     | 66   | GLN  |
| 2   | F     | 95   | HIS  |
| 2   | G     | 44   | ASN  |
| 2   | G     | 66   | GLN  |
| 2   | G     | 88   | HIS  |
| 2   | G     | 95   | HIS  |
| 2   | H     | 44   | ASN  |
| 2   | H     | 66   | GLN  |
| 2   | H     | 95   | HIS  |
| 1   | B     | 182  | HIS  |
| 1   | B     | 204  | ASN  |
| 1   | B     | 350  | GLN  |
| 1   | B     | 395  | GLN  |
| 1   | B     | 400  | GLN  |
| 1   | B     | 462  | HIS  |
| 1   | B     | 766  | GLN  |
| 1   | B     | 878  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 880  | HIS  |
| 1   | B     | 922  | ASN  |
| 1   | B     | 950  | ASN  |
| 1   | B     | 1485 | HIS  |
| 1   | B     | 1559 | HIS  |
| 1   | B     | 1564 | GLN  |
| 1   | B     | 1570 | GLN  |
| 1   | B     | 1826 | GLN  |
| 1   | B     | 1939 | GLN  |
| 1   | B     | 2030 | GLN  |
| 1   | B     | 2096 | GLN  |
| 1   | B     | 2254 | HIS  |
| 1   | B     | 2575 | HIS  |
| 1   | B     | 2757 | ASN  |
| 1   | B     | 2932 | GLN  |
| 1   | B     | 2977 | HIS  |
| 1   | B     | 3031 | HIS  |
| 1   | B     | 3326 | ASN  |
| 1   | B     | 3463 | ASN  |
| 1   | B     | 3598 | GLN  |
| 1   | B     | 3609 | GLN  |
| 1   | B     | 3809 | ASN  |
| 1   | B     | 3917 | ASN  |
| 1   | B     | 3963 | GLN  |
| 1   | B     | 3981 | GLN  |
| 1   | B     | 4097 | GLN  |
| 1   | B     | 4112 | GLN  |
| 1   | B     | 4212 | GLN  |
| 1   | B     | 4219 | GLN  |
| 1   | B     | 4226 | ASN  |
| 1   | B     | 4660 | ASN  |
| 1   | B     | 4855 | ASN  |
| 1   | C     | 182  | HIS  |
| 1   | C     | 204  | ASN  |
| 1   | C     | 350  | GLN  |
| 1   | C     | 395  | GLN  |
| 1   | C     | 400  | GLN  |
| 1   | C     | 462  | HIS  |
| 1   | C     | 766  | GLN  |
| 1   | C     | 878  | ASN  |
| 1   | C     | 880  | HIS  |
| 1   | C     | 922  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 950  | ASN  |
| 1   | C     | 1485 | HIS  |
| 1   | C     | 1559 | HIS  |
| 1   | C     | 1564 | GLN  |
| 1   | C     | 1570 | GLN  |
| 1   | C     | 1939 | GLN  |
| 1   | C     | 2030 | GLN  |
| 1   | C     | 2096 | GLN  |
| 1   | C     | 2575 | HIS  |
| 1   | C     | 2757 | ASN  |
| 1   | C     | 2932 | GLN  |
| 1   | C     | 2977 | HIS  |
| 1   | C     | 3031 | HIS  |
| 1   | C     | 3326 | ASN  |
| 1   | C     | 3463 | ASN  |
| 1   | C     | 3609 | GLN  |
| 1   | C     | 3809 | ASN  |
| 1   | C     | 3917 | ASN  |
| 1   | C     | 3963 | GLN  |
| 1   | C     | 3981 | GLN  |
| 1   | C     | 4097 | GLN  |
| 1   | C     | 4112 | GLN  |
| 1   | C     | 4219 | GLN  |
| 1   | C     | 4226 | ASN  |
| 1   | C     | 4660 | ASN  |
| 1   | C     | 4855 | ASN  |
| 1   | D     | 182  | HIS  |
| 1   | D     | 350  | GLN  |
| 1   | D     | 395  | GLN  |
| 1   | D     | 400  | GLN  |
| 1   | D     | 462  | HIS  |
| 1   | D     | 766  | GLN  |
| 1   | D     | 878  | ASN  |
| 1   | D     | 880  | HIS  |
| 1   | D     | 922  | ASN  |
| 1   | D     | 950  | ASN  |
| 1   | D     | 1485 | HIS  |
| 1   | D     | 1559 | HIS  |
| 1   | D     | 1564 | GLN  |
| 1   | D     | 1570 | GLN  |
| 1   | D     | 1826 | GLN  |
| 1   | D     | 1939 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 2030 | GLN  |
| 1   | D     | 2575 | HIS  |
| 1   | D     | 2757 | ASN  |
| 1   | D     | 2932 | GLN  |
| 1   | D     | 2977 | HIS  |
| 1   | D     | 3031 | HIS  |
| 1   | D     | 3326 | ASN  |
| 1   | D     | 3463 | ASN  |
| 1   | D     | 3598 | GLN  |
| 1   | D     | 3609 | GLN  |
| 1   | D     | 3917 | ASN  |
| 1   | D     | 3963 | GLN  |
| 1   | D     | 3981 | GLN  |
| 1   | D     | 4097 | GLN  |
| 1   | D     | 4112 | GLN  |
| 1   | D     | 4219 | GLN  |
| 1   | D     | 4226 | ASN  |
| 1   | D     | 4660 | ASN  |
| 1   | D     | 4855 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 8 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 | $\# Z  > 2$ |
| 8   | A1BYZ | B     | 8009 | -    | 32,32,32     | 0.45 | 0           | 40,47,47    | 2.04 | 5 (12%)     |
| 4   | CFF   | D     | 8002 | -    | 15,15,15     | 1.91 | 6 (40%)     | 23,23,23    | 2.92 | 12 (52%)    |
| 5   | ATP   | B     | 8003 | -    | 32,33,33     | 0.31 | 0           | 48,52,52    | 0.70 | 1 (2%)      |
| 8   | A1BYZ | A     | 8008 | -    | 32,32,32     | 0.78 | 1 (3%)      | 40,47,47    | 0.94 | 2 (5%)      |
| 8   | A1BYZ | A     | 8009 | -    | 32,32,32     | 0.45 | 0           | 40,47,47    | 2.04 | 5 (12%)     |
| 5   | ATP   | D     | 8007 | -    | 32,33,33     | 0.27 | 0           | 48,52,52    | 0.68 | 0           |
| 4   | CFF   | C     | 8002 | -    | 15,15,15     | 1.91 | 6 (40%)     | 23,23,23    | 2.93 | 12 (52%)    |
| 5   | ATP   | C     | 8007 | -    | 32,33,33     | 0.27 | 0           | 48,52,52    | 0.68 | 0           |
| 7   | PCW   | A     | 8006 | -    | 53,53,53     | 1.25 | 7 (13%)     | 59,61,61    | 1.11 | 4 (6%)      |
| 7   | PCW   | B     | 8006 | -    | 53,53,53     | 1.25 | 7 (13%)     | 59,61,61    | 1.11 | 4 (6%)      |
| 7   | PCW   | D     | 8006 | -    | 53,53,53     | 1.25 | 7 (13%)     | 59,61,61    | 1.11 | 4 (6%)      |
| 4   | CFF   | B     | 8002 | -    | 15,15,15     | 1.91 | 6 (40%)     | 23,23,23    | 2.92 | 12 (52%)    |
| 8   | A1BYZ | C     | 8008 | -    | 32,32,32     | 0.77 | 1 (3%)      | 40,47,47    | 0.94 | 2 (5%)      |
| 5   | ATP   | B     | 8007 | -    | 32,33,33     | 0.27 | 0           | 48,52,52    | 0.68 | 0           |
| 7   | PCW   | C     | 8006 | -    | 53,53,53     | 1.25 | 7 (13%)     | 59,61,61    | 1.11 | 4 (6%)      |
| 4   | CFF   | A     | 8002 | -    | 15,15,15     | 1.91 | 6 (40%)     | 23,23,23    | 2.92 | 12 (52%)    |
| 8   | A1BYZ | D     | 8009 | -    | 32,32,32     | 0.45 | 0           | 40,47,47    | 2.04 | 5 (12%)     |
| 7   | PCW   | C     | 8005 | -    | 53,53,53     | 1.23 | 7 (13%)     | 59,61,61    | 1.20 | 5 (8%)      |
| 5   | ATP   | D     | 8003 | -    | 32,33,33     | 0.30 | 0           | 48,52,52    | 0.70 | 1 (2%)      |
| 8   | A1BYZ | C     | 8009 | -    | 32,32,32     | 0.45 | 0           | 40,47,47    | 2.03 | 5 (12%)     |
| 8   | A1BYZ | B     | 8008 | -    | 32,32,32     | 0.78 | 1 (3%)      | 40,47,47    | 0.95 | 2 (5%)      |
| 5   | ATP   | C     | 8003 | -    | 32,33,33     | 0.30 | 0           | 48,52,52    | 0.70 | 1 (2%)      |
| 5   | ATP   | A     | 8003 | -    | 32,33,33     | 0.30 | 0           | 48,52,52    | 0.70 | 1 (2%)      |
| 5   | ATP   | A     | 8007 | -    | 32,33,33     | 0.27 | 0           | 48,52,52    | 0.68 | 0           |
| 7   | PCW   | A     | 8005 | -    | 53,53,53     | 1.23 | 7 (13%)     | 59,61,61    | 1.20 | 5 (8%)      |
| 7   | PCW   | B     | 8005 | -    | 53,53,53     | 1.23 | 7 (13%)     | 59,61,61    | 1.20 | 5 (8%)      |
| 7   | PCW   | D     | 8005 | -    | 53,53,53     | 1.23 | 7 (13%)     | 59,61,61    | 1.20 | 5 (8%)      |
| 8   | A1BYZ | D     | 8008 | -    | 32,32,32     | 0.78 | 1 (3%)      | 40,47,47    | 0.94 | 2 (5%)      |

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   |
|-----|-------|-------|------|------|---------|-------------|---------|
| 8   | A1BYZ | B     | 8009 | -    | -       | 5/18/59/59  | 0/3/3/3 |
| 4   | CFF   | D     | 8002 | -    | -       | -           | 0/2/2/2 |
| 5   | ATP   | B     | 8003 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 8   | A1BYZ | A     | 8008 | -    | -       | 5/18/59/59  | 0/3/3/3 |
| 8   | A1BYZ | A     | 8009 | -    | -       | 5/18/59/59  | 0/3/3/3 |
| 5   | ATP   | D     | 8007 | -    | -       | 8/22/38/38  | 0/3/3/3 |
| 4   | CFF   | C     | 8002 | -    | -       | -           | 0/2/2/2 |
| 5   | ATP   | C     | 8007 | -    | -       | 8/22/38/38  | 0/3/3/3 |
| 7   | PCW   | A     | 8006 | -    | -       | 28/57/57/57 | -       |
| 7   | PCW   | B     | 8006 | -    | -       | 28/57/57/57 | -       |
| 7   | PCW   | D     | 8006 | -    | -       | 28/57/57/57 | -       |
| 4   | CFF   | B     | 8002 | -    | -       | -           | 0/2/2/2 |
| 8   | A1BYZ | C     | 8008 | -    | -       | 5/18/59/59  | 0/3/3/3 |
| 5   | ATP   | B     | 8007 | -    | -       | 8/22/38/38  | 0/3/3/3 |
| 7   | PCW   | C     | 8006 | -    | -       | 28/57/57/57 | -       |
| 4   | CFF   | A     | 8002 | -    | -       | -           | 0/2/2/2 |
| 8   | A1BYZ | D     | 8009 | -    | -       | 5/18/59/59  | 0/3/3/3 |
| 7   | PCW   | C     | 8005 | -    | -       | 22/57/57/57 | -       |
| 5   | ATP   | D     | 8003 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 8   | A1BYZ | C     | 8009 | -    | -       | 5/18/59/59  | 0/3/3/3 |
| 8   | A1BYZ | B     | 8008 | -    | -       | 5/18/59/59  | 0/3/3/3 |
| 5   | ATP   | C     | 8003 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 5   | ATP   | A     | 8003 | -    | -       | 6/22/38/38  | 0/3/3/3 |
| 5   | ATP   | A     | 8007 | -    | -       | 8/22/38/38  | 0/3/3/3 |
| 7   | PCW   | A     | 8005 | -    | -       | 22/57/57/57 | -       |
| 7   | PCW   | B     | 8005 | -    | -       | 23/57/57/57 | -       |
| 7   | PCW   | D     | 8005 | -    | -       | 22/57/57/57 | -       |
| 8   | A1BYZ | D     | 8008 | -    | -       | 5/18/59/59  | 0/3/3/3 |

All (84) bond length outliers are listed below:

| Mol | Chain | Res  | Type  | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|-------|---------|-------|-------------|----------|
| 4   | A     | 8002 | CFF   | C6-N1   | -3.99 | 1.32        | 1.40     |
| 4   | D     | 8002 | CFF   | C6-N1   | -3.99 | 1.32        | 1.40     |
| 4   | C     | 8002 | CFF   | C6-N1   | -3.97 | 1.32        | 1.40     |
| 4   | B     | 8002 | CFF   | C6-N1   | -3.95 | 1.32        | 1.40     |
| 8   | D     | 8008 | A1BYZ | C16-C15 | -3.94 | 1.50        | 1.54     |
| 8   | A     | 8008 | A1BYZ | C16-C15 | -3.93 | 1.50        | 1.54     |

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| Mol | Chain | Res  | Type  | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|-------|---------|-------|-------------|----------|
| 8   | B     | 8008 | A1BYZ | C16-C15 | -3.90 | 1.50        | 1.54     |
| 8   | C     | 8008 | A1BYZ | C16-C15 | -3.86 | 1.50        | 1.54     |
| 7   | C     | 8006 | PCW   | O3-C11  | 3.03  | 1.42        | 1.33     |
| 7   | A     | 8006 | PCW   | O3-C11  | 3.03  | 1.42        | 1.33     |
| 7   | B     | 8006 | PCW   | O3-C11  | 3.03  | 1.42        | 1.33     |
| 7   | D     | 8006 | PCW   | O3-C11  | 3.03  | 1.42        | 1.33     |
| 7   | D     | 8005 | PCW   | O3-C11  | 2.95  | 1.41        | 1.33     |
| 7   | A     | 8005 | PCW   | O3-C11  | 2.94  | 1.41        | 1.33     |
| 7   | C     | 8005 | PCW   | O3-C11  | 2.93  | 1.41        | 1.33     |
| 7   | B     | 8005 | PCW   | O3-C11  | 2.93  | 1.41        | 1.33     |
| 7   | B     | 8005 | PCW   | O2-C31  | 2.86  | 1.42        | 1.34     |
| 7   | C     | 8005 | PCW   | O2-C31  | 2.85  | 1.42        | 1.34     |
| 7   | A     | 8005 | PCW   | O2-C31  | 2.83  | 1.42        | 1.34     |
| 7   | D     | 8005 | PCW   | O2-C31  | 2.82  | 1.42        | 1.34     |
| 7   | A     | 8006 | PCW   | O2-C31  | 2.69  | 1.41        | 1.34     |
| 4   | A     | 8002 | CFF   | C5-N7   | -2.67 | 1.33        | 1.38     |
| 4   | B     | 8002 | CFF   | C5-N7   | -2.67 | 1.33        | 1.38     |
| 4   | D     | 8002 | CFF   | C5-N7   | -2.67 | 1.33        | 1.38     |
| 7   | B     | 8006 | PCW   | O2-C31  | 2.67  | 1.41        | 1.34     |
| 7   | C     | 8006 | PCW   | O2-C31  | 2.67  | 1.41        | 1.34     |
| 7   | D     | 8006 | PCW   | O2-C31  | 2.67  | 1.41        | 1.34     |
| 4   | C     | 8002 | CFF   | C5-N7   | -2.66 | 1.33        | 1.38     |
| 7   | D     | 8006 | PCW   | P-O4P   | 2.60  | 1.69        | 1.59     |
| 7   | C     | 8006 | PCW   | P-O4P   | 2.59  | 1.69        | 1.59     |
| 7   | A     | 8006 | PCW   | P-O4P   | 2.58  | 1.69        | 1.59     |
| 7   | B     | 8006 | PCW   | P-O4P   | 2.58  | 1.69        | 1.59     |
| 7   | C     | 8005 | PCW   | P-O4P   | 2.53  | 1.69        | 1.59     |
| 7   | A     | 8005 | PCW   | P-O4P   | 2.52  | 1.69        | 1.59     |
| 7   | B     | 8005 | PCW   | P-O4P   | 2.52  | 1.69        | 1.59     |
| 7   | D     | 8005 | PCW   | P-O4P   | 2.51  | 1.69        | 1.59     |
| 7   | D     | 8006 | PCW   | O2-C2   | -2.49 | 1.40        | 1.46     |
| 7   | A     | 8006 | PCW   | O2-C2   | -2.47 | 1.40        | 1.46     |
| 4   | C     | 8002 | CFF   | C4-N3   | -2.46 | 1.34        | 1.38     |
| 7   | C     | 8006 | PCW   | O2-C2   | -2.45 | 1.40        | 1.46     |
| 7   | B     | 8006 | PCW   | O2-C2   | -2.44 | 1.40        | 1.46     |
| 4   | A     | 8002 | CFF   | C4-N3   | -2.43 | 1.34        | 1.38     |
| 4   | B     | 8002 | CFF   | C4-N3   | -2.43 | 1.34        | 1.38     |
| 7   | C     | 8005 | PCW   | O2-C2   | -2.42 | 1.40        | 1.46     |
| 4   | D     | 8002 | CFF   | C4-N3   | -2.38 | 1.34        | 1.38     |
| 7   | A     | 8005 | PCW   | O2-C2   | -2.38 | 1.41        | 1.46     |
| 7   | D     | 8005 | PCW   | O2-C2   | -2.38 | 1.41        | 1.46     |
| 7   | B     | 8005 | PCW   | O2-C2   | -2.37 | 1.41        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 7   | C     | 8006 | PCW  | C5-C4   | 2.34  | 1.58        | 1.51     |
| 7   | C     | 8005 | PCW  | C5-C4   | 2.34  | 1.58        | 1.51     |
| 7   | D     | 8006 | PCW  | C5-C4   | 2.33  | 1.58        | 1.51     |
| 7   | D     | 8005 | PCW  | C5-C4   | 2.32  | 1.58        | 1.51     |
| 7   | A     | 8006 | PCW  | C5-C4   | 2.32  | 1.58        | 1.51     |
| 7   | A     | 8005 | PCW  | C5-C4   | 2.32  | 1.58        | 1.51     |
| 7   | B     | 8005 | PCW  | C5-C4   | 2.31  | 1.58        | 1.51     |
| 7   | B     | 8006 | PCW  | C5-C4   | 2.31  | 1.58        | 1.51     |
| 7   | D     | 8005 | PCW  | C32-C31 | 2.18  | 1.57        | 1.50     |
| 7   | A     | 8005 | PCW  | C32-C31 | 2.16  | 1.57        | 1.50     |
| 7   | B     | 8005 | PCW  | C32-C31 | 2.15  | 1.56        | 1.50     |
| 7   | C     | 8005 | PCW  | C32-C31 | 2.15  | 1.56        | 1.50     |
| 7   | D     | 8006 | PCW  | C32-C31 | 2.15  | 1.56        | 1.50     |
| 4   | C     | 8002 | CFF  | O13-C6  | -2.15 | 1.18        | 1.23     |
| 4   | D     | 8002 | CFF  | O13-C6  | -2.15 | 1.18        | 1.23     |
| 4   | A     | 8002 | CFF  | O13-C6  | -2.14 | 1.18        | 1.23     |
| 7   | B     | 8005 | PCW  | P-O3P   | 2.14  | 1.67        | 1.59     |
| 4   | C     | 8002 | CFF  | C5-C6   | -2.14 | 1.37        | 1.43     |
| 7   | A     | 8006 | PCW  | P-O3P   | 2.13  | 1.67        | 1.59     |
| 4   | B     | 8002 | CFF  | O13-C6  | -2.13 | 1.18        | 1.23     |
| 7   | C     | 8006 | PCW  | C32-C31 | 2.12  | 1.56        | 1.50     |
| 4   | A     | 8002 | CFF  | C5-C6   | -2.12 | 1.37        | 1.43     |
| 4   | B     | 8002 | CFF  | C5-C6   | -2.12 | 1.37        | 1.43     |
| 7   | B     | 8006 | PCW  | P-O3P   | 2.12  | 1.67        | 1.59     |
| 7   | A     | 8005 | PCW  | P-O3P   | 2.12  | 1.67        | 1.59     |
| 7   | C     | 8005 | PCW  | P-O3P   | 2.12  | 1.67        | 1.59     |
| 7   | B     | 8006 | PCW  | C32-C31 | 2.12  | 1.56        | 1.50     |
| 7   | A     | 8006 | PCW  | C32-C31 | 2.11  | 1.56        | 1.50     |
| 4   | D     | 8002 | CFF  | C5-C6   | -2.11 | 1.37        | 1.43     |
| 7   | C     | 8006 | PCW  | P-O3P   | 2.11  | 1.67        | 1.59     |
| 7   | D     | 8006 | PCW  | P-O3P   | 2.11  | 1.67        | 1.59     |
| 7   | D     | 8005 | PCW  | P-O3P   | 2.10  | 1.67        | 1.59     |
| 4   | B     | 8002 | CFF  | O11-C2  | -2.09 | 1.18        | 1.22     |
| 4   | A     | 8002 | CFF  | O11-C2  | -2.07 | 1.18        | 1.22     |
| 4   | C     | 8002 | CFF  | O11-C2  | -2.07 | 1.18        | 1.22     |
| 4   | D     | 8002 | CFF  | O11-C2  | -2.05 | 1.18        | 1.22     |

All (116) bond angle outliers are listed below:

| Mol | Chain | Res  | Type  | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|-------|-------------|------|-------------|----------|
| 8   | D     | 8009 | A1BYZ | C14-C15-C16 | 9.69 | 115.84      | 110.70   |
| 8   | A     | 8009 | A1BYZ | C14-C15-C16 | 9.67 | 115.83      | 110.70   |

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| Mol | Chain | Res  | Type  | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|-------|-------------|-------|-------------|----------|
| 8   | B     | 8009 | A1BYZ | C14-C15-C16 | 9.63  | 115.81      | 110.70   |
| 8   | C     | 8009 | A1BYZ | C14-C15-C16 | 9.59  | 115.79      | 110.70   |
| 4   | C     | 8002 | CFF   | C14-N7-C8   | -8.11 | 111.11      | 126.28   |
| 4   | A     | 8002 | CFF   | C14-N7-C8   | -8.08 | 111.16      | 126.28   |
| 4   | B     | 8002 | CFF   | C14-N7-C8   | -8.07 | 111.17      | 126.28   |
| 4   | D     | 8002 | CFF   | C14-N7-C8   | -8.05 | 111.22      | 126.28   |
| 4   | C     | 8002 | CFF   | C14-N7-C5   | 5.49  | 140.83      | 127.77   |
| 4   | A     | 8002 | CFF   | C14-N7-C5   | 5.46  | 140.77      | 127.77   |
| 4   | B     | 8002 | CFF   | C14-N7-C5   | 5.45  | 140.74      | 127.77   |
| 4   | D     | 8002 | CFF   | C14-N7-C5   | 5.45  | 140.74      | 127.77   |
| 4   | D     | 8002 | CFF   | C5-C6-N1    | 4.41  | 120.14      | 112.06   |
| 4   | B     | 8002 | CFF   | C5-C6-N1    | 4.40  | 120.12      | 112.06   |
| 4   | A     | 8002 | CFF   | C5-C6-N1    | 4.40  | 120.11      | 112.06   |
| 8   | C     | 8009 | A1BYZ | C24-C25-C26 | -4.37 | 109.12      | 116.30   |
| 4   | C     | 8002 | CFF   | C5-C6-N1    | 4.36  | 120.05      | 112.06   |
| 8   | B     | 8009 | A1BYZ | C24-C25-C26 | -4.36 | 109.14      | 116.30   |
| 8   | A     | 8009 | A1BYZ | C24-C25-C26 | -4.35 | 109.15      | 116.30   |
| 8   | D     | 8009 | A1BYZ | C24-C25-C26 | -4.35 | 109.16      | 116.30   |
| 7   | A     | 8005 | PCW   | C21-C20-C19 | 4.22  | 156.42      | 124.83   |
| 7   | B     | 8005 | PCW   | C21-C20-C19 | 4.22  | 156.42      | 124.83   |
| 7   | D     | 8005 | PCW   | C21-C20-C19 | 4.21  | 156.41      | 124.83   |
| 7   | C     | 8005 | PCW   | C21-C20-C19 | 4.21  | 156.38      | 124.83   |
| 8   | C     | 8009 | A1BYZ | C15-C16-C17 | 4.10  | 113.37      | 110.88   |
| 8   | B     | 8009 | A1BYZ | C15-C16-C17 | 4.09  | 113.37      | 110.88   |
| 8   | A     | 8009 | A1BYZ | C15-C16-C17 | 4.05  | 113.35      | 110.88   |
| 8   | D     | 8009 | A1BYZ | C15-C16-C17 | 4.03  | 113.34      | 110.88   |
| 7   | C     | 8006 | PCW   | C21-C20-C19 | 3.96  | 154.53      | 124.83   |
| 7   | A     | 8006 | PCW   | C21-C20-C19 | 3.96  | 154.53      | 124.83   |
| 7   | B     | 8006 | PCW   | C21-C20-C19 | 3.96  | 154.52      | 124.83   |
| 7   | D     | 8006 | PCW   | C21-C20-C19 | 3.96  | 154.50      | 124.83   |
| 7   | A     | 8005 | PCW   | O2-C31-C32  | 3.80  | 119.69      | 111.48   |
| 7   | D     | 8005 | PCW   | O2-C31-C32  | 3.80  | 119.69      | 111.48   |
| 7   | C     | 8005 | PCW   | O2-C31-C32  | 3.79  | 119.68      | 111.48   |
| 7   | B     | 8005 | PCW   | O2-C31-C32  | 3.78  | 119.66      | 111.48   |
| 4   | C     | 8002 | CFF   | N3-C4-N9    | 3.76  | 132.19      | 126.27   |
| 4   | B     | 8002 | CFF   | N3-C4-N9    | 3.73  | 132.13      | 126.27   |
| 4   | A     | 8002 | CFF   | N3-C4-N9    | 3.72  | 132.12      | 126.27   |
| 4   | B     | 8002 | CFF   | C6-N1-C2    | -3.71 | 119.63      | 125.66   |
| 4   | D     | 8002 | CFF   | N3-C4-N9    | 3.71  | 132.09      | 126.27   |
| 4   | D     | 8002 | CFF   | C6-N1-C2    | -3.69 | 119.66      | 125.66   |
| 4   | A     | 8002 | CFF   | C6-N1-C2    | -3.69 | 119.66      | 125.66   |
| 4   | C     | 8002 | CFF   | C6-N1-C2    | -3.67 | 119.69      | 125.66   |

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| Mol | Chain | Res  | Type  | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|-------|-------------|-------|-------------|----------|
| 8   | C     | 8009 | A1BYZ | C15-C14-C13 | 3.54  | 113.95      | 110.21   |
| 8   | B     | 8009 | A1BYZ | C15-C14-C13 | 3.50  | 113.92      | 110.21   |
| 8   | A     | 8009 | A1BYZ | C15-C14-C13 | 3.50  | 113.91      | 110.21   |
| 8   | B     | 8008 | A1BYZ | C15-C16-C17 | -3.49 | 108.75      | 110.88   |
| 8   | D     | 8009 | A1BYZ | C15-C14-C13 | 3.48  | 113.89      | 110.21   |
| 8   | A     | 8008 | A1BYZ | C15-C16-C17 | -3.37 | 108.82      | 110.88   |
| 8   | C     | 8008 | A1BYZ | C15-C16-C17 | -3.36 | 108.83      | 110.88   |
| 8   | D     | 8008 | A1BYZ | C15-C16-C17 | -3.36 | 108.83      | 110.88   |
| 7   | C     | 8006 | PCW   | O2-C31-C32  | 3.28  | 118.58      | 111.48   |
| 7   | D     | 8006 | PCW   | O2-C31-C32  | 3.28  | 118.57      | 111.48   |
| 7   | A     | 8006 | PCW   | O2-C31-C32  | 3.27  | 118.55      | 111.48   |
| 7   | B     | 8006 | PCW   | O2-C31-C32  | 3.27  | 118.55      | 111.48   |
| 4   | D     | 8002 | CFF   | O13-C6-C5   | -3.17 | 119.88      | 126.38   |
| 4   | A     | 8002 | CFF   | O13-C6-C5   | -3.16 | 119.91      | 126.38   |
| 4   | C     | 8002 | CFF   | O13-C6-C5   | -3.14 | 119.94      | 126.38   |
| 4   | B     | 8002 | CFF   | O13-C6-C5   | -3.14 | 119.95      | 126.38   |
| 4   | B     | 8002 | CFF   | N7-C8-N9    | -3.09 | 107.88      | 113.48   |
| 4   | C     | 8002 | CFF   | N7-C8-N9    | -3.08 | 107.90      | 113.48   |
| 4   | A     | 8002 | CFF   | N7-C8-N9    | -3.07 | 107.92      | 113.48   |
| 4   | D     | 8002 | CFF   | N7-C8-N9    | -3.05 | 107.95      | 113.48   |
| 7   | D     | 8005 | PCW   | C18-C19-C20 | 2.93  | 146.76      | 124.83   |
| 7   | B     | 8005 | PCW   | C18-C19-C20 | 2.93  | 146.75      | 124.83   |
| 7   | C     | 8005 | PCW   | C18-C19-C20 | 2.93  | 146.75      | 124.83   |
| 7   | A     | 8005 | PCW   | C18-C19-C20 | 2.92  | 146.73      | 124.83   |
| 8   | D     | 8009 | A1BYZ | C20-C15-C16 | -2.63 | 111.18      | 112.87   |
| 8   | B     | 8009 | A1BYZ | C20-C15-C16 | -2.63 | 111.18      | 112.87   |
| 7   | B     | 8006 | PCW   | C18-C19-C20 | 2.62  | 144.48      | 124.83   |
| 7   | C     | 8006 | PCW   | C18-C19-C20 | 2.62  | 144.48      | 124.83   |
| 7   | A     | 8006 | PCW   | C18-C19-C20 | 2.62  | 144.45      | 124.83   |
| 7   | D     | 8006 | PCW   | C18-C19-C20 | 2.62  | 144.44      | 124.83   |
| 8   | A     | 8009 | A1BYZ | C20-C15-C16 | -2.60 | 111.20      | 112.87   |
| 8   | C     | 8009 | A1BYZ | C20-C15-C16 | -2.56 | 111.22      | 112.87   |
| 7   | B     | 8006 | PCW   | O3-C11-C12  | 2.53  | 119.54      | 111.83   |
| 7   | D     | 8006 | PCW   | O3-C11-C12  | 2.53  | 119.54      | 111.83   |
| 7   | A     | 8006 | PCW   | O3-C11-C12  | 2.52  | 119.51      | 111.83   |
| 7   | C     | 8006 | PCW   | O3-C11-C12  | 2.51  | 119.49      | 111.83   |
| 7   | B     | 8005 | PCW   | C2-O2-C31   | -2.46 | 111.90      | 117.80   |
| 7   | A     | 8005 | PCW   | C2-O2-C31   | -2.46 | 111.91      | 117.80   |
| 7   | D     | 8005 | PCW   | C2-O2-C31   | -2.46 | 111.92      | 117.80   |
| 7   | C     | 8005 | PCW   | C2-O2-C31   | -2.45 | 111.93      | 117.80   |
| 7   | D     | 8005 | PCW   | O3-C11-C12  | 2.42  | 119.22      | 111.83   |
| 7   | A     | 8005 | PCW   | O3-C11-C12  | 2.42  | 119.22      | 111.83   |

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| Mol | Chain | Res  | Type  | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|-------|-------------|-------|-------------|----------|
| 7   | C     | 8005 | PCW   | O3-C11-C12  | 2.42  | 119.21      | 111.83   |
| 7   | B     | 8005 | PCW   | O3-C11-C12  | 2.41  | 119.20      | 111.83   |
| 8   | B     | 8008 | A1BYZ | C24-C25-C26 | -2.40 | 112.35      | 116.30   |
| 8   | C     | 8008 | A1BYZ | C24-C25-C26 | -2.40 | 112.35      | 116.30   |
| 8   | A     | 8008 | A1BYZ | C24-C25-C26 | -2.40 | 112.36      | 116.30   |
| 8   | D     | 8008 | A1BYZ | C24-C25-C26 | -2.40 | 112.37      | 116.30   |
| 4   | B     | 8002 | CFF   | N3-C2-N1    | 2.39  | 120.12      | 117.14   |
| 4   | A     | 8002 | CFF   | N3-C2-N1    | 2.38  | 120.12      | 117.14   |
| 4   | D     | 8002 | CFF   | N3-C2-N1    | 2.38  | 120.12      | 117.14   |
| 4   | C     | 8002 | CFF   | N3-C2-N1    | 2.36  | 120.09      | 117.14   |
| 4   | D     | 8002 | CFF   | C6-C5-C4    | -2.25 | 120.08      | 122.92   |
| 4   | A     | 8002 | CFF   | C6-C5-C4    | -2.23 | 120.11      | 122.92   |
| 4   | B     | 8002 | CFF   | C6-C5-C4    | -2.23 | 120.11      | 122.92   |
| 4   | C     | 8002 | CFF   | C6-C5-C4    | -2.18 | 120.17      | 122.92   |
| 4   | B     | 8002 | CFF   | C10-N1-C2   | 2.15  | 121.07      | 117.33   |
| 4   | D     | 8002 | CFF   | C10-N1-C2   | 2.11  | 121.02      | 117.33   |
| 4   | A     | 8002 | CFF   | C10-N1-C2   | 2.11  | 121.01      | 117.33   |
| 4   | C     | 8002 | CFF   | C10-N1-C2   | 2.11  | 121.01      | 117.33   |
| 4   | C     | 8002 | CFF   | C8-N9-C4    | 2.08  | 107.98      | 102.98   |
| 4   | B     | 8002 | CFF   | C8-N9-C4    | 2.08  | 107.96      | 102.98   |
| 4   | A     | 8002 | CFF   | C8-N9-C4    | 2.07  | 107.94      | 102.98   |
| 4   | D     | 8002 | CFF   | C8-N9-C4    | 2.06  | 107.92      | 102.98   |
| 4   | B     | 8002 | CFF   | C5-C4-N9    | -2.05 | 108.03      | 112.10   |
| 4   | C     | 8002 | CFF   | C5-C4-N9    | -2.05 | 108.03      | 112.10   |
| 4   | A     | 8002 | CFF   | C5-C4-N9    | -2.05 | 108.03      | 112.10   |
| 4   | D     | 8002 | CFF   | C5-C4-N9    | -2.04 | 108.06      | 112.10   |
| 5   | B     | 8003 | ATP   | O3'-C3'-C2' | -2.02 | 105.33      | 111.82   |
| 5   | C     | 8003 | ATP   | O3'-C3'-C2' | -2.02 | 105.36      | 111.82   |
| 5   | A     | 8003 | ATP   | O3'-C3'-C2' | -2.01 | 105.37      | 111.82   |
| 5   | D     | 8003 | ATP   | O3'-C3'-C2' | -2.01 | 105.38      | 111.82   |

There are no chirality outliers.

All (297) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 5   | A     | 8003 | ATP  | C5'-O5'-PA-O1A |
| 5   | A     | 8003 | ATP  | C5'-O5'-PA-O3A |
| 5   | B     | 8003 | ATP  | C5'-O5'-PA-O1A |
| 5   | B     | 8003 | ATP  | C5'-O5'-PA-O3A |
| 5   | C     | 8003 | ATP  | C5'-O5'-PA-O1A |
| 5   | C     | 8003 | ATP  | C5'-O5'-PA-O3A |
| 5   | D     | 8003 | ATP  | C5'-O5'-PA-O1A |

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| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 5   | D     | 8003 | ATP   | C5'-O5'-PA-O3A  |
| 7   | A     | 8005 | PCW   | O3P-C1-C2-O2    |
| 7   | A     | 8005 | PCW   | C32-C31-O2-C2   |
| 7   | A     | 8006 | PCW   | O4P-C4-C5-N     |
| 7   | A     | 8006 | PCW   | C4-O4P-P-O3P    |
| 7   | B     | 8005 | PCW   | O3P-C1-C2-O2    |
| 7   | B     | 8005 | PCW   | C32-C31-O2-C2   |
| 7   | B     | 8006 | PCW   | O4P-C4-C5-N     |
| 7   | B     | 8006 | PCW   | C4-O4P-P-O3P    |
| 7   | C     | 8005 | PCW   | O3P-C1-C2-O2    |
| 7   | C     | 8005 | PCW   | C32-C31-O2-C2   |
| 7   | C     | 8006 | PCW   | O4P-C4-C5-N     |
| 7   | C     | 8006 | PCW   | C4-O4P-P-O3P    |
| 7   | D     | 8005 | PCW   | O3P-C1-C2-O2    |
| 7   | D     | 8005 | PCW   | C32-C31-O2-C2   |
| 7   | D     | 8006 | PCW   | O4P-C4-C5-N     |
| 7   | D     | 8006 | PCW   | C4-O4P-P-O3P    |
| 8   | A     | 8009 | A1BYZ | C3-C6-O8-C9     |
| 8   | A     | 8009 | A1BYZ | O7-C6-O8-C9     |
| 8   | B     | 8009 | A1BYZ | C3-C6-O8-C9     |
| 8   | B     | 8009 | A1BYZ | O7-C6-O8-C9     |
| 8   | C     | 8009 | A1BYZ | C3-C6-O8-C9     |
| 8   | C     | 8009 | A1BYZ | O7-C6-O8-C9     |
| 8   | D     | 8009 | A1BYZ | C3-C6-O8-C9     |
| 8   | D     | 8009 | A1BYZ | O7-C6-O8-C9     |
| 8   | A     | 8008 | A1BYZ | C10-C9-O8-C6    |
| 8   | B     | 8008 | A1BYZ | C10-C9-O8-C6    |
| 8   | C     | 8008 | A1BYZ | C10-C9-O8-C6    |
| 8   | D     | 8008 | A1BYZ | C10-C9-O8-C6    |
| 7   | A     | 8005 | PCW   | O31-C31-O2-C2   |
| 7   | B     | 8005 | PCW   | O31-C31-O2-C2   |
| 7   | C     | 8005 | PCW   | O31-C31-O2-C2   |
| 7   | D     | 8005 | PCW   | O31-C31-O2-C2   |
| 7   | A     | 8006 | PCW   | C32-C31-O2-C2   |
| 7   | B     | 8006 | PCW   | C32-C31-O2-C2   |
| 7   | C     | 8006 | PCW   | C32-C31-O2-C2   |
| 7   | D     | 8006 | PCW   | C32-C31-O2-C2   |
| 7   | A     | 8006 | PCW   | C22-C23-C24-C25 |
| 7   | B     | 8006 | PCW   | C22-C23-C24-C25 |
| 7   | C     | 8006 | PCW   | C22-C23-C24-C25 |
| 7   | D     | 8006 | PCW   | C22-C23-C24-C25 |
| 7   | A     | 8006 | PCW   | O31-C31-O2-C2   |

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| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 7   | B     | 8006 | PCW   | O31-C31-O2-C2   |
| 7   | C     | 8006 | PCW   | O31-C31-O2-C2   |
| 7   | D     | 8006 | PCW   | O31-C31-O2-C2   |
| 8   | A     | 8008 | A1BYZ | C15-C20-C21-C22 |
| 8   | B     | 8008 | A1BYZ | C15-C20-C21-C22 |
| 8   | C     | 8008 | A1BYZ | C15-C20-C21-C22 |
| 8   | D     | 8008 | A1BYZ | C15-C20-C21-C22 |
| 7   | A     | 8006 | PCW   | C11-C12-C13-C14 |
| 7   | B     | 8006 | PCW   | C11-C12-C13-C14 |
| 7   | C     | 8006 | PCW   | C11-C12-C13-C14 |
| 7   | D     | 8006 | PCW   | C11-C12-C13-C14 |
| 7   | A     | 8006 | PCW   | C36-C37-C38-C39 |
| 7   | B     | 8006 | PCW   | C36-C37-C38-C39 |
| 7   | C     | 8006 | PCW   | C36-C37-C38-C39 |
| 7   | D     | 8006 | PCW   | C36-C37-C38-C39 |
| 7   | A     | 8006 | PCW   | C33-C34-C35-C36 |
| 7   | B     | 8006 | PCW   | C33-C34-C35-C36 |
| 7   | C     | 8006 | PCW   | C33-C34-C35-C36 |
| 7   | D     | 8006 | PCW   | C33-C34-C35-C36 |
| 7   | B     | 8006 | PCW   | C12-C13-C14-C15 |
| 7   | C     | 8006 | PCW   | C12-C13-C14-C15 |
| 7   | A     | 8006 | PCW   | C12-C13-C14-C15 |
| 7   | D     | 8006 | PCW   | C12-C13-C14-C15 |
| 7   | A     | 8005 | PCW   | C12-C11-O3-C3   |
| 7   | B     | 8005 | PCW   | C12-C11-O3-C3   |
| 7   | C     | 8005 | PCW   | C12-C11-O3-C3   |
| 7   | D     | 8005 | PCW   | C12-C11-O3-C3   |
| 7   | B     | 8005 | PCW   | C35-C36-C37-C38 |
| 7   | C     | 8005 | PCW   | C35-C36-C37-C38 |
| 7   | A     | 8005 | PCW   | C35-C36-C37-C38 |
| 7   | D     | 8005 | PCW   | C35-C36-C37-C38 |
| 7   | A     | 8005 | PCW   | C41-C42-C43-C44 |
| 7   | D     | 8005 | PCW   | C41-C42-C43-C44 |
| 7   | B     | 8005 | PCW   | C41-C42-C43-C44 |
| 7   | C     | 8005 | PCW   | C41-C42-C43-C44 |
| 7   | A     | 8005 | PCW   | C24-C25-C26-C27 |
| 7   | B     | 8005 | PCW   | C24-C25-C26-C27 |
| 7   | C     | 8005 | PCW   | C24-C25-C26-C27 |
| 7   | D     | 8005 | PCW   | C24-C25-C26-C27 |
| 7   | A     | 8005 | PCW   | C43-C44-C45-C46 |
| 7   | B     | 8005 | PCW   | C43-C44-C45-C46 |
| 7   | D     | 8005 | PCW   | C43-C44-C45-C46 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 7   | C     | 8005 | PCW  | C43-C44-C45-C46 |
| 7   | A     | 8006 | PCW  | C23-C24-C25-C26 |
| 7   | B     | 8006 | PCW  | C23-C24-C25-C26 |
| 7   | C     | 8006 | PCW  | C23-C24-C25-C26 |
| 7   | D     | 8006 | PCW  | C23-C24-C25-C26 |
| 7   | A     | 8005 | PCW  | O11-C11-O3-C3   |
| 7   | B     | 8005 | PCW  | O11-C11-O3-C3   |
| 7   | C     | 8005 | PCW  | O11-C11-O3-C3   |
| 7   | D     | 8005 | PCW  | O11-C11-O3-C3   |
| 7   | A     | 8006 | PCW  | C21-C22-C23-C24 |
| 7   | B     | 8006 | PCW  | C21-C22-C23-C24 |
| 7   | C     | 8006 | PCW  | C21-C22-C23-C24 |
| 7   | D     | 8006 | PCW  | C21-C22-C23-C24 |
| 7   | A     | 8006 | PCW  | C16-C17-C18-C19 |
| 7   | B     | 8006 | PCW  | C16-C17-C18-C19 |
| 7   | C     | 8006 | PCW  | C16-C17-C18-C19 |
| 7   | D     | 8006 | PCW  | C16-C17-C18-C19 |
| 7   | A     | 8005 | PCW  | C42-C43-C44-C45 |
| 7   | C     | 8005 | PCW  | C42-C43-C44-C45 |
| 7   | D     | 8005 | PCW  | C42-C43-C44-C45 |
| 7   | B     | 8005 | PCW  | C42-C43-C44-C45 |
| 7   | A     | 8005 | PCW  | C32-C33-C34-C35 |
| 7   | B     | 8005 | PCW  | C32-C33-C34-C35 |
| 7   | C     | 8005 | PCW  | C32-C33-C34-C35 |
| 7   | D     | 8005 | PCW  | C32-C33-C34-C35 |
| 7   | D     | 8006 | PCW  | C35-C36-C37-C38 |
| 7   | A     | 8006 | PCW  | C35-C36-C37-C38 |
| 7   | B     | 8006 | PCW  | C35-C36-C37-C38 |
| 7   | C     | 8006 | PCW  | C35-C36-C37-C38 |
| 7   | A     | 8005 | PCW  | C20-C21-C22-C23 |
| 7   | B     | 8005 | PCW  | C20-C21-C22-C23 |
| 7   | C     | 8005 | PCW  | C20-C21-C22-C23 |
| 7   | D     | 8005 | PCW  | C20-C21-C22-C23 |
| 7   | D     | 8006 | PCW  | C17-C18-C19-C20 |
| 7   | A     | 8005 | PCW  | O3P-C1-C2-C3    |
| 7   | B     | 8005 | PCW  | O3P-C1-C2-C3    |
| 7   | C     | 8005 | PCW  | O3P-C1-C2-C3    |
| 7   | D     | 8005 | PCW  | O3P-C1-C2-C3    |
| 7   | A     | 8006 | PCW  | C17-C18-C19-C20 |
| 7   | B     | 8006 | PCW  | C17-C18-C19-C20 |
| 7   | C     | 8006 | PCW  | C17-C18-C19-C20 |
| 7   | C     | 8006 | PCW  | C42-C43-C44-C45 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 7   | B     | 8006 | PCW  | C42-C43-C44-C45 |
| 7   | A     | 8006 | PCW  | C42-C43-C44-C45 |
| 7   | D     | 8006 | PCW  | C42-C43-C44-C45 |
| 7   | A     | 8006 | PCW  | C19-C20-C21-C22 |
| 7   | B     | 8006 | PCW  | C19-C20-C21-C22 |
| 7   | C     | 8006 | PCW  | C19-C20-C21-C22 |
| 7   | D     | 8006 | PCW  | C19-C20-C21-C22 |
| 7   | B     | 8005 | PCW  | C45-C46-C47-C48 |
| 7   | C     | 8005 | PCW  | C45-C46-C47-C48 |
| 7   | D     | 8005 | PCW  | C45-C46-C47-C48 |
| 7   | A     | 8005 | PCW  | C45-C46-C47-C48 |
| 7   | A     | 8006 | PCW  | C45-C46-C47-C48 |
| 7   | C     | 8006 | PCW  | C45-C46-C47-C48 |
| 7   | D     | 8006 | PCW  | C45-C46-C47-C48 |
| 7   | A     | 8006 | PCW  | C31-C32-C33-C34 |
| 7   | B     | 8006 | PCW  | C31-C32-C33-C34 |
| 7   | C     | 8006 | PCW  | C31-C32-C33-C34 |
| 7   | B     | 8006 | PCW  | C45-C46-C47-C48 |
| 7   | D     | 8006 | PCW  | C31-C32-C33-C34 |
| 7   | A     | 8006 | PCW  | C25-C26-C27-C28 |
| 7   | B     | 8006 | PCW  | C25-C26-C27-C28 |
| 7   | C     | 8006 | PCW  | C25-C26-C27-C28 |
| 7   | D     | 8006 | PCW  | C25-C26-C27-C28 |
| 7   | C     | 8005 | PCW  | C13-C14-C15-C16 |
| 7   | A     | 8005 | PCW  | C13-C14-C15-C16 |
| 7   | B     | 8005 | PCW  | C13-C14-C15-C16 |
| 7   | D     | 8005 | PCW  | C13-C14-C15-C16 |
| 7   | B     | 8005 | PCW  | C21-C22-C23-C24 |
| 7   | A     | 8005 | PCW  | C21-C22-C23-C24 |
| 7   | B     | 8005 | PCW  | C15-C16-C17-C18 |
| 7   | C     | 8005 | PCW  | C21-C22-C23-C24 |
| 7   | D     | 8005 | PCW  | C21-C22-C23-C24 |
| 7   | A     | 8005 | PCW  | C15-C16-C17-C18 |
| 7   | C     | 8005 | PCW  | C15-C16-C17-C18 |
| 7   | D     | 8005 | PCW  | C15-C16-C17-C18 |
| 7   | A     | 8006 | PCW  | C5-C4-O4P-P     |
| 7   | B     | 8006 | PCW  | C5-C4-O4P-P     |
| 7   | C     | 8006 | PCW  | C5-C4-O4P-P     |
| 7   | D     | 8006 | PCW  | C5-C4-O4P-P     |
| 7   | D     | 8006 | PCW  | C34-C35-C36-C37 |
| 7   | A     | 8006 | PCW  | C34-C35-C36-C37 |
| 7   | B     | 8006 | PCW  | C34-C35-C36-C37 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 7   | C     | 8006 | PCW  | C34-C35-C36-C37 |
| 7   | A     | 8005 | PCW  | C34-C35-C36-C37 |
| 7   | B     | 8005 | PCW  | C34-C35-C36-C37 |
| 7   | C     | 8005 | PCW  | C34-C35-C36-C37 |
| 7   | D     | 8005 | PCW  | C34-C35-C36-C37 |
| 5   | A     | 8003 | ATP  | C5'-O5'-PA-O2A  |
| 5   | A     | 8007 | ATP  | C5'-O5'-PA-O1A  |
| 5   | A     | 8007 | ATP  | C5'-O5'-PA-O2A  |
| 5   | A     | 8007 | ATP  | C5'-O5'-PA-O3A  |
| 5   | B     | 8003 | ATP  | C5'-O5'-PA-O2A  |
| 5   | B     | 8007 | ATP  | C5'-O5'-PA-O1A  |
| 5   | B     | 8007 | ATP  | C5'-O5'-PA-O2A  |
| 5   | B     | 8007 | ATP  | C5'-O5'-PA-O3A  |
| 5   | C     | 8003 | ATP  | C5'-O5'-PA-O2A  |
| 5   | C     | 8007 | ATP  | C5'-O5'-PA-O1A  |
| 5   | C     | 8007 | ATP  | C5'-O5'-PA-O2A  |
| 5   | C     | 8007 | ATP  | C5'-O5'-PA-O3A  |
| 5   | D     | 8003 | ATP  | C5'-O5'-PA-O2A  |
| 5   | D     | 8007 | ATP  | C5'-O5'-PA-O1A  |
| 5   | D     | 8007 | ATP  | C5'-O5'-PA-O2A  |
| 5   | D     | 8007 | ATP  | C5'-O5'-PA-O3A  |
| 7   | A     | 8005 | PCW  | C4-O4P-P-O1P    |
| 7   | A     | 8006 | PCW  | C4-O4P-P-O2P    |
| 7   | B     | 8005 | PCW  | C4-O4P-P-O1P    |
| 7   | B     | 8006 | PCW  | C4-O4P-P-O2P    |
| 7   | C     | 8005 | PCW  | C4-O4P-P-O1P    |
| 7   | C     | 8006 | PCW  | C4-O4P-P-O2P    |
| 7   | D     | 8005 | PCW  | C4-O4P-P-O1P    |
| 7   | D     | 8006 | PCW  | C4-O4P-P-O2P    |
| 7   | A     | 8005 | PCW  | C25-C26-C27-C28 |
| 7   | B     | 8005 | PCW  | C25-C26-C27-C28 |
| 7   | D     | 8005 | PCW  | C25-C26-C27-C28 |
| 5   | A     | 8007 | ATP  | PB-O3A-PA-O1A   |
| 5   | A     | 8007 | ATP  | PB-O3A-PA-O2A   |
| 5   | B     | 8007 | ATP  | PB-O3A-PA-O1A   |
| 5   | B     | 8007 | ATP  | PB-O3A-PA-O2A   |
| 5   | C     | 8007 | ATP  | PB-O3A-PA-O1A   |
| 5   | C     | 8007 | ATP  | PB-O3A-PA-O2A   |
| 5   | D     | 8007 | ATP  | PB-O3A-PA-O1A   |
| 5   | D     | 8007 | ATP  | PB-O3A-PA-O2A   |
| 7   | C     | 8005 | PCW  | C25-C26-C27-C28 |
| 5   | A     | 8007 | ATP  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 5   | B     | 8007 | ATP   | C3'-C4'-C5'-O5' |
| 5   | C     | 8007 | ATP   | C3'-C4'-C5'-O5' |
| 5   | D     | 8007 | ATP   | C3'-C4'-C5'-O5' |
| 7   | D     | 8006 | PCW   | C41-C42-C43-C44 |
| 7   | B     | 8006 | PCW   | C41-C42-C43-C44 |
| 7   | A     | 8006 | PCW   | C41-C42-C43-C44 |
| 7   | C     | 8006 | PCW   | C41-C42-C43-C44 |
| 7   | A     | 8006 | PCW   | C12-C11-O3-C3   |
| 7   | B     | 8006 | PCW   | C12-C11-O3-C3   |
| 7   | C     | 8006 | PCW   | C12-C11-O3-C3   |
| 7   | D     | 8006 | PCW   | C12-C11-O3-C3   |
| 7   | A     | 8006 | PCW   | O11-C11-O3-C3   |
| 7   | B     | 8006 | PCW   | O11-C11-O3-C3   |
| 7   | D     | 8006 | PCW   | O11-C11-O3-C3   |
| 5   | A     | 8003 | ATP   | PA-O3A-PB-O3B   |
| 5   | B     | 8003 | ATP   | PA-O3A-PB-O3B   |
| 5   | C     | 8003 | ATP   | PA-O3A-PB-O3B   |
| 5   | D     | 8003 | ATP   | PA-O3A-PB-O3B   |
| 8   | A     | 8009 | A1BYZ | C15-C20-C21-C22 |
| 8   | B     | 8009 | A1BYZ | C15-C20-C21-C22 |
| 8   | C     | 8009 | A1BYZ | C15-C20-C21-C22 |
| 8   | D     | 8009 | A1BYZ | C15-C20-C21-C22 |
| 7   | C     | 8006 | PCW   | O11-C11-O3-C3   |
| 7   | A     | 8006 | PCW   | C39-C40-C41-C42 |
| 7   | B     | 8006 | PCW   | C39-C40-C41-C42 |
| 7   | C     | 8006 | PCW   | C39-C40-C41-C42 |
| 7   | D     | 8006 | PCW   | C39-C40-C41-C42 |
| 8   | A     | 8009 | A1BYZ | C16-C15-C20-C21 |
| 8   | B     | 8009 | A1BYZ | C16-C15-C20-C21 |
| 8   | C     | 8009 | A1BYZ | C16-C15-C20-C21 |
| 8   | D     | 8009 | A1BYZ | C16-C15-C20-C21 |
| 8   | A     | 8008 | A1BYZ | C2-C3-C6-O7     |
| 8   | A     | 8009 | A1BYZ | C2-C3-C6-O7     |
| 8   | B     | 8008 | A1BYZ | C2-C3-C6-O7     |
| 8   | B     | 8009 | A1BYZ | C2-C3-C6-O7     |
| 8   | C     | 8008 | A1BYZ | C2-C3-C6-O7     |
| 8   | C     | 8009 | A1BYZ | C2-C3-C6-O7     |
| 8   | D     | 8008 | A1BYZ | C2-C3-C6-O7     |
| 8   | D     | 8009 | A1BYZ | C2-C3-C6-O7     |
| 7   | A     | 8006 | PCW   | C32-C33-C34-C35 |
| 7   | B     | 8006 | PCW   | C32-C33-C34-C35 |
| 7   | D     | 8006 | PCW   | C32-C33-C34-C35 |

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| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 7   | C     | 8006 | PCW   | C32-C33-C34-C35 |
| 7   | A     | 8005 | PCW   | C17-C18-C19-C20 |
| 7   | B     | 8005 | PCW   | C17-C18-C19-C20 |
| 7   | C     | 8005 | PCW   | C17-C18-C19-C20 |
| 7   | D     | 8005 | PCW   | C17-C18-C19-C20 |
| 5   | A     | 8007 | ATP   | PB-O3B-PG-O3G   |
| 5   | B     | 8007 | ATP   | PB-O3B-PG-O3G   |
| 5   | C     | 8007 | ATP   | PB-O3B-PG-O3G   |
| 5   | D     | 8007 | ATP   | PB-O3B-PG-O3G   |
| 7   | D     | 8006 | PCW   | C15-C16-C17-C18 |
| 7   | A     | 8006 | PCW   | C15-C16-C17-C18 |
| 7   | B     | 8006 | PCW   | C15-C16-C17-C18 |
| 7   | C     | 8006 | PCW   | C15-C16-C17-C18 |
| 7   | B     | 8005 | PCW   | C5-C4-O4P-P     |
| 7   | A     | 8005 | PCW   | C39-C40-C41-C42 |
| 7   | B     | 8005 | PCW   | C39-C40-C41-C42 |
| 7   | C     | 8005 | PCW   | C39-C40-C41-C42 |
| 7   | D     | 8005 | PCW   | C39-C40-C41-C42 |
| 8   | A     | 8008 | A1BYZ | C4-C3-C6-O8     |
| 8   | B     | 8008 | A1BYZ | C4-C3-C6-O8     |
| 8   | C     | 8008 | A1BYZ | C4-C3-C6-O8     |
| 8   | D     | 8008 | A1BYZ | C4-C3-C6-O8     |
| 5   | A     | 8003 | ATP   | PA-O3A-PB-O1B   |
| 5   | B     | 8003 | ATP   | PA-O3A-PB-O1B   |
| 5   | C     | 8003 | ATP   | PA-O3A-PB-O1B   |
| 5   | D     | 8003 | ATP   | PA-O3A-PB-O1B   |
| 5   | A     | 8003 | ATP   | O4'-C4'-C5'-O5' |
| 5   | A     | 8007 | ATP   | O4'-C4'-C5'-O5' |
| 5   | B     | 8003 | ATP   | O4'-C4'-C5'-O5' |
| 5   | B     | 8007 | ATP   | O4'-C4'-C5'-O5' |
| 5   | C     | 8003 | ATP   | O4'-C4'-C5'-O5' |
| 5   | C     | 8007 | ATP   | O4'-C4'-C5'-O5' |
| 5   | D     | 8003 | ATP   | O4'-C4'-C5'-O5' |
| 5   | D     | 8007 | ATP   | O4'-C4'-C5'-O5' |
| 8   | A     | 8008 | A1BYZ | C4-C3-C6-O7     |
| 8   | B     | 8008 | A1BYZ | C4-C3-C6-O7     |
| 8   | C     | 8008 | A1BYZ | C4-C3-C6-O7     |
| 8   | D     | 8008 | A1BYZ | C4-C3-C6-O7     |

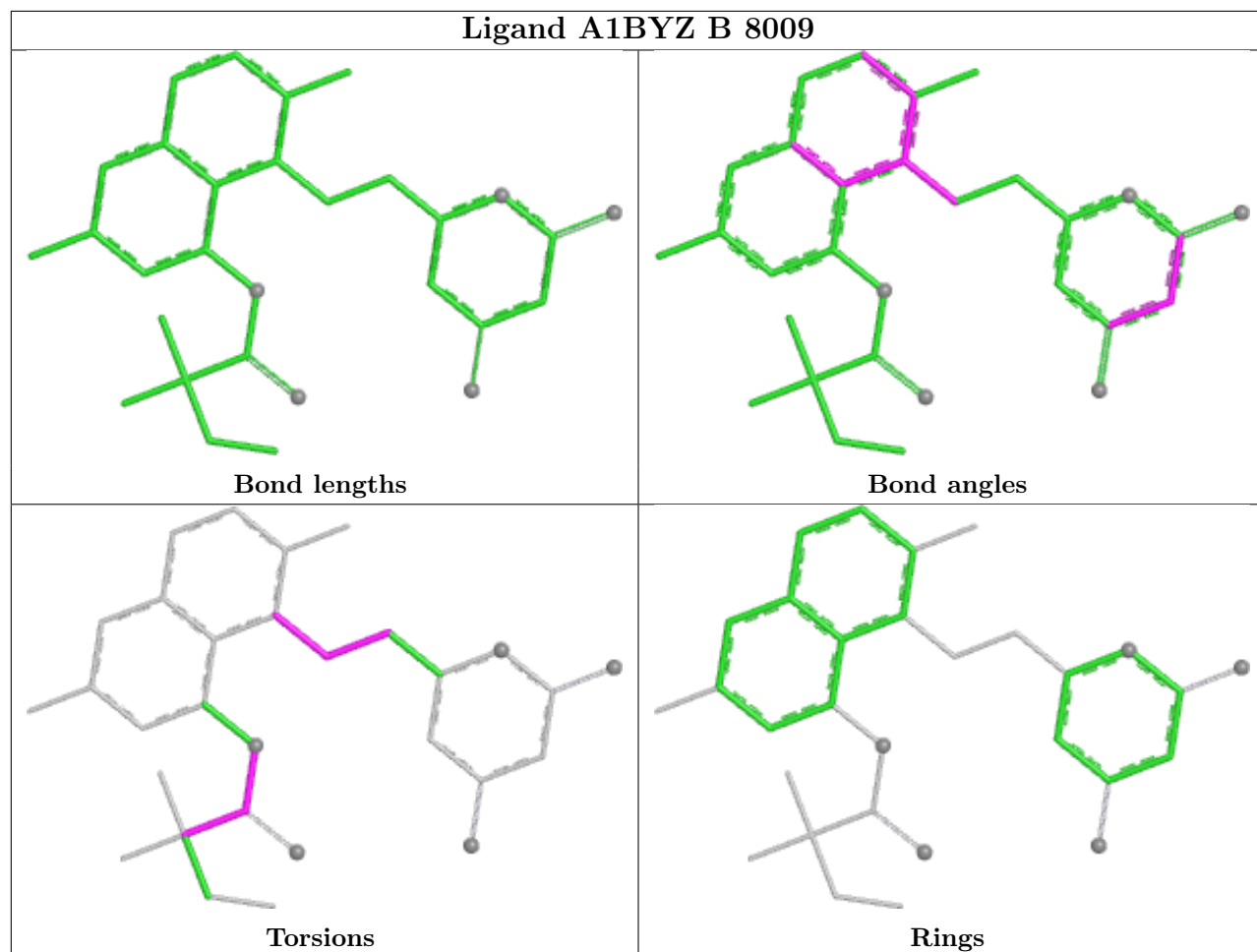
There are no ring outliers.

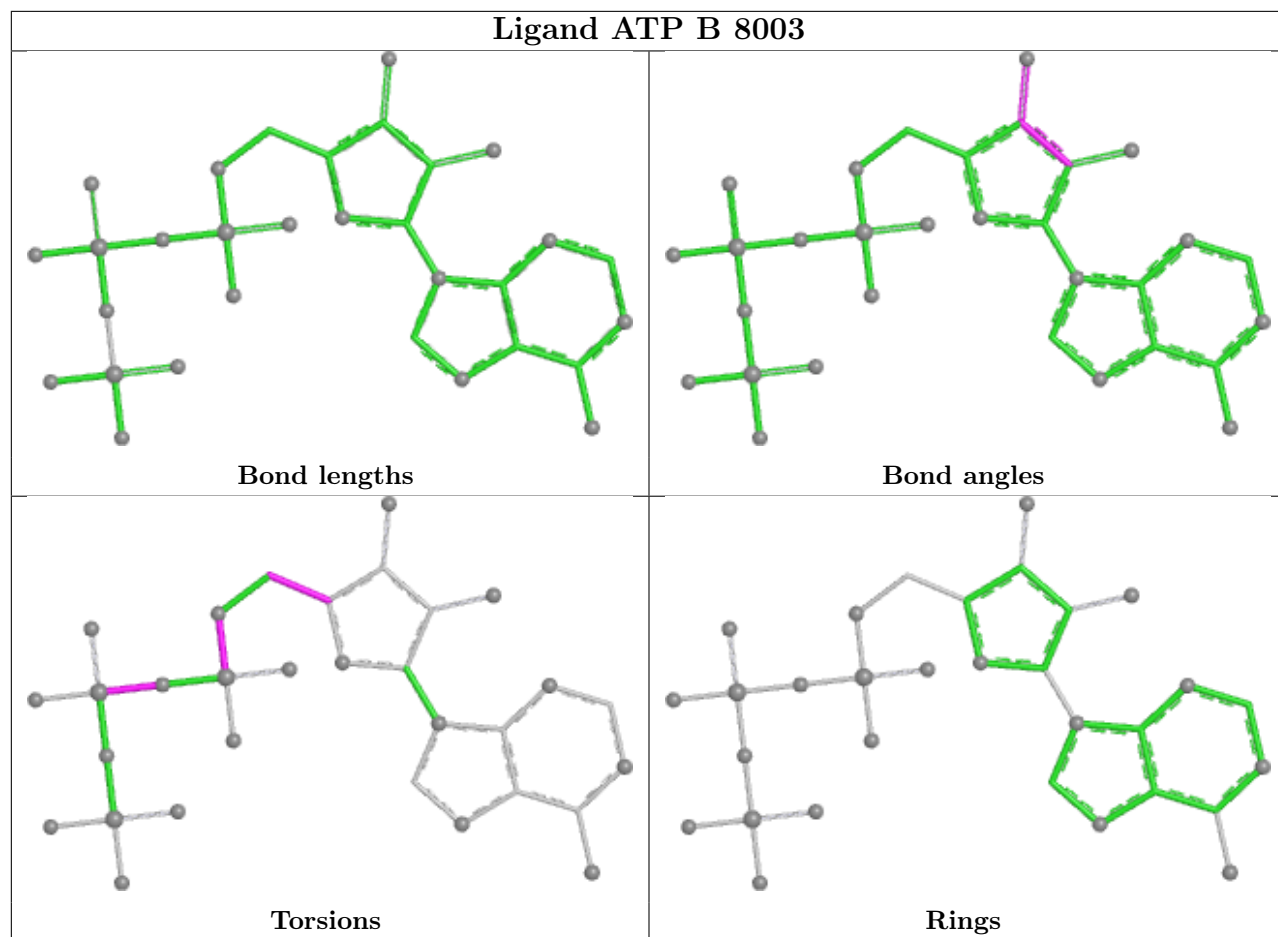
10 monomers are involved in 32 short contacts:

| Mol | Chain | Res  | Type  | Clashes | Symm-Clashes |
|-----|-------|------|-------|---------|--------------|
| 8   | B     | 8009 | A1BYZ | 2       | 0            |
| 8   | A     | 8009 | A1BYZ | 2       | 0            |
| 7   | A     | 8006 | PCW   | 5       | 0            |
| 7   | B     | 8006 | PCW   | 6       | 0            |
| 7   | D     | 8006 | PCW   | 5       | 0            |
| 7   | C     | 8006 | PCW   | 6       | 0            |
| 8   | D     | 8009 | A1BYZ | 2       | 0            |
| 8   | C     | 8009 | A1BYZ | 2       | 0            |
| 7   | B     | 8005 | PCW   | 1       | 0            |
| 7   | D     | 8005 | PCW   | 1       | 0            |

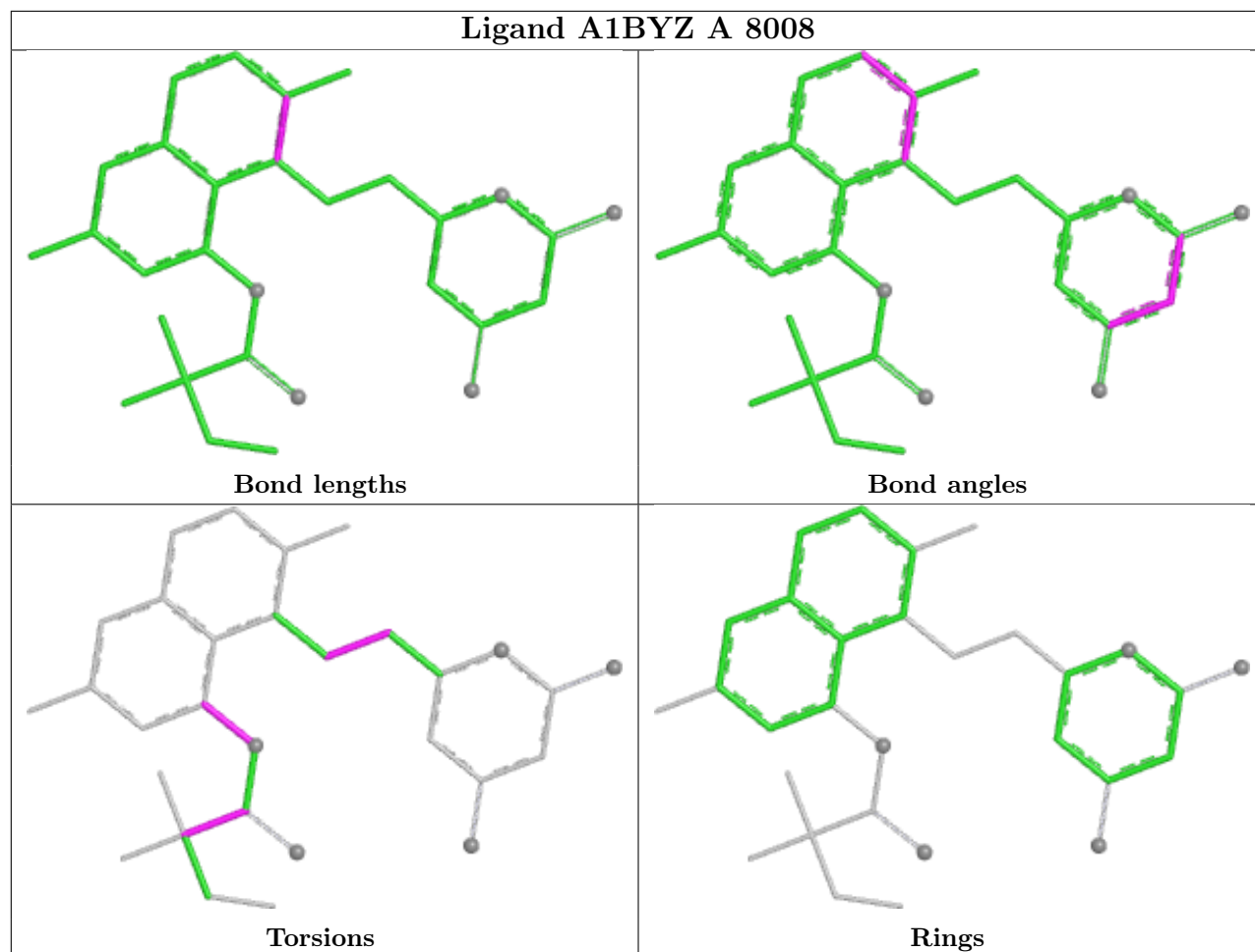
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A1BYZ B 8009

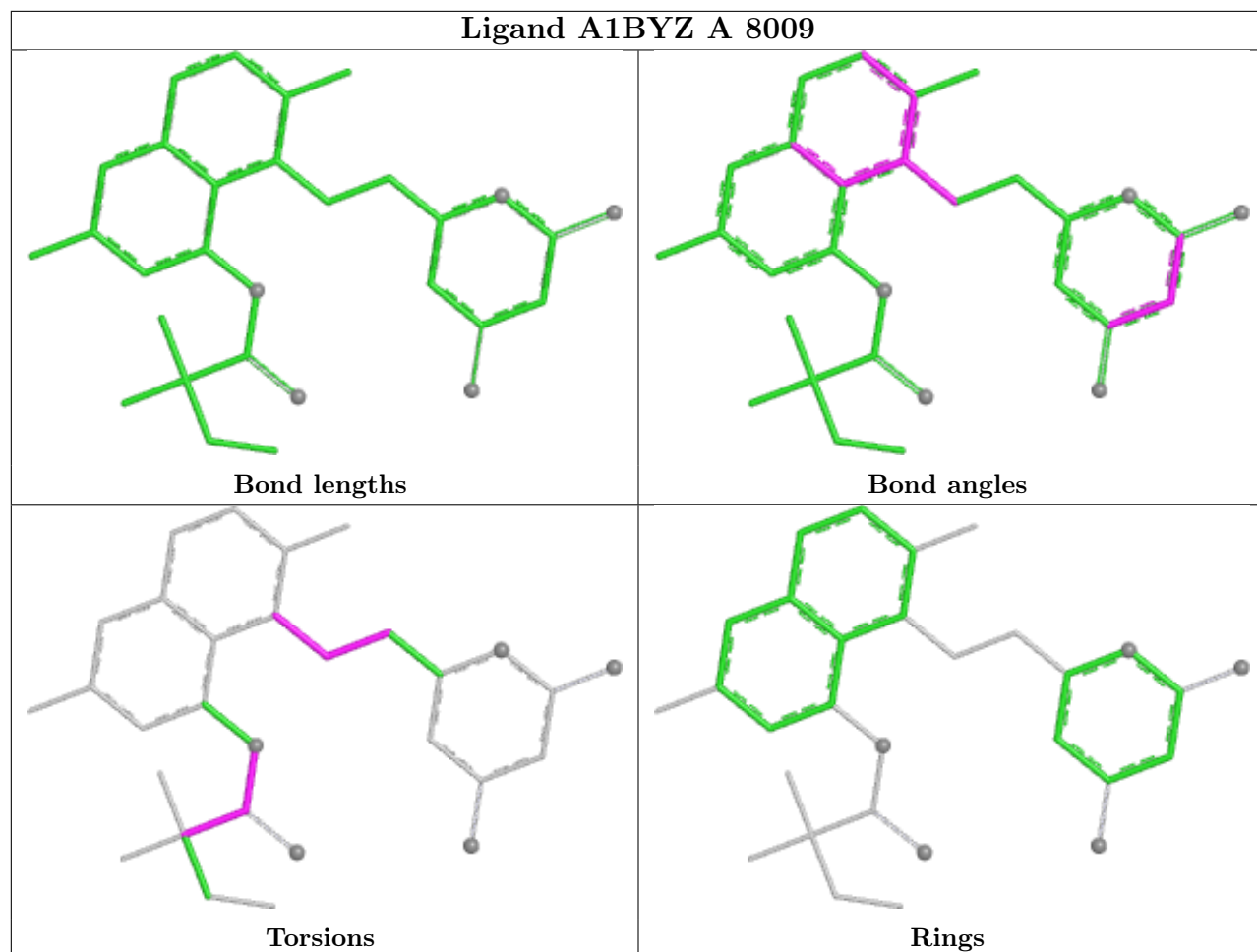


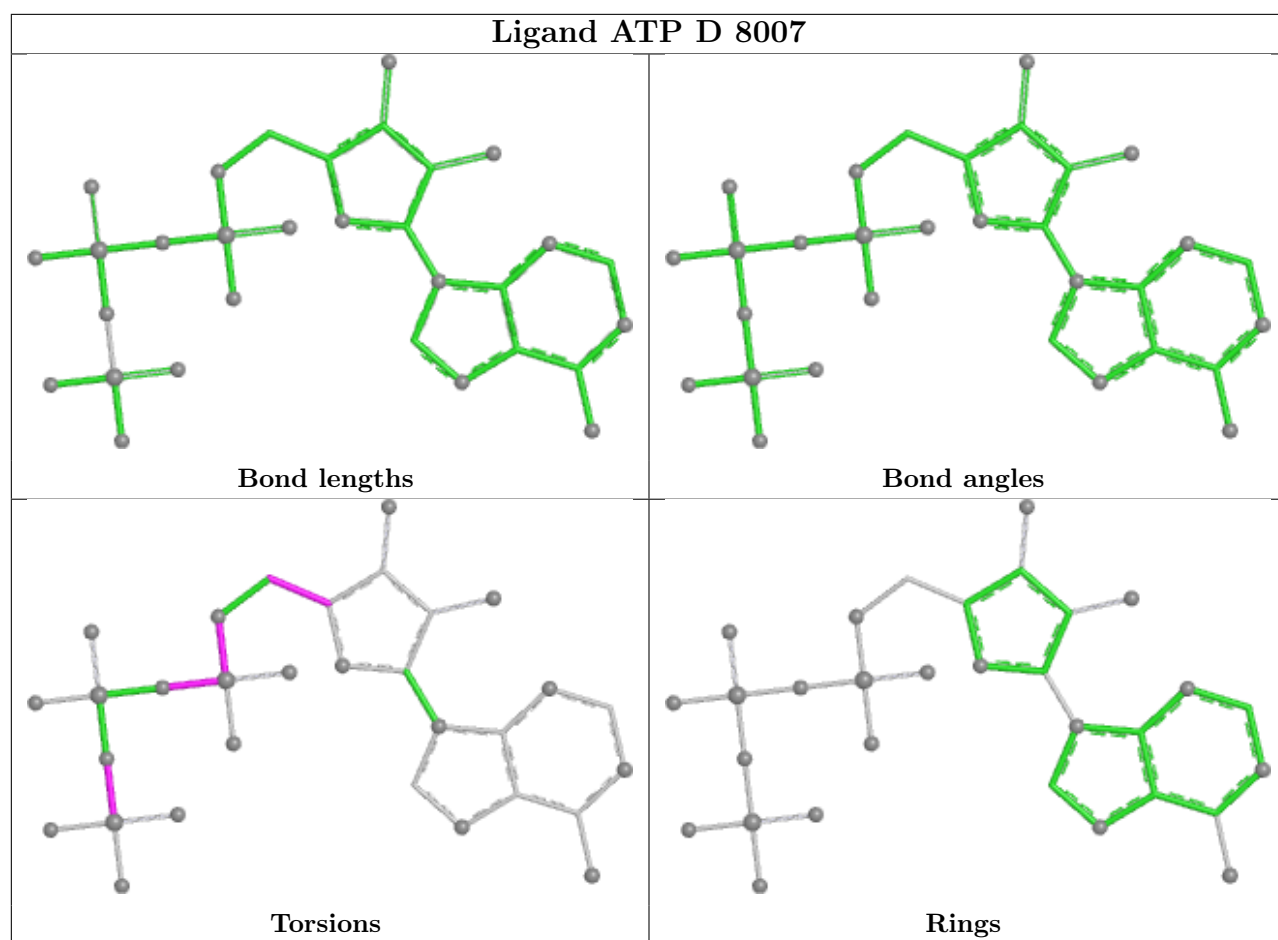


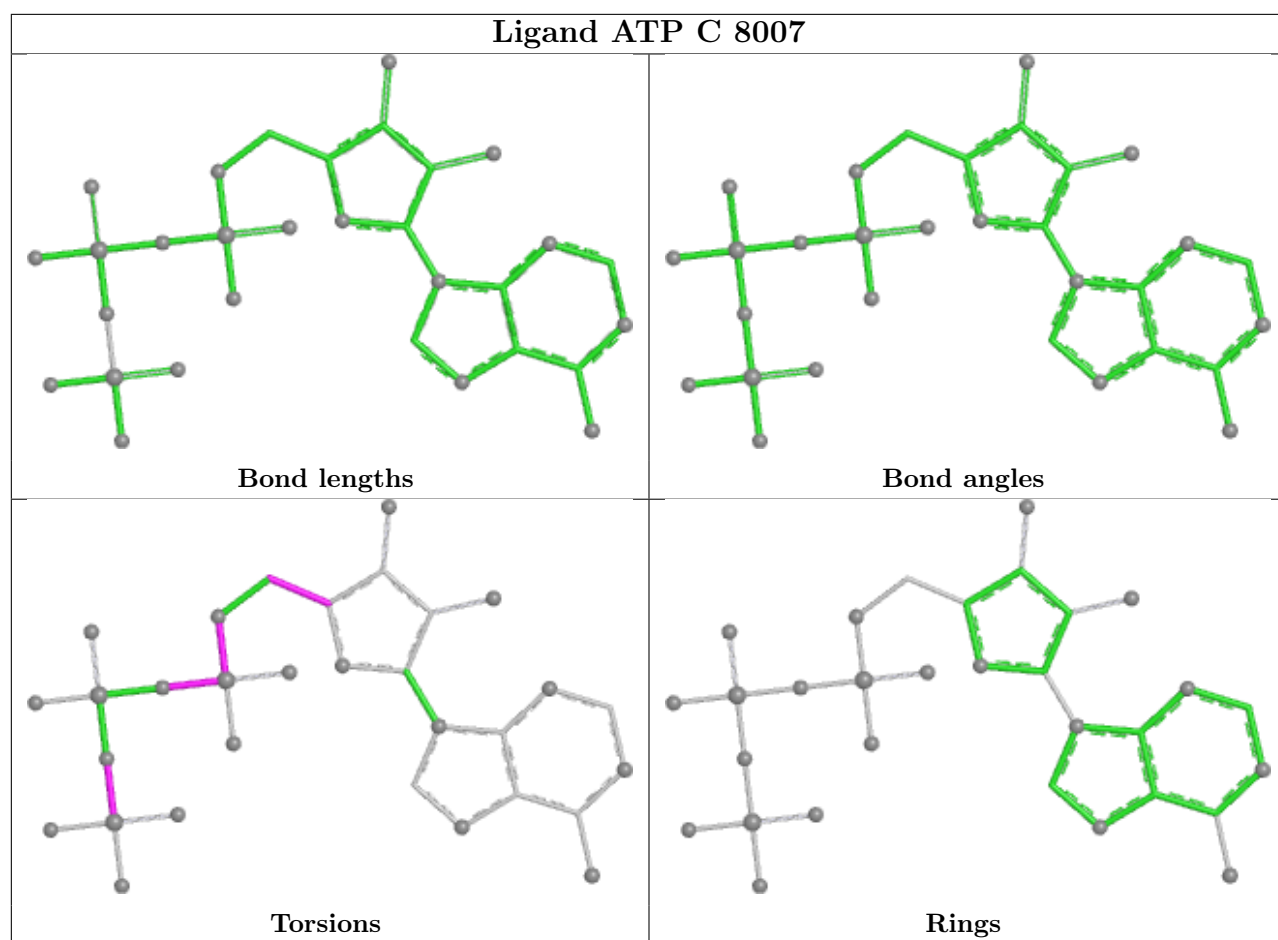
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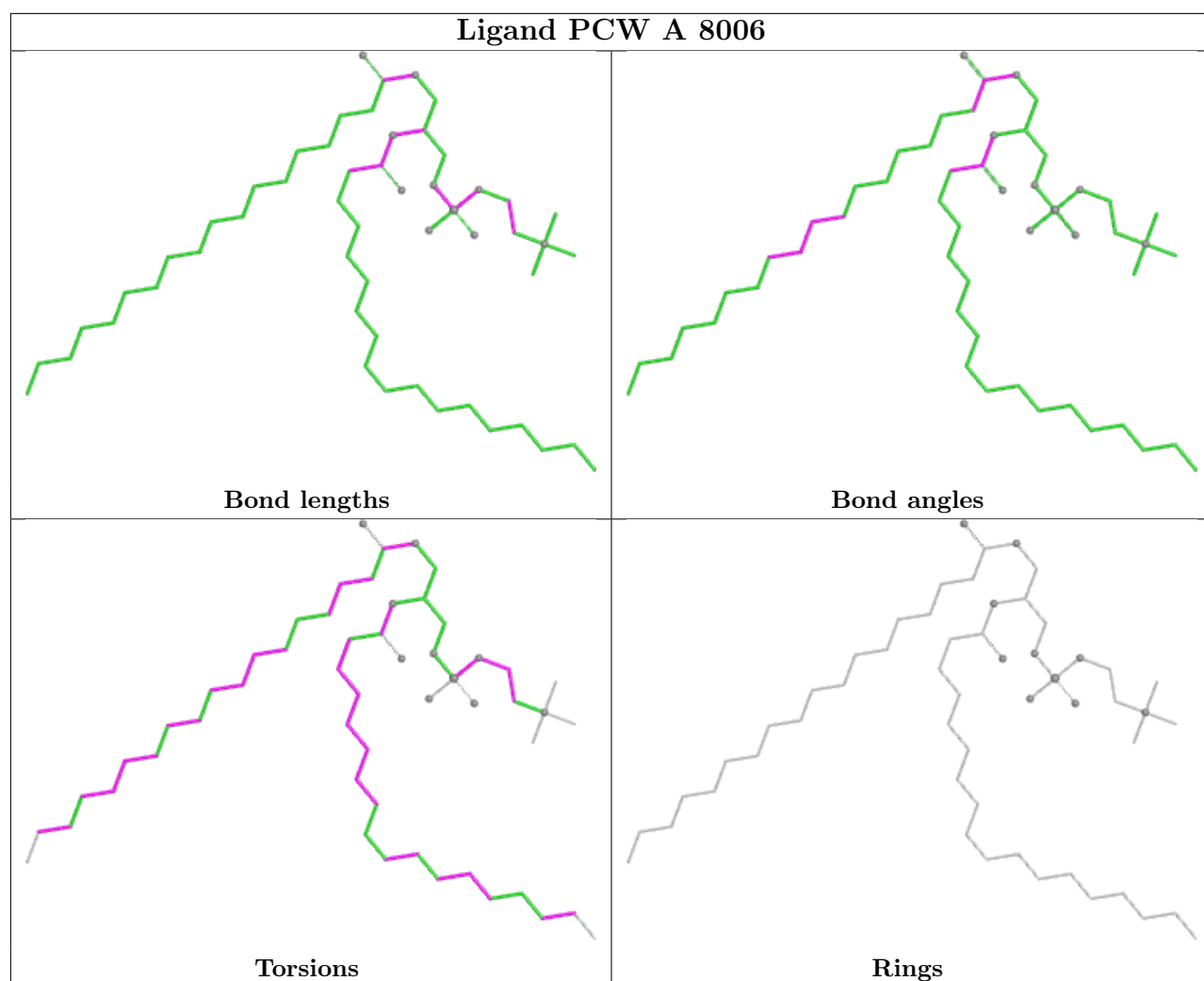


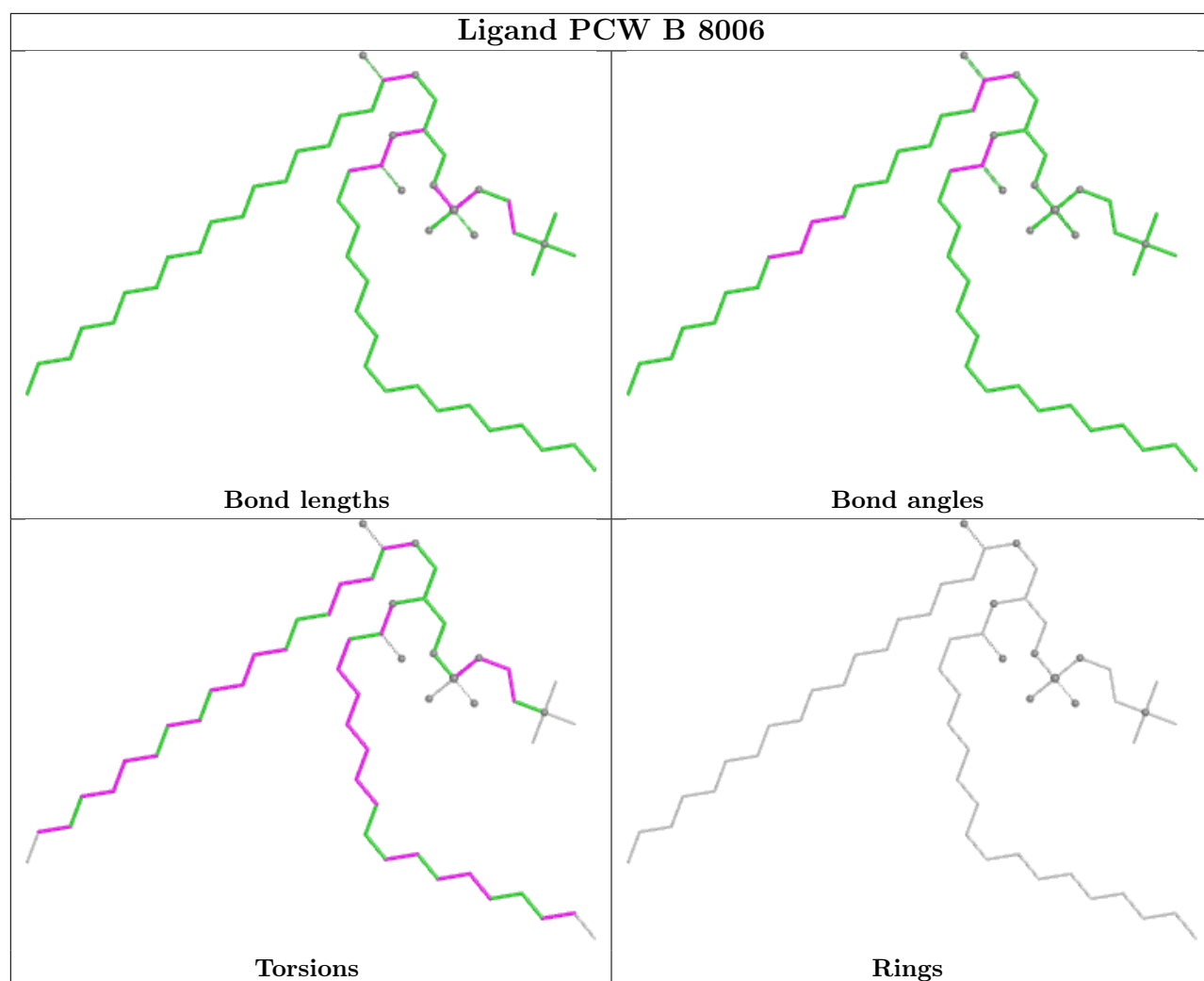
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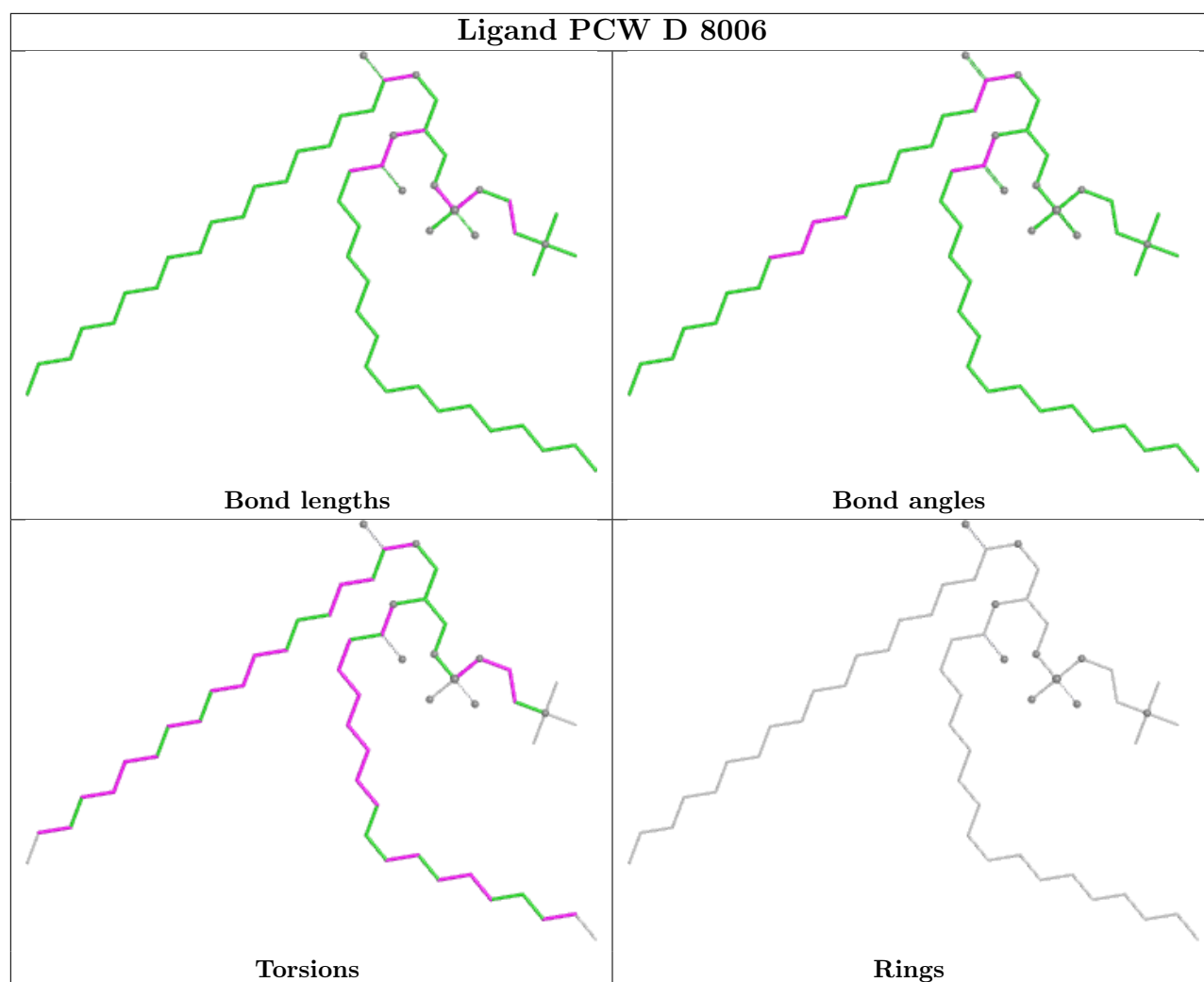




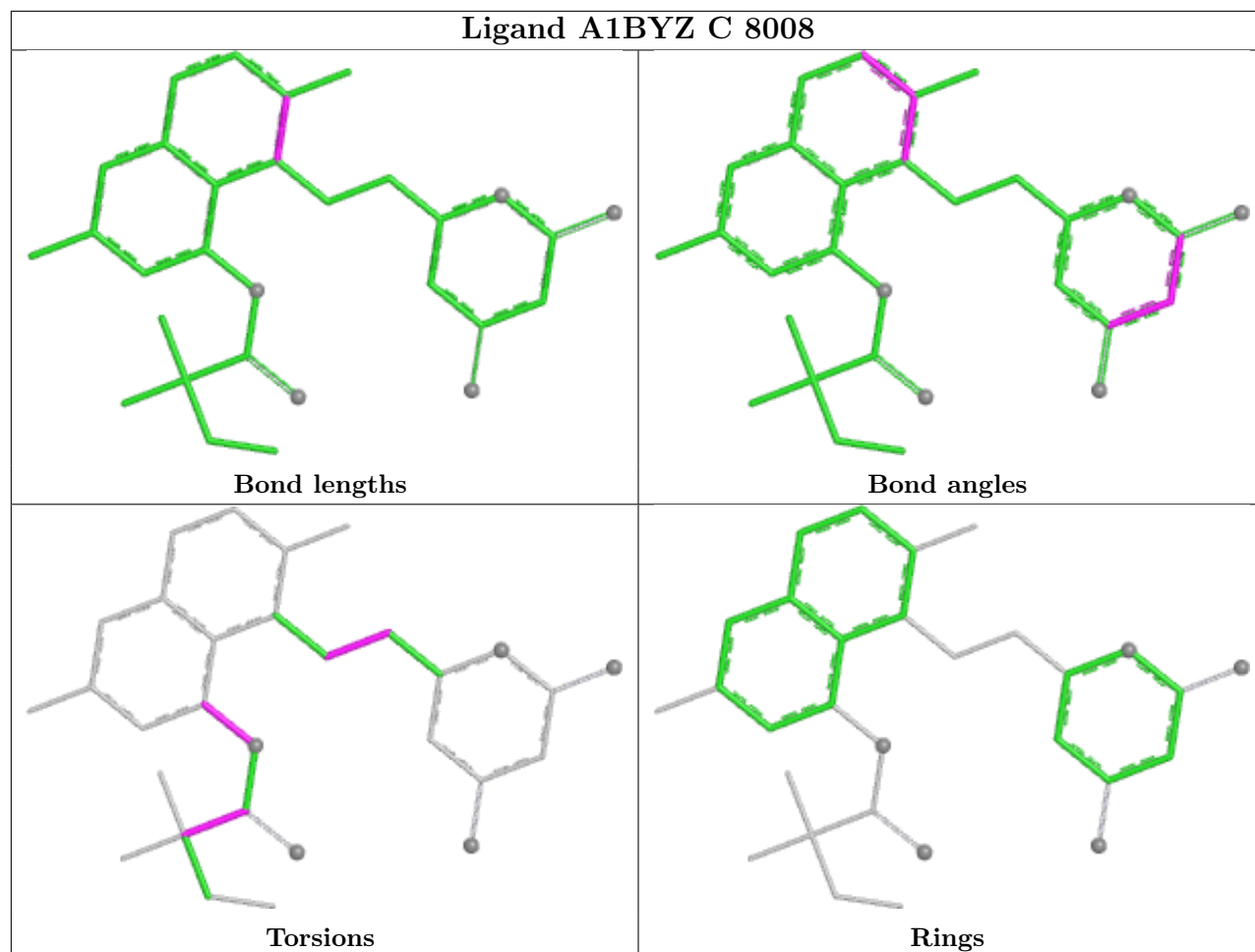


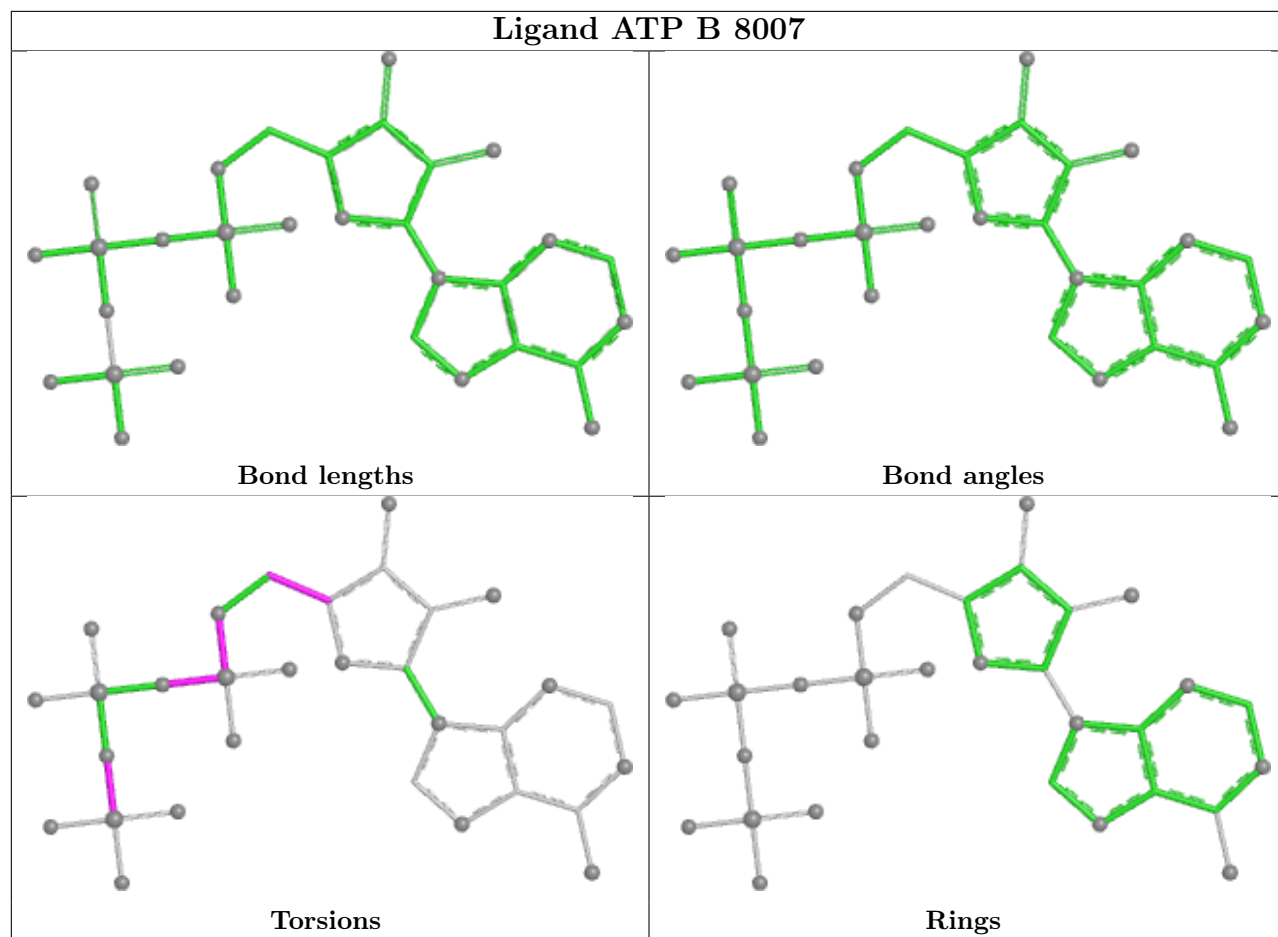


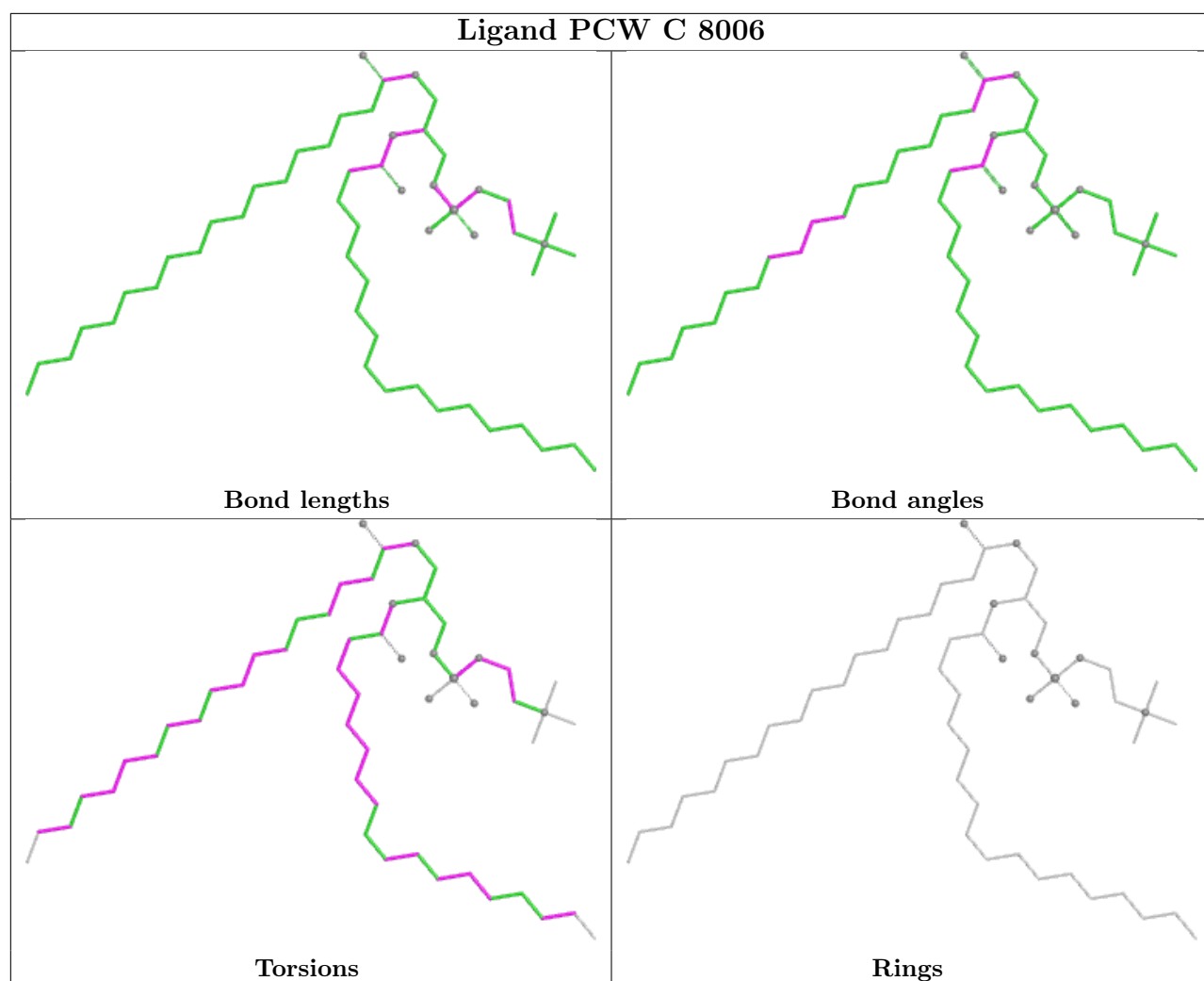




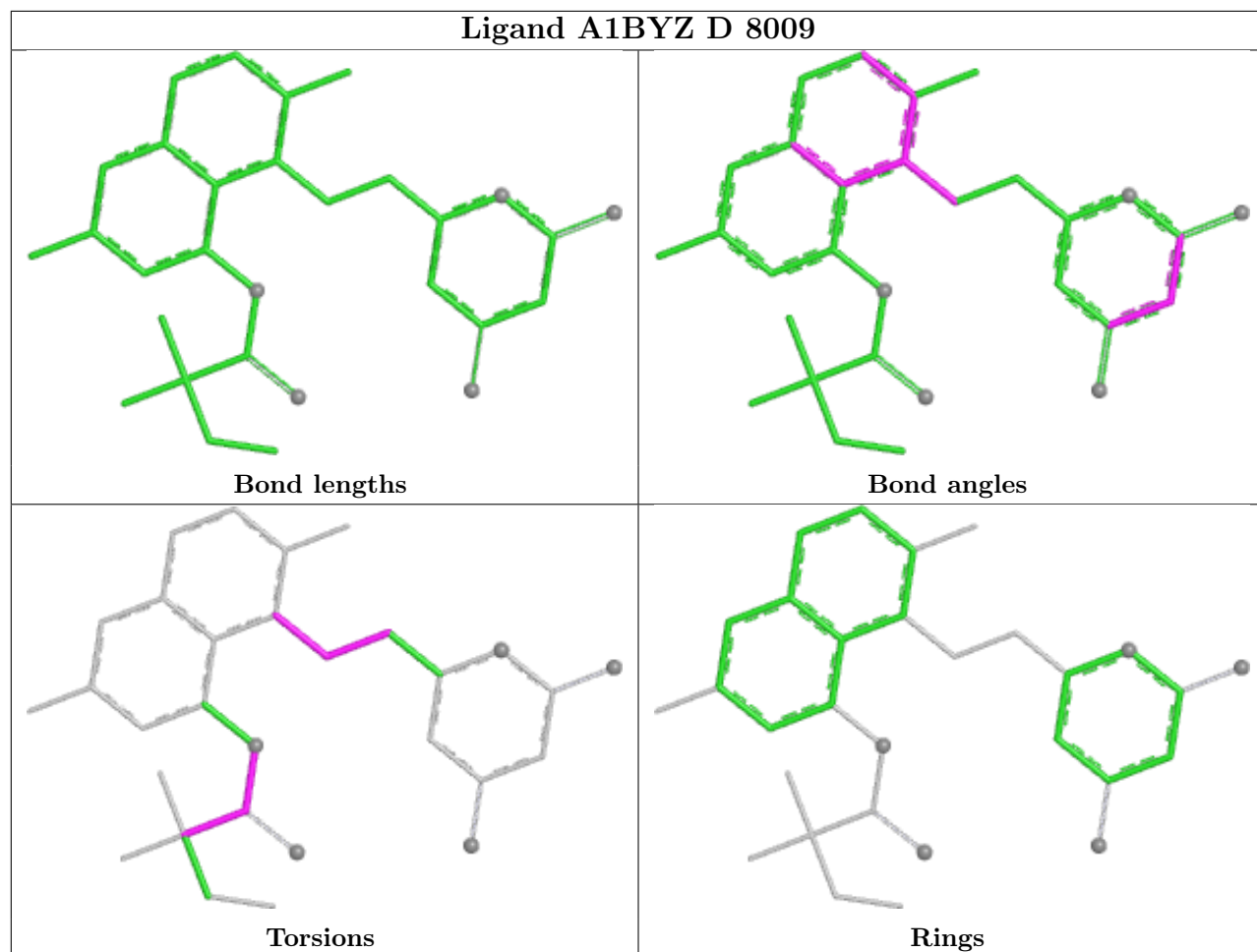
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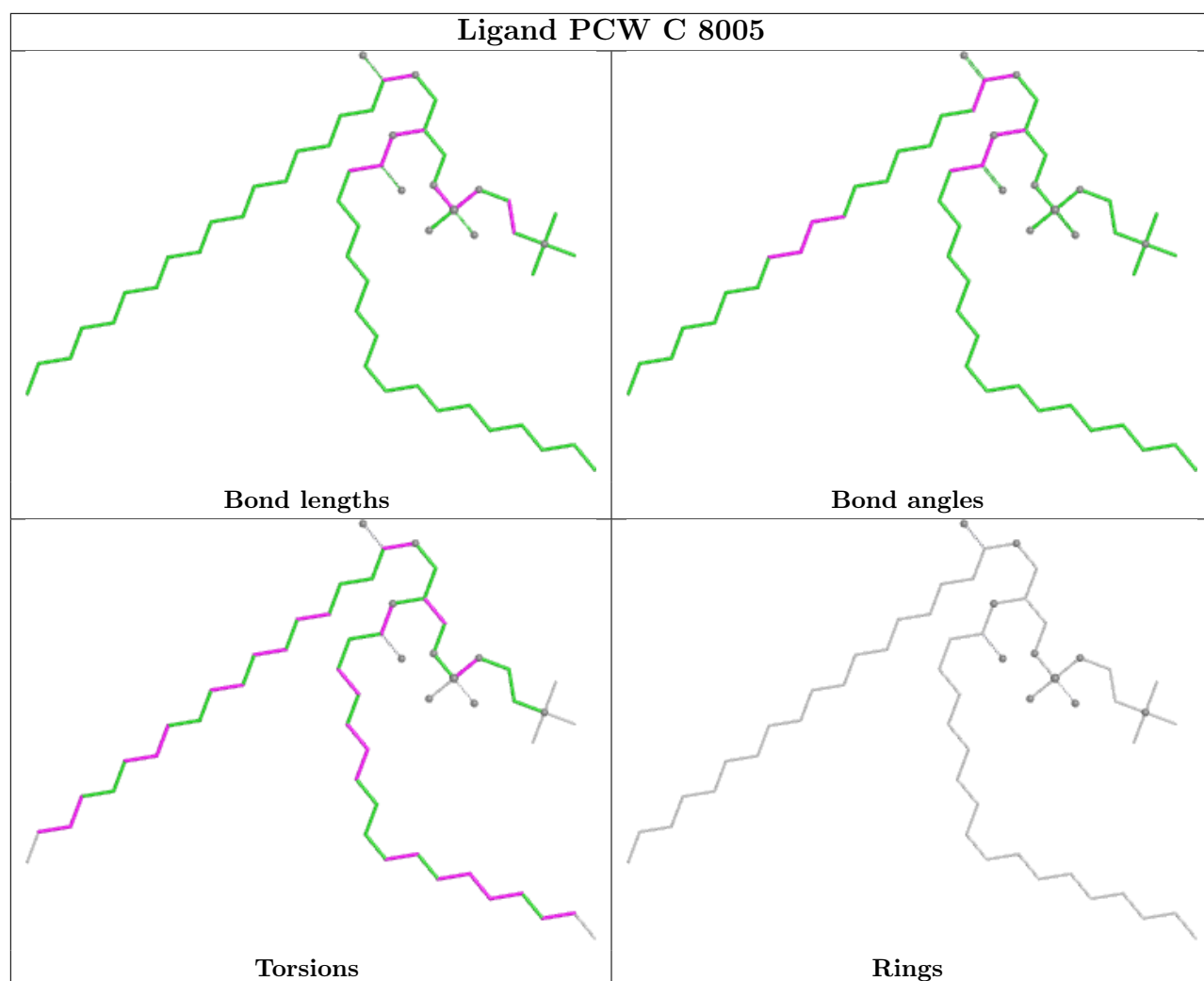


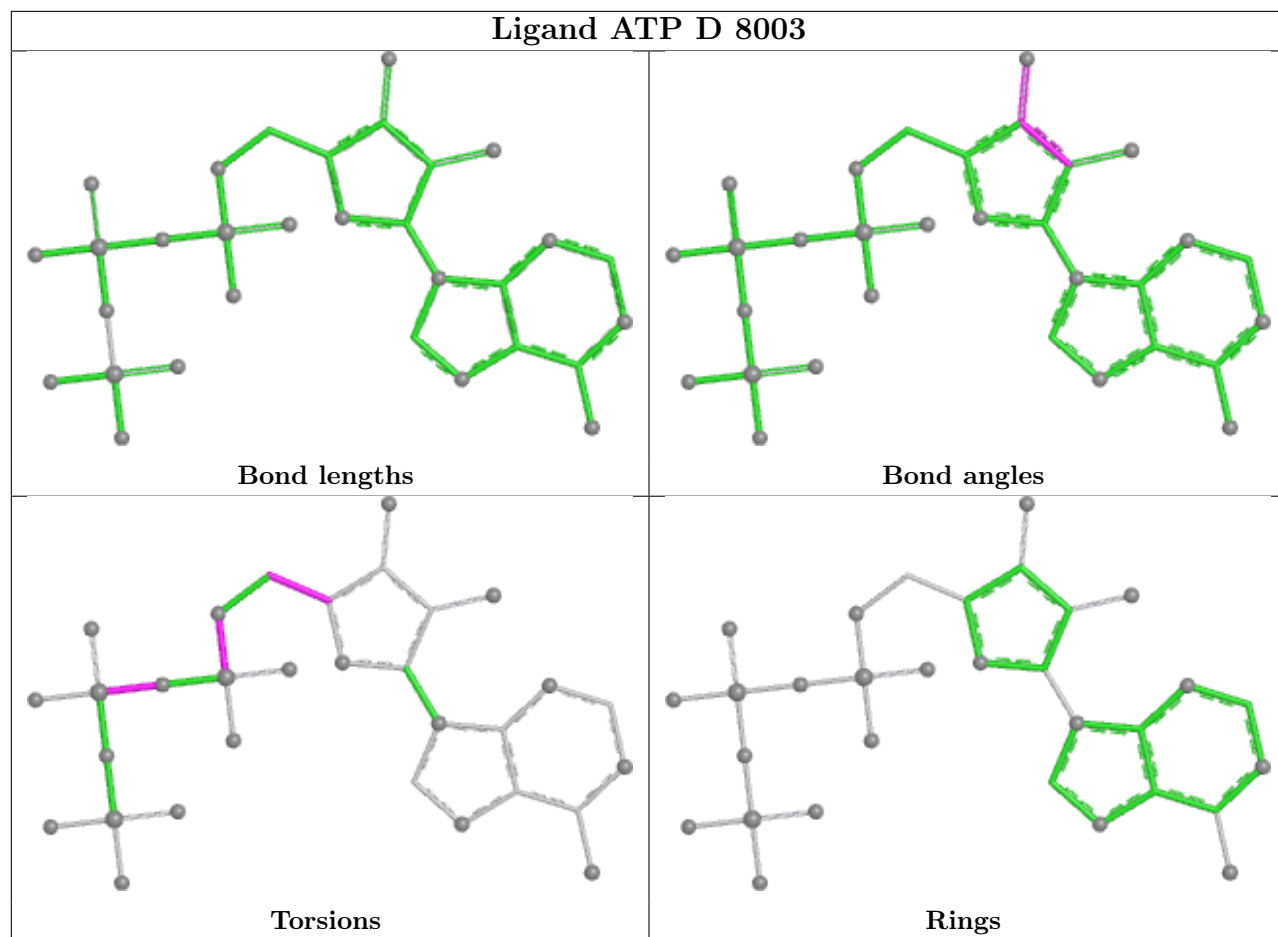




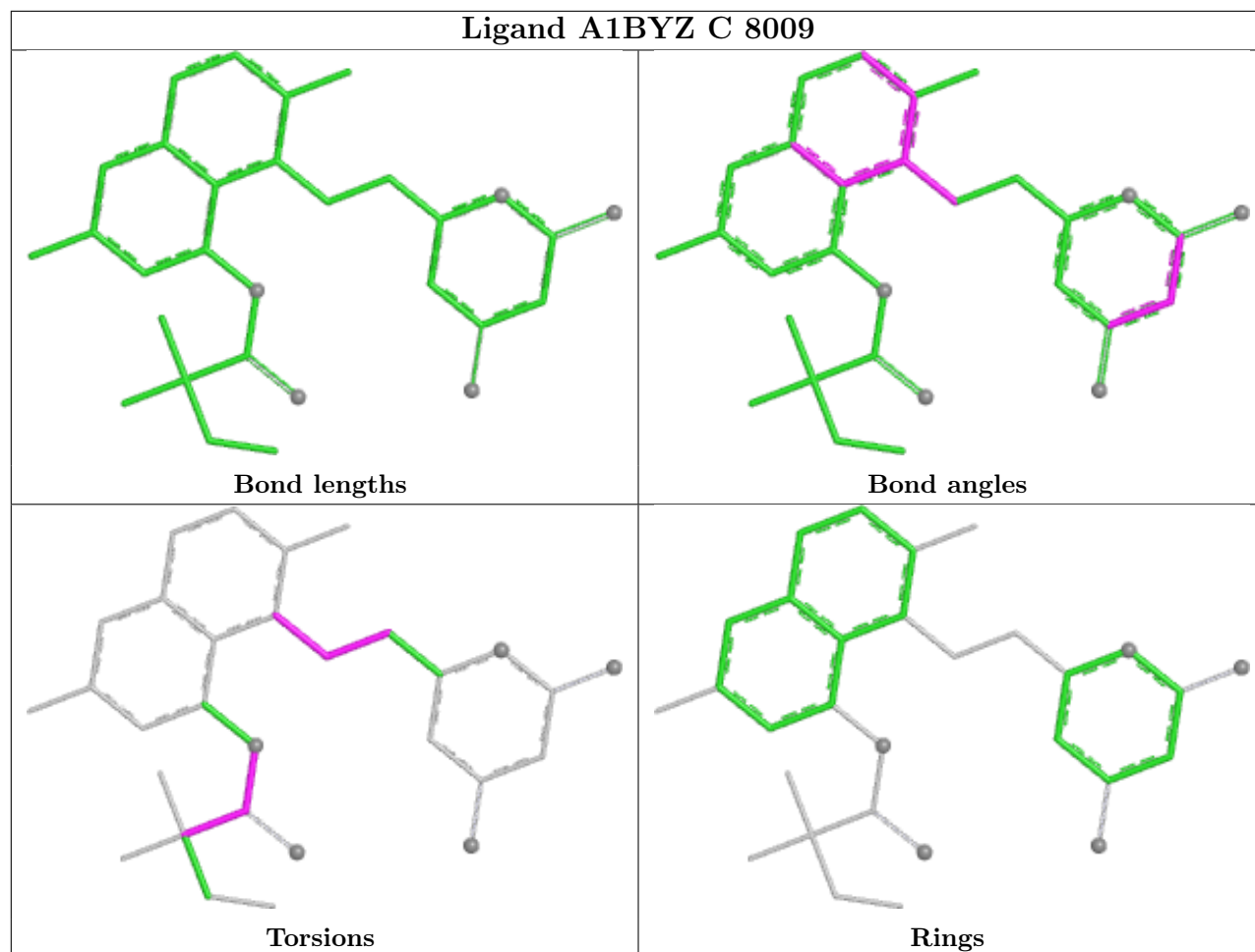
## Ligand A1BYZ D 8009



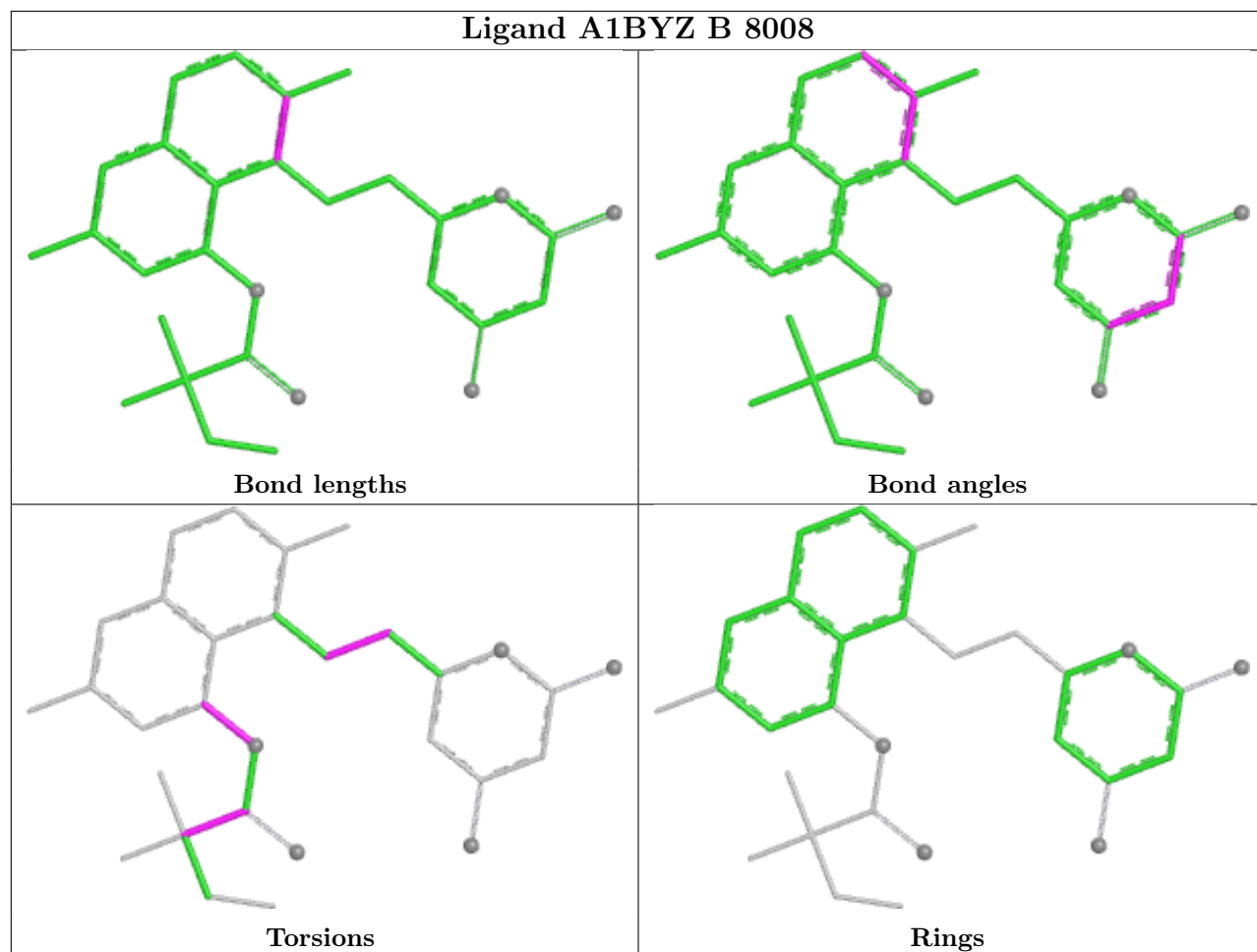


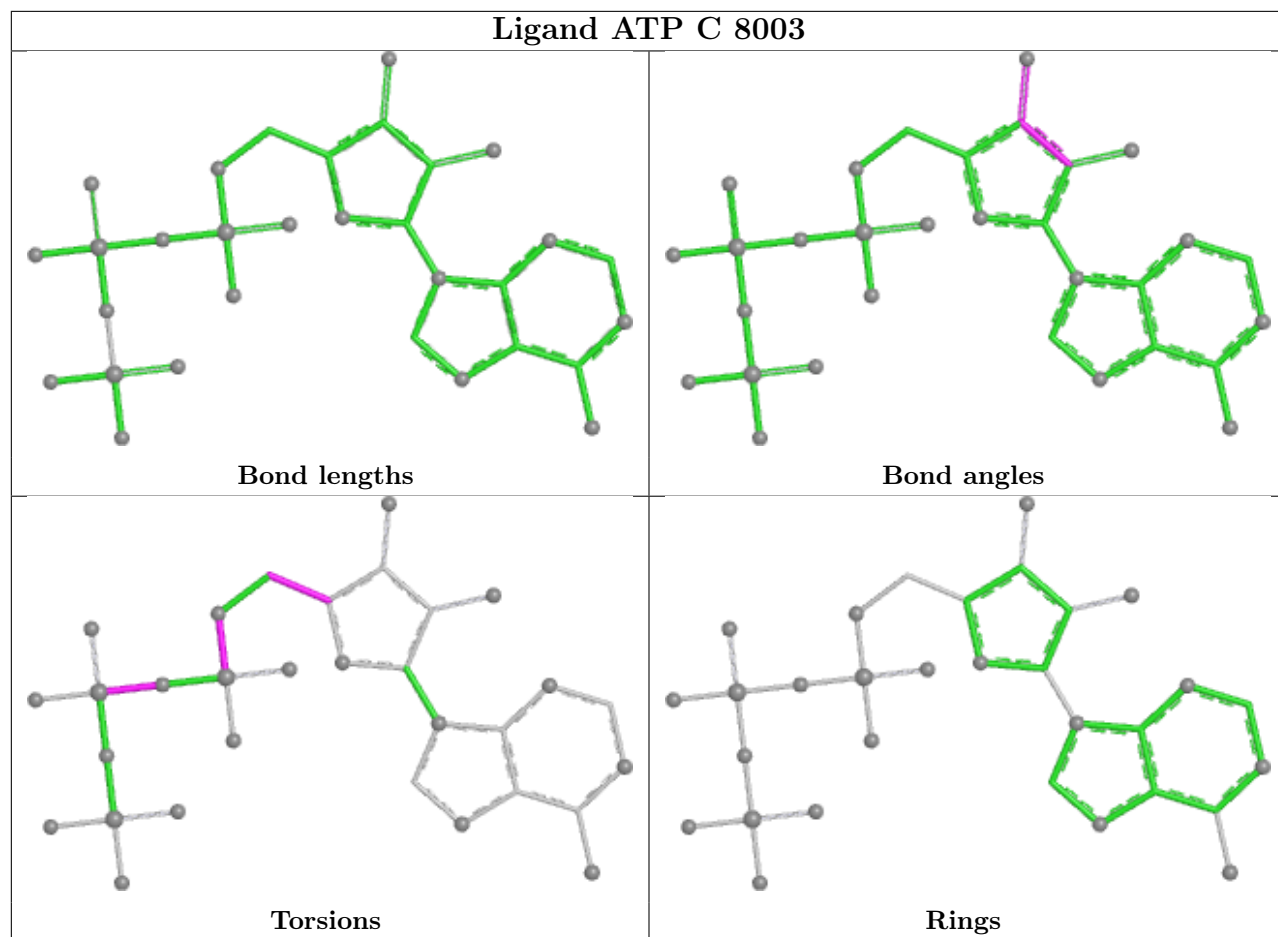


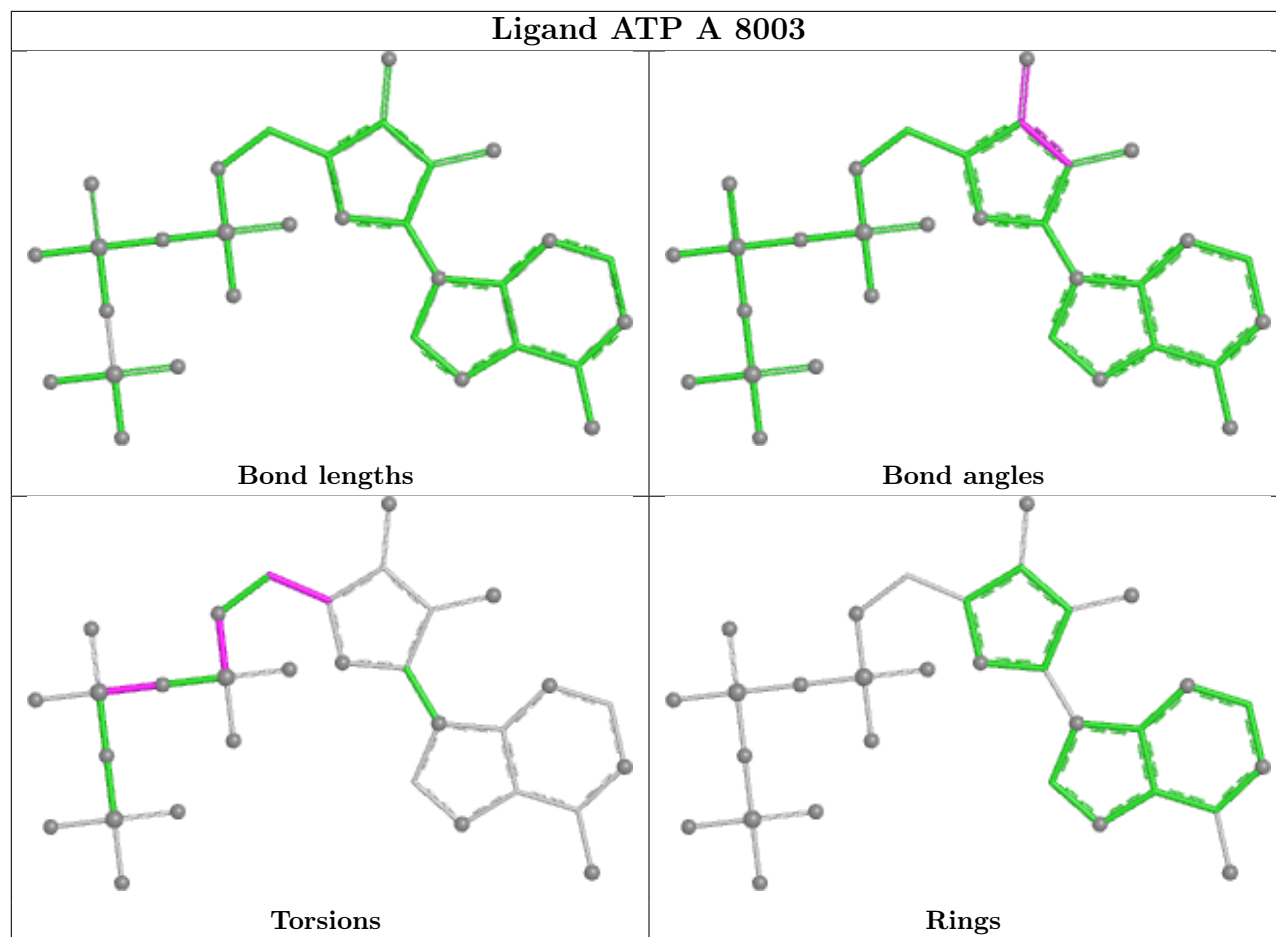
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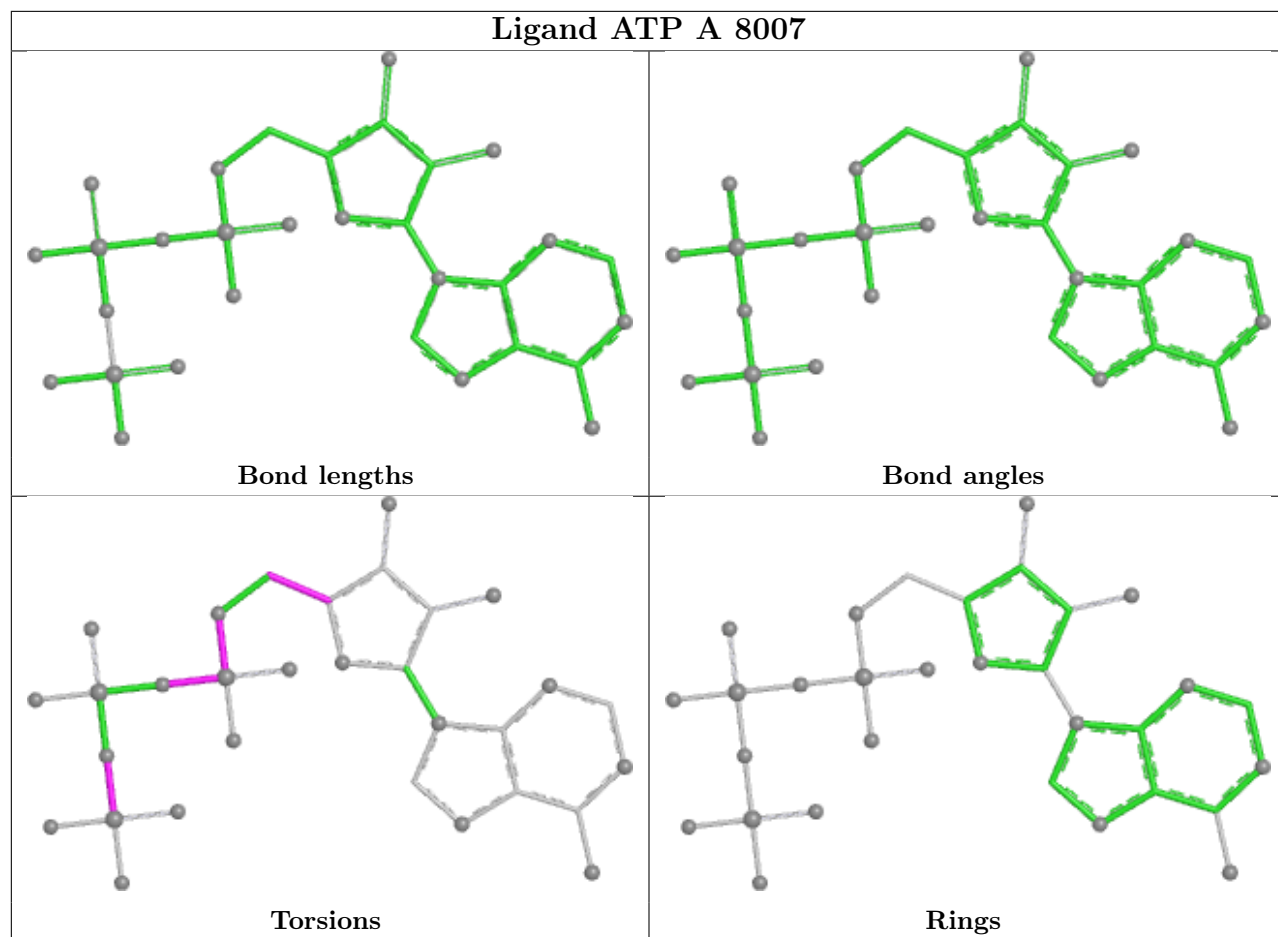


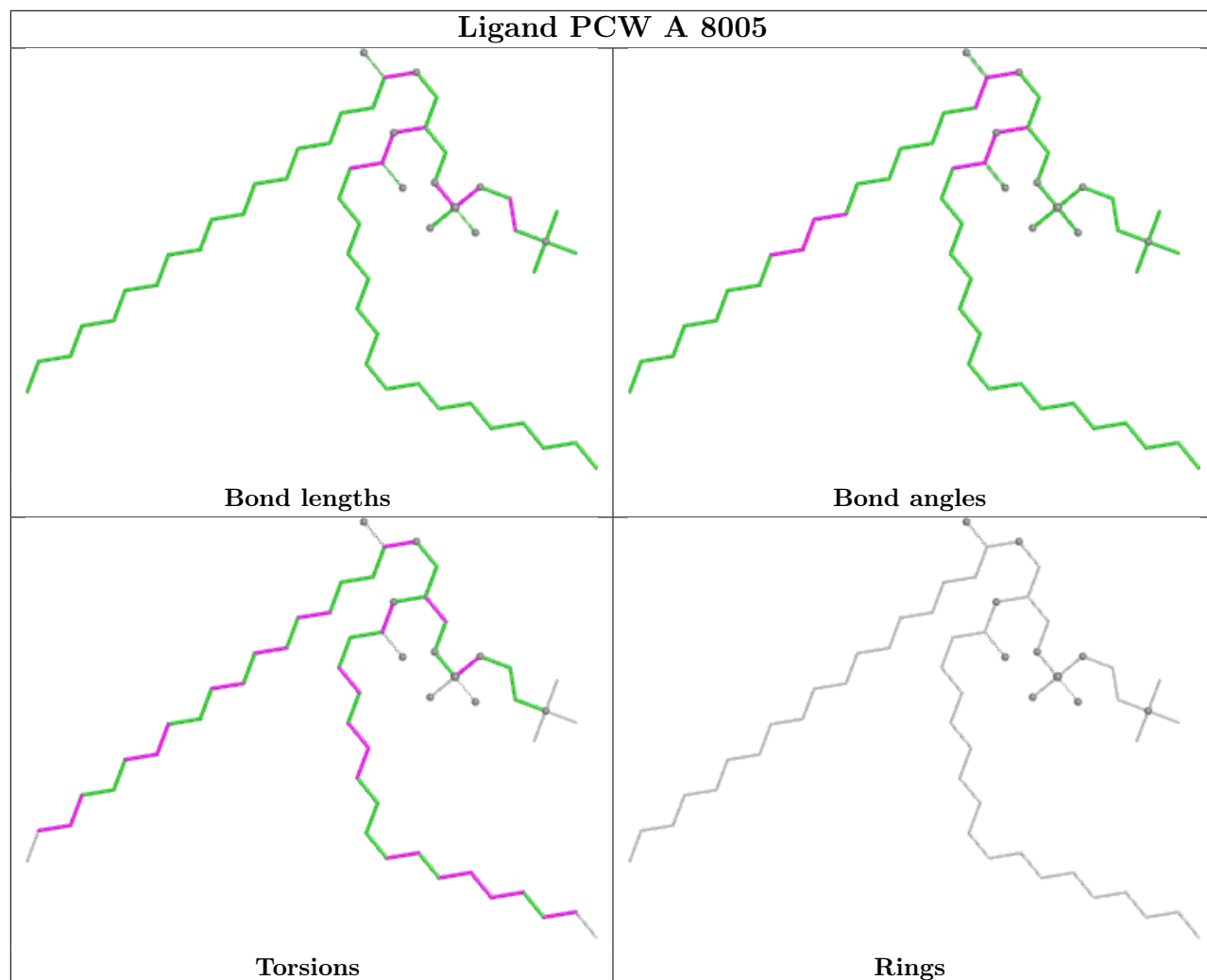
## Ligand A1BYZ B 8008

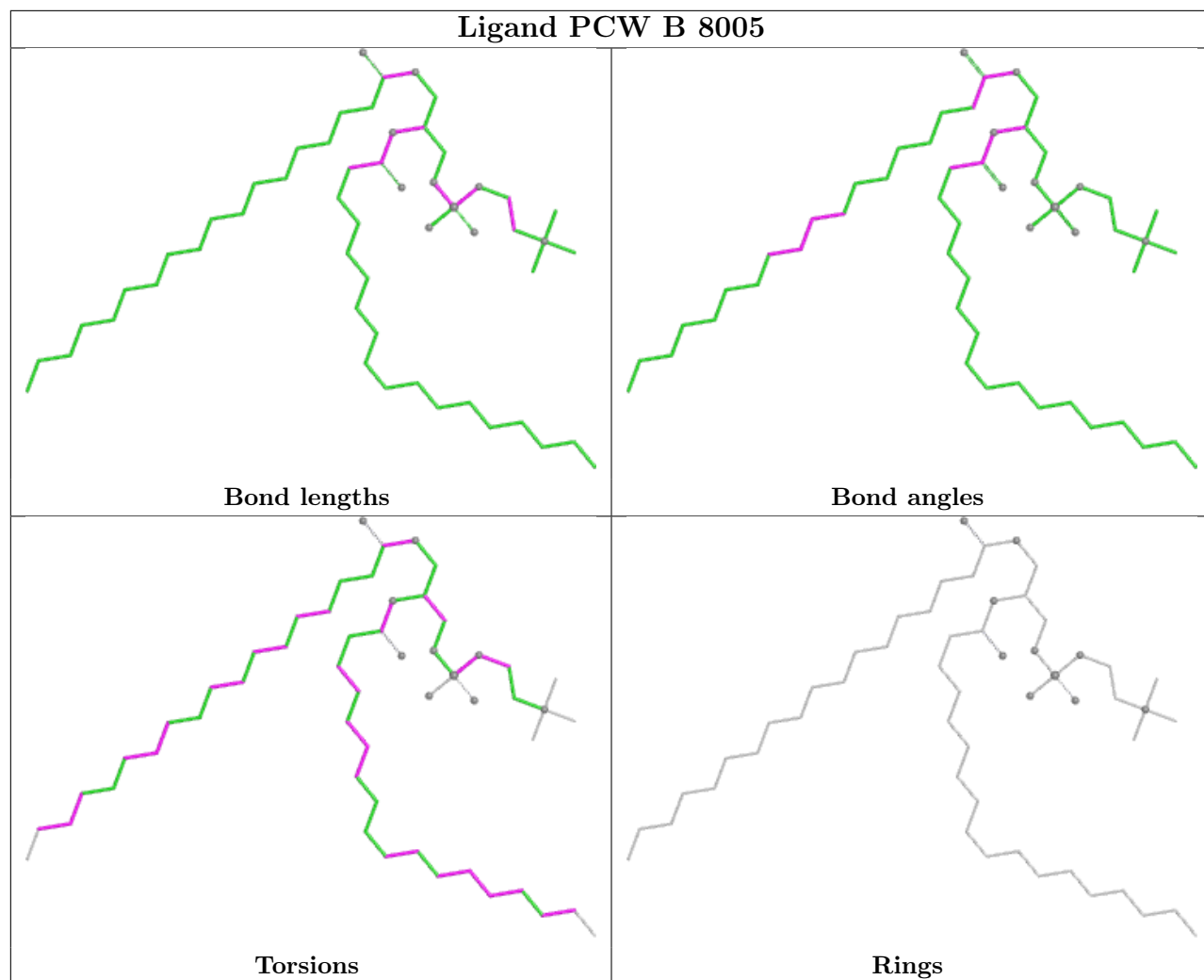


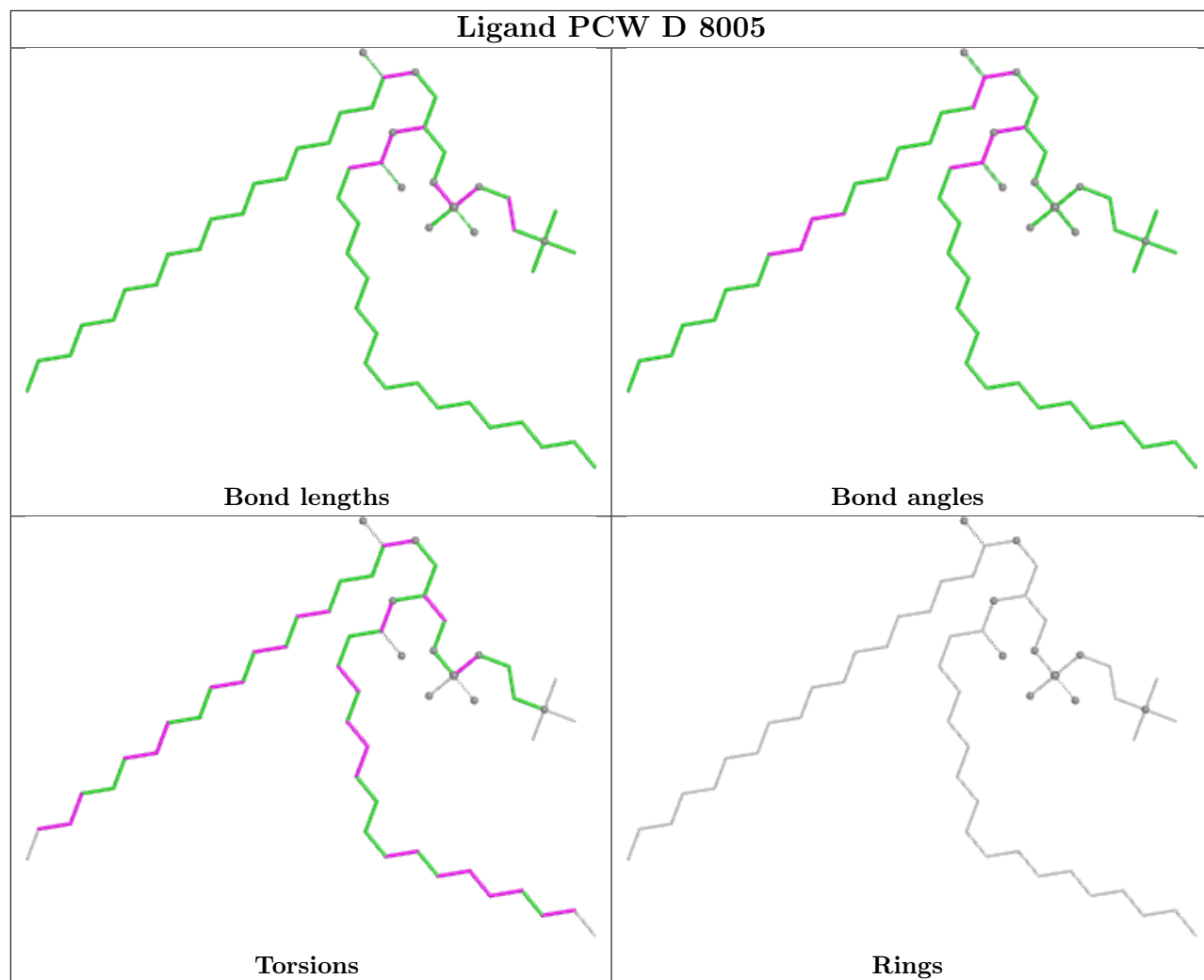


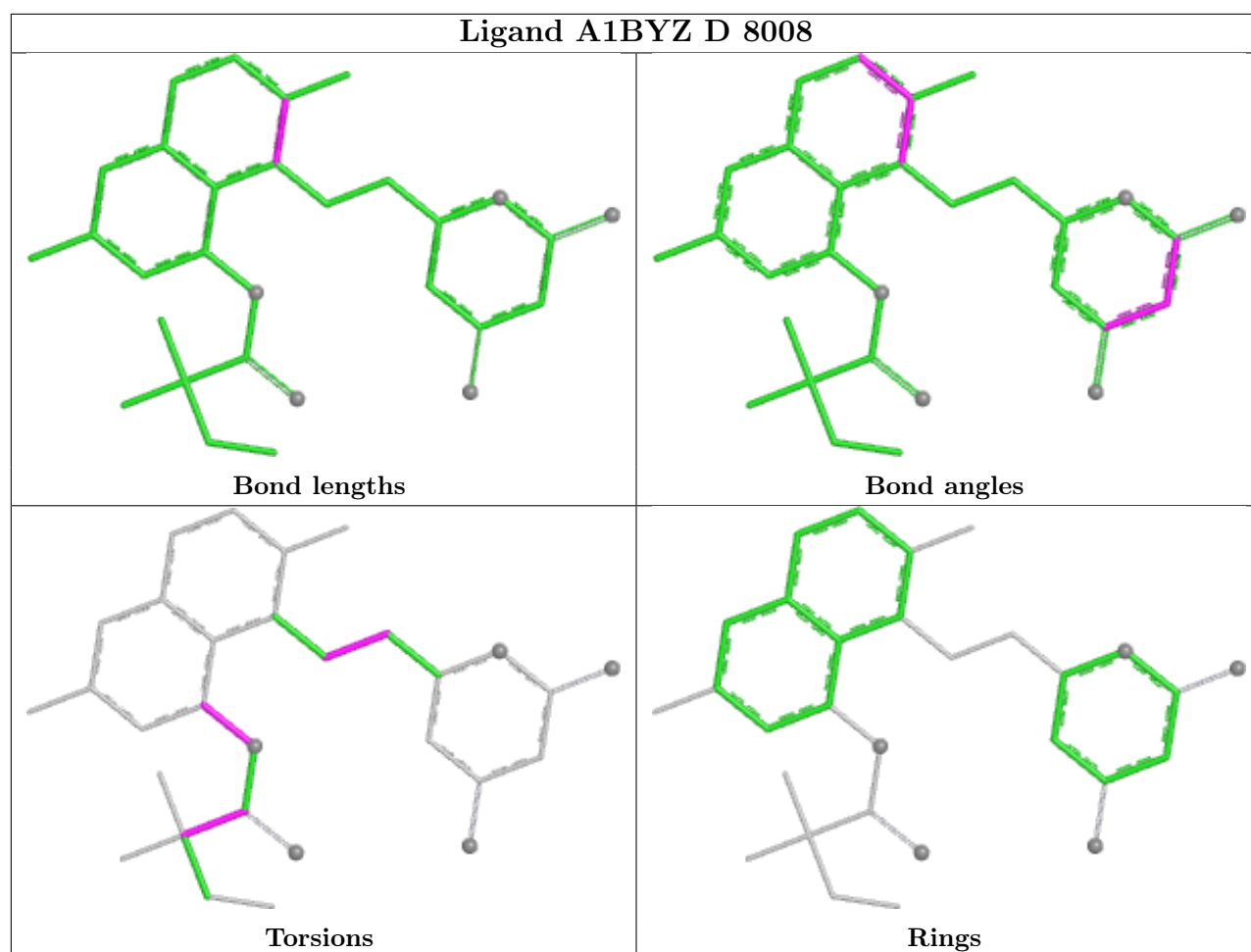












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

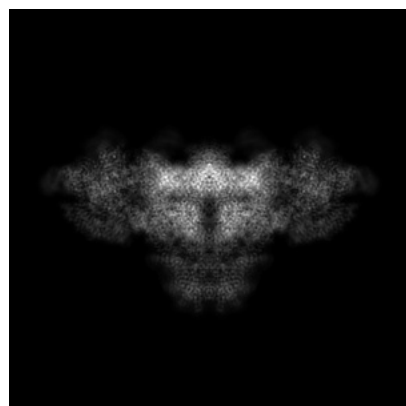
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49537. These allow visual inspection of the internal detail of the map and identification of artifacts.

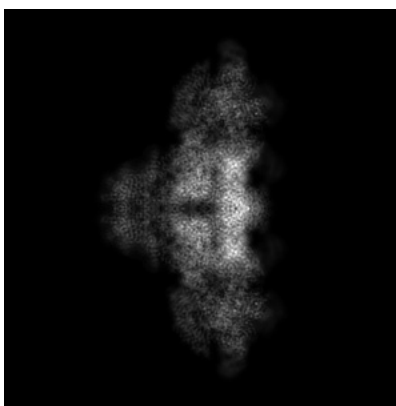
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

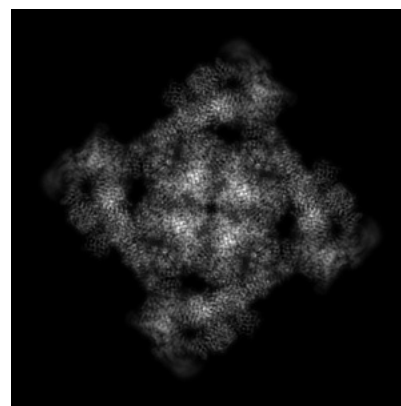
#### 6.1.1 Primary map



X

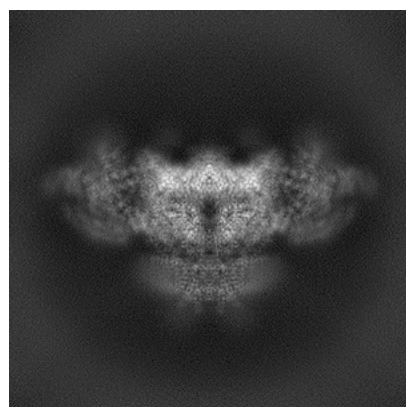


Y

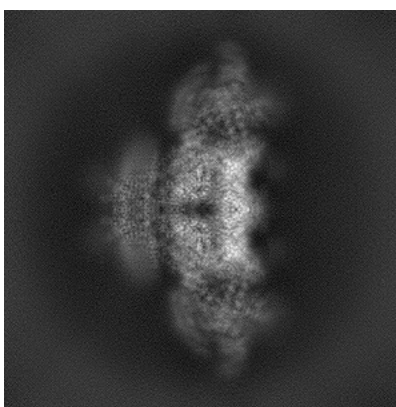


Z

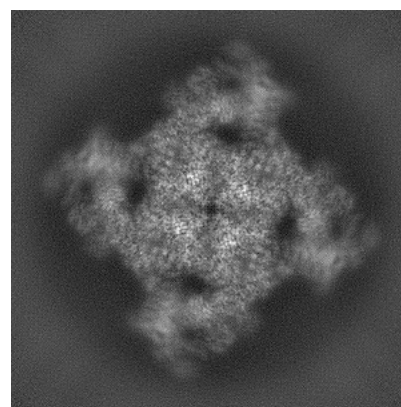
#### 6.1.2 Raw map



X



Y



Z

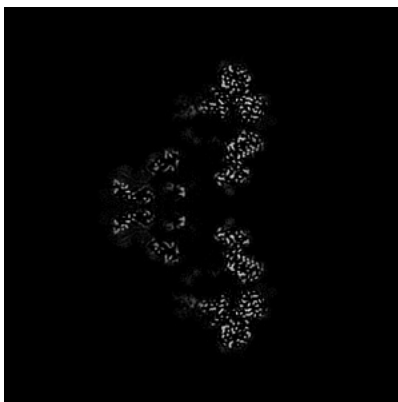
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

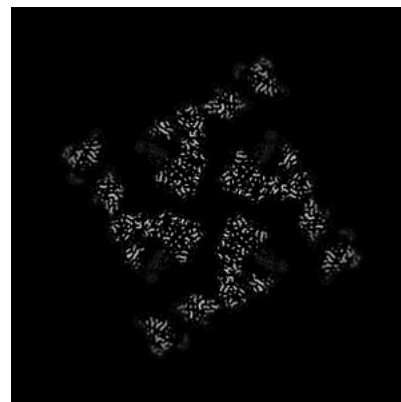
### 6.2.1 Primary map



X Index: 256

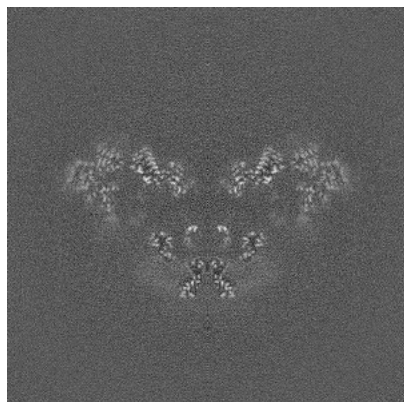


Y Index: 256

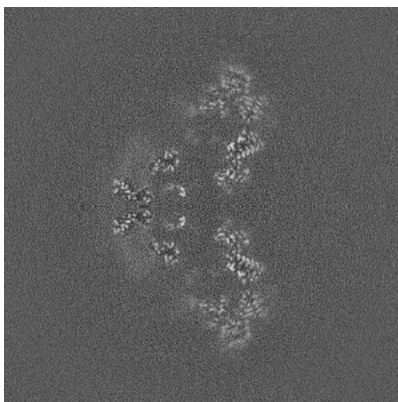


Z Index: 256

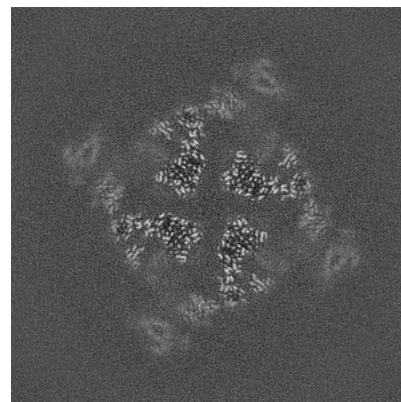
### 6.2.2 Raw map



X Index: 256



Y Index: 256

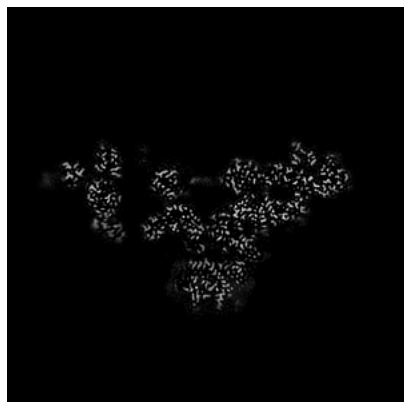


Z Index: 256

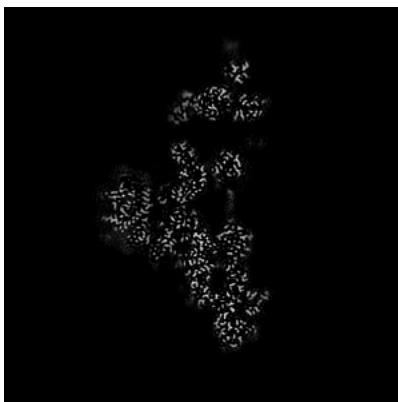
The images above show central slices of the map in three orthogonal directions.

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

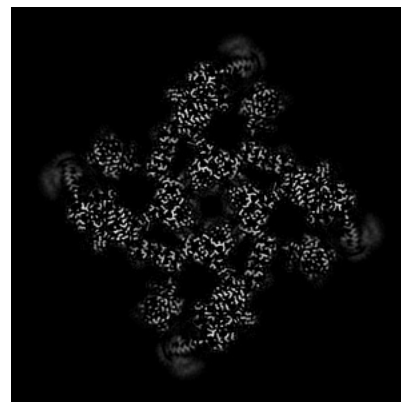
### 6.3.1 Primary map



X Index: 238

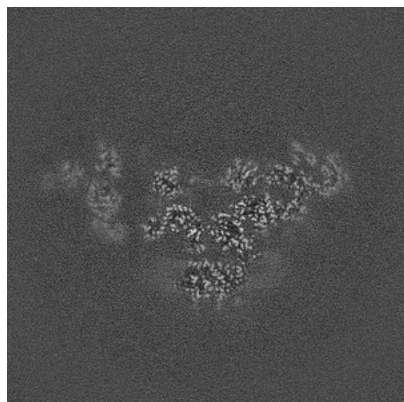


Y Index: 238

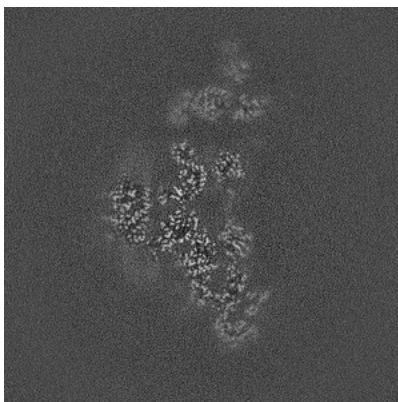


Z Index: 286

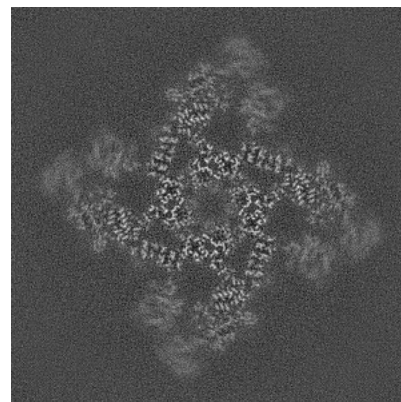
### 6.3.2 Raw map



X Index: 237



Y Index: 237

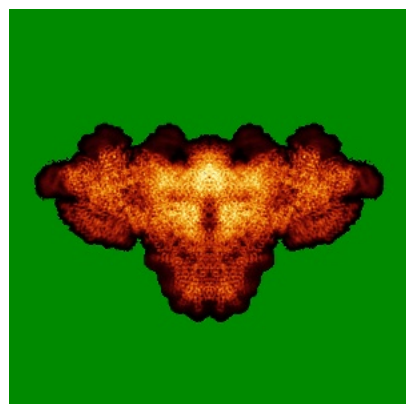


Z Index: 286

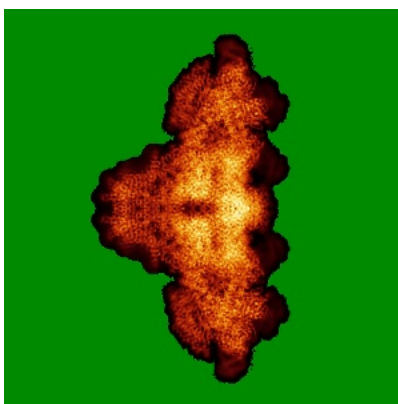
The images above show the largest variance slices of the map in three orthogonal directions.

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

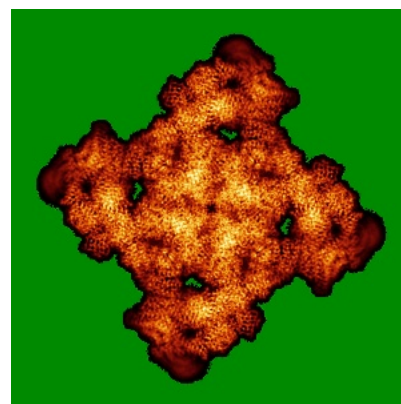
### 6.4.1 Primary map



X

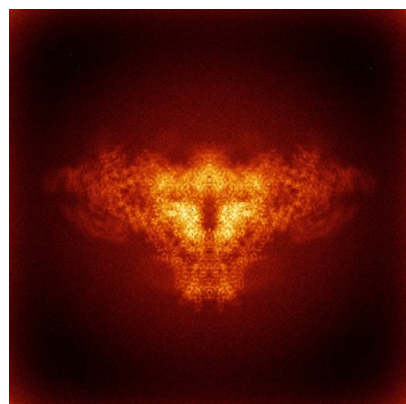


Y

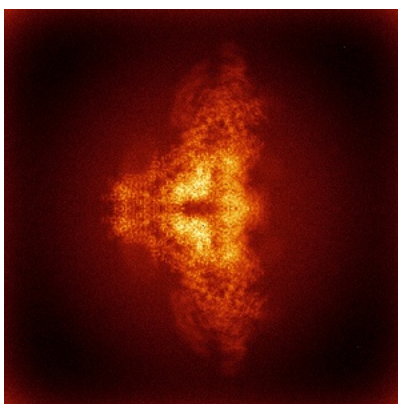


Z

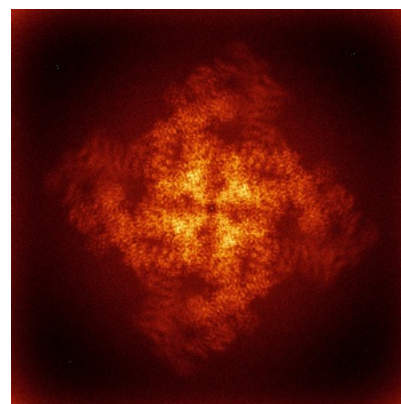
### 6.4.2 Raw map



X



Y

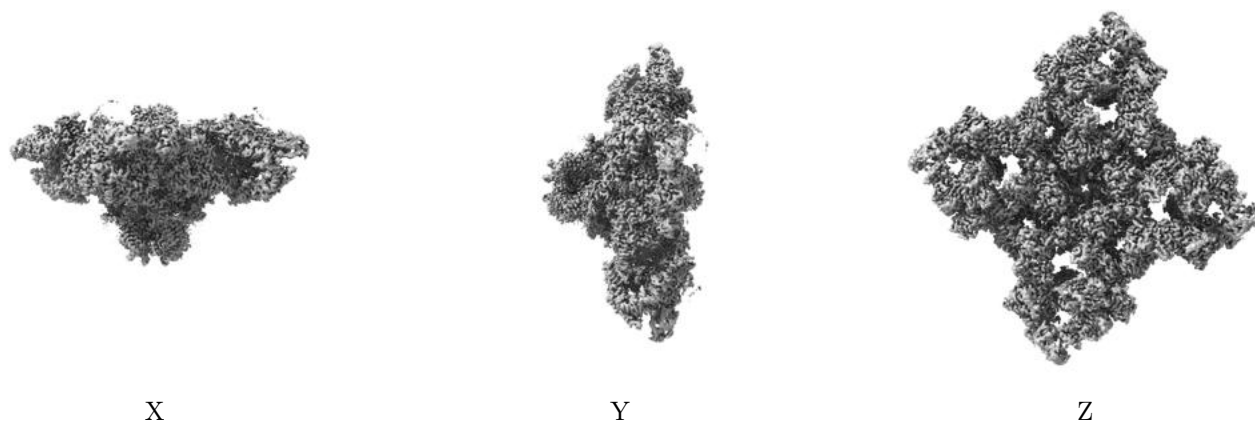


Z

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 [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

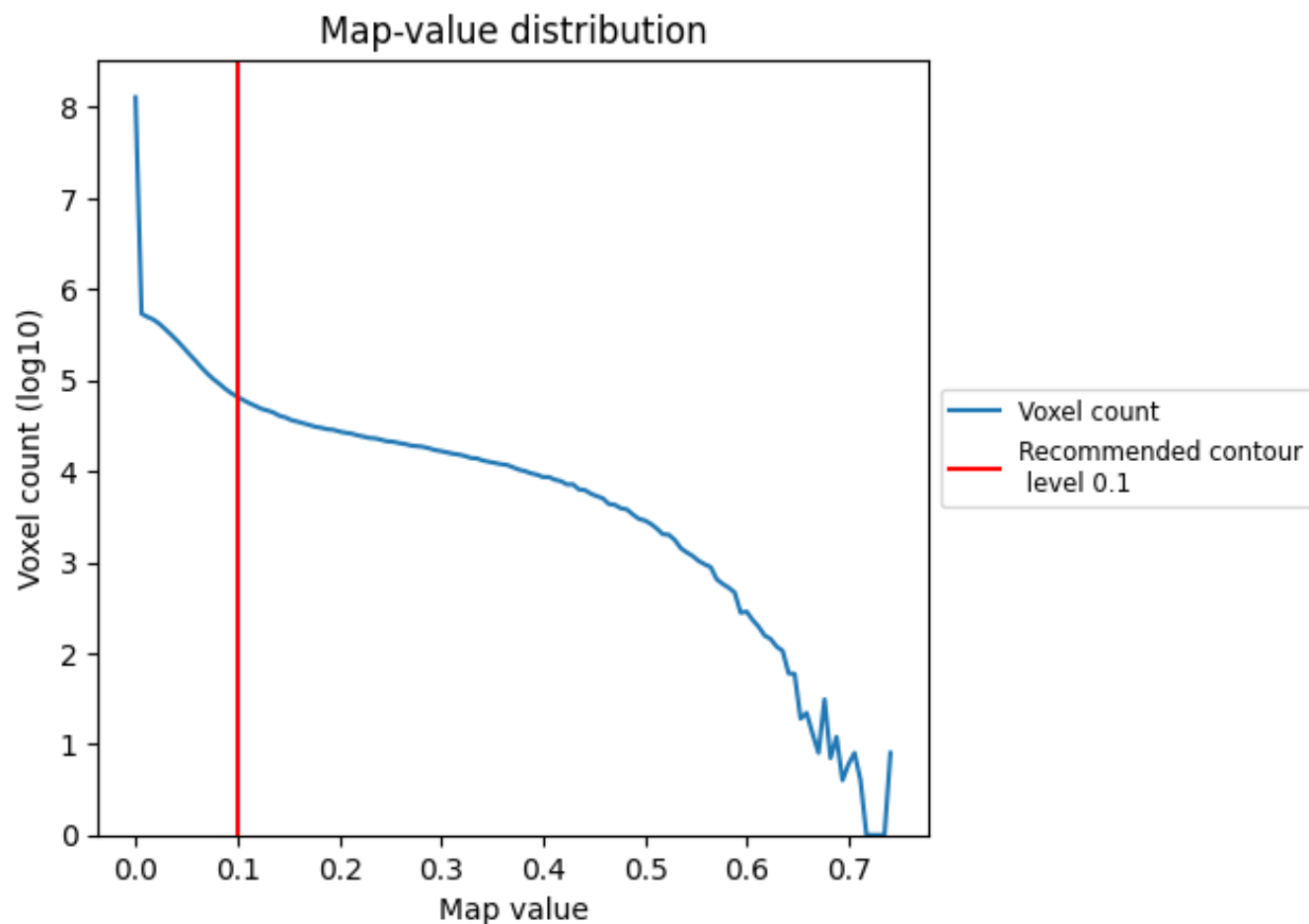
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

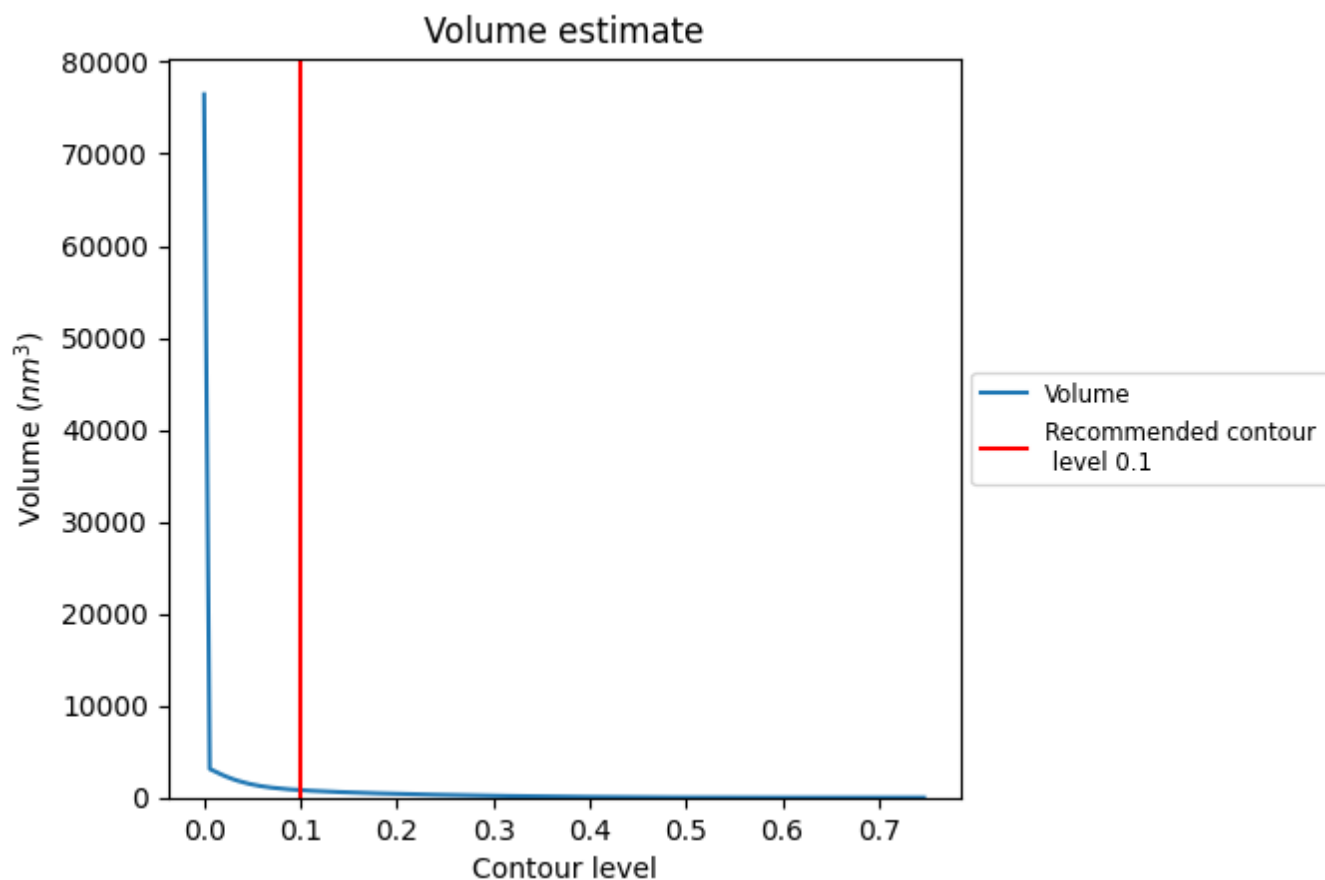
This section contains the results of statistical analysis of the map.

### 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.

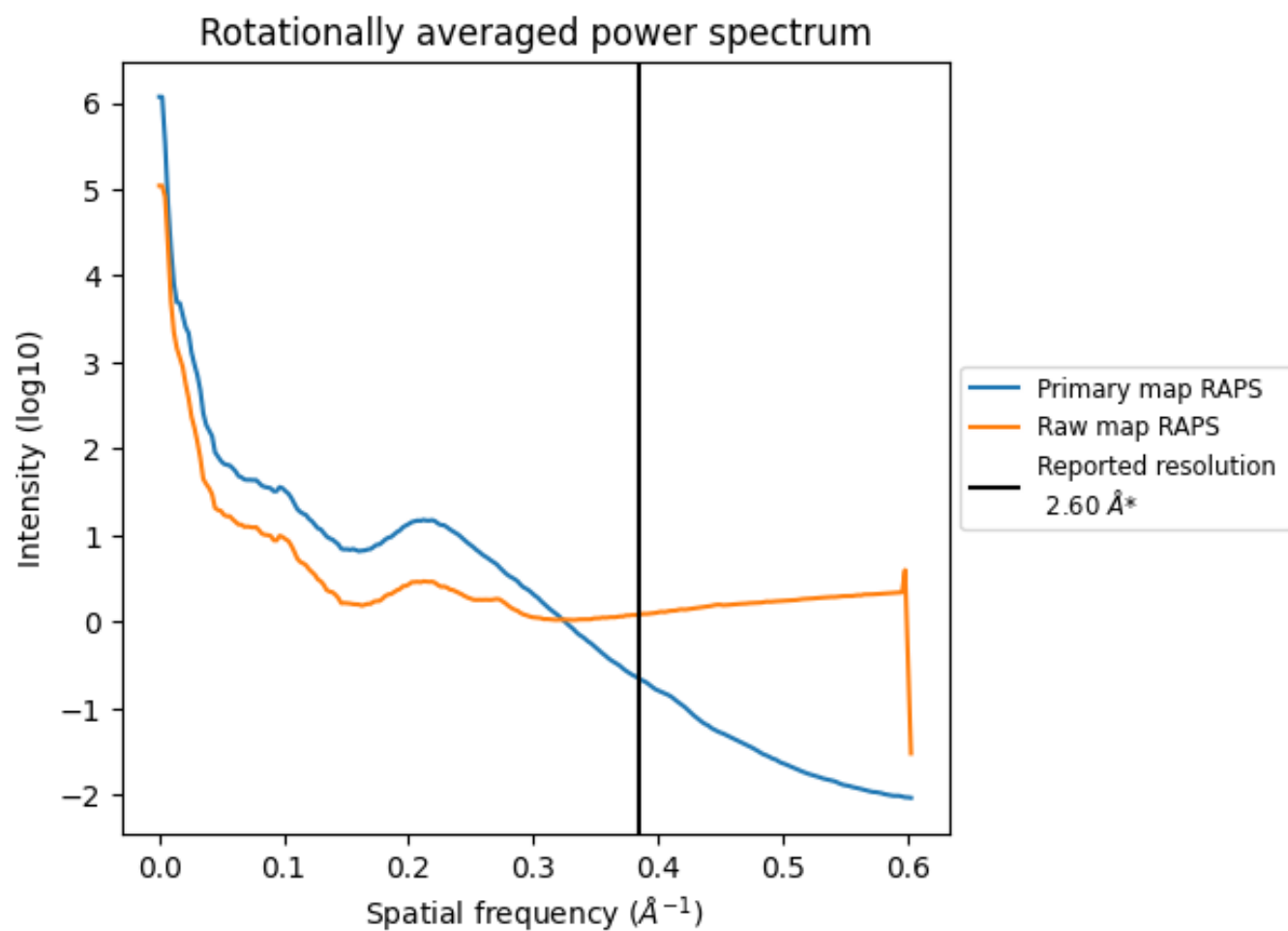
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 809 nm<sup>3</sup>; this corresponds to an approximate mass of 730 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 ⓘ

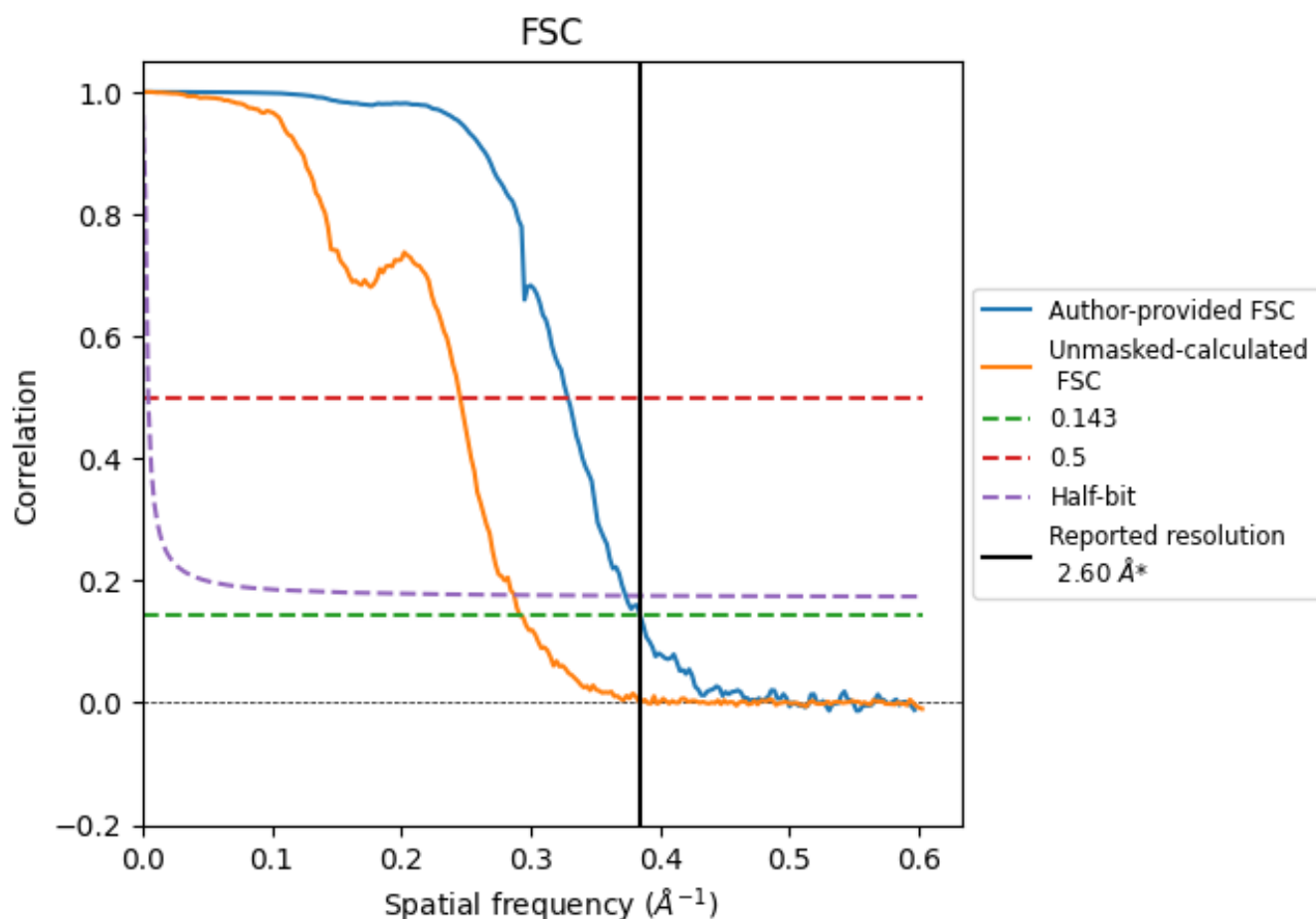


\*Reported resolution corresponds to spatial frequency of  $0.385 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.385  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.60                               | -    | -        |
| Author-provided FSC curve | 2.60                               | 3.04 | 2.68     |
| Unmasked-calculated*      | 3.43                               | 4.07 | 3.48     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.43 differs from the reported value 2.6 by more than 10 %

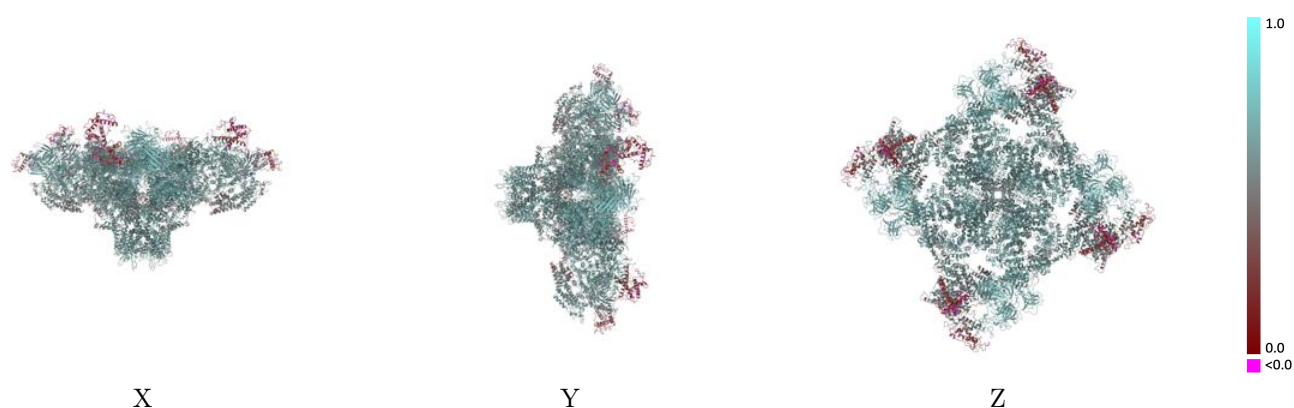
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49537 and PDB model 9NMQ. Per-residue inclusion information can be found in section 3 on page 9.

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

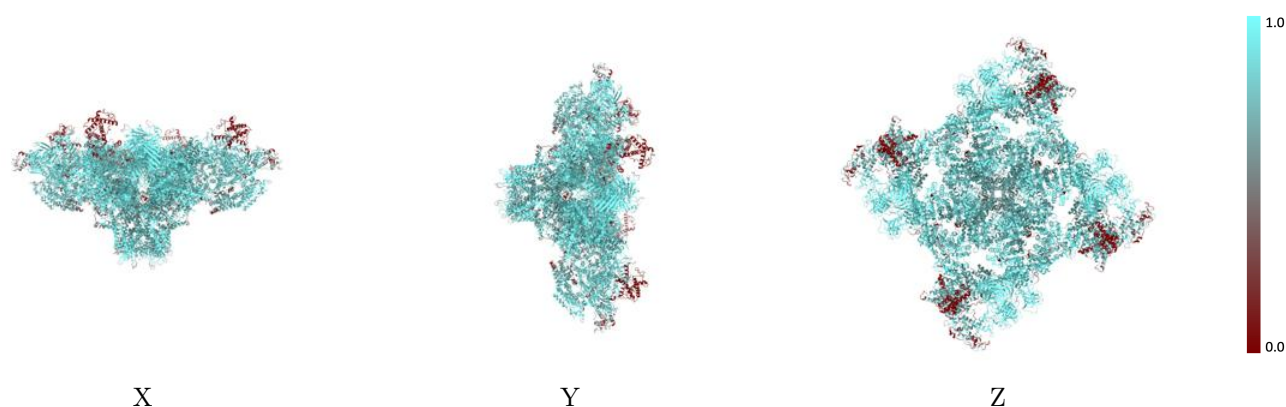
This section was not generated.

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



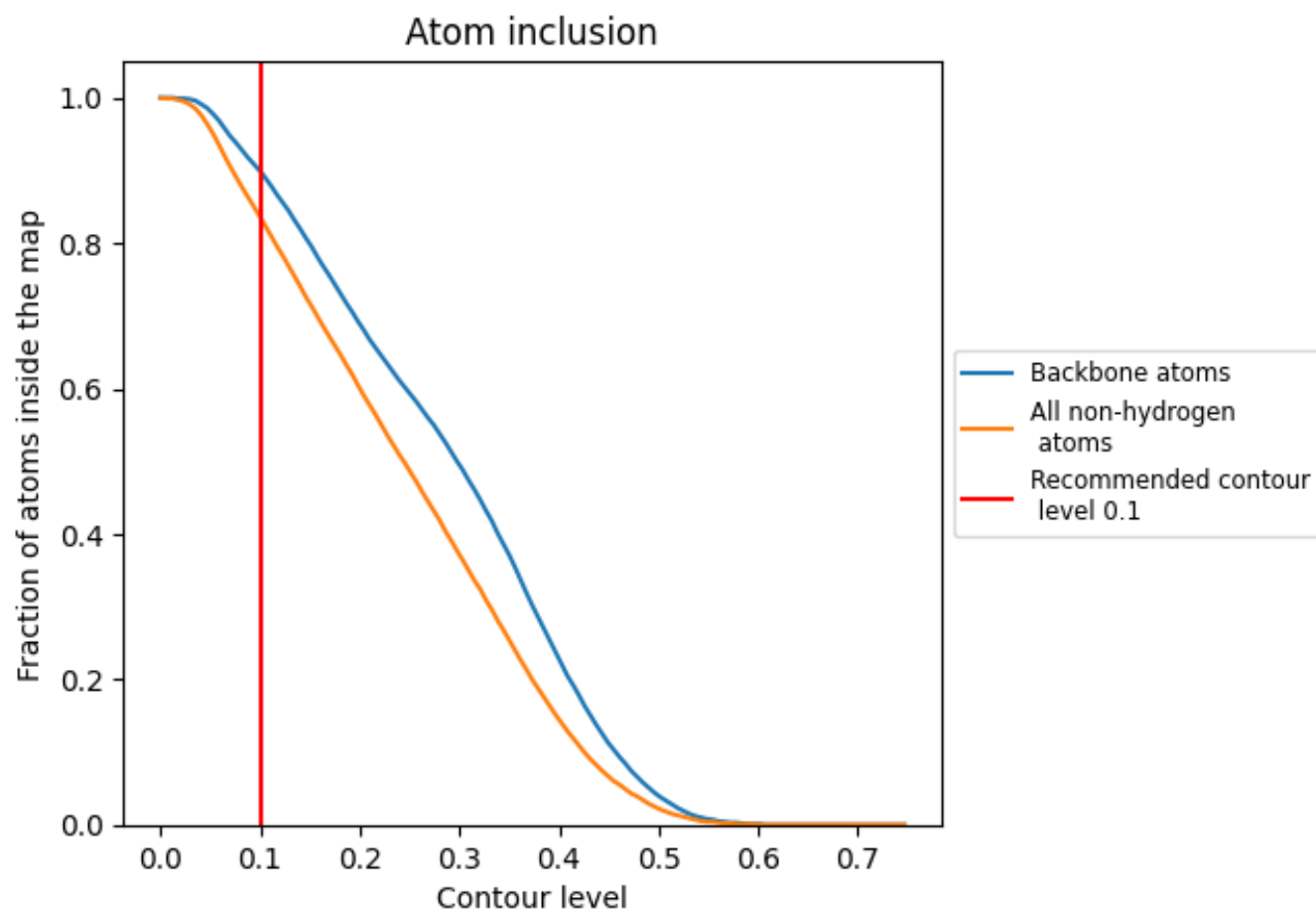
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.8360 | <div><div></div></div> 0.5810 |
| A     | <div><div></div></div> 0.8340 | <div><div></div></div> 0.5800 |
| B     | <div><div></div></div> 0.8330 | <div><div></div></div> 0.5780 |
| C     | <div><div></div></div> 0.8330 | <div><div></div></div> 0.5790 |
| D     | <div><div></div></div> 0.8330 | <div><div></div></div> 0.5780 |
| E     | <div><div></div></div> 0.9400 | <div><div></div></div> 0.6410 |
| F     | <div><div></div></div> 0.9400 | <div><div></div></div> 0.6440 |
| G     | <div><div></div></div> 0.9400 | <div><div></div></div> 0.6430 |
| H     | <div><div></div></div> 0.9400 | <div><div></div></div> 0.6430 |

1.0

0.0

<0.0