



## Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 08:57 PM UTC

PDB ID : 5MKF / pdb\_00005mkf  
EMDB ID : EMD-3524  
Title : cryoEM Structure of Polycystin-2 in complex with calcium and lipids  
Authors : Wilkes, M.; Madej, M.G.; Ziegler, C.  
Deposited on : 2016-12-04  
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

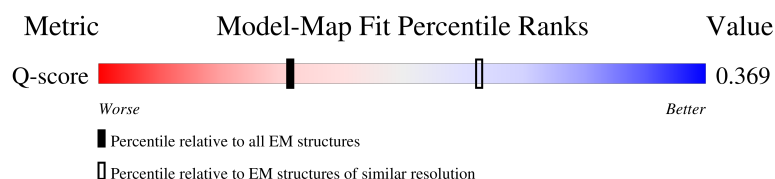
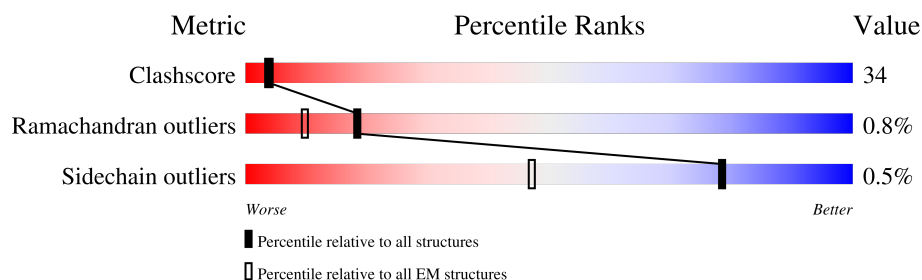
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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                       | 5410 ( 3.70 - 4.70 )                                     |

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     | 968    | <div> <div>16%</div> <div>20%</div> <div>29%</div> <div>50%</div> </div> |
| 1   | B     | 968    | <div> <div>15%</div> <div>20%</div> <div>29%</div> <div>50%</div> </div> |
| 1   | C     | 968    | <div> <div>15%</div> <div>20%</div> <div>29%</div> <div>50%</div> </div> |
| 1   | D     | 968    | <div> <div>16%</div> <div>19%</div> <div>30%</div> <div>50%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                    |
|-----|-------|--------|-------------------------------------------------------------------------------------|
| 2   | E     | 2      | <div> <div>100%</div> <div> <div></div> <div>50%</div> <div>50%</div> </div> </div> |
| 2   | F     | 2      | <div> <div>100%</div> <div> <div></div> </div> </div>                               |
| 2   | G     | 2      | <div> <div>100%</div> <div> <div></div> </div> </div>                               |
| 2   | H     | 2      | <div> <div>100%</div> <div> <div></div> </div> </div>                               |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | NAG  | A     | 1002 | -         | -        | X       | -                |
| 3   | NAG  | B     | 1002 | -         | -        | X       | -                |
| 3   | NAG  | C     | 1002 | -         | -        | X       | -                |
| 3   | NAG  | D     | 1002 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

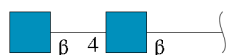
There are 7 unique types of molecules in this entry. The entry contains 16620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polycystin-2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 481      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3962  | 2612 | 629 | 702 | 19 |         |       |
| 1   | B     | 481      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3959  | 2610 | 629 | 702 | 18 |         |       |
| 1   | C     | 481      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3959  | 2610 | 629 | 702 | 18 |         |       |
| 1   | D     | 481      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3959  | 2610 | 629 | 702 | 18 |         |       |

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



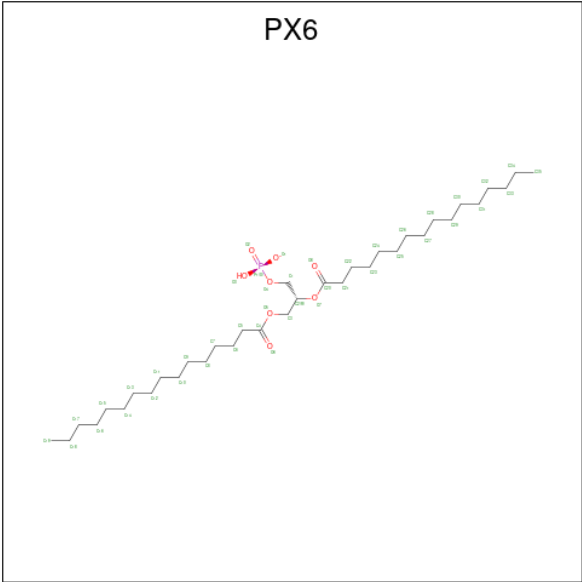
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 2   | E     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | F     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | G     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 2   | H     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



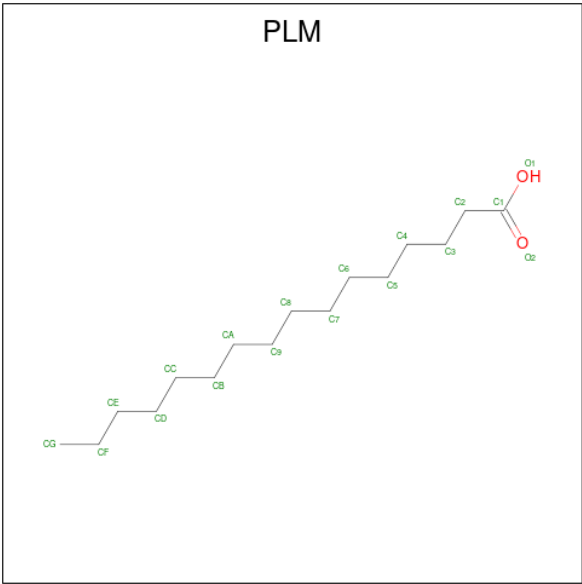
| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 3   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | D     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | D     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | D     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

- Molecule 4 is 1,2-DIPALMITOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX6) (formula: C<sub>35</sub>H<sub>68</sub>O<sub>8</sub>P).



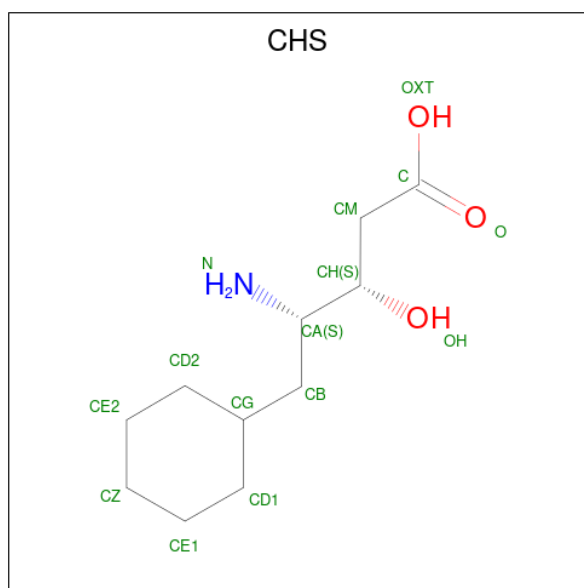
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 4   | A     | 1        | Total | C  | O | P | 0       |
|     |       |          | 40    | 31 | 8 | 1 |         |
| 4   | B     | 1        | Total | C  | O | P | 0       |
|     |       |          | 40    | 31 | 8 | 1 |         |
| 4   | C     | 1        | Total | C  | O | P | 0       |
|     |       |          | 40    | 31 | 8 | 1 |         |
| 4   | D     | 1        | Total | C  | O | P | 0       |
|     |       |          | 40    | 31 | 8 | 1 |         |

- Molecule 5 is PALMITIC ACID (CCD ID: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 5   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 5   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 5   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 5   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 5   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 5   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 5   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 5   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 5   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 5   | D     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 5   | D     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |
| 5   | D     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |

- Molecule 6 is 4-AMINO-5-CYCLOHEXYL-3-HYDROXY-PENTANOIC ACID (CCD ID: CHS) (formula:  $C_{11}H_{21}NO_3$ ).



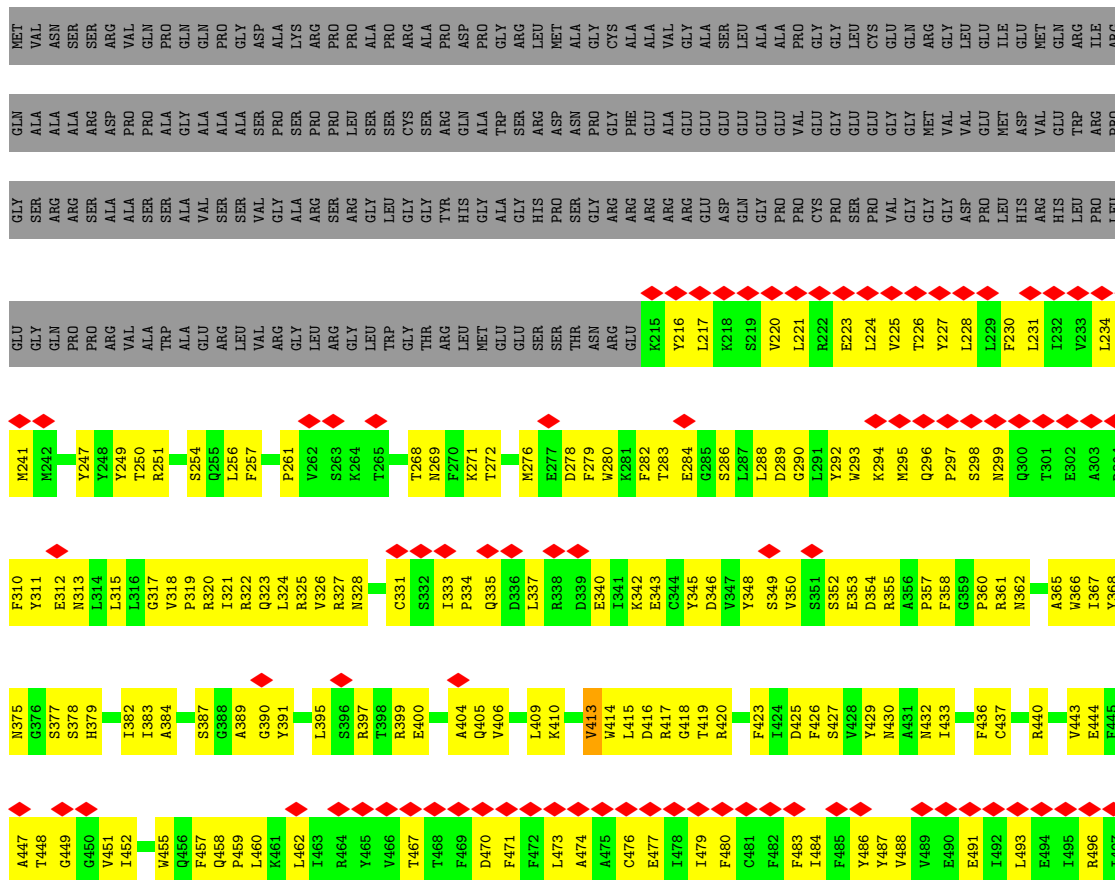
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 6   | A     | 1        | Total | C  | N | O | 0       |
|     |       |          | 15    | 11 | 1 | 3 |         |
| 6   | A     | 1        | Total | C  | N | O | 0       |
|     |       |          | 15    | 11 | 1 | 3 |         |
| 6   | B     | 1        | Total | C  | N | O | 0       |
|     |       |          | 15    | 11 | 1 | 3 |         |
| 6   | B     | 1        | Total | C  | N | O | 0       |
|     |       |          | 15    | 11 | 1 | 3 |         |
| 6   | C     | 1        | Total | C  | N | O | 0       |
|     |       |          | 15    | 11 | 1 | 3 |         |
| 6   | C     | 1        | Total | C  | N | O | 0       |
|     |       |          | 15    | 11 | 1 | 3 |         |
| 6   | D     | 1        | Total | C  | N | O | 0       |
|     |       |          | 15    | 11 | 1 | 3 |         |
| 6   | D     | 1        | Total | C  | N | O | 0       |
|     |       |          | 15    | 11 | 1 | 3 |         |

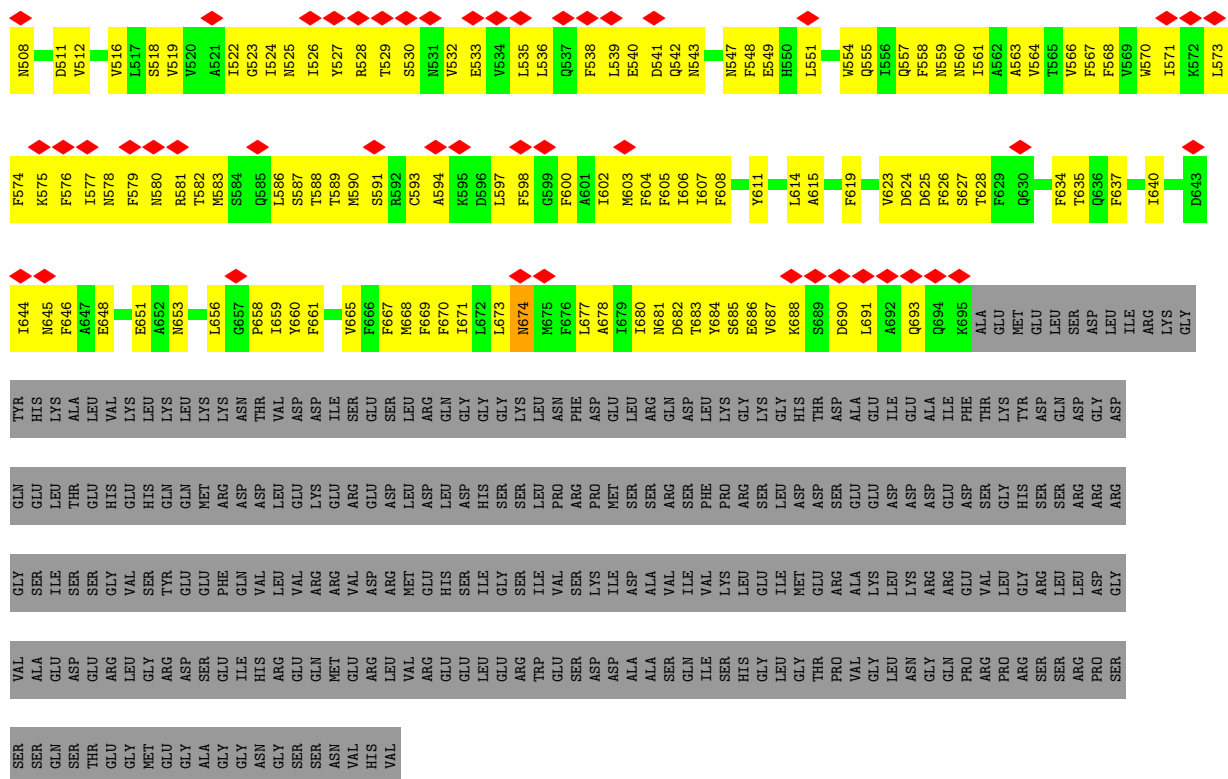
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

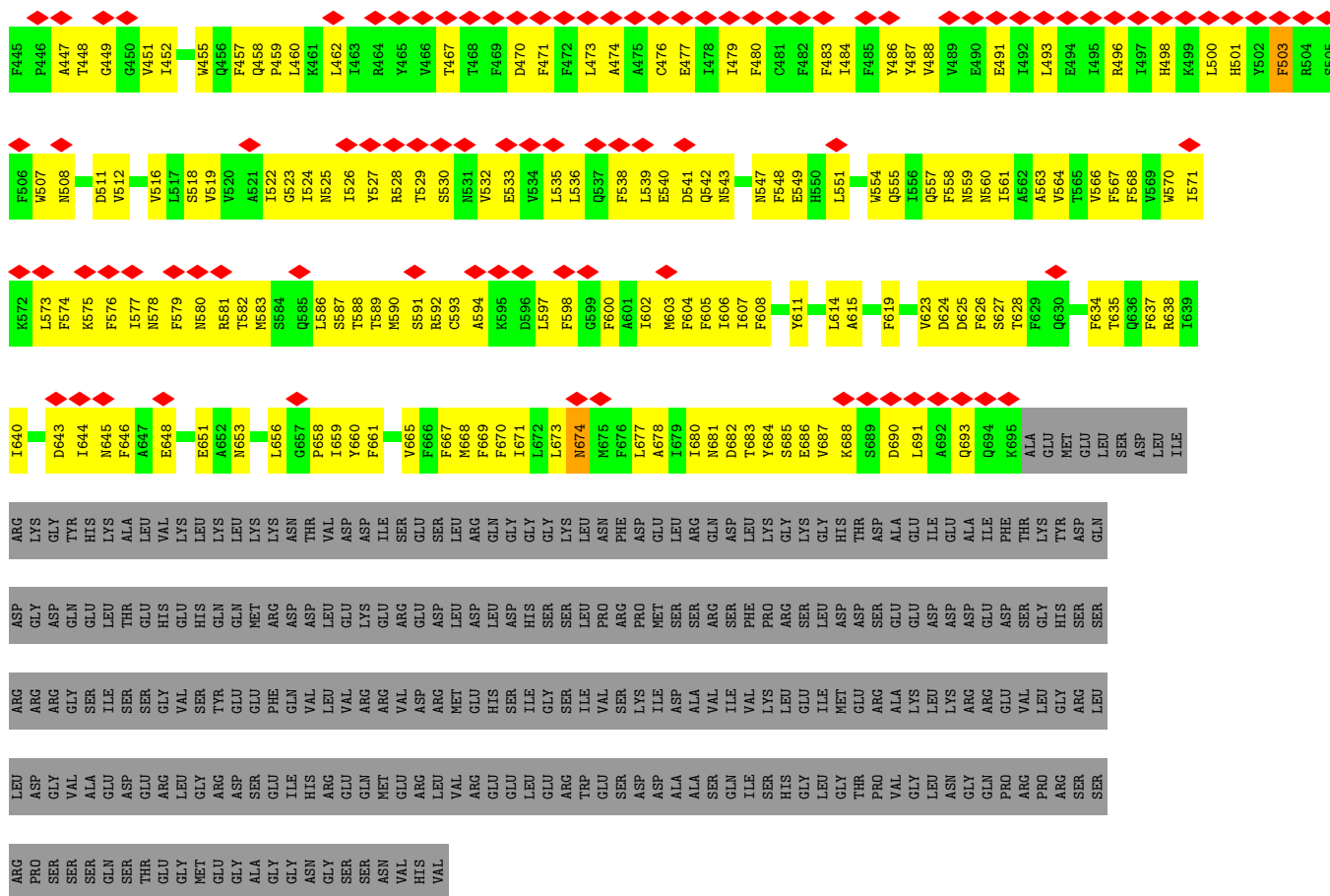
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 7   | A     | 4        | Total | Ca | 0       |
|     |       |          | 4     | 4  |         |
| 7   | B     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |











- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C4                               | Depositor |
| Number of particles used             | 35318                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | JEOL 3200FSC                            | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.8                                     | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.135                                   | Depositor |
| Minimum map value                    | -0.074                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.007                                   | Depositor |
| Recommended contour level            | 0.0354                                  | Depositor |
| Map size (Å)                         | 191.52, 191.52, 191.52                  | wwPDB     |
| Map dimensions                       | 168, 168, 168                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.14, 1.14, 1.14                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, NAG, CHS, CA, PX6

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     | 0.44         | 0/4068  | 0.61        | 0/5521  |
| 1   | B     | 0.44         | 0/4065  | 0.60        | 0/5518  |
| 1   | C     | 0.44         | 0/4065  | 0.60        | 0/5518  |
| 1   | D     | 0.44         | 0/4065  | 0.60        | 0/5518  |
| All | All   | 0.44         | 0/16263 | 0.61        | 0/22075 |

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                   | 1                   |
| 1   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 579 | PHE  | Peptide |
| 1   | B     | 579 | PHE  | Peptide |
| 1   | C     | 579 | PHE  | Peptide |
| 1   | D     | 579 | PHE  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3962  | 0        | 3898     | 291     | 0            |
| 1   | B     | 3959  | 0        | 3891     | 288     | 0            |
| 1   | C     | 3959  | 0        | 3891     | 283     | 0            |
| 1   | D     | 3959  | 0        | 3891     | 286     | 0            |
| 2   | E     | 28    | 0        | 25       | 0       | 0            |
| 2   | F     | 28    | 0        | 25       | 3       | 0            |
| 2   | G     | 28    | 0        | 25       | 3       | 0            |
| 2   | H     | 28    | 0        | 25       | 1       | 0            |
| 3   | A     | 42    | 0        | 39       | 15      | 0            |
| 3   | B     | 42    | 0        | 39       | 15      | 0            |
| 3   | C     | 42    | 0        | 39       | 15      | 0            |
| 3   | D     | 42    | 0        | 39       | 15      | 0            |
| 4   | A     | 40    | 0        | 56       | 2       | 0            |
| 4   | B     | 40    | 0        | 56       | 4       | 0            |
| 4   | C     | 40    | 0        | 56       | 5       | 0            |
| 4   | D     | 40    | 0        | 56       | 4       | 0            |
| 5   | A     | 54    | 0        | 93       | 5       | 0            |
| 5   | B     | 54    | 0        | 93       | 5       | 0            |
| 5   | C     | 54    | 0        | 93       | 4       | 0            |
| 5   | D     | 54    | 0        | 93       | 4       | 0            |
| 6   | A     | 30    | 0        | 40       | 2       | 0            |
| 6   | B     | 30    | 0        | 40       | 2       | 0            |
| 6   | C     | 30    | 0        | 40       | 1       | 0            |
| 6   | D     | 30    | 0        | 40       | 1       | 0            |
| 7   | A     | 4     | 0        | 0        | 0       | 0            |
| 7   | B     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 16620 | 0        | 16583    | 1113    | 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 34.

All (1113) 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:299:ASN:HD22 | 3:D:1005:NAG:C1 | 1.10                     | 1.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:299:ASN:HD22 | 3:C:1005:NAG:C1  | 1.17                     | 1.58              |
| 1:C:375:ASN:ND2  | 2:G:1:NAG:C1     | 1.68                     | 1.56              |
| 1:B:299:ASN:HD22 | 3:B:1005:NAG:C1  | 1.17                     | 1.55              |
| 1:B:375:ASN:ND2  | 2:F:1:NAG:C1     | 1.68                     | 1.55              |
| 1:A:299:ASN:HD22 | 3:A:1005:NAG:C1  | 1.17                     | 1.52              |
| 1:B:360:PRO:HB2  | 3:B:1002:NAG:C8  | 1.51                     | 1.39              |
| 1:A:360:PRO:HB2  | 3:A:1002:NAG:C8  | 1.51                     | 1.37              |
| 1:D:299:ASN:ND2  | 3:D:1005:NAG:C1  | 1.86                     | 1.37              |
| 1:D:360:PRO:HB2  | 3:D:1002:NAG:C8  | 1.53                     | 1.36              |
| 1:C:360:PRO:HB2  | 3:C:1002:NAG:C8  | 1.51                     | 1.36              |
| 1:B:299:ASN:ND2  | 3:B:1005:NAG:C1  | 1.92                     | 1.32              |
| 1:A:299:ASN:ND2  | 3:A:1005:NAG:C1  | 1.92                     | 1.32              |
| 1:C:299:ASN:ND2  | 3:C:1005:NAG:C1  | 1.92                     | 1.29              |
| 1:B:360:PRO:CB   | 3:B:1002:NAG:H81 | 1.72                     | 1.20              |
| 1:A:360:PRO:CB   | 3:A:1002:NAG:H81 | 1.72                     | 1.19              |
| 1:C:360:PRO:CB   | 3:C:1002:NAG:H81 | 1.72                     | 1.19              |
| 1:D:360:PRO:CB   | 3:D:1002:NAG:H81 | 1.75                     | 1.14              |
| 1:A:581:ARG:HB2  | 1:A:583:MET:HG2  | 1.18                     | 1.14              |
| 1:B:590:MET:SD   | 1:C:674:ASN:ND2  | 2.42                     | 0.92              |
| 1:C:645:ASN:HB3  | 1:C:648:GLU:OE2  | 1.71                     | 0.90              |
| 1:B:645:ASN:HB3  | 1:B:648:GLU:OE2  | 1.72                     | 0.89              |
| 1:A:645:ASN:HB3  | 1:A:648:GLU:OE2  | 1.72                     | 0.88              |
| 1:D:645:ASN:HB3  | 1:D:648:GLU:OE2  | 1.75                     | 0.86              |
| 1:A:458:GLN:NE2  | 1:A:459:PRO:O    | 2.08                     | 0.86              |
| 1:C:458:GLN:NE2  | 1:C:459:PRO:O    | 2.09                     | 0.86              |
| 1:B:309:ILE:HG13 | 1:B:310:PHE:H    | 1.40                     | 0.85              |
| 1:C:309:ILE:HG13 | 1:C:310:PHE:H    | 1.40                     | 0.85              |
| 1:A:309:ILE:HG13 | 1:A:310:PHE:H    | 1.40                     | 0.85              |
| 1:B:458:GLN:NE2  | 1:B:459:PRO:O    | 2.09                     | 0.85              |
| 1:D:458:GLN:NE2  | 1:D:459:PRO:O    | 2.08                     | 0.85              |
| 1:C:590:MET:SD   | 1:D:674:ASN:ND2  | 2.50                     | 0.85              |
| 1:A:674:ASN:ND2  | 1:D:590:MET:SD   | 2.50                     | 0.84              |
| 1:A:590:MET:SD   | 1:B:674:ASN:ND2  | 2.51                     | 0.84              |
| 1:D:309:ILE:HG13 | 1:D:310:PHE:H    | 1.41                     | 0.84              |
| 1:D:343:GLU:HA   | 3:D:1001:NAG:H62 | 1.60                     | 0.84              |
| 1:A:581:ARG:HB2  | 1:A:583:MET:CG   | 2.07                     | 0.82              |
| 1:B:343:GLU:HA   | 3:B:1001:NAG:H62 | 1.62                     | 0.81              |
| 1:A:343:GLU:HA   | 3:A:1001:NAG:H62 | 1.62                     | 0.81              |
| 3:B:1002:NAG:O7  | 3:B:1002:NAG:O3  | 1.99                     | 0.81              |
| 1:D:360:PRO:HB2  | 3:D:1002:NAG:H81 | 0.82                     | 0.81              |
| 3:A:1002:NAG:O7  | 3:A:1002:NAG:O3  | 1.99                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:525:ASN:OD1  | 1:C:526:ILE:N    | 2.14                     | 0.81              |
| 1:B:375:ASN:CG   | 2:F:1:NAG:C1     | 2.54                     | 0.80              |
| 1:B:525:ASN:OD1  | 1:B:526:ILE:N    | 2.14                     | 0.80              |
| 1:D:525:ASN:OD1  | 1:D:526:ILE:N    | 2.14                     | 0.80              |
| 1:A:323:GLN:HE22 | 1:A:414:TRP:HD1  | 1.30                     | 0.80              |
| 1:A:525:ASN:OD1  | 1:A:526:ILE:N    | 2.14                     | 0.79              |
| 1:A:360:PRO:CB   | 3:A:1002:NAG:C8  | 2.47                     | 0.79              |
| 3:D:1002:NAG:O7  | 3:D:1002:NAG:O3  | 1.99                     | 0.79              |
| 1:C:343:GLU:HA   | 3:C:1001:NAG:H62 | 1.62                     | 0.79              |
| 1:B:323:GLN:HE22 | 1:B:414:TRP:HD1  | 1.30                     | 0.79              |
| 1:C:375:ASN:CG   | 2:G:1:NAG:C1     | 2.54                     | 0.79              |
| 3:C:1002:NAG:O7  | 3:C:1002:NAG:O3  | 1.99                     | 0.79              |
| 1:B:397:ARG:HH11 | 1:B:543:ASN:HA   | 1.48                     | 0.79              |
| 1:A:674:ASN:HA   | 1:D:680:ILE:HG21 | 1.65                     | 0.78              |
| 1:D:397:ARG:HH11 | 1:D:543:ASN:HA   | 1.48                     | 0.78              |
| 1:C:397:ARG:HH11 | 1:C:543:ASN:HA   | 1.48                     | 0.78              |
| 1:C:680:ILE:HG21 | 1:D:674:ASN:HA   | 1.64                     | 0.78              |
| 1:D:323:GLN:HE22 | 1:D:414:TRP:HD1  | 1.30                     | 0.78              |
| 1:A:360:PRO:HB2  | 3:A:1002:NAG:H81 | 0.79                     | 0.77              |
| 1:C:323:GLN:HE22 | 1:C:414:TRP:HD1  | 1.30                     | 0.77              |
| 1:A:397:ARG:HH11 | 1:A:543:ASN:HA   | 1.48                     | 0.77              |
| 1:A:680:ILE:HG21 | 1:B:674:ASN:HA   | 1.67                     | 0.77              |
| 1:D:360:PRO:CB   | 3:D:1002:NAG:C8  | 2.49                     | 0.77              |
| 1:C:360:PRO:HB2  | 3:C:1002:NAG:H81 | 0.79                     | 0.77              |
| 1:C:360:PRO:CB   | 3:C:1002:NAG:C8  | 2.47                     | 0.77              |
| 1:B:677:LEU:HD21 | 1:C:673:LEU:HD22 | 1.66                     | 0.76              |
| 1:B:362:ASN:CB   | 3:B:1002:NAG:HN2 | 1.99                     | 0.76              |
| 1:B:360:PRO:HB2  | 3:B:1002:NAG:H81 | 0.79                     | 0.76              |
| 1:A:362:ASN:CB   | 3:A:1002:NAG:HN2 | 1.99                     | 0.75              |
| 1:A:268:THR:OG1  | 1:A:272:THR:O    | 2.05                     | 0.75              |
| 1:C:328:ASN:OD1  | 3:C:1001:NAG:O5  | 2.04                     | 0.75              |
| 1:B:328:ASN:OD1  | 3:B:1001:NAG:O5  | 2.04                     | 0.75              |
| 1:C:362:ASN:CB   | 3:C:1002:NAG:HN2 | 1.99                     | 0.75              |
| 1:C:677:LEU:HD21 | 1:D:673:LEU:HD22 | 1.69                     | 0.75              |
| 1:C:268:THR:OG1  | 1:C:272:THR:O    | 2.05                     | 0.74              |
| 1:A:328:ASN:OD1  | 3:A:1001:NAG:O5  | 2.04                     | 0.74              |
| 1:A:580:ASN:OD1  | 1:A:581:ARG:N    | 2.20                     | 0.74              |
| 1:D:268:THR:OG1  | 1:D:272:THR:O    | 2.05                     | 0.74              |
| 1:B:268:THR:OG1  | 1:B:272:THR:O    | 2.05                     | 0.74              |
| 1:D:362:ASN:CB   | 3:D:1002:NAG:HN2 | 2.00                     | 0.74              |
| 1:D:580:ASN:OD1  | 1:D:581:ARG:N    | 2.20                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:690:ASP:OD1  | 1:B:693:GLN:NE2  | 2.22                     | 0.73              |
| 1:A:673:LEU:HD22 | 1:D:677:LEU:HD21 | 1.69                     | 0.73              |
| 1:B:680:ILE:HG21 | 1:C:674:ASN:HA   | 1.69                     | 0.73              |
| 1:C:280:TRP:CG   | 1:C:410:LYS:HZ3  | 2.06                     | 0.73              |
| 1:A:690:ASP:OD1  | 1:A:693:GLN:NE2  | 2.22                     | 0.73              |
| 1:D:690:ASP:OD1  | 1:D:693:GLN:NE2  | 2.22                     | 0.73              |
| 1:B:360:PRO:CB   | 3:B:1002:NAG:C8  | 2.47                     | 0.73              |
| 1:A:323:GLN:OE1  | 1:A:414:TRP:NE1  | 2.22                     | 0.72              |
| 1:B:667:PHE:O    | 1:B:671:ILE:N    | 2.22                     | 0.72              |
| 1:D:328:ASN:OD1  | 3:D:1001:NAG:O5  | 2.04                     | 0.72              |
| 1:D:362:ASN:HB3  | 3:D:1002:NAG:HN2 | 1.54                     | 0.72              |
| 1:A:690:ASP:HA   | 1:A:693:GLN:HG2  | 1.71                     | 0.72              |
| 1:B:690:ASP:HA   | 1:B:693:GLN:HG2  | 1.72                     | 0.72              |
| 1:C:690:ASP:HA   | 1:C:693:GLN:HG2  | 1.72                     | 0.72              |
| 1:A:362:ASN:HB3  | 3:A:1002:NAG:HN2 | 1.55                     | 0.72              |
| 1:C:656:LEU:O    | 1:C:659:ILE:N    | 2.23                     | 0.72              |
| 1:A:667:PHE:O    | 1:A:671:ILE:N    | 2.22                     | 0.72              |
| 1:C:690:ASP:OD1  | 1:C:693:GLN:NE2  | 2.22                     | 0.72              |
| 1:D:656:LEU:O    | 1:D:659:ILE:N    | 2.23                     | 0.72              |
| 1:A:634:PHE:CZ   | 1:B:658:PRO:HB3  | 2.24                     | 0.72              |
| 1:D:323:GLN:OE1  | 1:D:414:TRP:NE1  | 2.22                     | 0.72              |
| 1:D:690:ASP:HA   | 1:D:693:GLN:HG2  | 1.72                     | 0.72              |
| 1:C:362:ASN:HB3  | 3:C:1002:NAG:HN2 | 1.55                     | 0.71              |
| 1:B:323:GLN:OE1  | 1:B:414:TRP:NE1  | 2.22                     | 0.71              |
| 1:B:580:ASN:OD1  | 1:B:581:ARG:N    | 2.20                     | 0.71              |
| 1:D:525:ASN:O    | 1:D:529:THR:OG1  | 2.08                     | 0.71              |
| 1:B:375:ASN:ND2  | 2:F:1:NAG:C2     | 2.54                     | 0.71              |
| 1:B:280:TRP:CG   | 1:B:410:LYS:HZ3  | 2.08                     | 0.71              |
| 1:B:362:ASN:HB3  | 3:B:1002:NAG:HN2 | 1.55                     | 0.71              |
| 1:C:580:ASN:OD1  | 1:C:581:ARG:N    | 2.20                     | 0.71              |
| 1:A:280:TRP:CG   | 1:A:410:LYS:HZ3  | 2.07                     | 0.71              |
| 1:C:323:GLN:OE1  | 1:C:414:TRP:NE1  | 2.22                     | 0.71              |
| 3:C:1002:NAG:O7  | 3:C:1002:NAG:C3  | 2.38                     | 0.71              |
| 1:A:656:LEU:O    | 1:A:659:ILE:N    | 2.23                     | 0.71              |
| 3:A:1002:NAG:O7  | 3:A:1002:NAG:C3  | 2.38                     | 0.71              |
| 1:B:656:LEU:O    | 1:B:659:ILE:N    | 2.23                     | 0.71              |
| 3:D:1002:NAG:O7  | 3:D:1002:NAG:C3  | 2.38                     | 0.71              |
| 1:C:667:PHE:O    | 1:C:671:ILE:N    | 2.22                     | 0.70              |
| 1:B:574:PHE:O    | 1:B:578:ASN:ND2  | 2.22                     | 0.70              |
| 3:B:1002:NAG:O7  | 3:B:1002:NAG:C3  | 2.38                     | 0.70              |
| 1:C:375:ASN:ND2  | 2:G:1:NAG:C2     | 2.54                     | 0.70              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:525:ASN:O    | 1:A:529:THR:OG1 | 2.08                     | 0.70              |
| 1:D:286:SER:O    | 1:D:290:GLY:N   | 2.25                     | 0.70              |
| 1:D:667:PHE:O    | 1:D:671:ILE:N   | 2.22                     | 0.70              |
| 1:D:280:TRP:CG   | 1:D:410:LYS:HZ3 | 2.10                     | 0.70              |
| 1:D:429:TYR:HD1  | 1:D:436:PHE:HD1 | 1.39                     | 0.70              |
| 1:C:419:THR:O    | 1:C:420:ARG:NH1 | 2.25                     | 0.69              |
| 1:B:322:ARG:HH21 | 1:B:423:PHE:HE2 | 1.40                     | 0.69              |
| 1:A:419:THR:O    | 1:A:420:ARG:NH1 | 2.25                     | 0.69              |
| 1:C:429:TYR:HD1  | 1:C:436:PHE:HD1 | 1.39                     | 0.69              |
| 1:C:322:ARG:HH21 | 1:C:423:PHE:HE2 | 1.40                     | 0.69              |
| 1:A:286:SER:O    | 1:A:290:GLY:N   | 2.25                     | 0.69              |
| 1:A:429:TYR:HD1  | 1:A:436:PHE:HD1 | 1.40                     | 0.69              |
| 1:B:286:SER:O    | 1:B:290:GLY:N   | 2.25                     | 0.69              |
| 1:A:455:TRP:NE1  | 1:B:651:GLU:OE2 | 2.25                     | 0.69              |
| 1:B:525:ASN:O    | 1:B:529:THR:OG1 | 2.08                     | 0.68              |
| 1:C:525:ASN:O    | 1:C:529:THR:OG1 | 2.08                     | 0.68              |
| 1:A:554:TRP:O    | 1:A:558:PHE:N   | 2.27                     | 0.68              |
| 1:C:286:SER:O    | 1:C:290:GLY:N   | 2.25                     | 0.68              |
| 1:B:429:TYR:HD1  | 1:B:436:PHE:HD1 | 1.40                     | 0.68              |
| 1:D:419:THR:O    | 1:D:420:ARG:NH1 | 2.25                     | 0.68              |
| 1:D:554:TRP:O    | 1:D:558:PHE:N   | 2.27                     | 0.68              |
| 1:A:290:GLY:O    | 1:A:293:TRP:NE1 | 2.27                     | 0.68              |
| 1:B:624:ASP:OD1  | 1:B:625:ASP:N   | 2.27                     | 0.68              |
| 1:D:322:ARG:HH21 | 1:D:423:PHE:HE2 | 1.40                     | 0.68              |
| 1:C:290:GLY:O    | 1:C:293:TRP:NE1 | 2.27                     | 0.68              |
| 1:D:624:ASP:OD1  | 1:D:625:ASP:N   | 2.27                     | 0.67              |
| 1:C:574:PHE:O    | 1:C:578:ASN:ND2 | 2.22                     | 0.67              |
| 1:D:409:LEU:HB3  | 1:D:414:TRP:CZ3 | 2.30                     | 0.67              |
| 1:A:223:GLU:O    | 1:A:226:THR:OG1 | 2.13                     | 0.67              |
| 1:A:322:ARG:HH21 | 1:A:423:PHE:HE2 | 1.40                     | 0.67              |
| 1:C:409:LEU:HB3  | 1:C:414:TRP:CZ3 | 2.30                     | 0.67              |
| 1:C:554:TRP:O    | 1:C:558:PHE:N   | 2.27                     | 0.67              |
| 1:D:290:GLY:O    | 1:D:293:TRP:NE1 | 2.27                     | 0.67              |
| 1:A:409:LEU:HB3  | 1:A:414:TRP:CZ3 | 2.30                     | 0.67              |
| 1:C:624:ASP:OD1  | 1:C:625:ASP:N   | 2.27                     | 0.67              |
| 1:D:223:GLU:O    | 1:D:226:THR:OG1 | 2.13                     | 0.67              |
| 1:B:409:LEU:HB3  | 1:B:414:TRP:CZ3 | 2.29                     | 0.67              |
| 1:B:223:GLU:O    | 1:B:226:THR:OG1 | 2.13                     | 0.67              |
| 1:B:290:GLY:O    | 1:B:293:TRP:NE1 | 2.27                     | 0.67              |
| 1:B:554:TRP:O    | 1:B:558:PHE:N   | 2.27                     | 0.67              |
| 1:A:624:ASP:OD1  | 1:A:625:ASP:N   | 2.27                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:677:LEU:HD21 | 1:B:673:LEU:HD22 | 1.76                     | 0.67              |
| 1:A:323:GLN:HE22 | 1:A:414:TRP:CD1  | 2.13                     | 0.66              |
| 1:B:493:LEU:HD22 | 1:B:496:ARG:HH11 | 1.61                     | 0.66              |
| 1:D:493:LEU:HD22 | 1:D:496:ARG:HH11 | 1.61                     | 0.66              |
| 1:A:405:GLN:O    | 1:A:409:LEU:N    | 2.29                     | 0.66              |
| 1:D:323:GLN:HE22 | 1:D:414:TRP:CD1  | 2.13                     | 0.66              |
| 1:A:493:LEU:HD22 | 1:A:496:ARG:HH11 | 1.61                     | 0.66              |
| 1:D:574:PHE:O    | 1:D:578:ASN:ND2  | 2.22                     | 0.66              |
| 1:C:405:GLN:O    | 1:C:409:LEU:N    | 2.29                     | 0.66              |
| 1:B:419:THR:O    | 1:B:420:ARG:NH1  | 2.25                     | 0.65              |
| 1:C:360:PRO:HB2  | 3:C:1002:NAG:H82 | 1.72                     | 0.65              |
| 1:A:360:PRO:HB2  | 3:A:1002:NAG:H82 | 1.72                     | 0.65              |
| 1:B:323:GLN:HE22 | 1:B:414:TRP:CD1  | 2.13                     | 0.65              |
| 1:C:323:GLN:HE22 | 1:C:414:TRP:CD1  | 2.13                     | 0.65              |
| 1:B:360:PRO:HB2  | 3:B:1002:NAG:H82 | 1.72                     | 0.65              |
| 1:C:493:LEU:HD22 | 1:C:496:ARG:HH11 | 1.61                     | 0.65              |
| 1:D:405:GLN:O    | 1:D:409:LEU:N    | 2.29                     | 0.65              |
| 1:B:405:GLN:O    | 1:B:409:LEU:N    | 2.29                     | 0.65              |
| 1:C:223:GLU:O    | 1:C:226:THR:OG1  | 2.13                     | 0.65              |
| 1:A:221:LEU:O    | 1:A:225:VAL:N    | 2.21                     | 0.64              |
| 1:B:668:MET:HA   | 1:B:671:ILE:HG22 | 1.80                     | 0.64              |
| 1:C:634:PHE:CZ   | 1:D:658:PRO:HB3  | 2.32                     | 0.64              |
| 1:A:668:MET:HA   | 1:A:671:ILE:HG22 | 1.80                     | 0.64              |
| 1:A:580:ASN:OD1  | 1:A:583:MET:SD   | 2.55                     | 0.64              |
| 1:C:644:ILE:HG23 | 1:C:646:PHE:H    | 1.63                     | 0.64              |
| 1:C:355:ARG:HG2  | 1:C:368:TYR:CZ   | 2.33                     | 0.64              |
| 1:D:355:ARG:HG2  | 1:D:368:TYR:CZ   | 2.33                     | 0.64              |
| 1:D:668:MET:HA   | 1:D:671:ILE:HG22 | 1.79                     | 0.64              |
| 1:A:355:ARG:HG2  | 1:A:368:TYR:CZ   | 2.33                     | 0.63              |
| 1:D:644:ILE:HG23 | 1:D:646:PHE:H    | 1.63                     | 0.63              |
| 1:B:355:ARG:HG2  | 1:B:368:TYR:CZ   | 2.33                     | 0.63              |
| 1:A:279:PHE:HE1  | 1:A:443:VAL:HG21 | 1.64                     | 0.63              |
| 1:C:279:PHE:HE1  | 1:C:443:VAL:HG21 | 1.64                     | 0.63              |
| 1:D:279:PHE:HE1  | 1:D:443:VAL:HG21 | 1.64                     | 0.63              |
| 1:D:637:PHE:O    | 1:D:640:ILE:N    | 2.32                     | 0.63              |
| 1:A:574:PHE:O    | 1:A:578:ASN:ND2  | 2.22                     | 0.63              |
| 1:C:586:LEU:O    | 1:C:589:THR:OG1  | 2.16                     | 0.63              |
| 1:B:296:GLN:HE22 | 1:C:417:ARG:HB2  | 1.63                     | 0.63              |
| 1:A:637:PHE:O    | 1:A:640:ILE:N    | 2.32                     | 0.62              |
| 1:A:644:ILE:HG23 | 1:A:646:PHE:H    | 1.63                     | 0.62              |
| 1:C:221:LEU:O    | 1:C:225:VAL:N    | 2.21                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:279:PHE:HE1  | 1:B:443:VAL:HG21 | 1.64                     | 0.62              |
| 1:B:634:PHE:CZ   | 1:C:658:PRO:HB3  | 2.35                     | 0.62              |
| 1:B:637:PHE:O    | 1:B:640:ILE:N    | 2.32                     | 0.62              |
| 1:B:644:ILE:HG23 | 1:B:646:PHE:H    | 1.63                     | 0.62              |
| 1:C:227:TYR:HA   | 1:C:230:PHE:HB3  | 1.81                     | 0.62              |
| 1:C:668:MET:HA   | 1:C:671:ILE:HG22 | 1.79                     | 0.62              |
| 1:B:227:TYR:HA   | 1:B:230:PHE:HB3  | 1.81                     | 0.62              |
| 1:A:227:TYR:HA   | 1:A:230:PHE:HB3  | 1.81                     | 0.62              |
| 1:C:637:PHE:O    | 1:C:640:ILE:N    | 2.32                     | 0.62              |
| 1:D:594:ALA:O    | 1:D:598:PHE:N    | 2.32                     | 0.62              |
| 1:A:594:ALA:O    | 1:A:598:PHE:N    | 2.32                     | 0.62              |
| 1:B:586:LEU:O    | 1:B:589:THR:OG1  | 2.16                     | 0.62              |
| 1:A:658:PRO:HB3  | 1:D:634:PHE:CZ   | 2.33                     | 0.61              |
| 1:D:343:GLU:HA   | 3:D:1001:NAG:C6  | 2.30                     | 0.61              |
| 1:B:519:VAL:HA   | 1:B:522:ILE:HD12 | 1.82                     | 0.61              |
| 1:D:586:LEU:O    | 1:D:589:THR:OG1  | 2.16                     | 0.61              |
| 1:D:227:TYR:HA   | 1:D:230:PHE:HB3  | 1.81                     | 0.61              |
| 1:C:535:LEU:HD12 | 1:C:536:LEU:HD12 | 1.83                     | 0.61              |
| 1:D:519:VAL:HA   | 1:D:522:ILE:HD12 | 1.81                     | 0.61              |
| 1:A:519:VAL:HA   | 1:A:522:ILE:HD12 | 1.81                     | 0.61              |
| 1:C:361:ARG:HA   | 1:C:366:TRP:HB3  | 1.83                     | 0.61              |
| 1:B:400:GLU:O    | 1:B:404:ALA:N    | 2.34                     | 0.60              |
| 1:C:594:ALA:O    | 1:C:598:PHE:N    | 2.32                     | 0.60              |
| 1:D:361:ARG:HA   | 1:D:366:TRP:HB3  | 1.83                     | 0.60              |
| 1:C:519:VAL:HA   | 1:C:522:ILE:HD12 | 1.81                     | 0.60              |
| 1:D:535:LEU:HD12 | 1:D:536:LEU:HD12 | 1.83                     | 0.60              |
| 1:A:586:LEU:O    | 1:A:589:THR:OG1  | 2.16                     | 0.60              |
| 1:A:383:ILE:HG13 | 1:A:384:ALA:H    | 1.67                     | 0.60              |
| 1:B:416:ASP:OD1  | 1:B:417:ARG:N    | 2.35                     | 0.60              |
| 1:C:498:HIS:HB3  | 1:C:501:HIS:HB3  | 1.84                     | 0.60              |
| 1:B:221:LEU:O    | 1:B:225:VAL:N    | 2.21                     | 0.60              |
| 1:C:416:ASP:OD1  | 1:C:417:ARG:N    | 2.35                     | 0.60              |
| 1:D:383:ILE:HG13 | 1:D:384:ALA:H    | 1.67                     | 0.60              |
| 1:A:440:ARG:HD2  | 1:A:549:GLU:HG3  | 1.84                     | 0.60              |
| 1:A:535:LEU:HD12 | 1:A:536:LEU:HD12 | 1.83                     | 0.60              |
| 1:B:383:ILE:HG13 | 1:B:384:ALA:H    | 1.67                     | 0.60              |
| 1:B:498:HIS:HB3  | 1:B:501:HIS:HB3  | 1.84                     | 0.60              |
| 1:D:500:LEU:HA   | 1:D:503:PHE:HB2  | 1.84                     | 0.60              |
| 1:B:294:LYS:HG2  | 1:B:295:MET:H    | 1.67                     | 0.59              |
| 1:B:535:LEU:HD12 | 1:B:536:LEU:HD12 | 1.83                     | 0.59              |
| 1:B:594:ALA:O    | 1:B:598:PHE:N    | 2.32                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:440:ARG:HD2  | 1:C:549:GLU:HG3  | 1.84                     | 0.59              |
| 1:A:409:LEU:HB3  | 1:A:414:TRP:HZ3  | 1.67                     | 0.59              |
| 1:A:500:LEU:HA   | 1:A:503:PHE:HB2  | 1.84                     | 0.59              |
| 1:D:294:LYS:HG2  | 1:D:295:MET:H    | 1.67                     | 0.59              |
| 1:D:440:ARG:HD2  | 1:D:549:GLU:HG3  | 1.84                     | 0.59              |
| 1:B:409:LEU:HB3  | 1:B:414:TRP:HZ3  | 1.67                     | 0.59              |
| 1:B:440:ARG:HD2  | 1:B:549:GLU:HG3  | 1.84                     | 0.59              |
| 1:B:500:LEU:HA   | 1:B:503:PHE:HB2  | 1.84                     | 0.59              |
| 1:C:400:GLU:O    | 1:C:404:ALA:N    | 2.34                     | 0.59              |
| 1:D:498:HIS:HB3  | 1:D:501:HIS:HB3  | 1.84                     | 0.59              |
| 1:A:349:SER:O    | 1:A:353:GLU:HG3  | 2.02                     | 0.59              |
| 1:B:293:TRP:CZ2  | 1:B:310:PHE:HD1  | 2.20                     | 0.59              |
| 1:B:656:LEU:HA   | 1:B:659:ILE:HG22 | 1.84                     | 0.59              |
| 1:D:349:SER:O    | 1:D:353:GLU:HG3  | 2.02                     | 0.59              |
| 1:A:293:TRP:CZ2  | 1:A:310:PHE:HD1  | 2.21                     | 0.59              |
| 1:A:400:GLU:O    | 1:A:404:ALA:N    | 2.34                     | 0.59              |
| 1:A:498:HIS:HB3  | 1:A:501:HIS:HB3  | 1.84                     | 0.59              |
| 1:C:383:ILE:HG13 | 1:C:384:ALA:H    | 1.67                     | 0.59              |
| 1:C:455:TRP:NE1  | 1:D:651:GLU:OE2  | 2.36                     | 0.59              |
| 1:D:360:PRO:HB2  | 3:D:1002:NAG:H82 | 1.75                     | 0.59              |
| 1:A:294:LYS:HG2  | 1:A:295:MET:H    | 1.67                     | 0.59              |
| 1:C:409:LEU:HB3  | 1:C:414:TRP:HZ3  | 1.67                     | 0.59              |
| 1:B:361:ARG:HA   | 1:B:366:TRP:HB3  | 1.83                     | 0.59              |
| 1:D:221:LEU:O    | 1:D:225:VAL:N    | 2.21                     | 0.59              |
| 1:A:361:ARG:HA   | 1:A:366:TRP:HB3  | 1.83                     | 0.59              |
| 1:C:343:GLU:HA   | 3:C:1001:NAG:C6  | 2.33                     | 0.59              |
| 6:A:1010:CHS:O   | 6:A:1010:CHS:OH  | 2.18                     | 0.59              |
| 1:B:619:PHE:HB2  | 1:B:626:PHE:HD2  | 1.68                     | 0.59              |
| 1:D:416:ASP:OD1  | 1:D:417:ARG:N    | 2.35                     | 0.59              |
| 1:A:656:LEU:HA   | 1:A:659:ILE:HG22 | 1.84                     | 0.58              |
| 1:C:500:LEU:HA   | 1:C:503:PHE:HB2  | 1.84                     | 0.58              |
| 1:B:349:SER:O    | 1:B:353:GLU:HG3  | 2.02                     | 0.58              |
| 1:D:619:PHE:HB2  | 1:D:626:PHE:HD2  | 1.68                     | 0.58              |
| 1:A:416:ASP:OD1  | 1:A:417:ARG:N    | 2.35                     | 0.58              |
| 1:A:619:PHE:HB2  | 1:A:626:PHE:HD2  | 1.68                     | 0.58              |
| 1:C:656:LEU:HA   | 1:C:659:ILE:HG22 | 1.84                     | 0.58              |
| 1:C:597:LEU:HA   | 1:C:600:PHE:HB3  | 1.84                     | 0.58              |
| 1:D:409:LEU:HB3  | 1:D:414:TRP:HZ3  | 1.67                     | 0.58              |
| 1:A:460:LEU:HD13 | 1:A:555:GLN:HG2  | 1.86                     | 0.58              |
| 1:B:455:TRP:NE1  | 1:C:651:GLU:OE2  | 2.36                     | 0.58              |
| 1:D:293:TRP:CZ2  | 1:D:310:PHE:HD1  | 2.20                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:651:GLU:OE2  | 1:D:455:TRP:NE1  | 2.37                     | 0.58              |
| 1:C:460:LEU:HD13 | 1:C:555:GLN:HG2  | 1.86                     | 0.58              |
| 1:C:293:TRP:CZ2  | 1:C:310:PHE:HD1  | 2.20                     | 0.58              |
| 1:D:250:THR:O    | 1:D:254:SER:N    | 2.23                     | 0.58              |
| 1:D:400:GLU:O    | 1:D:404:ALA:N    | 2.34                     | 0.58              |
| 1:D:656:LEU:HA   | 1:D:659:ILE:HG22 | 1.84                     | 0.58              |
| 1:C:335:GLN:OE1  | 1:C:335:GLN:N    | 2.34                     | 0.58              |
| 1:D:460:LEU:HD13 | 1:D:555:GLN:HG2  | 1.86                     | 0.58              |
| 1:A:597:LEU:HA   | 1:A:600:PHE:HB3  | 1.85                     | 0.58              |
| 1:B:343:GLU:HA   | 3:B:1001:NAG:C6  | 2.33                     | 0.58              |
| 1:C:294:LYS:HG2  | 1:C:295:MET:H    | 1.67                     | 0.58              |
| 1:C:619:PHE:HB2  | 1:C:626:PHE:HD2  | 1.68                     | 0.58              |
| 1:D:597:LEU:HA   | 1:D:600:PHE:HB3  | 1.85                     | 0.58              |
| 1:A:289:ASP:OD1  | 1:A:399:ARG:NH1  | 2.36                     | 0.57              |
| 1:A:523:GLY:O    | 1:A:527:TYR:N    | 2.36                     | 0.57              |
| 1:D:335:GLN:OE1  | 1:D:335:GLN:N    | 2.34                     | 0.57              |
| 1:B:460:LEU:HD13 | 1:B:555:GLN:HG2  | 1.86                     | 0.57              |
| 1:C:349:SER:O    | 1:C:353:GLU:HG3  | 2.02                     | 0.57              |
| 1:D:507:TRP:HB3  | 1:D:575:LYS:NZ   | 2.20                     | 0.57              |
| 1:A:583:MET:HA   | 1:A:586:LEU:HB2  | 1.87                     | 0.57              |
| 1:D:523:GLY:O    | 1:D:527:TYR:N    | 2.36                     | 0.57              |
| 6:B:1010:CHS:O   | 6:B:1010:CHS:OH  | 2.18                     | 0.57              |
| 1:A:296:GLN:HE22 | 1:B:417:ARG:HB2  | 1.69                     | 0.57              |
| 1:A:343:GLU:HA   | 3:A:1001:NAG:C6  | 2.33                     | 0.57              |
| 1:D:289:ASP:OD1  | 1:D:399:ARG:NH1  | 2.36                     | 0.57              |
| 1:B:597:LEU:HA   | 1:B:600:PHE:HB3  | 1.85                     | 0.56              |
| 1:D:524:ILE:O    | 1:D:528:ARG:HB2  | 2.05                     | 0.56              |
| 1:A:335:GLN:N    | 1:A:335:GLN:OE1  | 2.34                     | 0.56              |
| 1:A:507:TRP:HB3  | 1:A:575:LYS:NZ   | 2.20                     | 0.56              |
| 1:B:523:GLY:O    | 1:B:527:TYR:N    | 2.36                     | 0.56              |
| 1:C:250:THR:O    | 1:C:254:SER:N    | 2.23                     | 0.56              |
| 1:C:507:TRP:HB3  | 1:C:575:LYS:NZ   | 2.20                     | 0.56              |
| 1:B:382:ILE:HG23 | 1:B:383:ILE:H    | 1.71                     | 0.56              |
| 1:D:593:CYS:SG   | 1:D:594:ALA:N    | 2.79                     | 0.56              |
| 1:C:524:ILE:O    | 1:C:528:ARG:HB2  | 2.05                     | 0.56              |
| 1:D:382:ILE:HG23 | 1:D:383:ILE:H    | 1.71                     | 0.56              |
| 1:C:382:ILE:HG23 | 1:C:383:ILE:H    | 1.71                     | 0.56              |
| 1:A:593:CYS:SG   | 1:A:594:ALA:N    | 2.79                     | 0.56              |
| 1:B:289:ASP:OD1  | 1:B:399:ARG:NH1  | 2.36                     | 0.56              |
| 1:B:350:VAL:HA   | 1:B:353:GLU:CD   | 2.31                     | 0.56              |
| 1:C:523:GLY:O    | 1:C:527:TYR:N    | 2.36                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:365:ALA:HA   | 1:D:391:TYR:HB3  | 1.88                     | 0.56              |
| 6:D:1010:CHS:O   | 6:D:1010:CHS:OH  | 2.19                     | 0.56              |
| 1:A:382:ILE:HG23 | 1:A:383:ILE:H    | 1.71                     | 0.56              |
| 1:B:524:ILE:O    | 1:B:528:ARG:HB2  | 2.05                     | 0.56              |
| 1:B:686:GLU:O    | 1:B:690:ASP:N    | 2.39                     | 0.56              |
| 1:A:350:VAL:HA   | 1:A:353:GLU:CD   | 2.31                     | 0.55              |
| 1:A:365:ALA:HA   | 1:A:391:TYR:HB3  | 1.88                     | 0.55              |
| 1:C:289:ASP:OD1  | 1:C:399:ARG:NH1  | 2.36                     | 0.55              |
| 1:C:593:CYS:SG   | 1:C:594:ALA:N    | 2.79                     | 0.55              |
| 1:D:350:VAL:HA   | 1:D:353:GLU:CD   | 2.31                     | 0.55              |
| 1:B:507:TRP:HB3  | 1:B:575:LYS:NZ   | 2.20                     | 0.55              |
| 1:A:524:ILE:O    | 1:A:528:ARG:HB2  | 2.05                     | 0.55              |
| 1:A:686:GLU:O    | 1:A:690:ASP:N    | 2.39                     | 0.55              |
| 1:D:293:TRP:HZ2  | 1:D:310:PHE:HD1  | 1.54                     | 0.55              |
| 1:A:250:THR:O    | 1:A:254:SER:N    | 2.23                     | 0.55              |
| 1:B:335:GLN:N    | 1:B:335:GLN:OE1  | 2.34                     | 0.55              |
| 1:B:593:CYS:SG   | 1:B:594:ALA:N    | 2.79                     | 0.55              |
| 1:D:602:ILE:O    | 1:D:606:ILE:N    | 2.33                     | 0.55              |
| 1:A:417:ARG:HB2  | 1:D:296:GLN:HE22 | 1.72                     | 0.55              |
| 1:C:686:GLU:O    | 1:C:690:ASP:N    | 2.39                     | 0.55              |
| 1:D:331:CYS:HB3  | 1:D:346:ASP:HB3  | 1.89                     | 0.55              |
| 1:A:583:MET:O    | 1:A:587:SER:N    | 2.38                     | 0.55              |
| 1:B:583:MET:O    | 1:B:587:SER:N    | 2.40                     | 0.55              |
| 1:A:644:ILE:HG23 | 1:A:646:PHE:HB3  | 1.89                     | 0.55              |
| 1:C:331:CYS:HB3  | 1:C:346:ASP:HB3  | 1.89                     | 0.55              |
| 1:D:644:ILE:HG23 | 1:D:646:PHE:HB3  | 1.89                     | 0.55              |
| 1:B:293:TRP:HZ2  | 1:B:310:PHE:HD1  | 1.54                     | 0.55              |
| 1:C:644:ILE:HG23 | 1:C:646:PHE:HB3  | 1.89                     | 0.55              |
| 1:A:602:ILE:O    | 1:A:606:ILE:N    | 2.33                     | 0.54              |
| 1:B:337:LEU:O    | 1:B:340:GLU:N    | 2.40                     | 0.54              |
| 1:C:293:TRP:HZ2  | 1:C:310:PHE:HD1  | 1.54                     | 0.54              |
| 1:D:337:LEU:O    | 1:D:340:GLU:N    | 2.40                     | 0.54              |
| 1:B:331:CYS:HB3  | 1:B:346:ASP:HB3  | 1.89                     | 0.54              |
| 1:C:350:VAL:HA   | 1:C:353:GLU:CD   | 2.31                     | 0.54              |
| 1:D:686:GLU:O    | 1:D:690:ASP:N    | 2.39                     | 0.54              |
| 1:A:331:CYS:HB3  | 1:A:346:ASP:HB3  | 1.89                     | 0.54              |
| 1:C:337:LEU:O    | 1:C:340:GLU:N    | 2.40                     | 0.54              |
| 1:B:644:ILE:HG23 | 1:B:646:PHE:HB3  | 1.89                     | 0.54              |
| 1:C:365:ALA:HA   | 1:C:391:TYR:HB3  | 1.88                     | 0.54              |
| 1:A:337:LEU:O    | 1:A:340:GLU:N    | 2.40                     | 0.54              |
| 1:B:365:ALA:HA   | 1:B:391:TYR:HB3  | 1.88                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:293:TRP:HZ2  | 1:A:310:PHE:HD1  | 1.54                     | 0.54              |
| 1:C:600:PHE:HZ   | 1:C:603:MET:HE2  | 1.73                     | 0.54              |
| 1:D:323:GLN:NE2  | 1:D:414:TRP:HD1  | 2.03                     | 0.54              |
| 1:A:323:GLN:NE2  | 1:A:414:TRP:HD1  | 2.03                     | 0.54              |
| 1:D:583:MET:O    | 1:D:587:SER:N    | 2.40                     | 0.54              |
| 1:B:600:PHE:HZ   | 1:B:603:MET:HE2  | 1.73                     | 0.53              |
| 1:C:467:THR:HA   | 1:C:471:PHE:HE2  | 1.74                     | 0.53              |
| 1:D:467:THR:HA   | 1:D:471:PHE:HE2  | 1.74                     | 0.53              |
| 1:A:430:ASN:HD22 | 1:A:433:ILE:HG12 | 1.74                     | 0.53              |
| 1:A:467:THR:HA   | 1:A:471:PHE:HE2  | 1.74                     | 0.53              |
| 1:A:600:PHE:HZ   | 1:A:603:MET:HE2  | 1.73                     | 0.53              |
| 6:C:1010:CHS:O   | 6:C:1010:CHS:OH  | 2.18                     | 0.53              |
| 1:B:327:ARG:N    | 1:B:354:ASP:HB2  | 2.24                     | 0.53              |
| 1:C:292:TYR:HB3  | 1:C:399:ARG:HB2  | 1.91                     | 0.53              |
| 1:C:327:ARG:N    | 1:C:354:ASP:HB2  | 2.24                     | 0.53              |
| 1:D:600:PHE:HZ   | 1:D:603:MET:HE2  | 1.73                     | 0.53              |
| 1:B:665:VAL:O    | 1:B:669:PHE:HB3  | 2.09                     | 0.53              |
| 1:A:526:ILE:HA   | 1:A:530:SER:HB3  | 1.91                     | 0.53              |
| 1:C:309:ILE:HG13 | 1:C:310:PHE:N    | 2.18                     | 0.53              |
| 1:C:665:VAL:O    | 1:C:669:PHE:HB3  | 2.09                     | 0.53              |
| 1:A:665:VAL:O    | 1:A:669:PHE:HB3  | 2.09                     | 0.53              |
| 1:C:224:LEU:O    | 1:C:228:LEU:N    | 2.26                     | 0.53              |
| 1:C:430:ASN:HD22 | 1:C:433:ILE:HG12 | 1.74                     | 0.53              |
| 1:C:583:MET:O    | 1:C:587:SER:N    | 2.40                     | 0.53              |
| 1:A:680:ILE:HD13 | 1:B:674:ASN:HA   | 1.90                     | 0.53              |
| 1:B:322:ARG:HD2  | 1:B:389:ALA:HB2  | 1.91                     | 0.53              |
| 1:C:254:SER:HA   | 1:C:457:PHE:HE2  | 1.74                     | 0.53              |
| 1:D:292:TYR:HB3  | 1:D:399:ARG:HB2  | 1.91                     | 0.53              |
| 1:D:319:PRO:HG3  | 1:D:426:PHE:HB3  | 1.90                     | 0.53              |
| 1:D:322:ARG:HD2  | 1:D:389:ALA:HB2  | 1.91                     | 0.53              |
| 1:B:319:PRO:HG3  | 1:B:426:PHE:HB3  | 1.90                     | 0.53              |
| 1:A:280:TRP:CD1  | 1:A:410:LYS:HZ3  | 2.28                     | 0.52              |
| 1:A:309:ILE:HD11 | 1:A:313:ASN:HB2  | 1.91                     | 0.52              |
| 1:C:280:TRP:CD1  | 1:C:410:LYS:HZ3  | 2.27                     | 0.52              |
| 1:C:322:ARG:HD2  | 1:C:389:ALA:HB2  | 1.91                     | 0.52              |
| 1:C:541:ASP:OD1  | 1:C:542:GLN:N    | 2.42                     | 0.52              |
| 1:D:309:ILE:HG13 | 1:D:310:PHE:N    | 2.19                     | 0.52              |
| 1:D:526:ILE:HA   | 1:D:530:SER:HB3  | 1.91                     | 0.52              |
| 1:D:604:PHE:O    | 1:D:607:ILE:HG22 | 2.10                     | 0.52              |
| 1:D:665:VAL:O    | 1:D:669:PHE:HB3  | 2.09                     | 0.52              |
| 1:A:555:GLN:O    | 1:A:559:ASN:N    | 2.35                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:541:ASP:OD1  | 1:B:542:GLN:N    | 2.42                     | 0.52              |
| 1:C:296:GLN:HE22 | 1:D:417:ARG:HB2  | 1.74                     | 0.52              |
| 1:C:319:PRO:HB2  | 1:C:395:LEU:HD13 | 1.92                     | 0.52              |
| 1:D:319:PRO:HB2  | 1:D:395:LEU:HD13 | 1.92                     | 0.52              |
| 1:A:319:PRO:HB2  | 1:A:395:LEU:HD13 | 1.92                     | 0.52              |
| 1:A:604:PHE:O    | 1:A:607:ILE:HG22 | 2.09                     | 0.52              |
| 1:B:292:TYR:HB3  | 1:B:399:ARG:HB2  | 1.91                     | 0.52              |
| 1:B:430:ASN:HD22 | 1:B:433:ILE:HG12 | 1.73                     | 0.52              |
| 1:D:254:SER:HA   | 1:D:457:PHE:HE2  | 1.74                     | 0.52              |
| 1:D:430:ASN:HD22 | 1:D:433:ILE:HG12 | 1.74                     | 0.52              |
| 1:A:247:TYR:OH   | 1:B:624:ASP:HB3  | 2.09                     | 0.52              |
| 1:A:319:PRO:HG3  | 1:A:426:PHE:HB3  | 1.90                     | 0.52              |
| 1:B:250:THR:O    | 1:B:254:SER:N    | 2.23                     | 0.52              |
| 1:B:526:ILE:HA   | 1:B:530:SER:HB3  | 1.91                     | 0.52              |
| 1:C:634:PHE:O    | 1:C:637:PHE:N    | 2.41                     | 0.52              |
| 1:D:309:ILE:HD11 | 1:D:313:ASN:HB2  | 1.91                     | 0.52              |
| 1:D:555:GLN:O    | 1:D:559:ASN:N    | 2.35                     | 0.52              |
| 1:A:541:ASP:OD1  | 1:A:542:GLN:N    | 2.42                     | 0.52              |
| 1:B:319:PRO:HB2  | 1:B:395:LEU:HD13 | 1.92                     | 0.52              |
| 1:D:470:ASP:O    | 1:D:474:ALA:N    | 2.36                     | 0.52              |
| 1:A:292:TYR:HB3  | 1:A:399:ARG:HB2  | 1.91                     | 0.52              |
| 1:A:573:LEU:HA   | 1:A:576:PHE:HD2  | 1.75                     | 0.52              |
| 1:B:467:THR:HA   | 1:B:471:PHE:HE2  | 1.74                     | 0.52              |
| 1:C:319:PRO:HG3  | 1:C:426:PHE:HB3  | 1.90                     | 0.52              |
| 1:C:383:ILE:HG13 | 1:C:384:ALA:N    | 2.25                     | 0.52              |
| 1:A:322:ARG:HD2  | 1:A:389:ALA:HB2  | 1.91                     | 0.52              |
| 1:B:280:TRP:CD1  | 1:B:410:LYS:HZ3  | 2.28                     | 0.52              |
| 1:C:526:ILE:HA   | 1:C:530:SER:HB3  | 1.91                     | 0.52              |
| 1:D:283:THR:OG1  | 1:D:284:GLU:N    | 2.43                     | 0.52              |
| 1:A:327:ARG:N    | 1:A:354:ASP:HB2  | 2.24                     | 0.52              |
| 1:A:473:LEU:O    | 1:A:477:GLU:N    | 2.43                     | 0.52              |
| 1:B:323:GLN:NE2  | 1:B:414:TRP:HD1  | 2.03                     | 0.52              |
| 1:B:573:LEU:HA   | 1:B:576:PHE:HD2  | 1.75                     | 0.52              |
| 1:C:283:THR:OG1  | 1:C:284:GLU:N    | 2.43                     | 0.52              |
| 1:D:541:ASP:OD1  | 1:D:542:GLN:N    | 2.42                     | 0.52              |
| 1:D:573:LEU:HA   | 1:D:576:PHE:HD2  | 1.75                     | 0.52              |
| 1:A:383:ILE:HG13 | 1:A:384:ALA:N    | 2.25                     | 0.51              |
| 1:A:447:ALA:O    | 1:D:432:ASN:ND2  | 2.38                     | 0.51              |
| 1:B:254:SER:HA   | 1:B:457:PHE:HE2  | 1.74                     | 0.51              |
| 1:C:217:LEU:HA   | 1:C:220:VAL:HB   | 1.92                     | 0.51              |
| 1:A:254:SER:HA   | 1:A:457:PHE:HE2  | 1.74                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:280:TRP:NE1  | 1:D:415:LEU:HD12 | 2.26                     | 0.51              |
| 1:D:327:ARG:N    | 1:D:354:ASP:HB2  | 2.24                     | 0.51              |
| 1:D:634:PHE:O    | 1:D:637:PHE:N    | 2.41                     | 0.51              |
| 1:D:688:LYS:HD2  | 1:D:691:LEU:HD11 | 1.92                     | 0.51              |
| 1:A:254:SER:HA   | 1:A:457:PHE:CE2  | 2.45                     | 0.51              |
| 1:C:309:ILE:HD11 | 1:C:313:ASN:HB2  | 1.91                     | 0.51              |
| 1:C:323:GLN:NE2  | 1:C:414:TRP:HD1  | 2.03                     | 0.51              |
| 1:A:280:TRP:NE1  | 1:A:415:LEU:HD12 | 2.26                     | 0.51              |
| 1:A:283:THR:OG1  | 1:A:284:GLU:N    | 2.43                     | 0.51              |
| 1:B:309:ILE:HD11 | 1:B:313:ASN:HB2  | 1.91                     | 0.51              |
| 1:B:349:SER:N    | 1:B:352:SER:OG   | 2.43                     | 0.51              |
| 1:C:604:PHE:O    | 1:C:607:ILE:HG22 | 2.09                     | 0.51              |
| 1:C:688:LYS:HD2  | 1:C:691:LEU:HD11 | 1.92                     | 0.51              |
| 1:B:602:ILE:O    | 1:B:606:ILE:N    | 2.33                     | 0.51              |
| 1:B:688:LYS:HD2  | 1:B:691:LEU:HD11 | 1.93                     | 0.51              |
| 1:C:362:ASN:HB2  | 3:C:1002:NAG:HN2 | 1.75                     | 0.51              |
| 1:C:526:ILE:O    | 1:C:530:SER:OG   | 2.25                     | 0.51              |
| 1:D:296:GLN:HG2  | 1:D:311:TYR:CD1  | 2.46                     | 0.51              |
| 1:A:217:LEU:HA   | 1:A:220:VAL:HB   | 1.92                     | 0.51              |
| 1:B:594:ALA:HB1  | 1:B:598:PHE:HB2  | 1.93                     | 0.51              |
| 1:B:604:PHE:O    | 1:B:607:ILE:HG22 | 2.09                     | 0.51              |
| 1:C:279:PHE:CE1  | 1:C:443:VAL:HG21 | 2.46                     | 0.51              |
| 1:C:280:TRP:NE1  | 1:C:415:LEU:HD12 | 2.26                     | 0.51              |
| 1:C:573:LEU:HA   | 1:C:576:PHE:HD2  | 1.75                     | 0.51              |
| 1:D:254:SER:HA   | 1:D:457:PHE:CE2  | 2.45                     | 0.51              |
| 1:D:526:ILE:O    | 1:D:530:SER:OG   | 2.25                     | 0.51              |
| 1:A:349:SER:N    | 1:A:352:SER:OG   | 2.43                     | 0.51              |
| 1:A:594:ALA:HB1  | 1:A:598:PHE:HB2  | 1.93                     | 0.51              |
| 1:B:280:TRP:NE1  | 1:B:415:LEU:HD12 | 2.26                     | 0.51              |
| 1:C:349:SER:N    | 1:C:352:SER:OG   | 2.43                     | 0.51              |
| 1:D:217:LEU:HA   | 1:D:220:VAL:HB   | 1.92                     | 0.51              |
| 1:D:406:VAL:HA   | 1:D:409:LEU:HB2  | 1.93                     | 0.51              |
| 1:C:406:VAL:HA   | 1:C:409:LEU:HB2  | 1.93                     | 0.51              |
| 1:D:280:TRP:CD1  | 1:D:410:LYS:HZ3  | 2.29                     | 0.51              |
| 1:A:309:ILE:HG13 | 1:A:310:PHE:N    | 2.18                     | 0.51              |
| 1:A:634:PHE:O    | 1:A:637:PHE:N    | 2.41                     | 0.51              |
| 1:A:678:ALA:O    | 1:A:681:ASN:N    | 2.44                     | 0.51              |
| 1:B:254:SER:HA   | 1:B:457:PHE:CE2  | 2.45                     | 0.51              |
| 1:C:432:ASN:ND2  | 1:D:447:ALA:O    | 2.38                     | 0.51              |
| 1:A:430:ASN:ND2  | 1:A:433:ILE:HG12 | 2.26                     | 0.50              |
| 1:B:296:GLN:HG2  | 1:B:311:TYR:CD1  | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:678:ALA:O    | 1:B:681:ASN:N    | 2.44                     | 0.50              |
| 1:C:247:TYR:OH   | 1:D:624:ASP:HB3  | 2.11                     | 0.50              |
| 1:C:254:SER:HA   | 1:C:457:PHE:CE2  | 2.45                     | 0.50              |
| 1:A:624:ASP:HB3  | 1:D:247:TYR:OH   | 2.11                     | 0.50              |
| 1:C:261:PRO:HG3  | 1:C:269:ASN:HA   | 1.93                     | 0.50              |
| 1:D:427:SER:OG   | 1:D:437:CYS:O    | 2.25                     | 0.50              |
| 1:D:473:LEU:O    | 1:D:477:GLU:N    | 2.43                     | 0.50              |
| 1:A:261:PRO:HG3  | 1:A:269:ASN:HA   | 1.93                     | 0.50              |
| 1:A:406:VAL:HA   | 1:A:409:LEU:HB2  | 1.93                     | 0.50              |
| 1:B:406:VAL:HA   | 1:B:409:LEU:HB2  | 1.93                     | 0.50              |
| 1:C:216:TYR:O    | 1:C:220:VAL:N    | 2.39                     | 0.50              |
| 1:C:296:GLN:HG2  | 1:C:311:TYR:CD1  | 2.46                     | 0.50              |
| 1:A:427:SER:OG   | 1:A:437:CYS:O    | 2.25                     | 0.50              |
| 1:B:554:TRP:HA   | 1:B:557:GLN:HB2  | 1.94                     | 0.50              |
| 1:C:470:ASP:O    | 1:C:474:ALA:N    | 2.36                     | 0.50              |
| 1:A:296:GLN:HG2  | 1:A:311:TYR:CD1  | 2.46                     | 0.50              |
| 1:B:234:LEU:HD21 | 1:B:480:PHE:CE1  | 2.47                     | 0.50              |
| 1:B:261:PRO:HG3  | 1:B:269:ASN:HA   | 1.93                     | 0.50              |
| 1:B:279:PHE:CE1  | 1:B:443:VAL:HG21 | 2.46                     | 0.50              |
| 1:C:473:LEU:O    | 1:C:477:GLU:N    | 2.43                     | 0.50              |
| 1:C:554:TRP:HA   | 1:C:557:GLN:HB2  | 1.94                     | 0.50              |
| 1:D:261:PRO:HG3  | 1:D:269:ASN:HA   | 1.93                     | 0.50              |
| 1:D:349:SER:N    | 1:D:352:SER:OG   | 2.43                     | 0.50              |
| 1:D:383:ILE:HG13 | 1:D:384:ALA:N    | 2.25                     | 0.50              |
| 1:D:582:THR:O    | 1:D:586:LEU:N    | 2.34                     | 0.50              |
| 1:D:678:ALA:O    | 1:D:681:ASN:N    | 2.44                     | 0.50              |
| 1:A:234:LEU:HD21 | 1:A:480:PHE:CE1  | 2.47                     | 0.50              |
| 1:A:476:CYS:HA   | 1:A:479:ILE:HD12 | 1.94                     | 0.50              |
| 1:A:688:LYS:HD2  | 1:A:691:LEU:HD11 | 1.92                     | 0.50              |
| 1:B:237:LEU:O    | 1:B:241:MET:N    | 2.35                     | 0.50              |
| 1:C:430:ASN:ND2  | 1:C:433:ILE:HG12 | 2.26                     | 0.50              |
| 1:B:217:LEU:HA   | 1:B:220:VAL:HB   | 1.92                     | 0.50              |
| 1:B:283:THR:OG1  | 1:B:284:GLU:N    | 2.43                     | 0.50              |
| 1:B:383:ILE:HG13 | 1:B:384:ALA:N    | 2.25                     | 0.50              |
| 1:D:234:LEU:HD21 | 1:D:480:PHE:CE1  | 2.47                     | 0.50              |
| 1:A:432:ASN:ND2  | 1:B:447:ALA:O    | 2.37                     | 0.50              |
| 1:B:555:GLN:O    | 1:B:559:ASN:N    | 2.35                     | 0.50              |
| 1:C:427:SER:OG   | 1:C:437:CYS:O    | 2.25                     | 0.50              |
| 1:C:583:MET:HA   | 1:C:586:LEU:HB2  | 1.94                     | 0.50              |
| 1:C:678:ALA:O    | 1:C:681:ASN:N    | 2.44                     | 0.50              |
| 1:D:554:TRP:HA   | 1:D:557:GLN:HB2  | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:570:TRP:O    | 1:D:573:LEU:HG   | 2.12                     | 0.50              |
| 1:D:594:ALA:HB1  | 1:D:598:PHE:HB2  | 1.93                     | 0.50              |
| 1:A:570:TRP:O    | 1:A:573:LEU:HG   | 2.12                     | 0.49              |
| 1:B:430:ASN:ND2  | 1:B:433:ILE:HG12 | 2.26                     | 0.49              |
| 1:B:583:MET:HA   | 1:B:586:LEU:HB2  | 1.94                     | 0.49              |
| 1:C:234:LEU:HD21 | 1:C:480:PHE:CE1  | 2.47                     | 0.49              |
| 1:C:570:TRP:O    | 1:C:573:LEU:HG   | 2.12                     | 0.49              |
| 1:C:594:ALA:HB1  | 1:C:598:PHE:HB2  | 1.93                     | 0.49              |
| 1:C:597:LEU:HD12 | 1:C:600:PHE:HB3  | 1.94                     | 0.49              |
| 1:D:430:ASN:ND2  | 1:D:433:ILE:HG12 | 2.26                     | 0.49              |
| 1:D:597:LEU:HD12 | 1:D:600:PHE:HB3  | 1.94                     | 0.49              |
| 1:A:536:LEU:HA   | 1:A:539:LEU:HB3  | 1.94                     | 0.49              |
| 1:A:554:TRP:HA   | 1:A:557:GLN:HB2  | 1.94                     | 0.49              |
| 1:B:473:LEU:O    | 1:B:477:GLU:N    | 2.43                     | 0.49              |
| 1:B:476:CYS:HA   | 1:B:479:ILE:HD12 | 1.94                     | 0.49              |
| 1:B:536:LEU:HA   | 1:B:539:LEU:HB3  | 1.94                     | 0.49              |
| 1:B:570:TRP:O    | 1:B:573:LEU:HG   | 2.12                     | 0.49              |
| 1:B:611:TYR:O    | 1:B:615:ALA:N    | 2.45                     | 0.49              |
| 1:C:684:TYR:HA   | 1:C:687:VAL:HG22 | 1.95                     | 0.49              |
| 1:A:597:LEU:HD12 | 1:A:600:PHE:HB3  | 1.94                     | 0.49              |
| 1:B:247:TYR:OH   | 1:C:624:ASP:HB3  | 2.12                     | 0.49              |
| 1:B:597:LEU:HD12 | 1:B:600:PHE:HB3  | 1.94                     | 0.49              |
| 1:D:357:PRO:HB2  | 1:D:361:ARG:HE   | 1.77                     | 0.49              |
| 1:D:611:TYR:O    | 1:D:615:ALA:N    | 2.45                     | 0.49              |
| 1:A:357:PRO:HB2  | 1:A:361:ARG:HE   | 1.77                     | 0.49              |
| 1:D:378:SER:HA   | 1:D:387:SER:HA   | 1.94                     | 0.49              |
| 1:A:682:ASP:OD1  | 1:A:683:THR:N    | 2.43                     | 0.49              |
| 1:B:325:ARG:NH2  | 1:B:358:PHE:HB2  | 2.28                     | 0.49              |
| 1:B:357:PRO:HB2  | 1:B:361:ARG:HE   | 1.78                     | 0.49              |
| 1:B:460:LEU:HD23 | 1:B:548:PHE:HZ   | 1.78                     | 0.49              |
| 1:B:684:TYR:HA   | 1:B:687:VAL:HG22 | 1.95                     | 0.49              |
| 1:C:460:LEU:HD23 | 1:C:548:PHE:HZ   | 1.78                     | 0.49              |
| 1:C:476:CYS:HA   | 1:C:479:ILE:HD12 | 1.94                     | 0.49              |
| 1:D:476:CYS:HA   | 1:D:479:ILE:HD12 | 1.94                     | 0.49              |
| 1:D:532:VAL:HG11 | 1:D:551:LEU:HB3  | 1.95                     | 0.49              |
| 1:A:325:ARG:NH2  | 1:A:358:PHE:HB2  | 2.28                     | 0.49              |
| 1:A:532:VAL:HG11 | 1:A:551:LEU:HB3  | 1.95                     | 0.49              |
| 1:A:583:MET:O    | 1:A:586:LEU:N    | 2.45                     | 0.49              |
| 1:B:378:SER:HA   | 1:B:387:SER:HA   | 1.94                     | 0.49              |
| 1:D:460:LEU:HD23 | 1:D:548:PHE:HZ   | 1.78                     | 0.49              |
| 1:D:583:MET:HA   | 1:D:586:LEU:HB2  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:328:ASN:HA   | 1:A:345:TYR:CE2  | 2.48                     | 0.49              |
| 1:B:560:ASN:HB2  | 1:C:656:LEU:HD11 | 1.94                     | 0.49              |
| 1:B:682:ASP:OD1  | 1:B:682:ASP:N    | 2.46                     | 0.49              |
| 1:C:682:ASP:OD1  | 1:C:683:THR:N    | 2.43                     | 0.49              |
| 1:D:484:ILE:O    | 1:D:488:VAL:HG23 | 2.13                     | 0.49              |
| 1:D:566:VAL:HG12 | 1:D:570:TRP:CZ3  | 2.48                     | 0.49              |
| 1:B:566:VAL:HG12 | 1:B:570:TRP:CZ3  | 2.48                     | 0.49              |
| 1:C:328:ASN:HA   | 1:C:345:TYR:CE2  | 2.48                     | 0.49              |
| 1:D:216:TYR:O    | 1:D:220:VAL:N    | 2.39                     | 0.49              |
| 1:D:323:GLN:OE1  | 1:D:414:TRP:CD1  | 2.66                     | 0.49              |
| 1:D:626:PHE:O    | 1:D:627:SER:C    | 2.56                     | 0.49              |
| 1:D:684:TYR:HA   | 1:D:687:VAL:HG22 | 1.95                     | 0.49              |
| 1:A:224:LEU:HD22 | 1:A:577:ILE:HD11 | 1.95                     | 0.49              |
| 1:A:367:ILE:O    | 1:A:367:ILE:CG2  | 2.61                     | 0.49              |
| 1:B:328:ASN:HA   | 1:B:345:TYR:CE2  | 2.48                     | 0.49              |
| 1:B:427:SER:OG   | 1:B:437:CYS:O    | 2.25                     | 0.49              |
| 1:C:357:PRO:HB2  | 1:C:361:ARG:HE   | 1.77                     | 0.49              |
| 1:D:362:ASN:H    | 1:D:366:TRP:HB2  | 1.78                     | 0.49              |
| 1:B:224:LEU:O    | 1:B:228:LEU:N    | 2.26                     | 0.48              |
| 1:B:362:ASN:H    | 1:B:366:TRP:HB2  | 1.78                     | 0.48              |
| 1:C:237:LEU:O    | 1:C:241:MET:N    | 2.35                     | 0.48              |
| 1:A:216:TYR:O    | 1:A:220:VAL:N    | 2.39                     | 0.48              |
| 1:A:368:TYR:HA   | 1:A:390:GLY:O    | 2.14                     | 0.48              |
| 1:A:484:ILE:O    | 1:A:488:VAL:HG23 | 2.13                     | 0.48              |
| 1:C:325:ARG:NH2  | 1:C:358:PHE:HB2  | 2.28                     | 0.48              |
| 1:C:378:SER:HA   | 1:C:387:SER:HA   | 1.94                     | 0.48              |
| 1:C:582:THR:O    | 1:C:586:LEU:N    | 2.34                     | 0.48              |
| 1:D:367:ILE:O    | 1:D:367:ILE:CG2  | 2.61                     | 0.48              |
| 1:D:536:LEU:HA   | 1:D:539:LEU:HB3  | 1.94                     | 0.48              |
| 1:A:378:SER:HA   | 1:A:387:SER:HA   | 1.94                     | 0.48              |
| 1:B:367:ILE:O    | 1:B:367:ILE:CG2  | 2.61                     | 0.48              |
| 1:C:269:ASN:OD1  | 1:C:271:LYS:N    | 2.47                     | 0.48              |
| 1:C:323:GLN:OE1  | 1:C:414:TRP:CD1  | 2.66                     | 0.48              |
| 1:A:566:VAL:HG12 | 1:A:570:TRP:CZ3  | 2.48                     | 0.48              |
| 1:A:670:PHE:HA   | 1:A:673:LEU:HD12 | 1.96                     | 0.48              |
| 1:B:224:LEU:HD22 | 1:B:577:ILE:HD11 | 1.95                     | 0.48              |
| 1:B:368:TYR:HA   | 1:B:390:GLY:O    | 2.14                     | 0.48              |
| 1:C:600:PHE:CZ   | 1:C:603:MET:HE2  | 2.48                     | 0.48              |
| 1:D:586:LEU:HA   | 1:D:589:THR:HG23 | 1.95                     | 0.48              |
| 1:B:247:TYR:OH   | 1:B:251:ARG:HD2  | 2.14                     | 0.48              |
| 1:B:280:TRP:O    | 1:B:284:GLU:HG2  | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:484:ILE:O    | 1:B:488:VAL:HG23 | 2.13                     | 0.48              |
| 1:C:367:ILE:O    | 1:C:367:ILE:CG2  | 2.61                     | 0.48              |
| 1:C:484:ILE:O    | 1:C:488:VAL:HG23 | 2.13                     | 0.48              |
| 1:C:532:VAL:HG11 | 1:C:551:LEU:HB3  | 1.95                     | 0.48              |
| 1:C:555:GLN:O    | 1:C:559:ASN:N    | 2.35                     | 0.48              |
| 1:C:566:VAL:HG12 | 1:C:570:TRP:CZ3  | 2.48                     | 0.48              |
| 1:D:644:ILE:HG23 | 1:D:646:PHE:N    | 2.28                     | 0.48              |
| 1:D:682:ASP:OD1  | 1:D:683:THR:N    | 2.43                     | 0.48              |
| 1:A:280:TRP:O    | 1:A:284:GLU:HG2  | 2.14                     | 0.48              |
| 1:A:319:PRO:HB2  | 1:A:395:LEU:HD22 | 1.95                     | 0.48              |
| 1:A:600:PHE:CZ   | 1:A:603:MET:HE2  | 2.48                     | 0.48              |
| 1:B:362:ASN:HB2  | 3:B:1002:NAG:HN2 | 1.75                     | 0.48              |
| 1:B:532:VAL:HG11 | 1:B:551:LEU:HB3  | 1.95                     | 0.48              |
| 1:D:237:LEU:O    | 1:D:241:MET:N    | 2.35                     | 0.48              |
| 1:D:269:ASN:OD1  | 1:D:271:LYS:N    | 2.47                     | 0.48              |
| 1:A:684:TYR:HA   | 1:A:687:VAL:HG22 | 1.95                     | 0.48              |
| 1:B:600:PHE:CZ   | 1:B:603:MET:HE2  | 2.48                     | 0.48              |
| 1:B:682:ASP:O    | 1:B:685:SER:OG   | 2.22                     | 0.48              |
| 1:C:626:PHE:O    | 1:C:627:SER:C    | 2.56                     | 0.48              |
| 1:C:682:ASP:OD1  | 1:C:682:ASP:N    | 2.46                     | 0.48              |
| 1:A:323:GLN:OE1  | 1:A:414:TRP:CD1  | 2.66                     | 0.48              |
| 1:A:460:LEU:HD23 | 1:A:548:PHE:HZ   | 1.78                     | 0.48              |
| 1:A:493:LEU:HD23 | 1:A:496:ARG:HE   | 1.79                     | 0.48              |
| 1:B:560:ASN:CB   | 1:C:656:LEU:HD11 | 2.44                     | 0.48              |
| 1:C:536:LEU:HA   | 1:C:539:LEU:HB3  | 1.94                     | 0.48              |
| 1:D:224:LEU:HD22 | 1:D:577:ILE:HD11 | 1.95                     | 0.48              |
| 1:D:328:ASN:HA   | 1:D:345:TYR:CE2  | 2.48                     | 0.48              |
| 1:A:276:MET:O    | 1:A:279:PHE:HB3  | 2.14                     | 0.48              |
| 1:A:362:ASN:H    | 1:A:366:TRP:HB2  | 1.77                     | 0.48              |
| 1:A:611:TYR:O    | 1:A:615:ALA:N    | 2.45                     | 0.48              |
| 1:A:644:ILE:HG23 | 1:A:646:PHE:N    | 2.28                     | 0.48              |
| 1:B:309:ILE:HG13 | 1:B:310:PHE:N    | 2.19                     | 0.48              |
| 1:C:362:ASN:H    | 1:C:366:TRP:HB2  | 1.78                     | 0.48              |
| 1:C:602:ILE:O    | 1:C:606:ILE:N    | 2.33                     | 0.48              |
| 1:C:644:ILE:HG23 | 1:C:646:PHE:N    | 2.28                     | 0.48              |
| 1:D:280:TRP:O    | 1:D:284:GLU:HG2  | 2.14                     | 0.48              |
| 1:D:600:PHE:CZ   | 1:D:603:MET:HE2  | 2.48                     | 0.48              |
| 1:D:682:ASP:O    | 1:D:685:SER:OG   | 2.22                     | 0.48              |
| 1:A:682:ASP:OD1  | 1:A:682:ASP:N    | 2.46                     | 0.48              |
| 1:B:323:GLN:OE1  | 1:B:414:TRP:CD1  | 2.66                     | 0.48              |
| 1:B:493:LEU:HD23 | 1:B:496:ARG:HE   | 1.79                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:634:PHE:O    | 1:B:637:PHE:N    | 2.41                     | 0.48              |
| 1:C:586:LEU:HA   | 1:C:589:THR:HG23 | 1.95                     | 0.48              |
| 1:D:325:ARG:NH2  | 1:D:358:PHE:HB2  | 2.28                     | 0.48              |
| 1:D:368:TYR:HA   | 1:D:390:GLY:O    | 2.13                     | 0.48              |
| 1:A:256:LEU:HD22 | 1:A:257:PHE:CZ   | 2.49                     | 0.47              |
| 1:A:269:ASN:OD1  | 1:A:271:LYS:N    | 2.47                     | 0.47              |
| 1:A:317:GLY:O    | 1:A:318:VAL:HG13 | 2.14                     | 0.47              |
| 1:B:586:LEU:HA   | 1:B:589:THR:HG23 | 1.95                     | 0.47              |
| 1:A:247:TYR:OH   | 1:A:251:ARG:HD2  | 2.14                     | 0.47              |
| 1:B:269:ASN:OD1  | 1:B:271:LYS:N    | 2.47                     | 0.47              |
| 1:B:644:ILE:HG23 | 1:B:646:PHE:N    | 2.28                     | 0.47              |
| 1:B:670:PHE:HA   | 1:B:673:LEU:HD12 | 1.96                     | 0.47              |
| 1:C:256:LEU:HD22 | 1:C:257:PHE:CZ   | 2.49                     | 0.47              |
| 1:C:280:TRP:O    | 1:C:284:GLU:HG2  | 2.14                     | 0.47              |
| 1:C:317:GLY:O    | 1:C:318:VAL:HG13 | 2.14                     | 0.47              |
| 1:C:670:PHE:HA   | 1:C:673:LEU:HD12 | 1.96                     | 0.47              |
| 1:A:310:PHE:HD2  | 1:A:311:TYR:CD2  | 2.33                     | 0.47              |
| 1:A:362:ASN:HB2  | 3:A:1002:NAG:HN2 | 1.75                     | 0.47              |
| 1:A:586:LEU:HA   | 1:A:589:THR:HG23 | 1.95                     | 0.47              |
| 1:C:276:MET:O    | 1:C:279:PHE:HB3  | 2.14                     | 0.47              |
| 1:D:319:PRO:HB2  | 1:D:395:LEU:HD22 | 1.95                     | 0.47              |
| 1:D:493:LEU:HD23 | 1:D:496:ARG:HE   | 1.79                     | 0.47              |
| 1:D:690:ASP:O    | 1:D:693:GLN:HG2  | 2.15                     | 0.47              |
| 1:B:249:TYR:HD1  | 1:C:448:THR:HB   | 1.80                     | 0.47              |
| 1:B:276:MET:O    | 1:B:279:PHE:HB3  | 2.14                     | 0.47              |
| 1:B:310:PHE:HD2  | 1:B:311:TYR:CD2  | 2.32                     | 0.47              |
| 1:B:317:GLY:O    | 1:B:318:VAL:HG13 | 2.14                     | 0.47              |
| 1:B:432:ASN:ND2  | 1:C:447:ALA:O    | 2.37                     | 0.47              |
| 1:A:487:TYR:HB3  | 1:A:491:GLU:CD   | 2.40                     | 0.47              |
| 1:A:626:PHE:O    | 1:A:627:SER:C    | 2.56                     | 0.47              |
| 1:A:634:PHE:CE1  | 1:B:658:PRO:HB3  | 2.49                     | 0.47              |
| 1:A:681:ASN:HA   | 1:B:678:ALA:HB2  | 1.94                     | 0.47              |
| 1:C:319:PRO:HB2  | 1:C:395:LEU:HD22 | 1.95                     | 0.47              |
| 1:C:626:PHE:HE1  | 1:C:635:THR:HG21 | 1.80                     | 0.47              |
| 1:D:325:ARG:HG2  | 1:D:326:VAL:N    | 2.30                     | 0.47              |
| 1:D:626:PHE:HE1  | 1:D:635:THR:HG21 | 1.80                     | 0.47              |
| 1:B:296:GLN:OE1  | 1:C:417:ARG:NH1  | 2.48                     | 0.47              |
| 1:C:325:ARG:HG2  | 1:C:326:VAL:N    | 2.30                     | 0.47              |
| 1:C:532:VAL:HG13 | 1:C:551:LEU:HD13 | 1.97                     | 0.47              |
| 1:D:256:LEU:HD22 | 1:D:257:PHE:CZ   | 2.49                     | 0.47              |
| 1:D:317:GLY:O    | 1:D:318:VAL:HG13 | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:532:VAL:HG13 | 1:A:551:LEU:HD13 | 1.97                     | 0.47              |
| 1:A:690:ASP:O    | 1:A:693:GLN:HG2  | 2.15                     | 0.47              |
| 1:B:256:LEU:HD22 | 1:B:257:PHE:CZ   | 2.49                     | 0.47              |
| 1:B:487:TYR:HB3  | 1:B:491:GLU:CD   | 2.40                     | 0.47              |
| 1:B:532:VAL:HG13 | 1:B:551:LEU:HD13 | 1.97                     | 0.47              |
| 1:B:626:PHE:O    | 1:B:627:SER:C    | 2.56                     | 0.47              |
| 1:C:322:ARG:HB3  | 1:C:423:PHE:HB2  | 1.97                     | 0.47              |
| 1:C:368:TYR:HA   | 1:C:390:GLY:O    | 2.14                     | 0.47              |
| 1:C:487:TYR:HB3  | 1:C:491:GLU:CD   | 2.40                     | 0.47              |
| 1:C:493:LEU:HD23 | 1:C:496:ARG:HE   | 1.79                     | 0.47              |
| 1:C:690:ASP:O    | 1:C:693:GLN:HG2  | 2.15                     | 0.47              |
| 1:D:247:TYR:OH   | 1:D:251:ARG:HD2  | 2.14                     | 0.47              |
| 1:D:487:TYR:HB3  | 1:D:491:GLU:CD   | 2.40                     | 0.47              |
| 1:A:605:PHE:HA   | 1:A:608:PHE:HB3  | 1.97                     | 0.47              |
| 1:C:224:LEU:HD22 | 1:C:577:ILE:HD11 | 1.95                     | 0.47              |
| 1:C:312:GLU:OE1  | 1:D:449:GLY:N    | 2.48                     | 0.47              |
| 1:C:560:ASN:HB2  | 1:D:656:LEU:HD11 | 1.96                     | 0.47              |
| 1:D:276:MET:O    | 1:D:279:PHE:HB3  | 2.14                     | 0.47              |
| 1:D:279:PHE:CE1  | 1:D:443:VAL:HG21 | 2.46                     | 0.47              |
| 1:D:532:VAL:HG13 | 1:D:551:LEU:HD13 | 1.97                     | 0.47              |
| 4:A:1006:PX6:H61 | 4:A:1006:PX6:H54 | 1.70                     | 0.47              |
| 1:B:547:ASN:O    | 1:B:549:GLU:N    | 2.48                     | 0.47              |
| 1:D:518:SER:O    | 1:D:522:ILE:HG13 | 2.15                     | 0.47              |
| 1:D:605:PHE:HA   | 1:D:608:PHE:HB3  | 1.97                     | 0.47              |
| 1:A:235:CYS:O    | 1:A:238:THR:OG1  | 2.32                     | 0.47              |
| 1:A:325:ARG:HG2  | 1:A:326:VAL:N    | 2.30                     | 0.47              |
| 1:A:449:GLY:N    | 1:D:312:GLU:OE1  | 2.48                     | 0.47              |
| 1:C:611:TYR:O    | 1:C:615:ALA:N    | 2.45                     | 0.47              |
| 1:D:536:LEU:HD12 | 1:D:539:LEU:HD23 | 1.97                     | 0.47              |
| 1:A:518:SER:O    | 1:A:522:ILE:HG13 | 2.16                     | 0.46              |
| 1:A:536:LEU:HD12 | 1:A:539:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:626:PHE:HE1  | 1:A:635:THR:HG21 | 1.80                     | 0.46              |
| 1:B:297:PRO:O    | 1:B:298:SER:OG   | 2.28                     | 0.46              |
| 1:B:319:PRO:HB2  | 1:B:395:LEU:HD22 | 1.95                     | 0.46              |
| 1:B:536:LEU:HD12 | 1:B:539:LEU:HD23 | 1.97                     | 0.46              |
| 1:B:538:PHE:HA   | 1:B:541:ASP:CG   | 2.40                     | 0.46              |
| 1:C:247:TYR:OH   | 1:C:251:ARG:HD2  | 2.14                     | 0.46              |
| 1:C:677:LEU:HD21 | 1:D:673:LEU:HB3  | 1.97                     | 0.46              |
| 1:D:322:ARG:HB3  | 1:D:423:PHE:HB2  | 1.97                     | 0.46              |
| 1:B:320:ARG:N    | 1:B:425:ASP:O    | 2.44                     | 0.46              |
| 1:B:322:ARG:HB3  | 1:B:423:PHE:HB2  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:626:PHE:HE1  | 1:B:635:THR:HG21 | 1.80                     | 0.46              |
| 1:C:310:PHE:HD2  | 1:C:311:TYR:CD2  | 2.32                     | 0.46              |
| 1:C:605:PHE:HA   | 1:C:608:PHE:HB3  | 1.97                     | 0.46              |
| 4:C:1006:PX6:H49 | 4:C:1006:PX6:H42 | 1.53                     | 0.46              |
| 1:D:547:ASN:O    | 1:D:549:GLU:N    | 2.48                     | 0.46              |
| 1:D:687:VAL:HA   | 1:D:690:ASP:HB3  | 1.97                     | 0.46              |
| 1:A:656:LEU:HD11 | 1:D:560:ASN:HB2  | 1.95                     | 0.46              |
| 1:A:687:VAL:HA   | 1:A:690:ASP:HB3  | 1.97                     | 0.46              |
| 1:C:518:SER:O    | 1:C:522:ILE:HG13 | 2.16                     | 0.46              |
| 1:C:538:PHE:HA   | 1:C:541:ASP:CG   | 2.40                     | 0.46              |
| 4:C:1006:PX6:H46 | 4:C:1006:PX6:H53 | 1.47                     | 0.46              |
| 1:A:279:PHE:CE1  | 1:A:443:VAL:HG21 | 2.46                     | 0.46              |
| 1:C:349:SER:H    | 1:C:352:SER:HG   | 1.62                     | 0.46              |
| 1:C:536:LEU:HD12 | 1:C:539:LEU:HD23 | 1.97                     | 0.46              |
| 1:D:310:PHE:HD2  | 1:D:311:TYR:CD2  | 2.33                     | 0.46              |
| 1:D:670:PHE:HA   | 1:D:673:LEU:HD12 | 1.96                     | 0.46              |
| 1:A:296:GLN:OE1  | 1:B:417:ARG:NH1  | 2.49                     | 0.46              |
| 1:A:507:TRP:HB3  | 1:A:575:LYS:HZ3  | 1.79                     | 0.46              |
| 1:B:216:TYR:O    | 1:B:220:VAL:N    | 2.39                     | 0.46              |
| 1:C:634:PHE:CE1  | 1:D:658:PRO:HB3  | 2.51                     | 0.46              |
| 1:A:470:ASP:O    | 1:A:474:ALA:N    | 2.36                     | 0.46              |
| 1:A:538:PHE:HA   | 1:A:541:ASP:CG   | 2.40                     | 0.46              |
| 1:B:410:LYS:O    | 1:B:413:VAL:N    | 2.49                     | 0.46              |
| 1:C:342:LYS:HB3  | 1:C:343:GLU:CD   | 2.41                     | 0.46              |
| 1:A:547:ASN:O    | 1:A:549:GLU:N    | 2.48                     | 0.46              |
| 1:B:605:PHE:HA   | 1:B:608:PHE:HB3  | 1.97                     | 0.46              |
| 1:C:547:ASN:O    | 1:C:549:GLU:N    | 2.48                     | 0.46              |
| 1:A:619:PHE:HB2  | 1:A:626:PHE:CD2  | 2.51                     | 0.46              |
| 1:B:325:ARG:HG2  | 1:B:326:VAL:N    | 2.30                     | 0.46              |
| 5:B:1007:PLM:HF1 | 5:B:1007:PLM:HC2 | 1.75                     | 0.46              |
| 1:D:538:PHE:HA   | 1:D:541:ASP:CG   | 2.40                     | 0.46              |
| 1:B:349:SER:H    | 1:B:352:SER:HG   | 1.64                     | 0.46              |
| 1:B:470:ASP:O    | 1:B:474:ALA:N    | 2.36                     | 0.46              |
| 1:D:342:LYS:HB3  | 1:D:343:GLU:CD   | 2.41                     | 0.46              |
| 1:D:349:SER:O    | 1:D:353:GLU:N    | 2.49                     | 0.46              |
| 1:A:342:LYS:HB3  | 1:A:343:GLU:CD   | 2.41                     | 0.46              |
| 1:B:568:PHE:HD1  | 1:B:571:ILE:HD11 | 1.80                     | 0.46              |
| 1:B:690:ASP:O    | 1:B:693:GLN:HG2  | 2.15                     | 0.46              |
| 1:D:619:PHE:HB2  | 1:D:626:PHE:CD2  | 2.51                     | 0.46              |
| 1:A:448:THR:HB   | 1:D:249:TYR:HD1  | 1.81                     | 0.45              |
| 1:A:677:LEU:HD21 | 1:B:673:LEU:HB3  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:322:ARG:HB3  | 1:A:423:PHE:HB2  | 1.97                     | 0.45              |
| 1:A:645:ASN:CB   | 1:A:648:GLU:OE2  | 2.56                     | 0.45              |
| 1:A:658:PRO:HB3  | 1:D:634:PHE:CE1  | 2.51                     | 0.45              |
| 1:B:349:SER:O    | 1:B:353:GLU:N    | 2.49                     | 0.45              |
| 4:B:1006:PX6:H49 | 4:B:1006:PX6:H42 | 1.53                     | 0.45              |
| 1:C:323:GLN:NE2  | 1:C:414:TRP:CD1  | 2.82                     | 0.45              |
| 1:C:597:LEU:O    | 1:C:600:PHE:N    | 2.50                     | 0.45              |
| 1:A:224:LEU:O    | 1:A:228:LEU:N    | 2.26                     | 0.45              |
| 1:A:656:LEU:HD11 | 1:D:560:ASN:CB   | 2.46                     | 0.45              |
| 1:B:342:LYS:HB3  | 1:B:343:GLU:CD   | 2.41                     | 0.45              |
| 5:B:1007:PLM:HA2 | 5:B:1007:PLM:HD1 | 1.67                     | 0.45              |
| 1:C:687:VAL:HA   | 1:C:690:ASP:HB3  | 1.97                     | 0.45              |
| 5:C:1008:PLM:H52 | 5:C:1008:PLM:H21 | 1.83                     | 0.45              |
| 1:D:597:LEU:O    | 1:D:600:PHE:N    | 2.50                     | 0.45              |
| 1:D:560:ASN:O    | 1:D:563:ALA:N    | 2.50                     | 0.45              |
| 1:A:410:LYS:O    | 1:A:413:VAL:N    | 2.49                     | 0.45              |
| 1:A:568:PHE:HD1  | 1:A:571:ILE:HD11 | 1.80                     | 0.45              |
| 1:B:687:VAL:HA   | 1:B:690:ASP:HB3  | 1.97                     | 0.45              |
| 1:C:568:PHE:HD1  | 1:C:571:ILE:HD11 | 1.80                     | 0.45              |
| 1:D:682:ASP:OD1  | 1:D:682:ASP:N    | 2.46                     | 0.45              |
| 1:A:278:ASP:O    | 1:A:282:PHE:N    | 2.49                     | 0.45              |
| 1:C:410:LYS:O    | 1:C:413:VAL:N    | 2.49                     | 0.45              |
| 4:C:1006:PX6:H67 | 4:C:1006:PX6:H60 | 1.73                     | 0.45              |
| 1:A:673:LEU:HB3  | 1:D:677:LEU:HD21 | 1.98                     | 0.45              |
| 1:B:611:TYR:HA   | 1:B:614:LEU:HB3  | 1.99                     | 0.45              |
| 1:C:249:TYR:HD1  | 1:D:448:THR:HB   | 1.82                     | 0.45              |
| 1:A:349:SER:H    | 1:A:352:SER:HG   | 1.65                     | 0.45              |
| 1:A:406:VAL:HA   | 1:A:409:LEU:HD12 | 1.99                     | 0.45              |
| 1:A:682:ASP:CG   | 1:A:683:THR:H    | 2.24                     | 0.45              |
| 1:D:349:SER:H    | 1:D:352:SER:HG   | 1.63                     | 0.45              |
| 1:D:410:LYS:O    | 1:D:413:VAL:N    | 2.49                     | 0.45              |
| 5:A:1007:PLM:H91 | 1:B:667:PHE:CE2  | 2.52                     | 0.45              |
| 1:B:518:SER:O    | 1:B:522:ILE:HG13 | 2.16                     | 0.45              |
| 1:C:349:SER:O    | 1:C:353:GLU:N    | 2.49                     | 0.45              |
| 1:C:681:ASN:HA   | 1:D:678:ALA:HB2  | 1.98                     | 0.45              |
| 1:D:362:ASN:HB2  | 3:D:1002:NAG:HN2 | 1.78                     | 0.45              |
| 1:D:682:ASP:CG   | 1:D:683:THR:H    | 2.24                     | 0.45              |
| 4:D:1006:PX6:H67 | 4:D:1006:PX6:H60 | 1.71                     | 0.45              |
| 1:A:349:SER:O    | 1:A:353:GLU:N    | 2.49                     | 0.45              |
| 1:C:560:ASN:O    | 1:C:563:ALA:N    | 2.50                     | 0.45              |
| 1:D:406:VAL:HA   | 1:D:409:LEU:HD12 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:568:PHE:HD1  | 1:D:571:ILE:HD11 | 1.81                     | 0.45              |
| 1:C:296:GLN:HG2  | 1:C:311:TYR:HD1  | 1.82                     | 0.44              |
| 1:A:237:LEU:O    | 1:A:241:MET:N    | 2.35                     | 0.44              |
| 1:A:568:PHE:CD1  | 1:A:571:ILE:HD11 | 2.52                     | 0.44              |
| 1:A:582:THR:O    | 1:A:586:LEU:N    | 2.34                     | 0.44              |
| 5:A:1007:PLM:HD1 | 5:A:1007:PLM:HA2 | 1.71                     | 0.44              |
| 1:C:321:ILE:HG13 | 1:C:395:LEU:HD11 | 1.99                     | 0.44              |
| 1:D:224:LEU:O    | 1:D:228:LEU:N    | 2.26                     | 0.44              |
| 1:D:484:ILE:O    | 1:D:488:VAL:N    | 2.48                     | 0.44              |
| 1:B:308:PHE:HB3  | 1:B:315:LEU:H    | 1.83                     | 0.44              |
| 1:B:321:ILE:HG13 | 1:B:395:LEU:HD11 | 1.99                     | 0.44              |
| 1:B:570:TRP:O    | 1:B:573:LEU:N    | 2.51                     | 0.44              |
| 1:C:382:ILE:HG23 | 1:C:383:ILE:N    | 2.32                     | 0.44              |
| 1:C:570:TRP:O    | 1:C:573:LEU:N    | 2.51                     | 0.44              |
| 1:D:611:TYR:HA   | 1:D:614:LEU:HB3  | 1.99                     | 0.44              |
| 1:A:667:PHE:CE2  | 5:D:1007:PLM:H91 | 2.53                     | 0.44              |
| 1:A:677:LEU:O    | 1:A:681:ASN:N    | 2.46                     | 0.44              |
| 1:B:296:GLN:HG2  | 1:B:311:TYR:HD1  | 1.83                     | 0.44              |
| 1:C:226:THR:HB   | 1:C:483:PHE:HZ   | 1.83                     | 0.44              |
| 1:C:320:ARG:N    | 1:C:425:ASP:O    | 2.44                     | 0.44              |
| 1:C:568:PHE:CD1  | 1:C:571:ILE:HD11 | 2.52                     | 0.44              |
| 1:D:235:CYS:O    | 1:D:238:THR:OG1  | 2.32                     | 0.44              |
| 1:D:568:PHE:CD1  | 1:D:571:ILE:HD11 | 2.52                     | 0.44              |
| 1:D:677:LEU:O    | 1:D:681:ASN:N    | 2.46                     | 0.44              |
| 1:A:574:PHE:HE1  | 1:B:603:MET:HG3  | 1.82                     | 0.44              |
| 1:C:560:ASN:CB   | 1:D:656:LEU:HD11 | 2.47                     | 0.44              |
| 1:A:296:GLN:HG2  | 1:A:311:TYR:HD1  | 1.83                     | 0.44              |
| 1:A:308:PHE:HB3  | 1:A:315:LEU:H    | 1.83                     | 0.44              |
| 1:A:537:GLN:HE22 | 1:B:336:ASP:CG   | 2.24                     | 0.44              |
| 1:A:570:TRP:O    | 1:A:573:LEU:N    | 2.51                     | 0.44              |
| 1:B:406:VAL:HA   | 1:B:409:LEU:HD12 | 1.99                     | 0.44              |
| 1:B:451:VAL:O    | 1:B:452:ILE:HD13 | 2.18                     | 0.44              |
| 1:C:308:PHE:HB3  | 1:C:315:LEU:H    | 1.83                     | 0.44              |
| 1:C:645:ASN:CB   | 1:C:648:GLU:OE2  | 2.56                     | 0.44              |
| 1:D:226:THR:HB   | 1:D:483:PHE:HZ   | 1.83                     | 0.44              |
| 4:D:1006:PX6:H46 | 4:D:1006:PX6:H53 | 1.47                     | 0.44              |
| 1:A:564:VAL:O    | 1:A:567:PHE:HB3  | 2.18                     | 0.44              |
| 1:B:597:LEU:O    | 1:B:600:PHE:N    | 2.50                     | 0.44              |
| 1:C:238:THR:OG1  | 1:C:239:TYR:N    | 2.51                     | 0.44              |
| 1:C:451:VAL:O    | 1:C:452:ILE:HD13 | 2.18                     | 0.44              |
| 5:C:1007:PLM:H91 | 1:D:667:PHE:CE2  | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:228:LEU:HA   | 1:D:231:LEU:HD23 | 2.00                     | 0.44              |
| 1:A:310:PHE:HD2  | 1:A:311:TYR:HD2  | 1.65                     | 0.44              |
| 1:A:484:ILE:O    | 1:A:488:VAL:N    | 2.48                     | 0.44              |
| 1:A:611:TYR:HA   | 1:A:614:LEU:HB3  | 1.99                     | 0.44              |
| 4:A:1006:PX6:H53 | 4:A:1006:PX6:H46 | 1.47                     | 0.44              |
| 1:B:226:THR:HB   | 1:B:483:PHE:HZ   | 1.83                     | 0.44              |
| 1:B:560:ASN:O    | 1:B:563:ALA:N    | 2.50                     | 0.44              |
| 1:C:235:CYS:O    | 1:C:238:THR:OG1  | 2.32                     | 0.44              |
| 1:C:560:ASN:OD1  | 1:C:561:ILE:N    | 2.51                     | 0.44              |
| 1:A:228:LEU:HA   | 1:A:231:LEU:HD23 | 2.00                     | 0.44              |
| 1:A:560:ASN:O    | 1:A:563:ALA:N    | 2.50                     | 0.44              |
| 1:B:568:PHE:CD1  | 1:B:571:ILE:HD11 | 2.52                     | 0.44              |
| 5:B:1007:PLM:H91 | 1:C:667:PHE:CE2  | 2.53                     | 0.44              |
| 1:C:247:TYR:CZ   | 1:C:251:ARG:HB2  | 2.53                     | 0.44              |
| 1:C:611:TYR:HA   | 1:C:614:LEU:HB3  | 1.99                     | 0.44              |
| 1:D:656:LEU:HA   | 1:D:656:LEU:HD23 | 1.72                     | 0.44              |
| 1:A:312:GLU:OE1  | 1:B:449:GLY:N    | 2.50                     | 0.43              |
| 1:B:634:PHE:CE1  | 1:C:658:PRO:HB3  | 2.53                     | 0.43              |
| 1:C:680:ILE:HD13 | 1:D:674:ASN:HA   | 2.00                     | 0.43              |
| 1:D:570:TRP:O    | 1:D:573:LEU:N    | 2.51                     | 0.43              |
| 1:A:323:GLN:NE2  | 1:A:414:TRP:CD1  | 2.82                     | 0.43              |
| 1:A:382:ILE:HG23 | 1:A:383:ILE:N    | 2.32                     | 0.43              |
| 1:A:638:ARG:NE   | 1:A:643:ASP:OD2  | 2.48                     | 0.43              |
| 1:B:319:PRO:HA   | 1:B:425:ASP:O    | 2.18                     | 0.43              |
| 1:C:319:PRO:HA   | 1:C:425:ASP:O    | 2.18                     | 0.43              |
| 1:D:247:TYR:CZ   | 1:D:251:ARG:HB2  | 2.53                     | 0.43              |
| 1:A:321:ILE:HG13 | 1:A:395:LEU:HD11 | 1.99                     | 0.43              |
| 5:A:1007:PLM:HF1 | 5:A:1007:PLM:HC2 | 1.76                     | 0.43              |
| 1:B:564:VAL:O    | 1:B:567:PHE:HB3  | 2.18                     | 0.43              |
| 1:C:564:VAL:O    | 1:C:567:PHE:HB3  | 2.18                     | 0.43              |
| 1:D:308:PHE:HB3  | 1:D:315:LEU:H    | 1.83                     | 0.43              |
| 1:A:326:VAL:HG13 | 1:A:352:SER:O    | 2.19                     | 0.43              |
| 1:B:235:CYS:O    | 1:B:238:THR:OG1  | 2.32                     | 0.43              |
| 1:B:560:ASN:N    | 1:B:560:ASN:OD1  | 2.51                     | 0.43              |
| 1:C:406:VAL:HA   | 1:C:409:LEU:HD12 | 1.99                     | 0.43              |
| 1:D:321:ILE:HG13 | 1:D:395:LEU:HD11 | 1.99                     | 0.43              |
| 1:D:326:VAL:HG13 | 1:D:352:SER:O    | 2.19                     | 0.43              |
| 1:A:249:TYR:HD1  | 1:B:448:THR:HB   | 1.84                     | 0.43              |
| 1:A:451:VAL:O    | 1:A:452:ILE:HD13 | 2.18                     | 0.43              |
| 1:A:678:ALA:HB2  | 1:D:681:ASN:HA   | 2.00                     | 0.43              |
| 1:B:608:PHE:O    | 1:B:636:GLN:NE2  | 2.25                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:560:ASN:OD1  | 1:D:560:ASN:N    | 2.51                     | 0.43              |
| 5:D:1007:PLM:HF1 | 5:D:1007:PLM:HC2 | 1.76                     | 0.43              |
| 1:A:226:THR:HB   | 1:A:483:PHE:HZ   | 1.83                     | 0.43              |
| 1:A:247:TYR:CZ   | 1:A:251:ARG:HB2  | 2.53                     | 0.43              |
| 1:A:597:LEU:O    | 1:A:600:PHE:N    | 2.50                     | 0.43              |
| 1:B:238:THR:OG1  | 1:B:239:TYR:N    | 2.51                     | 0.43              |
| 1:B:382:ILE:HG23 | 1:B:383:ILE:N    | 2.32                     | 0.43              |
| 1:C:682:ASP:O    | 1:C:685:SER:OG   | 2.22                     | 0.43              |
| 1:C:682:ASP:CG   | 1:C:683:THR:H    | 2.24                     | 0.43              |
| 1:D:278:ASP:O    | 1:D:282:PHE:N    | 2.49                     | 0.43              |
| 1:D:451:VAL:O    | 1:D:452:ILE:HD13 | 2.18                     | 0.43              |
| 1:A:379:HIS:HB2  | 1:A:440:ARG:HH22 | 1.84                     | 0.43              |
| 1:A:677:LEU:HA   | 1:A:677:LEU:HD23 | 1.74                     | 0.43              |
| 1:A:684:TYR:HE2  | 1:B:682:ASP:OD2  | 2.02                     | 0.43              |
| 1:B:310:PHE:HD2  | 1:B:311:TYR:HD2  | 1.65                     | 0.43              |
| 1:B:508:ASN:HA   | 1:B:511:ASP:OD2  | 2.19                     | 0.43              |
| 1:B:682:ASP:CG   | 1:B:683:THR:H    | 2.24                     | 0.43              |
| 1:C:228:LEU:HA   | 1:C:231:LEU:HD23 | 2.00                     | 0.43              |
| 1:C:293:TRP:CH2  | 1:C:310:PHE:HB3  | 2.54                     | 0.43              |
| 1:C:405:GLN:O    | 1:C:409:LEU:HG   | 2.19                     | 0.43              |
| 1:D:319:PRO:HA   | 1:D:425:ASP:O    | 2.18                     | 0.43              |
| 1:B:293:TRP:CH2  | 1:B:310:PHE:HB3  | 2.54                     | 0.43              |
| 1:B:379:HIS:HB2  | 1:B:440:ARG:HH22 | 1.84                     | 0.43              |
| 1:B:582:THR:O    | 1:B:586:LEU:N    | 2.34                     | 0.43              |
| 1:B:677:LEU:HA   | 1:B:677:LEU:HD23 | 1.74                     | 0.43              |
| 1:C:508:ASN:HA   | 1:C:511:ASP:OD2  | 2.19                     | 0.43              |
| 1:D:238:THR:OG1  | 1:D:239:TYR:N    | 2.51                     | 0.43              |
| 1:D:564:VAL:O    | 1:D:567:PHE:HB3  | 2.18                     | 0.43              |
| 1:A:656:LEU:HA   | 1:A:656:LEU:HD23 | 1.72                     | 0.43              |
| 1:B:247:TYR:CZ   | 1:B:251:ARG:HB2  | 2.53                     | 0.43              |
| 1:B:611:TYR:HB3  | 1:B:660:TYR:HE1  | 1.84                     | 0.43              |
| 1:B:686:GLU:O    | 1:B:689:SER:OG   | 2.26                     | 0.43              |
| 1:C:560:ASN:OD1  | 1:C:560:ASN:N    | 2.51                     | 0.43              |
| 1:D:382:ILE:HG23 | 1:D:383:ILE:N    | 2.32                     | 0.43              |
| 1:A:319:PRO:HA   | 1:A:425:ASP:O    | 2.18                     | 0.43              |
| 1:A:690:ASP:CA   | 1:A:693:GLN:HG2  | 2.46                     | 0.43              |
| 1:C:532:VAL:O    | 1:C:535:LEU:HG   | 2.19                     | 0.43              |
| 1:C:677:LEU:CD2  | 1:D:673:LEU:HB3  | 2.49                     | 0.43              |
| 1:D:310:PHE:HD2  | 1:D:311:TYR:HD2  | 1.65                     | 0.43              |
| 1:A:293:TRP:CH2  | 1:A:310:PHE:HB3  | 2.54                     | 0.42              |
| 1:A:508:ASN:HA   | 1:A:511:ASP:OD2  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:532:VAL:O    | 1:B:535:LEU:HG   | 2.19                     | 0.42              |
| 1:B:656:LEU:HA   | 1:B:656:LEU:HD23 | 1.72                     | 0.42              |
| 1:C:297:PRO:O    | 1:C:298:SER:OG   | 2.28                     | 0.42              |
| 1:C:326:VAL:HG13 | 1:C:352:SER:O    | 2.19                     | 0.42              |
| 1:D:405:GLN:O    | 1:D:409:LEU:HG   | 2.19                     | 0.42              |
| 1:A:682:ASP:CG   | 1:A:683:THR:N    | 2.77                     | 0.42              |
| 1:B:326:VAL:HG13 | 1:B:352:SER:O    | 2.19                     | 0.42              |
| 1:C:611:TYR:HB3  | 1:C:660:TYR:HE1  | 1.84                     | 0.42              |
| 1:D:611:TYR:HB3  | 1:D:660:TYR:HE1  | 1.84                     | 0.42              |
| 1:A:536:LEU:HD23 | 1:A:540:GLU:HB3  | 2.02                     | 0.42              |
| 1:A:611:TYR:HB3  | 1:A:660:TYR:HE1  | 1.84                     | 0.42              |
| 1:B:592:ARG:HA   | 1:B:592:ARG:HD2  | 1.85                     | 0.42              |
| 1:D:226:THR:HB   | 1:D:483:PHE:CZ   | 2.55                     | 0.42              |
| 1:D:293:TRP:CH2  | 1:D:310:PHE:HB3  | 2.54                     | 0.42              |
| 1:D:324:LEU:HD13 | 1:D:348:TYR:CZ   | 2.55                     | 0.42              |
| 1:D:690:ASP:CA   | 1:D:693:GLN:HG2  | 2.46                     | 0.42              |
| 1:A:418:GLY:O    | 1:A:420:ARG:HG2  | 2.19                     | 0.42              |
| 1:A:532:VAL:O    | 1:A:535:LEU:HG   | 2.19                     | 0.42              |
| 1:B:228:LEU:HA   | 1:B:231:LEU:HD23 | 2.00                     | 0.42              |
| 1:B:588:THR:HA   | 1:B:591:SER:HB3  | 2.01                     | 0.42              |
| 5:B:1007:PLM:H91 | 1:C:667:PHE:HE2  | 1.84                     | 0.42              |
| 5:B:1008:PLM:H52 | 5:B:1008:PLM:H21 | 1.83                     | 0.42              |
| 1:C:324:LEU:HD13 | 1:C:348:TYR:CZ   | 2.55                     | 0.42              |
| 1:C:379:HIS:HB2  | 1:C:440:ARG:HH22 | 1.84                     | 0.42              |
| 1:D:379:HIS:HB2  | 1:D:440:ARG:HH22 | 1.84                     | 0.42              |
| 4:D:1006:PX6:H49 | 4:D:1006:PX6:H42 | 1.53                     | 0.42              |
| 1:A:588:THR:HA   | 1:A:591:SER:HB3  | 2.01                     | 0.42              |
| 1:A:673:LEU:HB3  | 1:D:677:LEU:CD2  | 2.49                     | 0.42              |
| 1:B:470:ASP:O    | 1:B:473:LEU:N    | 2.53                     | 0.42              |
| 1:C:310:PHE:HD2  | 1:C:311:TYR:HD2  | 1.65                     | 0.42              |
| 1:C:484:ILE:O    | 1:C:488:VAL:N    | 2.48                     | 0.42              |
| 1:D:536:LEU:HD23 | 1:D:540:GLU:HB3  | 2.02                     | 0.42              |
| 1:D:682:ASP:CG   | 1:D:683:THR:N    | 2.77                     | 0.42              |
| 1:A:405:GLN:O    | 1:A:409:LEU:HG   | 2.19                     | 0.42              |
| 1:A:653:ASN:ND2  | 1:A:656:LEU:HD12 | 2.35                     | 0.42              |
| 1:B:226:THR:HB   | 1:B:483:PHE:CZ   | 2.55                     | 0.42              |
| 1:B:418:GLY:O    | 1:B:420:ARG:HG2  | 2.19                     | 0.42              |
| 1:D:470:ASP:O    | 1:D:473:LEU:N    | 2.53                     | 0.42              |
| 1:A:226:THR:HB   | 1:A:483:PHE:CZ   | 2.55                     | 0.42              |
| 1:A:560:ASN:OD1  | 1:A:561:ILE:N    | 2.51                     | 0.42              |
| 1:B:312:GLU:OE1  | 1:C:449:GLY:N    | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:324:LEU:HD13 | 1:B:348:TYR:CZ   | 2.54                     | 0.42              |
| 1:B:653:ASN:ND2  | 1:B:656:LEU:HD12 | 2.35                     | 0.42              |
| 1:C:226:THR:HB   | 1:C:483:PHE:CZ   | 2.55                     | 0.42              |
| 1:D:508:ASN:HA   | 1:D:511:ASP:OD2  | 2.19                     | 0.42              |
| 1:D:532:VAL:O    | 1:D:535:LEU:HG   | 2.19                     | 0.42              |
| 1:A:238:THR:OG1  | 1:A:239:TYR:N    | 2.51                     | 0.42              |
| 1:A:574:PHE:CE1  | 1:B:603:MET:HG3  | 2.55                     | 0.42              |
| 1:B:405:GLN:O    | 1:B:409:LEU:HG   | 2.19                     | 0.42              |
| 1:C:418:GLY:O    | 1:C:420:ARG:HG2  | 2.19                     | 0.42              |
| 1:C:653:ASN:ND2  | 1:C:656:LEU:HD12 | 2.35                     | 0.42              |
| 4:C:1006:PX6:H54 | 4:C:1006:PX6:H61 | 1.65                     | 0.42              |
| 1:D:333:ILE:HG13 | 1:D:334:PRO:HD2  | 2.01                     | 0.42              |
| 1:A:297:PRO:O    | 1:A:298:SER:OG   | 2.28                     | 0.42              |
| 1:A:324:LEU:HD13 | 1:A:348:TYR:CZ   | 2.54                     | 0.42              |
| 1:B:310:PHE:HB2  | 1:B:311:TYR:CD2  | 2.55                     | 0.42              |
| 1:B:323:GLN:NE2  | 1:B:414:TRP:CD1  | 2.82                     | 0.42              |
| 1:B:619:PHE:HB2  | 1:B:626:PHE:CD2  | 2.51                     | 0.42              |
| 1:D:418:GLY:O    | 1:D:420:ARG:HG2  | 2.19                     | 0.42              |
| 1:D:653:ASN:ND2  | 1:D:656:LEU:HD12 | 2.35                     | 0.42              |
| 1:B:681:ASN:HA   | 1:C:678:ALA:HB2  | 2.02                     | 0.42              |
| 1:B:682:ASP:CG   | 1:B:683:THR:N    | 2.78                     | 0.42              |
| 1:C:536:LEU:HD23 | 1:C:540:GLU:HB3  | 2.02                     | 0.42              |
| 1:A:470:ASP:O    | 1:A:473:LEU:N    | 2.53                     | 0.41              |
| 1:A:512:VAL:O    | 1:A:516:VAL:HG23 | 2.20                     | 0.41              |
| 1:B:512:VAL:O    | 1:B:516:VAL:HG23 | 2.20                     | 0.41              |
| 1:B:645:ASN:CB   | 1:B:648:GLU:OE2  | 2.56                     | 0.41              |
| 1:B:682:ASP:OD1  | 1:B:683:THR:N    | 2.43                     | 0.41              |
| 1:C:470:ASP:O    | 1:C:473:LEU:N    | 2.53                     | 0.41              |
| 5:C:1007:PLM:H91 | 1:D:667:PHE:HE2  | 1.85                     | 0.41              |
| 1:D:588:THR:HA   | 1:D:591:SER:HB3  | 2.01                     | 0.41              |
| 1:A:310:PHE:HB2  | 1:A:311:TYR:CD2  | 2.55                     | 0.41              |
| 1:A:644:ILE:HG23 | 1:A:646:PHE:CB   | 2.50                     | 0.41              |
| 1:B:560:ASN:ND2  | 4:B:1006:PX6:H43 | 2.35                     | 0.41              |
| 4:B:1006:PX6:H67 | 4:B:1006:PX6:H60 | 1.71                     | 0.41              |
| 1:C:682:ASP:CG   | 1:C:683:THR:N    | 2.78                     | 0.41              |
| 1:D:323:GLN:NE2  | 1:D:414:TRP:CD1  | 2.82                     | 0.41              |
| 1:B:278:ASP:O    | 1:B:282:PHE:N    | 2.49                     | 0.41              |
| 1:B:333:ILE:HG13 | 1:B:334:PRO:HD2  | 2.01                     | 0.41              |
| 1:B:420:ARG:HA   | 1:B:420:ARG:HD3  | 1.88                     | 0.41              |
| 1:B:638:ARG:NE   | 1:B:643:ASP:OD2  | 2.49                     | 0.41              |
| 1:C:588:THR:HA   | 1:C:591:SER:HB3  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:677:LEU:O    | 1:C:681:ASN:N    | 2.46                     | 0.41              |
| 5:A:1007:PLM:H91 | 1:B:667:PHE:HE2  | 1.86                     | 0.41              |
| 1:B:417:ARG:HG2  | 1:B:418:GLY:N    | 2.36                     | 0.41              |
| 1:B:536:LEU:HD23 | 1:B:540:GLU:HB3  | 2.02                     | 0.41              |
| 1:C:333:ILE:HG13 | 1:C:334:PRO:HD2  | 2.01                     | 0.41              |
| 1:D:560:ASN:ND2  | 4:D:1006:PX6:H43 | 2.35                     | 0.41              |
| 1:A:560:ASN:OD1  | 1:A:560:ASN:N    | 2.51                     | 0.41              |
| 1:C:644:ILE:HG23 | 1:C:646:PHE:CB   | 2.50                     | 0.41              |
| 1:D:320:ARG:N    | 1:D:425:ASP:O    | 2.44                     | 0.41              |
| 1:D:644:ILE:HG23 | 1:D:646:PHE:CB   | 2.50                     | 0.41              |
| 1:A:683:THR:O    | 1:A:687:VAL:HG22 | 2.21                     | 0.41              |
| 1:C:310:PHE:HB2  | 1:C:311:TYR:CD2  | 2.55                     | 0.41              |
| 1:C:405:GLN:C    | 1:C:409:LEU:HG   | 2.45                     | 0.41              |
| 1:D:274:SER:OG   | 1:D:275:SER:N    | 2.54                     | 0.41              |
| 1:D:310:PHE:HB2  | 1:D:311:TYR:CD2  | 2.55                     | 0.41              |
| 1:A:274:SER:OG   | 1:A:275:SER:N    | 2.54                     | 0.41              |
| 1:A:320:ARG:N    | 1:A:425:ASP:O    | 2.43                     | 0.41              |
| 1:A:409:LEU:HB3  | 1:A:414:TRP:CH2  | 2.56                     | 0.41              |
| 1:B:644:ILE:HG23 | 1:B:646:PHE:CB   | 2.50                     | 0.41              |
| 1:D:284:GLU:HA   | 1:D:288:LEU:HD13 | 2.03                     | 0.41              |
| 1:D:296:GLN:HG2  | 1:D:311:TYR:HD1  | 1.83                     | 0.41              |
| 1:D:568:PHE:HA   | 1:D:571:ILE:HG12 | 2.03                     | 0.41              |
| 1:B:310:PHE:CD2  | 1:B:311:TYR:CD2  | 3.09                     | 0.41              |
| 1:C:568:PHE:HA   | 1:C:571:ILE:HG12 | 2.03                     | 0.41              |
| 1:C:619:PHE:HB2  | 1:C:626:PHE:CD2  | 2.51                     | 0.41              |
| 1:D:405:GLN:C    | 1:D:409:LEU:HG   | 2.45                     | 0.41              |
| 1:A:284:GLU:HA   | 1:A:288:LEU:HD13 | 2.03                     | 0.41              |
| 1:A:310:PHE:CD2  | 1:A:311:TYR:CD2  | 3.09                     | 0.41              |
| 1:A:333:ILE:HG13 | 1:A:334:PRO:HD2  | 2.01                     | 0.41              |
| 1:A:377:SER:OG   | 1:A:378:SER:N    | 2.54                     | 0.41              |
| 1:A:405:GLN:C    | 1:A:409:LEU:HG   | 2.45                     | 0.41              |
| 1:A:483:PHE:O    | 1:A:486:TYR:HB3  | 2.21                     | 0.41              |
| 1:A:677:LEU:CD2  | 1:B:673:LEU:HB3  | 2.51                     | 0.41              |
| 5:A:1008:PLM:H52 | 5:A:1008:PLM:H21 | 1.87                     | 0.41              |
| 1:B:405:GLN:C    | 1:B:409:LEU:HG   | 2.46                     | 0.41              |
| 1:B:683:THR:O    | 1:B:687:VAL:HG22 | 2.21                     | 0.41              |
| 1:C:417:ARG:HG2  | 1:C:418:GLY:N    | 2.36                     | 0.41              |
| 1:C:444:GLU:HB2  | 1:C:452:ILE:HB   | 2.03                     | 0.41              |
| 1:C:512:VAL:O    | 1:C:516:VAL:HG23 | 2.20                     | 0.41              |
| 1:C:560:ASN:ND2  | 4:C:1006:PX6:H43 | 2.36                     | 0.41              |
| 1:C:656:LEU:HA   | 1:C:656:LEU:HD23 | 1.72                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:681:ASN:HD22  | 1:D:678:ALA:CB   | 2.34                     | 0.41              |
| 1:D:483:PHE:O     | 1:D:486:TYR:HB3  | 2.21                     | 0.41              |
| 1:D:512:VAL:O     | 1:D:516:VAL:HG23 | 2.20                     | 0.41              |
| 1:D:560:ASN:OD1   | 1:D:561:ILE:N    | 2.51                     | 0.41              |
| 1:B:444:GLU:HB2   | 1:B:452:ILE:HB   | 2.03                     | 0.41              |
| 1:C:483:PHE:O     | 1:C:486:TYR:HB3  | 2.21                     | 0.41              |
| 1:D:417:ARG:HG2   | 1:D:418:GLY:N    | 2.36                     | 0.41              |
| 1:A:462:LEU:CD1   | 1:A:533:GLU:HG2  | 2.51                     | 0.40              |
| 1:A:674:ASN:HA    | 1:D:680:ILE:HD13 | 2.02                     | 0.40              |
| 1:B:280:TRP:HE1   | 1:B:415:LEU:HD12 | 1.86                     | 0.40              |
| 1:B:483:PHE:O     | 1:B:486:TYR:HB3  | 2.21                     | 0.40              |
| 1:B:526:ILE:O     | 1:B:530:SER:OG   | 2.25                     | 0.40              |
| 1:B:568:PHE:HA    | 1:B:571:ILE:HG12 | 2.03                     | 0.40              |
| 1:C:462:LEU:CD1   | 1:C:533:GLU:HG2  | 2.51                     | 0.40              |
| 1:C:683:THR:O     | 1:C:687:VAL:HG22 | 2.21                     | 0.40              |
| 1:D:592:ARG:HA    | 1:D:592:ARG:HD2  | 1.85                     | 0.40              |
| 5:D:1009:PLM:H42  | 5:D:1009:PLM:H72 | 1.95                     | 0.40              |
| 1:B:409:LEU:HB3   | 1:B:414:TRP:CH2  | 2.56                     | 0.40              |
| 1:C:278:ASP:O     | 1:C:282:PHE:N    | 2.49                     | 0.40              |
| 1:C:284:GLU:HA    | 1:C:288:LEU:HD13 | 2.03                     | 0.40              |
| 1:C:661:PHE:O     | 1:C:665:VAL:HG12 | 2.21                     | 0.40              |
| 1:D:444:GLU:HB2   | 1:D:452:ILE:HB   | 2.03                     | 0.40              |
| 1:D:638:ARG:NE    | 1:D:643:ASP:OD2  | 2.48                     | 0.40              |
| 1:D:661:PHE:O     | 1:D:665:VAL:HG12 | 2.21                     | 0.40              |
| 1:A:452:ILE:HD11  | 1:D:248:TYR:CD1  | 2.56                     | 0.40              |
| 1:A:661:PHE:O     | 1:A:665:VAL:HG12 | 2.21                     | 0.40              |
| 1:A:667:PHE:HE2   | 5:D:1007:PLM:H91 | 1.85                     | 0.40              |
| 6:A:1011:CHS:HD13 | 6:A:1011:CHS:HA  | 1.92                     | 0.40              |
| 1:B:377:SER:OG    | 1:B:378:SER:N    | 2.54                     | 0.40              |
| 1:B:536:LEU:HB3   | 1:B:540:GLU:CD   | 2.47                     | 0.40              |
| 4:B:1006:PX6:H54  | 4:B:1006:PX6:H61 | 1.68                     | 0.40              |
| 1:C:677:LEU:HA    | 1:C:677:LEU:HD23 | 1.74                     | 0.40              |
| 5:C:1007:PLM:HA2  | 5:C:1007:PLM:HD1 | 1.69                     | 0.40              |
| 1:D:302:GLU:O     | 1:D:306:ARG:HA   | 2.21                     | 0.40              |
| 1:D:310:PHE:CD2   | 1:D:311:TYR:CD2  | 3.09                     | 0.40              |
| 1:D:374:LEU:HA    | 2:H:1:NAG:H82    | 2.03                     | 0.40              |
| 1:D:377:SER:OG    | 1:D:378:SER:N    | 2.54                     | 0.40              |
| 1:D:462:LEU:CD1   | 1:D:533:GLU:HG2  | 2.51                     | 0.40              |
| 1:A:644:ILE:HA    | 1:A:644:ILE:HD13 | 1.86                     | 0.40              |
| 6:B:1011:CHS:HD13 | 6:B:1011:CHS:HA  | 1.84                     | 0.40              |
| 1:C:377:SER:OG    | 1:C:378:SER:N    | 2.54                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:683:THR:O   | 1:D:687:VAL:HG22 | 2.21                     | 0.40              |
| 1:A:417:ARG:HG2 | 1:A:418:GLY:N    | 2.36                     | 0.40              |
| 1:A:568:PHE:HA  | 1:A:571:ILE:HG12 | 2.03                     | 0.40              |
| 1:B:484:ILE:O   | 1:B:488:VAL:N    | 2.48                     | 0.40              |
| 1:C:536:LEU:HB3 | 1:C:540:GLU:CD   | 2.47                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 479/968 (50%)   | 419 (88%)  | 56 (12%)  | 4 (1%)   | 16          | 52 |
| 1   | B     | 479/968 (50%)   | 419 (88%)  | 56 (12%)  | 4 (1%)   | 16          | 52 |
| 1   | C     | 479/968 (50%)   | 419 (88%)  | 56 (12%)  | 4 (1%)   | 16          | 52 |
| 1   | D     | 479/968 (50%)   | 419 (88%)  | 56 (12%)  | 4 (1%)   | 16          | 52 |
| All | All   | 1916/3872 (50%) | 1676 (88%) | 224 (12%) | 16 (1%)  | 18          | 52 |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 628 | THR  |
| 1   | B     | 628 | THR  |
| 1   | C     | 628 | THR  |
| 1   | D     | 628 | THR  |
| 1   | A     | 674 | ASN  |
| 1   | B     | 674 | ASN  |
| 1   | C     | 674 | ASN  |
| 1   | D     | 674 | ASN  |
| 1   | A     | 309 | ILE  |
| 1   | B     | 309 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 309 | ILE  |
| 1   | D     | 309 | ILE  |
| 1   | A     | 413 | VAL  |
| 1   | B     | 413 | VAL  |
| 1   | C     | 413 | VAL  |
| 1   | D     | 413 | VAL  |

### 5.3.2 Protein sidechains [i](#)

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     | 432/837 (52%)   | 429 (99%)   | 3 (1%)   | 76          | 78 |
| 1   | B     | 431/837 (52%)   | 429 (100%)  | 2 (0%)   | 81          | 81 |
| 1   | C     | 431/837 (52%)   | 429 (100%)  | 2 (0%)   | 81          | 81 |
| 1   | D     | 431/837 (52%)   | 429 (100%)  | 2 (0%)   | 81          | 81 |
| All | All   | 1725/3348 (52%) | 1716 (100%) | 9 (0%)   | 78          | 81 |

All (9) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 503 | PHE  |
| 1   | A     | 583 | MET  |
| 1   | A     | 623 | VAL  |
| 1   | B     | 503 | PHE  |
| 1   | B     | 623 | VAL  |
| 1   | C     | 503 | PHE  |
| 1   | C     | 623 | VAL  |
| 1   | D     | 503 | PHE  |
| 1   | D     | 623 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 299 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 379 | HIS  |
| 1   | A     | 430 | ASN  |
| 1   | B     | 299 | ASN  |
| 1   | B     | 379 | HIS  |
| 1   | B     | 430 | ASN  |
| 1   | C     | 299 | ASN  |
| 1   | C     | 379 | HIS  |
| 1   | C     | 430 | ASN  |
| 1   | D     | 299 | ASN  |
| 1   | D     | 379 | HIS  |
| 1   | D     | 430 | ASN  |
| 1   | D     | 630 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

8 monosaccharides are modelled in this entry.

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 | $\# Z  > 2$ |
| 2   | NAG  | E     | 1   | 2    | 14,14,15     | 0.33 | 0           | 17,19,21    | 0.61 | 0           |
| 2   | NAG  | E     | 2   | 2    | 14,14,15     | 1.00 | 1 (7%)      | 17,19,21    | 0.64 | 0           |
| 2   | NAG  | F     | 1   | 2    | 14,14,15     | 0.34 | 0           | 17,19,21    | 0.60 | 0           |
| 2   | NAG  | F     | 2   | 2    | 14,14,15     | 1.01 | 1 (7%)      | 17,19,21    | 0.65 | 0           |
| 2   | NAG  | G     | 1   | 2    | 14,14,15     | 0.34 | 0           | 17,19,21    | 0.61 | 0           |
| 2   | NAG  | G     | 2   | 2    | 14,14,15     | 1.00 | 1 (7%)      | 17,19,21    | 0.64 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | NAG  | H     | 1   | 2    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.60 | 0        |
| 2   | NAG  | H     | 2   | 2    | 14,14,15     | 1.01 | 1 (7%)   | 17,19,21    | 0.64 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | NAG  | E     | 1   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | E     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | F     | 1   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | F     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | G     | 1   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | G     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | H     | 1   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | H     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | F     | 2   | NAG  | C1-C2 | 3.36 | 1.56        | 1.52     |
| 2   | H     | 2   | NAG  | C1-C2 | 3.32 | 1.56        | 1.52     |
| 2   | E     | 2   | NAG  | C1-C2 | 3.31 | 1.56        | 1.52     |
| 2   | G     | 2   | NAG  | C1-C2 | 3.28 | 1.56        | 1.52     |

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

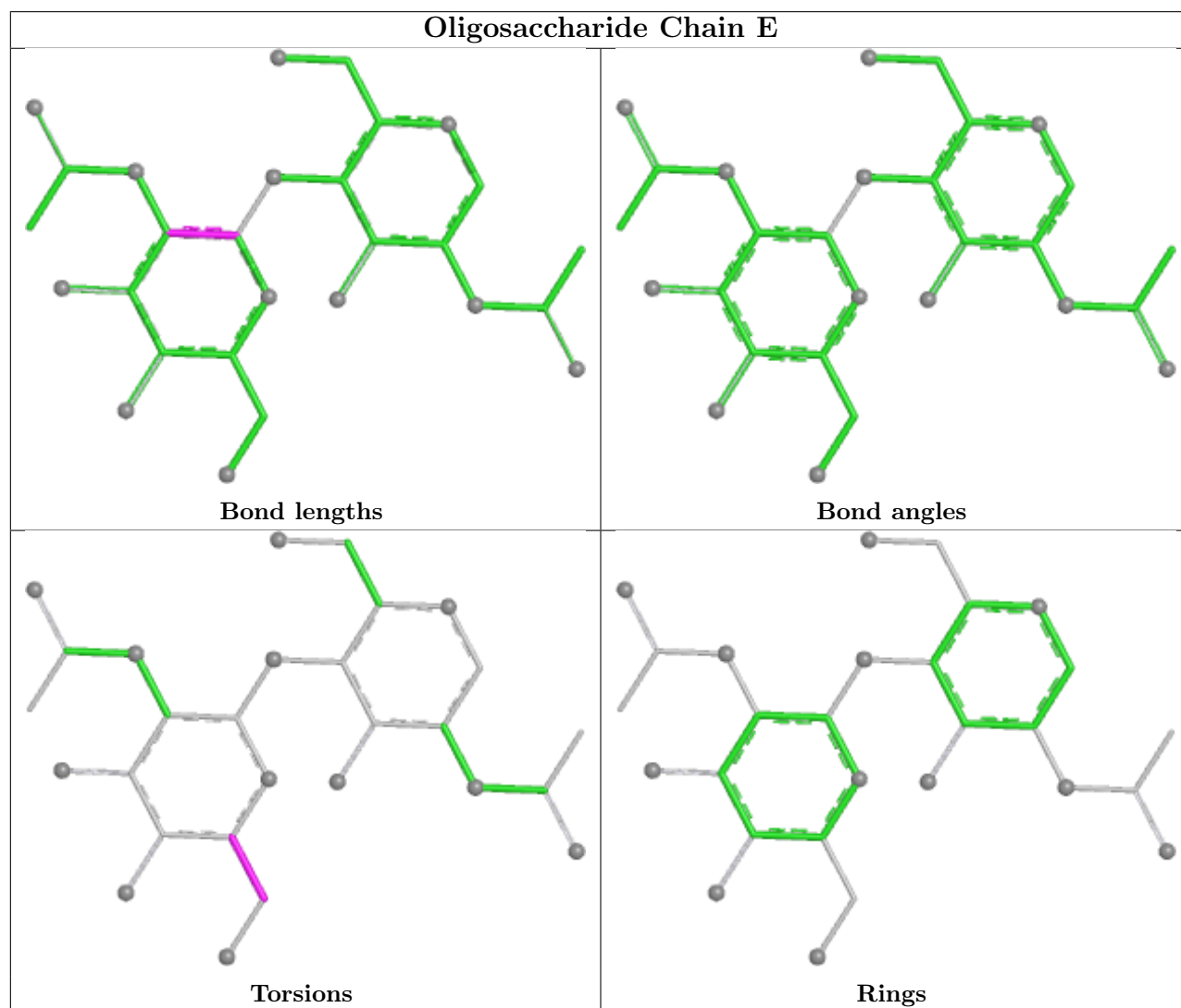
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | E     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | F     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | G     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | H     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | E     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | F     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | G     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | H     | 2   | NAG  | C4-C5-C6-O6 |

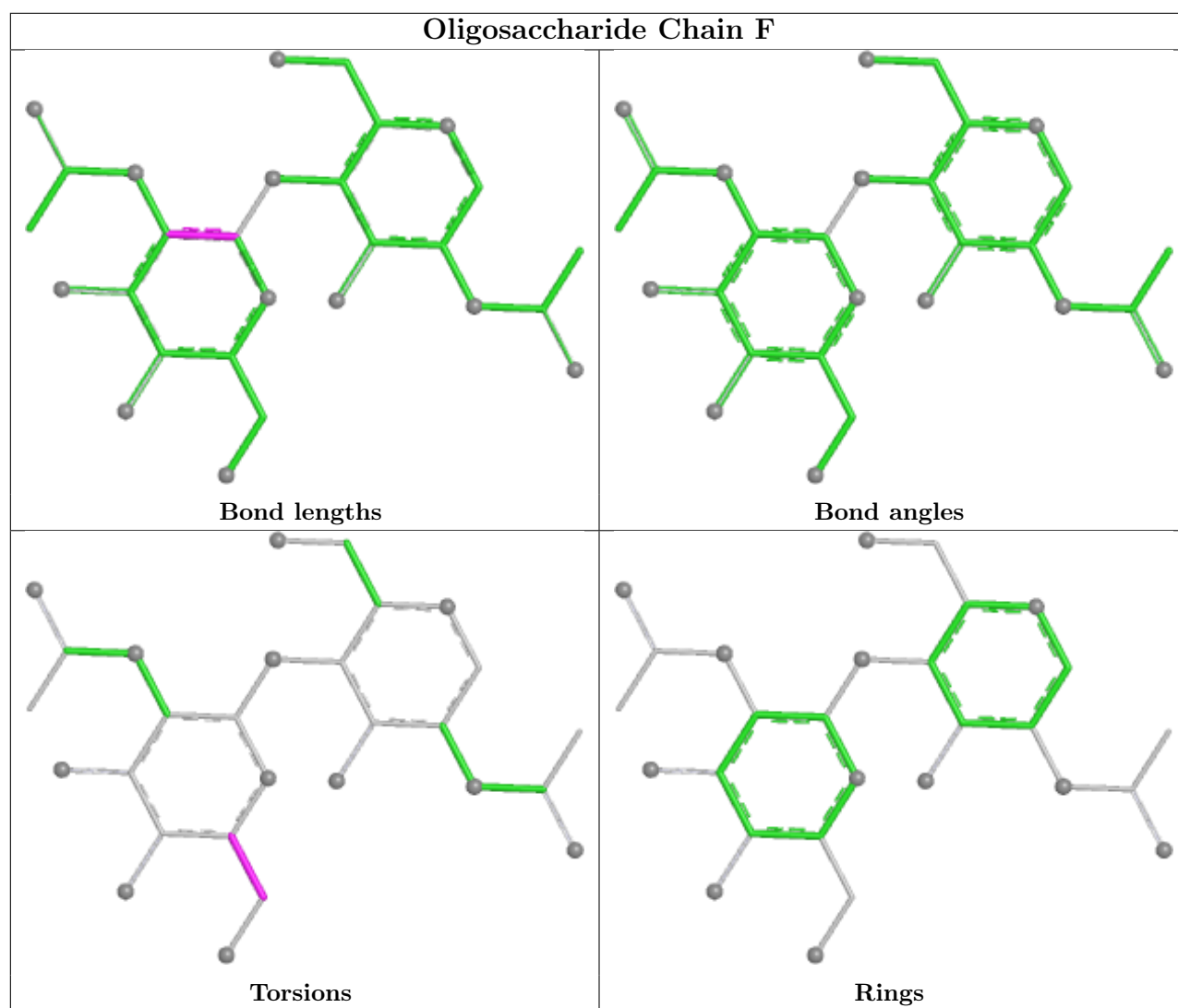
There are no ring outliers.

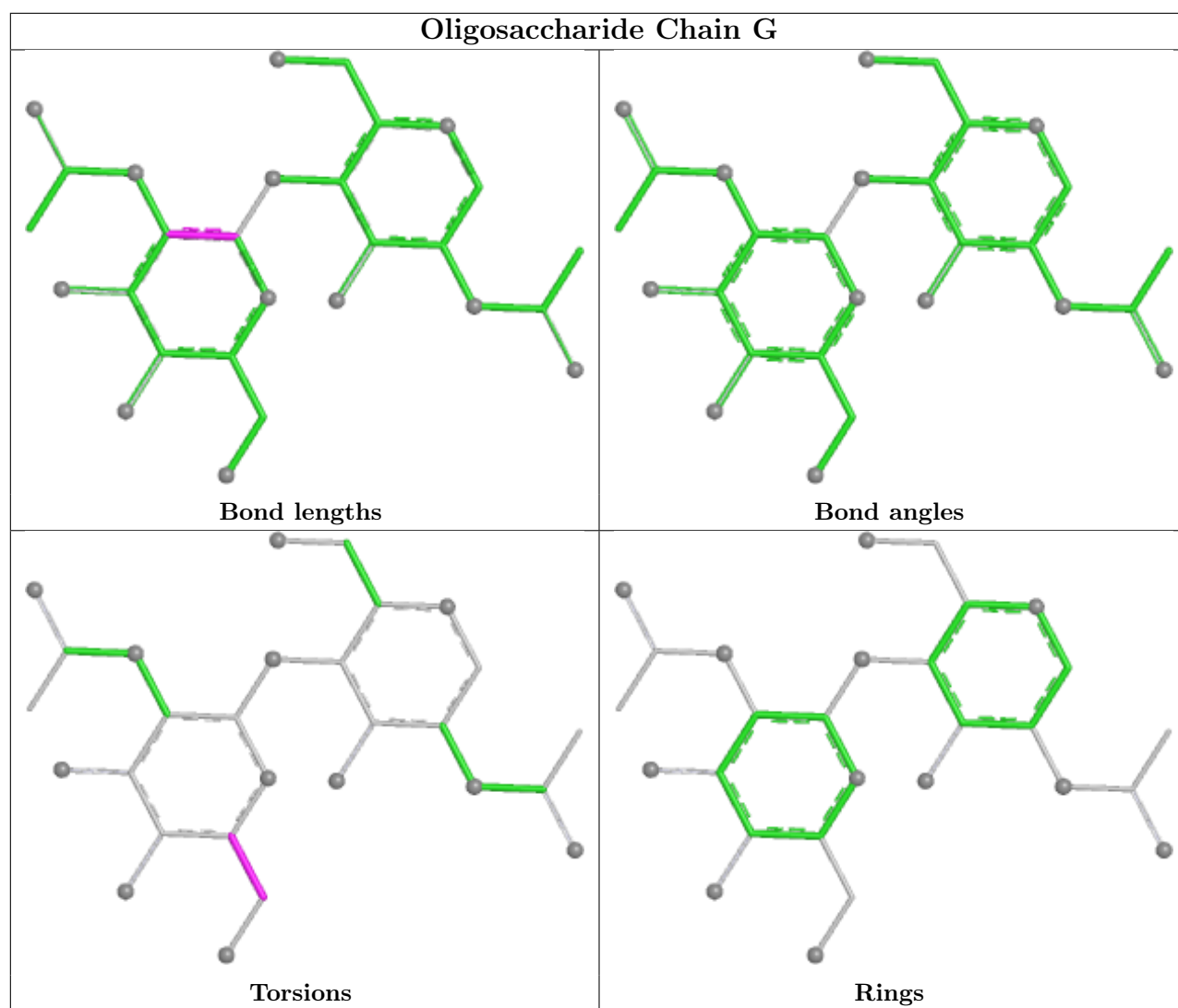
3 monomers are involved in 7 short contacts:

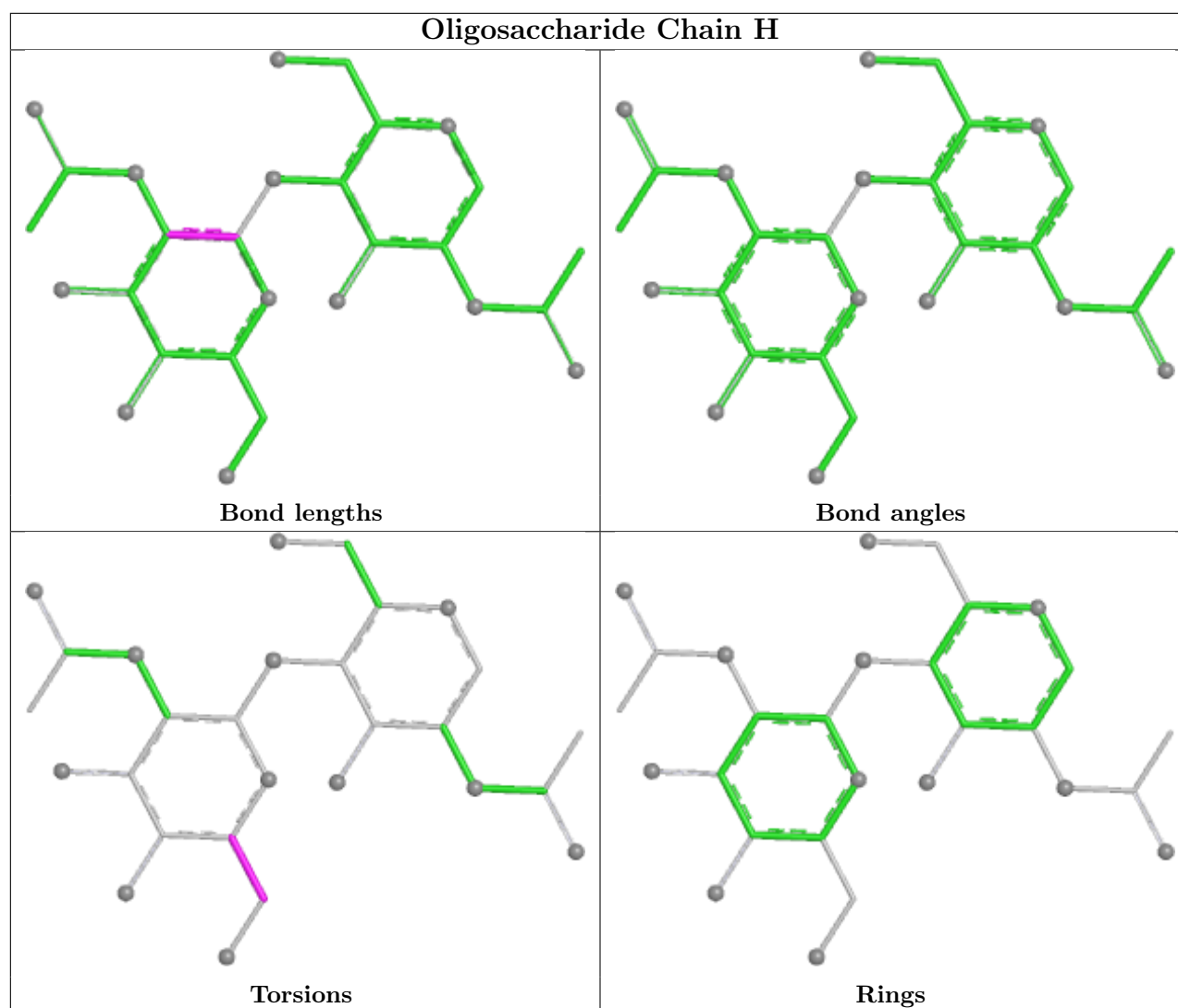
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | H     | 1   | NAG  | 1       | 0            |
| 2   | G     | 1   | NAG  | 3       | 0            |
| 2   | F     | 1   | NAG  | 3       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









## 5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 5 are monoatomic - leaving 36 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 | $\# Z  > 2$ |
| 5   | PLM  | C     | 1008 | -    | 17,17,17     | 0.52 | 0           | 17,17,17    | 0.89 | 0           |
| 3   | NAG  | C     | 1001 | 1    | 14,14,15     | 0.34 | 0           | 17,19,21    | 0.49 | 0           |
| 5   | PLM  | B     | 1008 | -    | 17,17,17     | 0.52 | 0           | 17,17,17    | 0.90 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | PLM  | D     | 1007 | -    | 17,17,17     | 0.55 | 0        | 17,17,17    | 0.78 | 1 (5%)   |
| 3   | NAG  | C     | 1005 | -    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.38 | 0        |
| 4   | PX6  | A     | 1006 | -    | 39,39,43     | 1.46 | 6 (15%)  | 42,44,48    | 1.49 | 3 (7%)   |
| 6   | CHS  | D     | 1010 | -    | 15,15,15     | 0.65 | 0        | 15,19,19    | 0.90 | 1 (6%)   |
| 6   | CHS  | D     | 1011 | -    | 15,15,15     | 0.59 | 0        | 15,19,19    | 0.94 | 1 (6%)   |
| 3   | NAG  | C     | 1002 | 1    | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.36 | 0        |
| 5   | PLM  | A     | 1008 | -    | 17,17,17     | 0.52 | 0        | 17,17,17    | 0.90 | 0        |
| 6   | CHS  | A     | 1011 | -    | 15,15,15     | 0.58 | 0        | 15,19,19    | 0.94 | 1 (6%)   |
| 5   | PLM  | D     | 1009 | -    | 17,17,17     | 0.55 | 0        | 17,17,17    | 0.76 | 0        |
| 3   | NAG  | A     | 1001 | 1    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.48 | 0        |
| 3   | NAG  | B     | 1002 | 1    | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.36 | 0        |
| 3   | NAG  | B     | 1005 | -    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.38 | 0        |
| 5   | PLM  | A     | 1009 | -    | 17,17,17     | 0.55 | 0        | 17,17,17    | 0.77 | 0        |
| 6   | CHS  | A     | 1010 | -    | 15,15,15     | 0.66 | 0        | 15,19,19    | 0.90 | 0        |
| 4   | PX6  | B     | 1006 | -    | 39,39,43     | 1.47 | 6 (15%)  | 42,44,48    | 1.48 | 3 (7%)   |
| 4   | PX6  | C     | 1006 | -    | 39,39,43     | 1.47 | 6 (15%)  | 42,44,48    | 1.48 | 3 (7%)   |
| 5   | PLM  | B     | 1007 | -    | 17,17,17     | 0.55 | 0        | 17,17,17    | 0.77 | 1 (5%)   |
| 3   | NAG  | A     | 1002 | 1    | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.36 | 0        |
| 5   | PLM  | B     | 1009 | -    | 17,17,17     | 0.55 | 0        | 17,17,17    | 0.76 | 0        |
| 3   | NAG  | D     | 1005 | -    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.38 | 0        |
| 6   | CHS  | C     | 1011 | -    | 15,15,15     | 0.58 | 0        | 15,19,19    | 0.95 | 1 (6%)   |
| 5   | PLM  | C     | 1009 | -    | 17,17,17     | 0.56 | 0        | 17,17,17    | 0.76 | 0        |
| 5   | PLM  | A     | 1007 | -    | 17,17,17     | 0.55 | 0        | 17,17,17    | 0.78 | 1 (5%)   |
| 3   | NAG  | B     | 1001 | 1    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.47 | 0        |
| 4   | PX6  | D     | 1006 | -    | 39,39,43     | 1.47 | 6 (15%)  | 42,44,48    | 1.48 | 3 (7%)   |
| 5   | PLM  | C     | 1007 | -    | 17,17,17     | 0.56 | 0        | 17,17,17    | 0.78 | 1 (5%)   |
| 5   | PLM  | D     | 1008 | -    | 17,17,17     | 0.52 | 0        | 17,17,17    | 0.89 | 0        |
| 3   | NAG  | D     | 1002 | 1    | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.36 | 0        |
| 6   | CHS  | B     | 1010 | -    | 15,15,15     | 0.65 | 0        | 15,19,19    | 0.90 | 1 (6%)   |
| 6   | CHS  | B     | 1011 | -    | 15,15,15     | 0.57 | 0        | 15,19,19    | 0.93 | 1 (6%)   |
| 3   | NAG  | D     | 1001 | 1    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.48 | 0        |
| 6   | CHS  | C     | 1010 | -    | 15,15,15     | 0.65 | 0        | 15,19,19    | 0.90 | 0        |
| 3   | NAG  | A     | 1005 | -    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.38 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|------|------|---------|-------------|---------|
| 5   | PLM  | C     | 1008 | -    | -       | 7/15/15/15  | -       |
| 3   | NAG  | C     | 1001 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 5   | PLM  | B     | 1008 | -    | -       | 6/15/15/15  | -       |
| 5   | PLM  | D     | 1007 | -    | -       | 11/15/15/15 | -       |
| 3   | NAG  | C     | 1005 | -    | -       | 2/6/23/26   | 0/1/1/1 |
| 4   | PX6  | A     | 1006 | -    | -       | 19/41/41/45 | -       |
| 6   | CHS  | D     | 1010 | -    | -       | 3/12/20/20  | 0/1/1/1 |
| 6   | CHS  | D     | 1011 | -    | -       | 2/12/20/20  | 0/1/1/1 |
| 3   | NAG  | C     | 1002 | 1    | -       | 3/6/23/26   | 0/1/1/1 |
| 5   | PLM  | A     | 1008 | -    | -       | 6/15/15/15  | -       |
| 6   | CHS  | A     | 1011 | -    | -       | 2/12/20/20  | 0/1/1/1 |
| 5   | PLM  | D     | 1009 | -    | -       | 8/15/15/15  | -       |
| 3   | NAG  | A     | 1001 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 3   | NAG  | B     | 1002 | 1    | -       | 3/6/23/26   | 0/1/1/1 |
| 3   | NAG  | B     | 1005 | -    | -       | 2/6/23/26   | 0/1/1/1 |
| 5   | PLM  | A     | 1009 | -    | -       | 6/15/15/15  | -       |
| 6   | CHS  | A     | 1010 | -    | -       | 3/12/20/20  | 0/1/1/1 |
| 4   | PX6  | B     | 1006 | -    | -       | 19/41/41/45 | -       |
| 4   | PX6  | C     | 1006 | -    | -       | 18/41/41/45 | -       |
| 5   | PLM  | B     | 1007 | -    | -       | 11/15/15/15 | -       |
| 3   | NAG  | A     | 1002 | 1    | -       | 3/6/23/26   | 0/1/1/1 |
| 5   | PLM  | B     | 1009 | -    | -       | 8/15/15/15  | -       |
| 3   | NAG  | D     | 1005 | -    | -       | 2/6/23/26   | 0/1/1/1 |
| 6   | CHS  | C     | 1011 | -    | -       | 2/12/20/20  | 0/1/1/1 |
| 5   | PLM  | C     | 1009 | -    | -       | 8/15/15/15  | -       |
| 5   | PLM  | A     | 1007 | -    | -       | 11/15/15/15 | -       |
| 3   | NAG  | B     | 1001 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 4   | PX6  | D     | 1006 | -    | -       | 18/41/41/45 | -       |
| 5   | PLM  | C     | 1007 | -    | -       | 11/15/15/15 | -       |
| 5   | PLM  | D     | 1008 | -    | -       | 6/15/15/15  | -       |
| 3   | NAG  | D     | 1002 | 1    | -       | 3/6/23/26   | 0/1/1/1 |
| 6   | CHS  | B     | 1010 | -    | -       | 3/12/20/20  | 0/1/1/1 |
| 6   | CHS  | B     | 1011 | -    | -       | 4/12/20/20  | 0/1/1/1 |
| 3   | NAG  | D     | 1001 | 1    | -       | 2/6/23/26   | 0/1/1/1 |
| 6   | CHS  | C     | 1010 | -    | -       | 3/12/20/20  | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | NAG  | A     | 1005 | -    | -       | 2/6/23/26 | 0/1/1/1 |

All (24) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4   | C     | 1006 | PX6  | P1-O2  | 4.79  | 1.65        | 1.50     |
| 4   | D     | 1006 | PX6  | P1-O2  | 4.78  | 1.65        | 1.50     |
| 4   | B     | 1006 | PX6  | P1-O2  | 4.78  | 1.65        | 1.50     |
| 4   | A     | 1006 | PX6  | P1-O2  | 4.77  | 1.65        | 1.50     |
| 4   | C     | 1006 | PX6  | O7-C2  | -3.26 | 1.38        | 1.46     |
| 4   | B     | 1006 | PX6  | O7-C2  | -3.25 | 1.38        | 1.46     |
| 4   | D     | 1006 | PX6  | O7-C2  | -3.22 | 1.39        | 1.46     |
| 4   | A     | 1006 | PX6  | O7-C2  | -3.21 | 1.39        | 1.46     |
| 4   | C     | 1006 | PX6  | O5-C4  | 2.91  | 1.41        | 1.33     |
| 4   | B     | 1006 | PX6  | O5-C4  | 2.91  | 1.41        | 1.33     |
| 4   | D     | 1006 | PX6  | O5-C4  | 2.89  | 1.41        | 1.33     |
| 4   | A     | 1006 | PX6  | O5-C4  | 2.89  | 1.41        | 1.33     |
| 4   | C     | 1006 | PX6  | O7-C20 | 2.47  | 1.41        | 1.34     |
| 4   | B     | 1006 | PX6  | O7-C20 | 2.46  | 1.41        | 1.34     |
| 4   | A     | 1006 | PX6  | O7-C20 | 2.46  | 1.41        | 1.34     |
| 4   | D     | 1006 | PX6  | O7-C20 | 2.45  | 1.41        | 1.34     |
| 4   | D     | 1006 | PX6  | P1-O3  | -2.36 | 1.46        | 1.54     |
| 4   | C     | 1006 | PX6  | P1-O3  | -2.36 | 1.46        | 1.54     |
| 4   | B     | 1006 | PX6  | P1-O3  | -2.36 | 1.46        | 1.54     |
| 4   | A     | 1006 | PX6  | P1-O3  | -2.36 | 1.46        | 1.54     |
| 4   | D     | 1006 | PX6  | P1-O1  | -2.29 | 1.46        | 1.54     |
| 4   | B     | 1006 | PX6  | P1-O1  | -2.26 | 1.46        | 1.54     |
| 4   | C     | 1006 | PX6  | P1-O1  | -2.26 | 1.46        | 1.54     |
| 4   | A     | 1006 | PX6  | P1-O1  | -2.23 | 1.46        | 1.54     |

All (22) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 4   | A     | 1006 | PX6  | O5-C3-C2   | 7.08 | 128.82      | 108.40   |
| 4   | D     | 1006 | PX6  | O5-C3-C2   | 7.07 | 128.78      | 108.40   |
| 4   | B     | 1006 | PX6  | O5-C3-C2   | 7.05 | 128.73      | 108.40   |
| 4   | C     | 1006 | PX6  | O5-C3-C2   | 7.04 | 128.70      | 108.40   |
| 4   | A     | 1006 | PX6  | O7-C20-C21 | 3.36 | 118.76      | 111.48   |
| 4   | C     | 1006 | PX6  | O7-C20-C21 | 3.35 | 118.74      | 111.48   |
| 4   | B     | 1006 | PX6  | O7-C20-C21 | 3.35 | 118.74      | 111.48   |
| 4   | D     | 1006 | PX6  | O7-C20-C21 | 3.32 | 118.67      | 111.48   |
| 4   | A     | 1006 | PX6  | O5-C4-C5   | 2.57 | 119.66      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4   | B     | 1006 | PX6  | O5-C4-C5 | 2.54  | 119.58      | 111.83   |
| 4   | C     | 1006 | PX6  | O5-C4-C5 | 2.53  | 119.56      | 111.83   |
| 4   | D     | 1006 | PX6  | O5-C4-C5 | 2.53  | 119.54      | 111.83   |
| 6   | C     | 1011 | CHS  | CH-CM-C  | -2.17 | 109.14      | 113.93   |
| 6   | D     | 1011 | CHS  | CH-CM-C  | -2.17 | 109.14      | 113.93   |
| 6   | A     | 1011 | CHS  | CH-CM-C  | -2.14 | 109.20      | 113.93   |
| 6   | B     | 1011 | CHS  | CH-CM-C  | -2.12 | 109.25      | 113.93   |
| 5   | B     | 1007 | PLM  | O1-C1-C2 | 2.07  | 120.54      | 114.00   |
| 5   | C     | 1007 | PLM  | O1-C1-C2 | 2.07  | 120.54      | 114.00   |
| 5   | D     | 1007 | PLM  | O1-C1-C2 | 2.06  | 120.52      | 114.00   |
| 5   | A     | 1007 | PLM  | O1-C1-C2 | 2.06  | 120.52      | 114.00   |
| 6   | D     | 1010 | CHS  | CH-CM-C  | -2.01 | 109.49      | 113.93   |
| 6   | B     | 1010 | CHS  | CH-CM-C  | -2.01 | 109.50      | 113.93   |

There are no chirality outliers.

All (223) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 3   | A     | 1002 | NAG  | C3-C2-N2-C7  |
| 3   | B     | 1002 | NAG  | C3-C2-N2-C7  |
| 3   | C     | 1002 | NAG  | C3-C2-N2-C7  |
| 3   | D     | 1002 | NAG  | C3-C2-N2-C7  |
| 4   | A     | 1006 | PX6  | O7-C2-C3-O5  |
| 4   | D     | 1006 | PX6  | O7-C2-C3-O5  |
| 6   | A     | 1010 | CHS  | N-CA-CB-CG   |
| 6   | A     | 1010 | CHS  | CA-CH-CM-C   |
| 6   | A     | 1010 | CHS  | OH-CH-CM-C   |
| 6   | A     | 1011 | CHS  | CA-CB-CG-CD1 |
| 6   | B     | 1010 | CHS  | N-CA-CB-CG   |
| 6   | B     | 1010 | CHS  | CA-CH-CM-C   |
| 6   | B     | 1010 | CHS  | OH-CH-CM-C   |
| 6   | B     | 1011 | CHS  | CA-CB-CG-CD1 |
| 6   | B     | 1011 | CHS  | CA-CB-CG-CD2 |
| 6   | C     | 1010 | CHS  | N-CA-CB-CG   |
| 6   | C     | 1010 | CHS  | CA-CH-CM-C   |
| 6   | C     | 1010 | CHS  | OH-CH-CM-C   |
| 6   | C     | 1011 | CHS  | CA-CB-CG-CD1 |
| 6   | D     | 1010 | CHS  | N-CA-CB-CG   |
| 6   | D     | 1010 | CHS  | CA-CH-CM-C   |
| 6   | D     | 1010 | CHS  | OH-CH-CM-C   |
| 6   | D     | 1011 | CHS  | CA-CB-CG-CD1 |
| 3   | A     | 1001 | NAG  | O5-C5-C6-O6  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | B     | 1001 | NAG  | O5-C5-C6-O6     |
| 3   | C     | 1001 | NAG  | O5-C5-C6-O6     |
| 3   | D     | 1001 | NAG  | O5-C5-C6-O6     |
| 3   | A     | 1001 | NAG  | C4-C5-C6-O6     |
| 3   | B     | 1001 | NAG  | C4-C5-C6-O6     |
| 3   | C     | 1001 | NAG  | C4-C5-C6-O6     |
| 3   | D     | 1001 | NAG  | C4-C5-C6-O6     |
| 3   | A     | 1005 | NAG  | O5-C5-C6-O6     |
| 3   | B     | 1005 | NAG  | O5-C5-C6-O6     |
| 3   | C     | 1005 | NAG  | O5-C5-C6-O6     |
| 3   | D     | 1005 | NAG  | O5-C5-C6-O6     |
| 3   | A     | 1005 | NAG  | C4-C5-C6-O6     |
| 3   | B     | 1005 | NAG  | C4-C5-C6-O6     |
| 3   | C     | 1005 | NAG  | C4-C5-C6-O6     |
| 3   | D     | 1005 | NAG  | C4-C5-C6-O6     |
| 5   | D     | 1009 | PLM  | C4-C5-C6-C7     |
| 4   | D     | 1006 | PX6  | C25-C26-C27-C28 |
| 4   | C     | 1006 | PX6  | C25-C26-C27-C28 |
| 5   | B     | 1009 | PLM  | C4-C5-C6-C7     |
| 5   | C     | 1009 | PLM  | C4-C5-C6-C7     |
| 4   | B     | 1006 | PX6  | C25-C26-C27-C28 |
| 5   | A     | 1009 | PLM  | C4-C5-C6-C7     |
| 5   | B     | 1008 | PLM  | C4-C5-C6-C7     |
| 5   | C     | 1008 | PLM  | C4-C5-C6-C7     |
| 4   | A     | 1006 | PX6  | C25-C26-C27-C28 |
| 5   | A     | 1008 | PLM  | C4-C5-C6-C7     |
| 4   | B     | 1006 | PX6  | O7-C2-C3-O5     |
| 4   | C     | 1006 | PX6  | O7-C2-C3-O5     |
| 5   | B     | 1007 | PLM  | CA-CB-CC-CD     |
| 3   | A     | 1002 | NAG  | O5-C5-C6-O6     |
| 3   | B     | 1002 | NAG  | O5-C5-C6-O6     |
| 3   | C     | 1002 | NAG  | O5-C5-C6-O6     |
| 3   | D     | 1002 | NAG  | O5-C5-C6-O6     |
| 5   | D     | 1007 | PLM  | CA-CB-CC-CD     |
| 5   | C     | 1007 | PLM  | CA-CB-CC-CD     |
| 5   | A     | 1007 | PLM  | CA-CB-CC-CD     |
| 5   | D     | 1008 | PLM  | C4-C5-C6-C7     |
| 4   | B     | 1006 | PX6  | C23-C24-C25-C26 |
| 4   | C     | 1006 | PX6  | C23-C24-C25-C26 |
| 4   | D     | 1006 | PX6  | C23-C24-C25-C26 |
| 4   | D     | 1006 | PX6  | C27-C28-C29-C30 |
| 4   | C     | 1006 | PX6  | C27-C28-C29-C30 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | A     | 1006 | PX6  | C23-C24-C25-C26 |
| 4   | B     | 1006 | PX6  | C27-C28-C29-C30 |
| 4   | A     | 1006 | PX6  | C27-C28-C29-C30 |
| 4   | A     | 1006 | PX6  | C21-C20-O7-C2   |
| 5   | A     | 1007 | PLM  | CC-CD-CE-CF     |
| 5   | B     | 1007 | PLM  | CC-CD-CE-CF     |
| 5   | D     | 1007 | PLM  | CC-CD-CE-CF     |
| 4   | A     | 1006 | PX6  | O8-C20-O7-C2    |
| 4   | B     | 1006 | PX6  | C21-C20-O7-C2   |
| 4   | C     | 1006 | PX6  | C21-C20-O7-C2   |
| 4   | D     | 1006 | PX6  | C21-C20-O7-C2   |
| 5   | C     | 1007 | PLM  | CC-CD-CE-CF     |
| 6   | A     | 1011 | CHS  | CA-CB-CG-CD2    |
| 6   | C     | 1011 | CHS  | CA-CB-CG-CD2    |
| 6   | D     | 1011 | CHS  | CA-CB-CG-CD2    |
| 5   | A     | 1007 | PLM  | C6-C7-C8-C9     |
| 4   | A     | 1006 | PX6  | C28-C29-C30-C31 |
| 4   | B     | 1006 | PX6  | C28-C29-C30-C31 |
| 4   | C     | 1006 | PX6  | C28-C29-C30-C31 |
| 4   | D     | 1006 | PX6  | C28-C29-C30-C31 |
| 5   | C     | 1007 | PLM  | C6-C7-C8-C9     |
| 5   | D     | 1007 | PLM  | C6-C7-C8-C9     |
| 4   | B     | 1006 | PX6  | O8-C20-O7-C2    |
| 4   | C     | 1006 | PX6  | O8-C20-O7-C2    |
| 4   | D     | 1006 | PX6  | O8-C20-O7-C2    |
| 5   | B     | 1007 | PLM  | C6-C7-C8-C9     |
| 4   | A     | 1006 | PX6  | C22-C23-C24-C25 |
| 4   | B     | 1006 | PX6  | C26-C27-C28-C29 |
| 4   | A     | 1006 | PX6  | C26-C27-C28-C29 |
| 4   | C     | 1006 | PX6  | C22-C23-C24-C25 |
| 4   | C     | 1006 | PX6  | C26-C27-C28-C29 |
| 4   | D     | 1006 | PX6  | C26-C27-C28-C29 |
| 4   | B     | 1006 | PX6  | C22-C23-C24-C25 |
| 4   | D     | 1006 | PX6  | C22-C23-C24-C25 |
| 5   | B     | 1007 | PLM  | C2-C3-C4-C5     |
| 4   | C     | 1006 | PX6  | C7-C8-C9-C10    |
| 5   | D     | 1007 | PLM  | C2-C3-C4-C5     |
| 5   | A     | 1007 | PLM  | C2-C3-C4-C5     |
| 4   | A     | 1006 | PX6  | C7-C8-C9-C10    |
| 4   | B     | 1006 | PX6  | C7-C8-C9-C10    |
| 5   | C     | 1007 | PLM  | C2-C3-C4-C5     |
| 4   | A     | 1006 | PX6  | C21-C22-C23-C24 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | B     | 1007 | PLM  | C4-C5-C6-C7     |
| 4   | D     | 1006 | PX6  | C7-C8-C9-C10    |
| 5   | D     | 1008 | PLM  | C2-C3-C4-C5     |
| 5   | D     | 1007 | PLM  | C4-C5-C6-C7     |
| 5   | C     | 1007 | PLM  | C4-C5-C6-C7     |
| 4   | B     | 1006 | PX6  | C21-C22-C23-C24 |
| 4   | C     | 1006 | PX6  | C21-C22-C23-C24 |
| 5   | A     | 1007 | PLM  | C4-C5-C6-C7     |
| 4   | A     | 1006 | PX6  | C31-C32-C33-C34 |
| 4   | D     | 1006 | PX6  | C21-C22-C23-C24 |
| 4   | D     | 1006 | PX6  | C20-C21-C22-C23 |
| 4   | B     | 1006 | PX6  | C31-C32-C33-C34 |
| 4   | D     | 1006 | PX6  | C31-C32-C33-C34 |
| 4   | C     | 1006 | PX6  | C20-C21-C22-C23 |
| 4   | C     | 1006 | PX6  | C29-C30-C31-C32 |
| 4   | B     | 1006 | PX6  | C20-C21-C22-C23 |
| 5   | C     | 1009 | PLM  | C6-C7-C8-C9     |
| 4   | A     | 1006 | PX6  | C32-C33-C34-C35 |
| 5   | A     | 1007 | PLM  | C3-C4-C5-C6     |
| 5   | D     | 1009 | PLM  | C6-C7-C8-C9     |
| 4   | B     | 1006 | PX6  | C32-C33-C34-C35 |
| 4   | D     | 1006 | PX6  | C32-C33-C34-C35 |
| 4   | D     | 1006 | PX6  | C29-C30-C31-C32 |
| 5   | B     | 1009 | PLM  | C6-C7-C8-C9     |
| 4   | C     | 1006 | PX6  | C32-C33-C34-C35 |
| 5   | C     | 1007 | PLM  | C3-C4-C5-C6     |
| 5   | D     | 1007 | PLM  | C3-C4-C5-C6     |
| 4   | C     | 1006 | PX6  | C31-C32-C33-C34 |
| 4   | B     | 1006 | PX6  | C29-C30-C31-C32 |
| 5   | B     | 1007 | PLM  | C3-C4-C5-C6     |
| 5   | A     | 1008 | PLM  | CD-CE-CF-CG     |
| 5   | D     | 1008 | PLM  | CD-CE-CF-CG     |
| 5   | C     | 1008 | PLM  | C1-C2-C3-C4     |
| 5   | C     | 1008 | PLM  | CD-CE-CF-CG     |
| 5   | B     | 1008 | PLM  | CD-CE-CF-CG     |
| 4   | A     | 1006 | PX6  | C20-C21-C22-C23 |
| 4   | A     | 1006 | PX6  | C29-C30-C31-C32 |
| 4   | A     | 1006 | PX6  | C1-C2-C3-O5     |
| 4   | B     | 1006 | PX6  | C1-C2-C3-O5     |
| 4   | C     | 1006 | PX6  | C1-C2-C3-O5     |
| 4   | D     | 1006 | PX6  | C1-C2-C3-O5     |
| 5   | B     | 1008 | PLM  | C1-C2-C3-C4     |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 5   | A     | 1007 | PLM  | CB-CC-CD-CE |
| 5   | C     | 1007 | PLM  | CB-CC-CD-CE |
| 5   | D     | 1007 | PLM  | CB-CC-CD-CE |
| 5   | B     | 1007 | PLM  | CB-CC-CD-CE |
| 5   | A     | 1008 | PLM  | C1-C2-C3-C4 |
| 5   | D     | 1007 | PLM  | C8-C9-CA-CB |
| 5   | C     | 1007 | PLM  | C8-C9-CA-CB |
| 5   | A     | 1009 | PLM  | C7-C8-C9-CA |
| 4   | B     | 1006 | PX6  | C1-O4-P1-O3 |
| 5   | B     | 1007 | PLM  | C8-C9-CA-CB |
| 5   | D     | 1007 | PLM  | C9-CA-CB-CC |
| 5   | B     | 1007 | PLM  | C9-CA-CB-CC |
| 5   | D     | 1009 | PLM  | C7-C8-C9-CA |
| 5   | C     | 1009 | PLM  | C7-C8-C9-CA |
| 5   | C     | 1007 | PLM  | C9-CA-CB-CC |
| 5   | A     | 1007 | PLM  | C8-C9-CA-CB |
| 6   | B     | 1011 | CHS  | N-CA-CB-CG  |
| 5   | B     | 1009 | PLM  | C7-C8-C9-CA |
| 5   | B     | 1009 | PLM  | C5-C6-C7-C8 |
| 4   | D     | 1006 | PX6  | C5-C6-C7-C8 |
| 4   | B     | 1006 | PX6  | C5-C6-C7-C8 |
| 5   | A     | 1009 | PLM  | C6-C7-C8-C9 |
| 5   | A     | 1009 | PLM  | CB-CC-CD-CE |
| 4   | C     | 1006 | PX6  | C5-C6-C7-C8 |
| 5   | A     | 1007 | PLM  | C9-CA-CB-CC |
| 5   | B     | 1009 | PLM  | CB-CC-CD-CE |
| 5   | C     | 1007 | PLM  | O2-C1-C2-C3 |
| 5   | D     | 1007 | PLM  | O2-C1-C2-C3 |
| 5   | A     | 1007 | PLM  | O2-C1-C2-C3 |
| 5   | B     | 1007 | PLM  | O2-C1-C2-C3 |
| 3   | B     | 1002 | NAG  | C4-C5-C6-O6 |
| 3   | D     | 1002 | NAG  | C4-C5-C6-O6 |
| 5   | D     | 1009 | PLM  | CB-CC-CD-CE |
| 5   | C     | 1009 | PLM  | CB-CC-CD-CE |
| 3   | A     | 1002 | NAG  | C4-C5-C6-O6 |
| 3   | C     | 1002 | NAG  | C4-C5-C6-O6 |
| 5   | A     | 1008 | PLM  | O2-C1-C2-C3 |
| 5   | A     | 1007 | PLM  | O1-C1-C2-C3 |
| 5   | B     | 1008 | PLM  | O1-C1-C2-C3 |
| 5   | A     | 1009 | PLM  | O1-C1-C2-C3 |
| 5   | C     | 1007 | PLM  | O1-C1-C2-C3 |
| 5   | C     | 1009 | PLM  | C5-C6-C7-C8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | D     | 1006 | PX6  | C24-C25-C26-C27 |
| 5   | B     | 1008 | PLM  | O2-C1-C2-C3     |
| 5   | B     | 1009 | PLM  | O1-C1-C2-C3     |
| 5   | D     | 1007 | PLM  | O1-C1-C2-C3     |
| 5   | C     | 1008 | PLM  | C6-C7-C8-C9     |
| 4   | B     | 1006 | PX6  | C24-C25-C26-C27 |
| 4   | C     | 1006 | PX6  | C24-C25-C26-C27 |
| 5   | D     | 1009 | PLM  | O1-C1-C2-C3     |
| 5   | B     | 1008 | PLM  | C6-C7-C8-C9     |
| 5   | B     | 1007 | PLM  | O1-C1-C2-C3     |
| 5   | C     | 1008 | PLM  | O1-C1-C2-C3     |
| 5   | C     | 1009 | PLM  | O1-C1-C2-C3     |
| 5   | C     | 1009 | PLM  | O2-C1-C2-C3     |
| 5   | D     | 1009 | PLM  | O2-C1-C2-C3     |
| 5   | A     | 1008 | PLM  | O1-C1-C2-C3     |
| 5   | A     | 1009 | PLM  | O2-C1-C2-C3     |
| 5   | B     | 1009 | PLM  | O2-C1-C2-C3     |
| 5   | C     | 1008 | PLM  | O2-C1-C2-C3     |
| 5   | A     | 1008 | PLM  | C6-C7-C8-C9     |
| 4   | A     | 1006 | PX6  | C5-C6-C7-C8     |
| 5   | D     | 1009 | PLM  | C5-C6-C7-C8     |
| 4   | A     | 1006 | PX6  | C24-C25-C26-C27 |
| 5   | D     | 1008 | PLM  | C7-C8-C9-CA     |
| 6   | B     | 1011 | CHS  | CH-CA-CB-CG     |
| 5   | B     | 1009 | PLM  | CC-CD-CE-CF     |
| 5   | C     | 1009 | PLM  | CC-CD-CE-CF     |
| 5   | D     | 1009 | PLM  | CC-CD-CE-CF     |
| 4   | A     | 1006 | PX6  | C10-C11-C12-C13 |
| 5   | D     | 1008 | PLM  | O1-C1-C2-C3     |
| 5   | C     | 1008 | PLM  | C5-C6-C7-C8     |
| 5   | D     | 1008 | PLM  | O2-C1-C2-C3     |

There are no ring outliers.

30 monomers are involved in 99 short contacts:

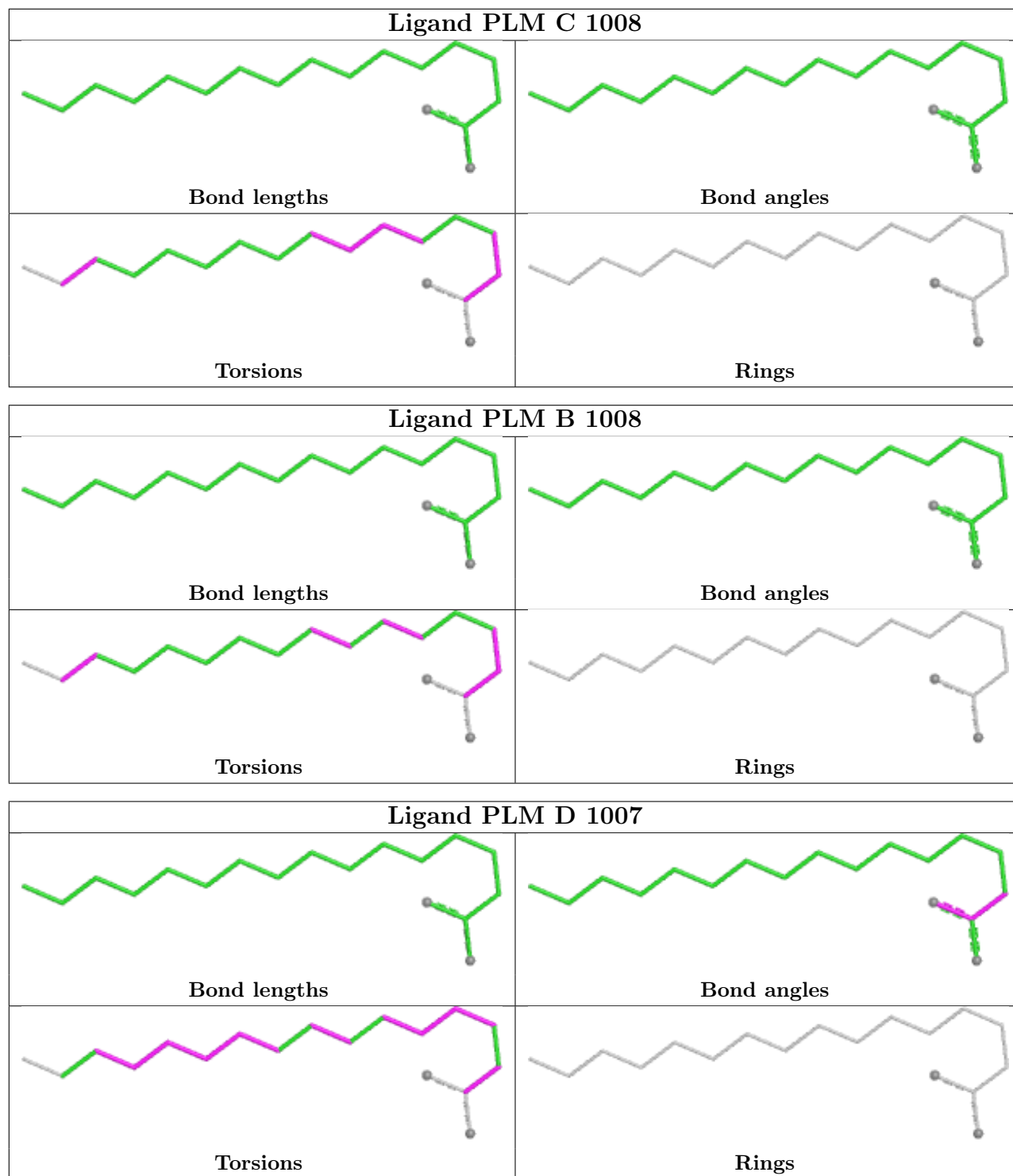
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | C     | 1008 | PLM  | 1       | 0            |
| 3   | C     | 1001 | NAG  | 3       | 0            |
| 5   | B     | 1008 | PLM  | 1       | 0            |
| 5   | D     | 1007 | PLM  | 3       | 0            |
| 3   | C     | 1005 | NAG  | 2       | 0            |
| 4   | A     | 1006 | PX6  | 2       | 0            |

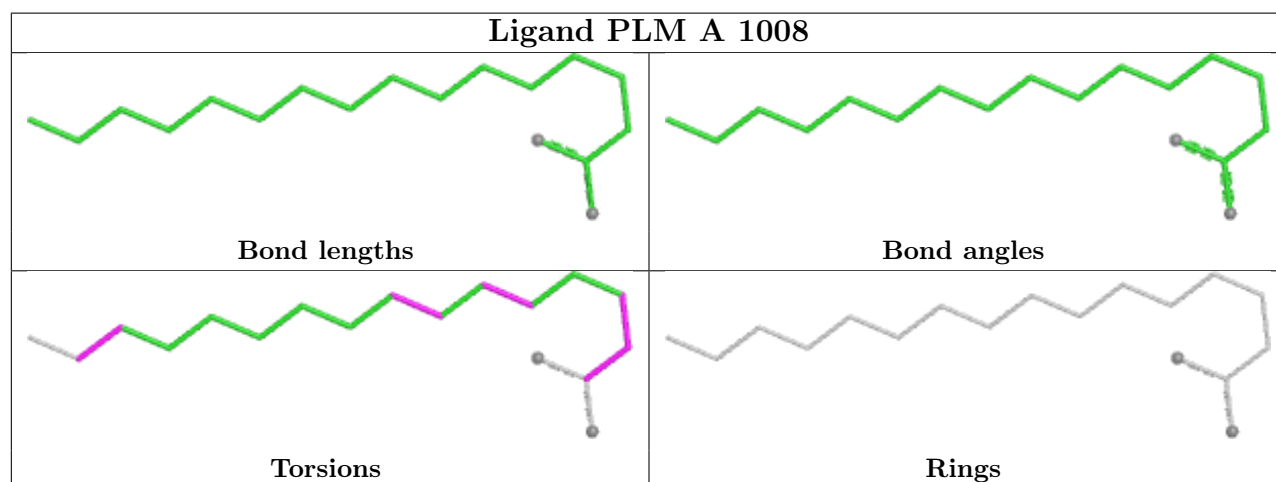
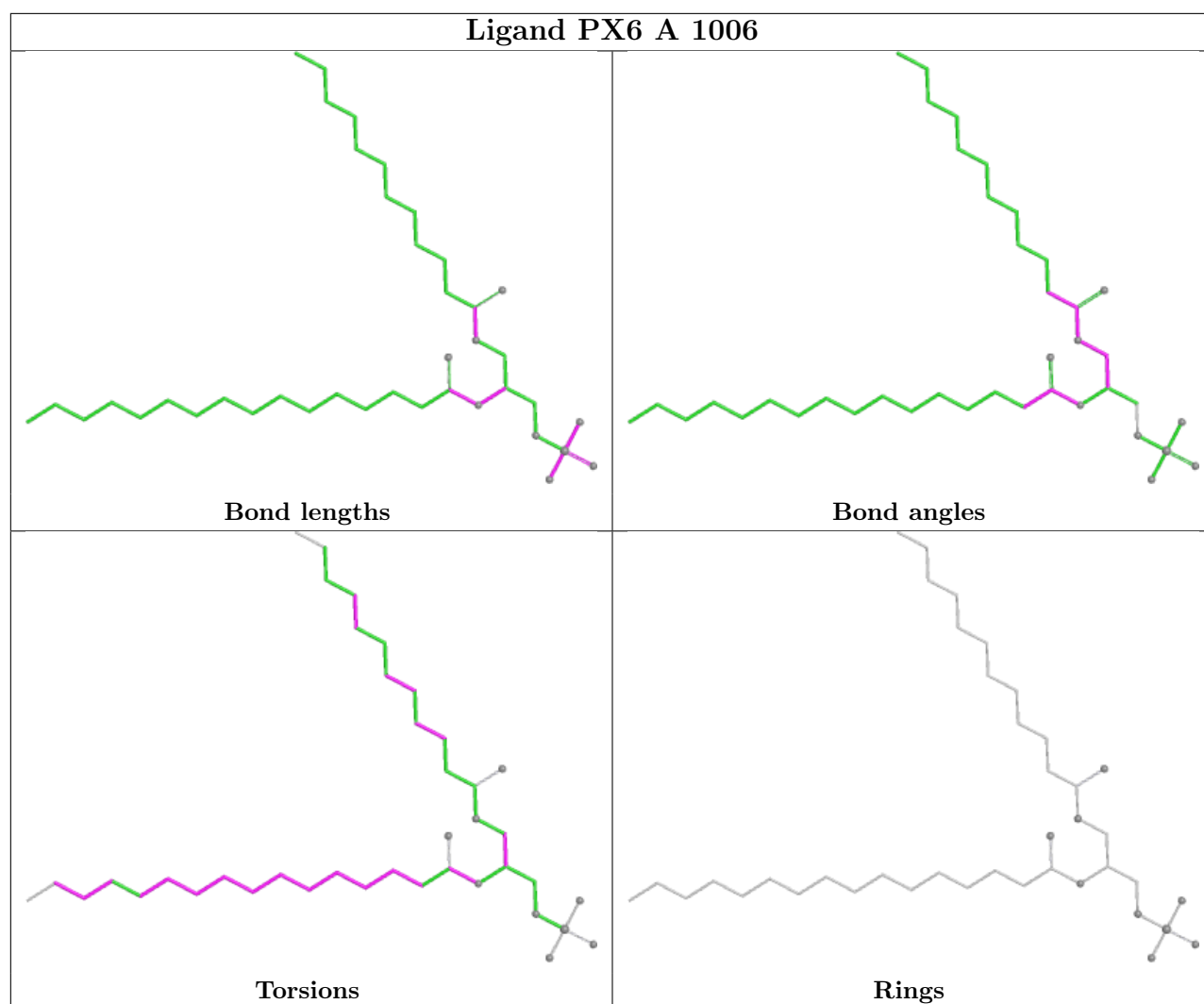
*Continued on next page...*

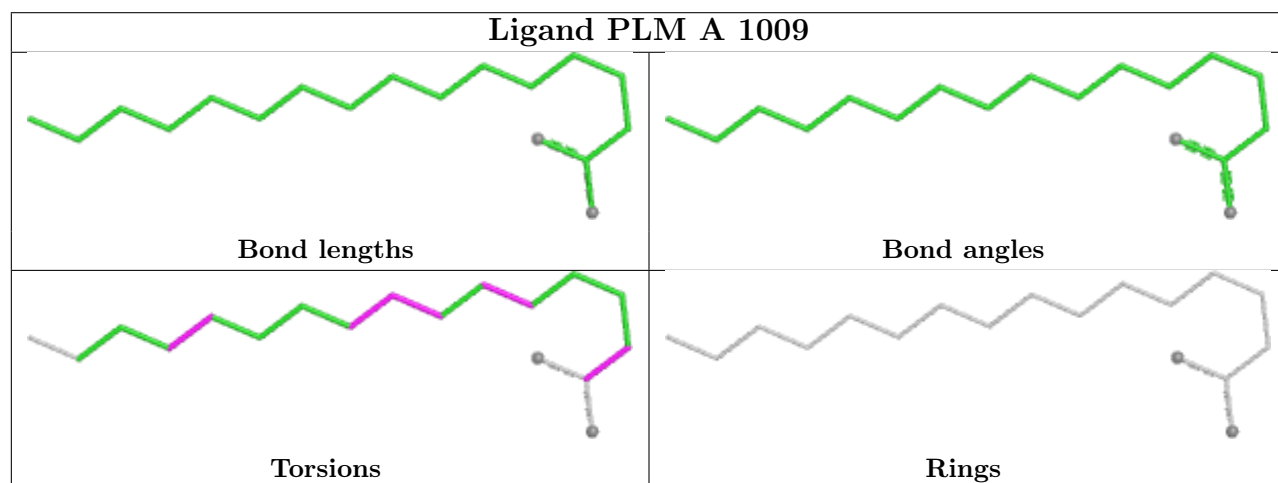
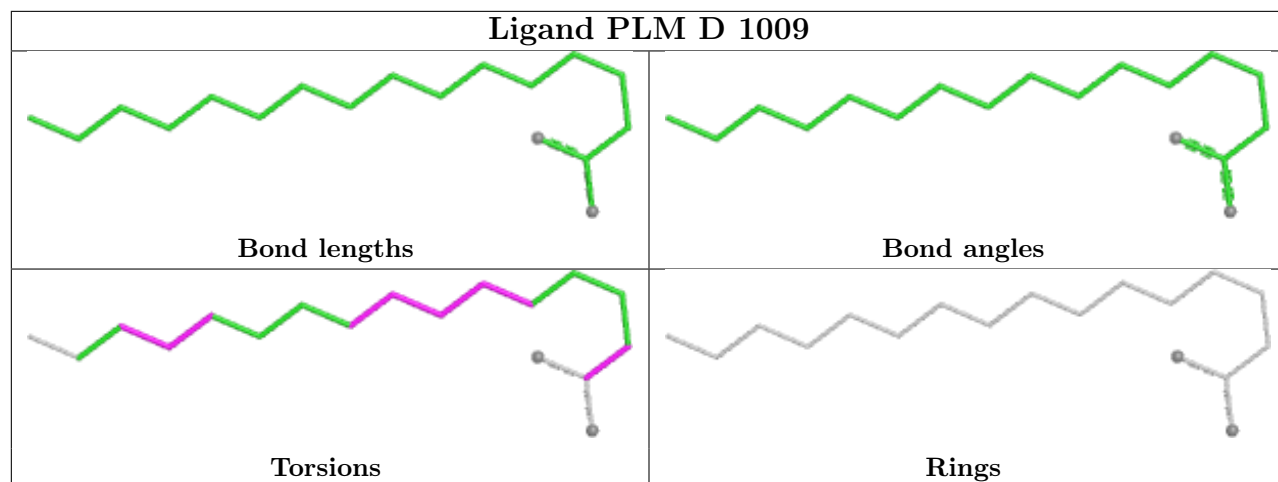
*Continued from previous page...*

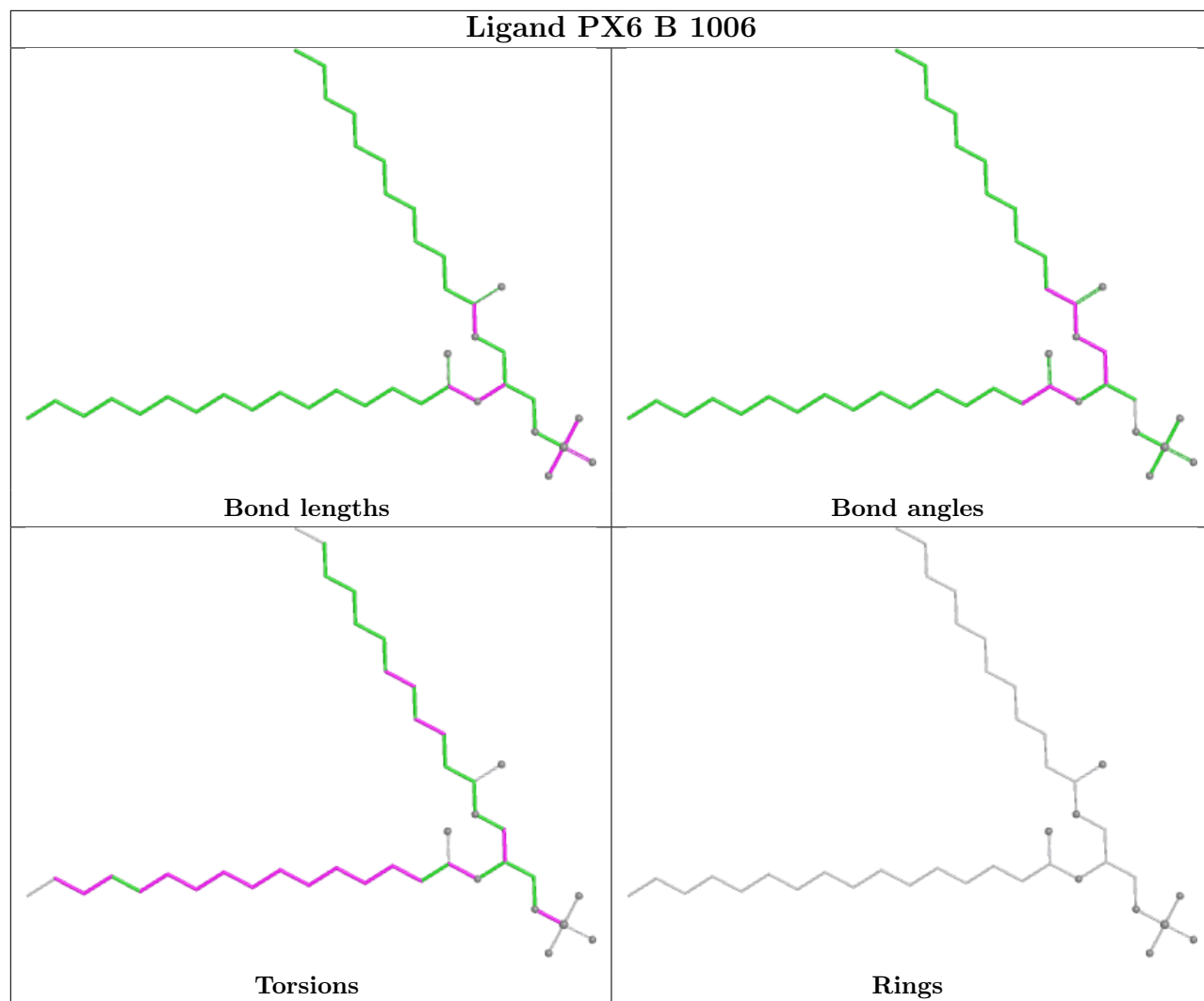
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6   | D     | 1010 | CHS  | 1       | 0            |
| 3   | C     | 1002 | NAG  | 10      | 0            |
| 5   | A     | 1008 | PLM  | 1       | 0            |
| 6   | A     | 1011 | CHS  | 1       | 0            |
| 5   | D     | 1009 | PLM  | 1       | 0            |
| 3   | A     | 1001 | NAG  | 3       | 0            |
| 3   | B     | 1002 | NAG  | 10      | 0            |
| 3   | B     | 1005 | NAG  | 2       | 0            |
| 6   | A     | 1010 | CHS  | 1       | 0            |
| 4   | B     | 1006 | PX6  | 4       | 0            |
| 4   | C     | 1006 | PX6  | 5       | 0            |
| 5   | B     | 1007 | PLM  | 4       | 0            |
| 3   | A     | 1002 | NAG  | 10      | 0            |
| 3   | D     | 1005 | NAG  | 2       | 0            |
| 5   | A     | 1007 | PLM  | 4       | 0            |
| 3   | B     | 1001 | NAG  | 3       | 0            |
| 4   | D     | 1006 | PX6  | 4       | 0            |
| 5   | C     | 1007 | PLM  | 3       | 0            |
| 3   | D     | 1002 | NAG  | 10      | 0            |
| 6   | B     | 1010 | CHS  | 1       | 0            |
| 6   | B     | 1011 | CHS  | 1       | 0            |
| 3   | D     | 1001 | NAG  | 3       | 0            |
| 6   | C     | 1010 | CHS  | 1       | 0            |
| 3   | A     | 1005 | NAG  | 2       | 0            |

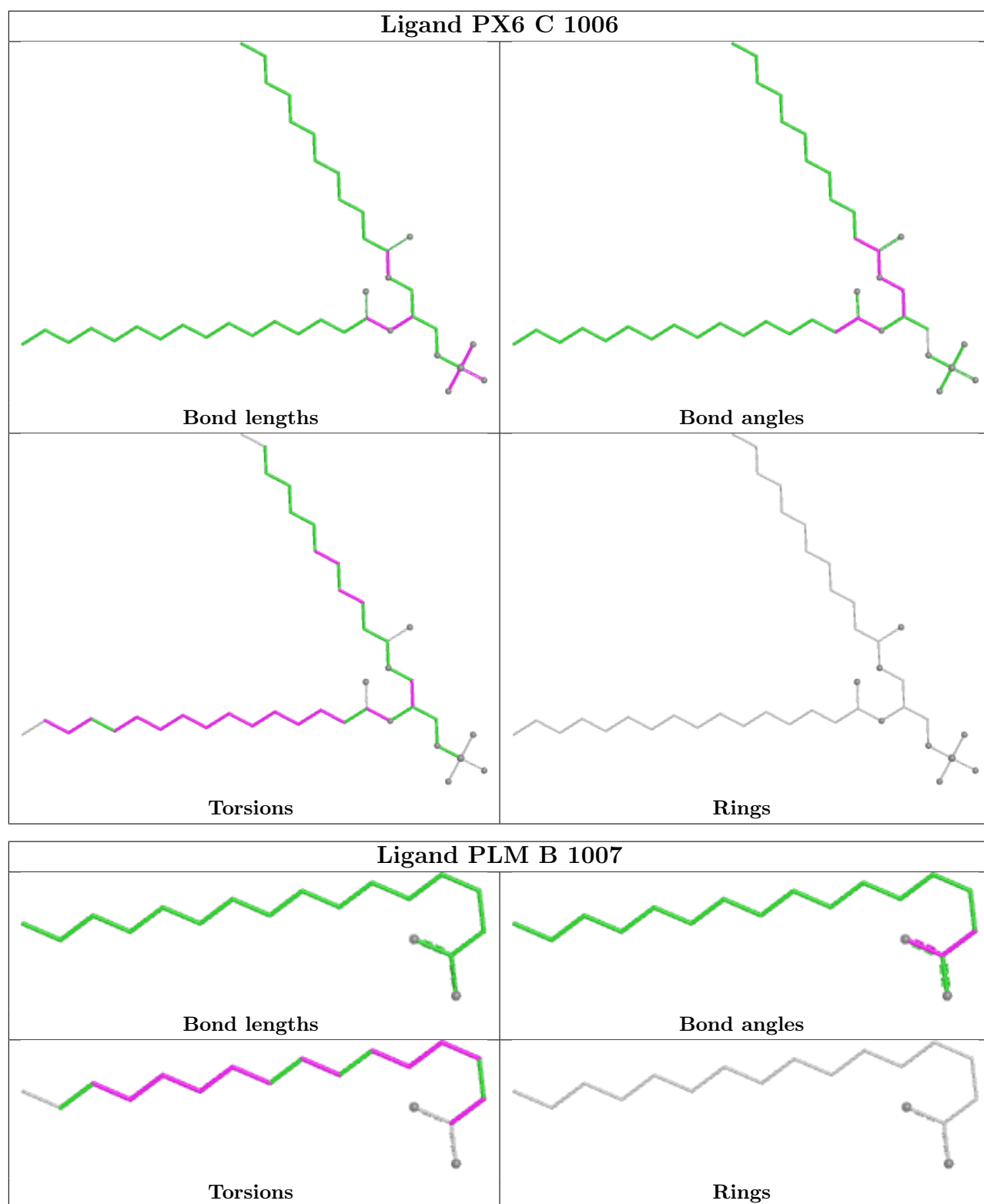
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

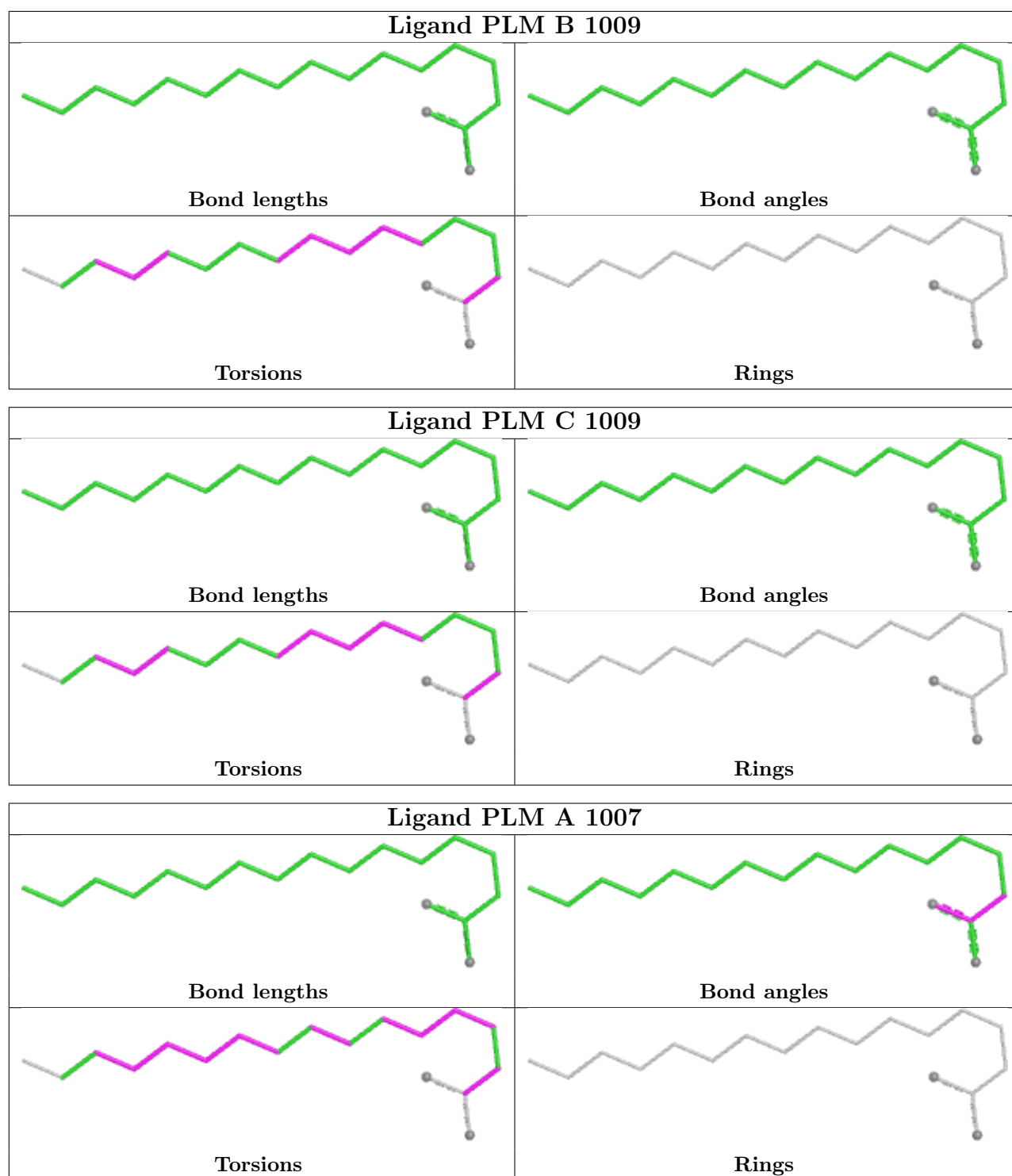


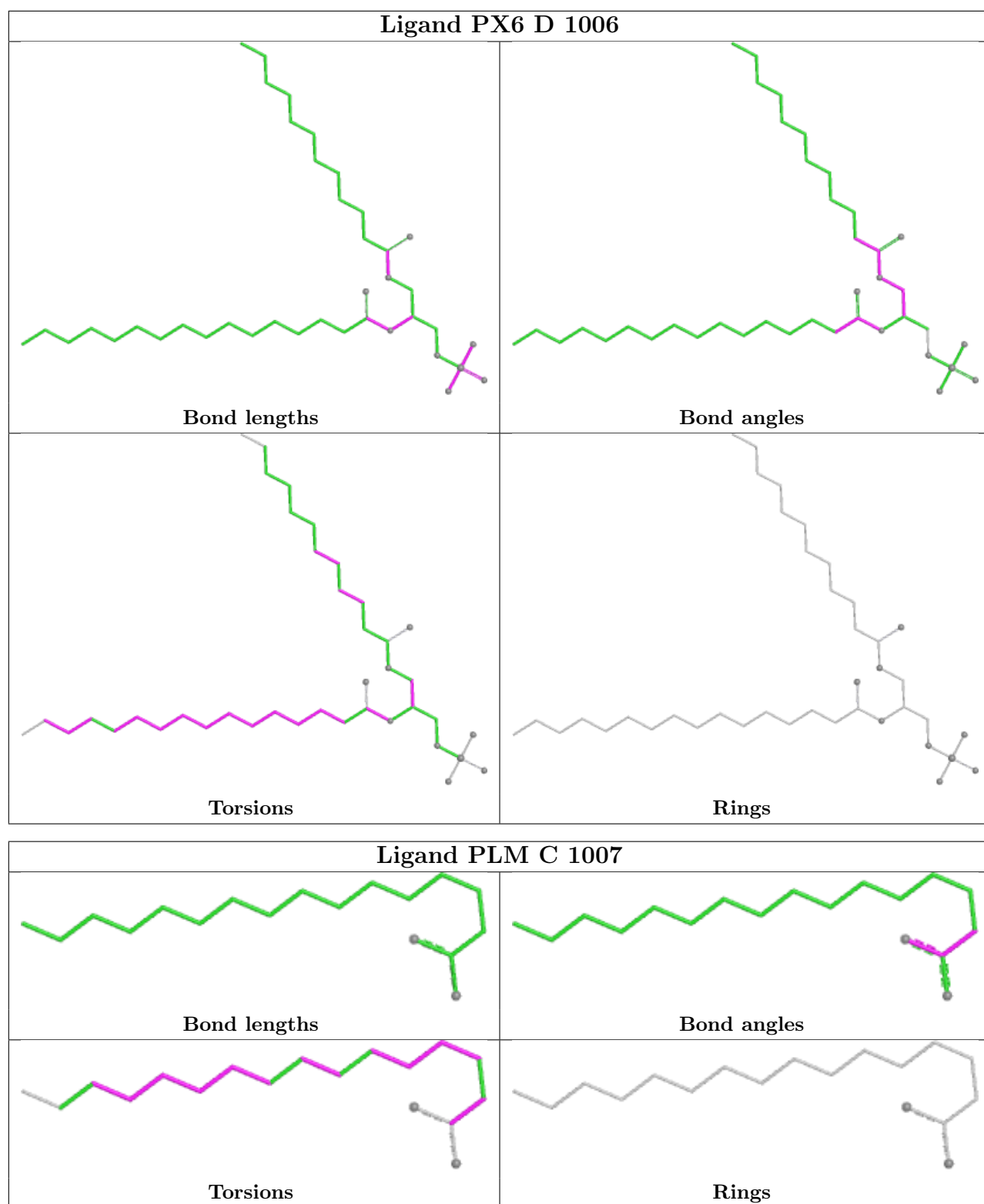


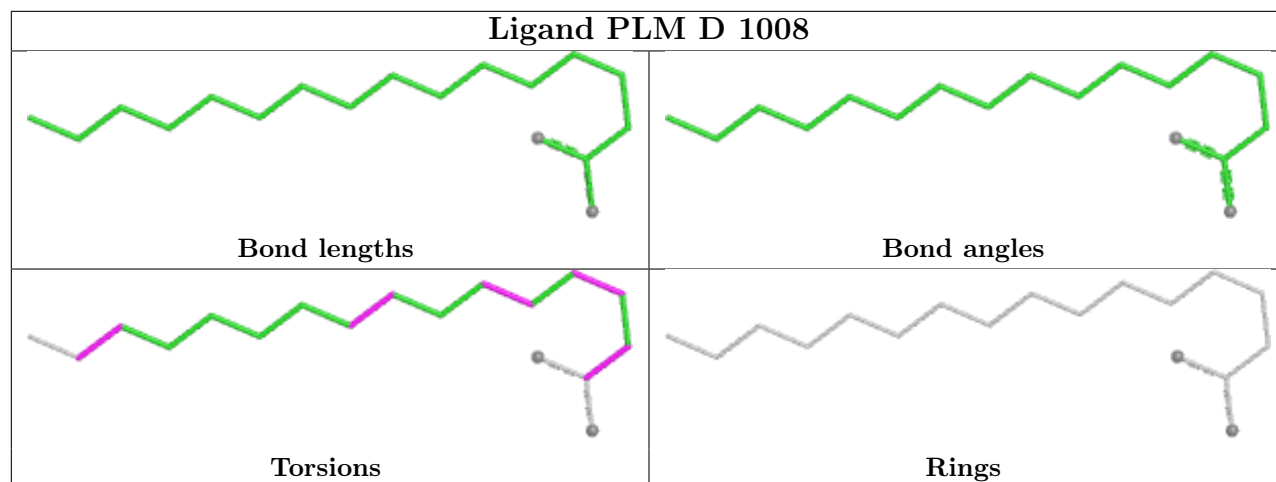












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

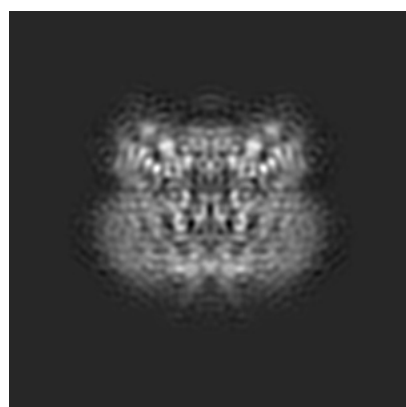
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3524. These allow visual inspection of the internal detail of the map and identification of artifacts.

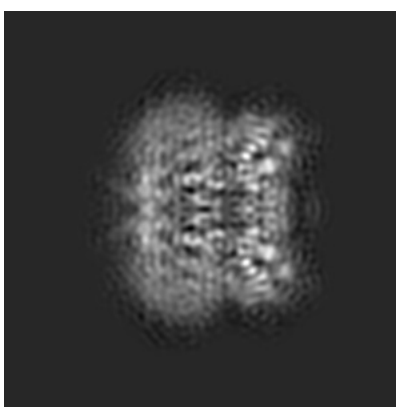
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

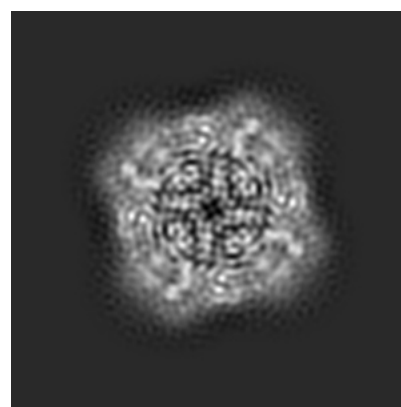
#### 6.1.1 Primary map



X



Y

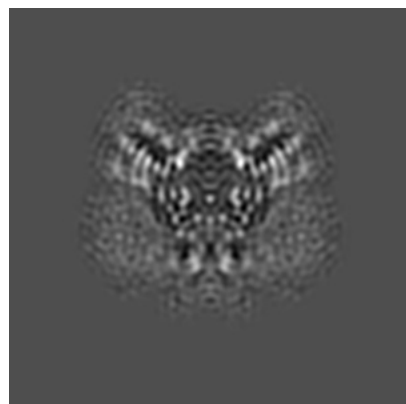


Z

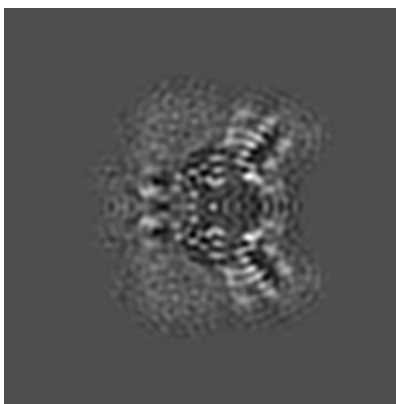
The images above show the map projected in three orthogonal directions.

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

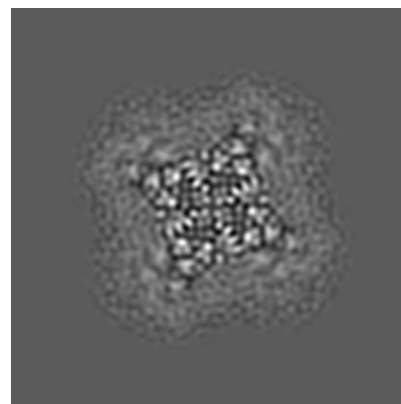
#### 6.2.1 Primary map



X Index: 84



Y Index: 84

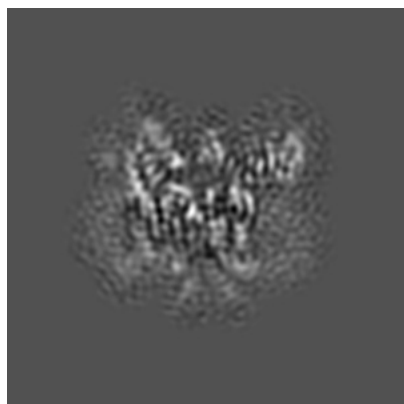


Z Index: 84

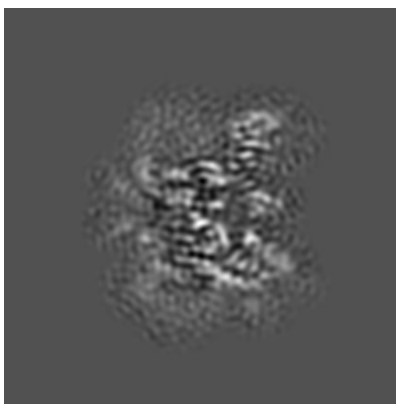
The images above show central slices of the map in three orthogonal directions.

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

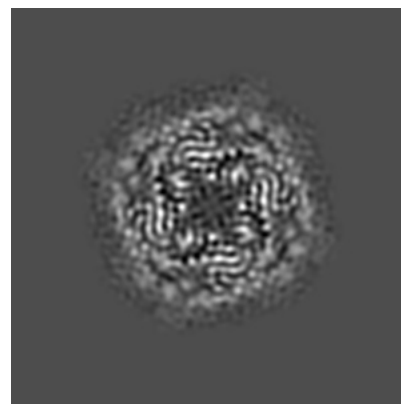
### 6.3.1 Primary map



X Index: 74



Y Index: 94

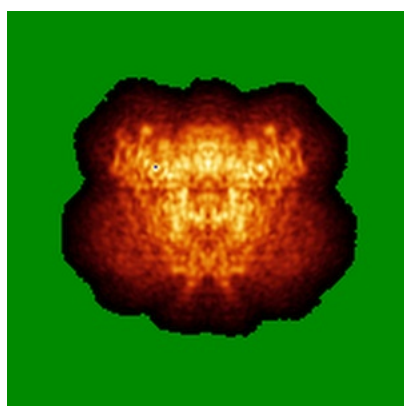


Z Index: 102

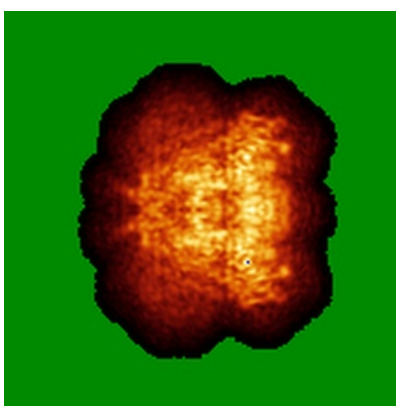
The images above show the largest variance slices of the map in three orthogonal directions.

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

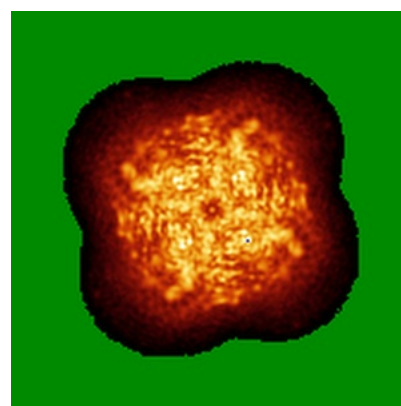
### 6.4.1 Primary map



X



Y

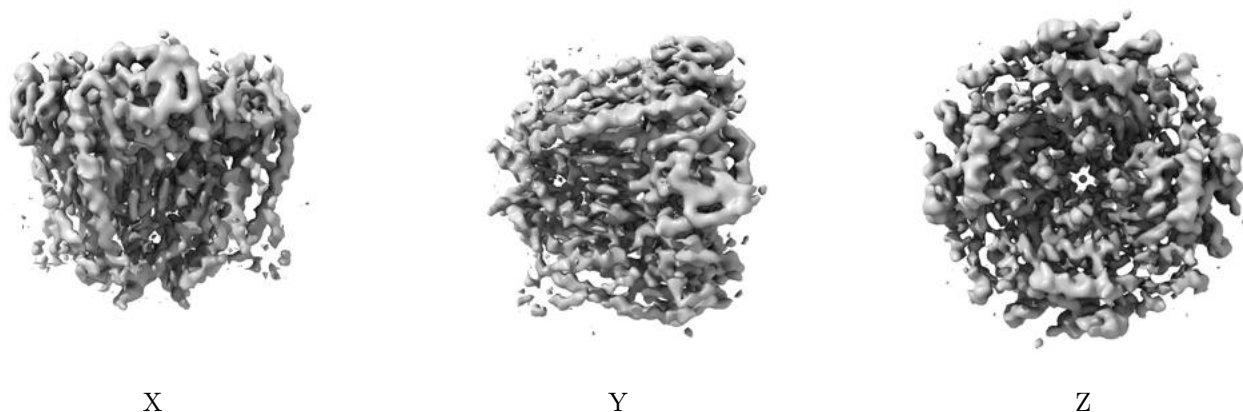


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0354. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

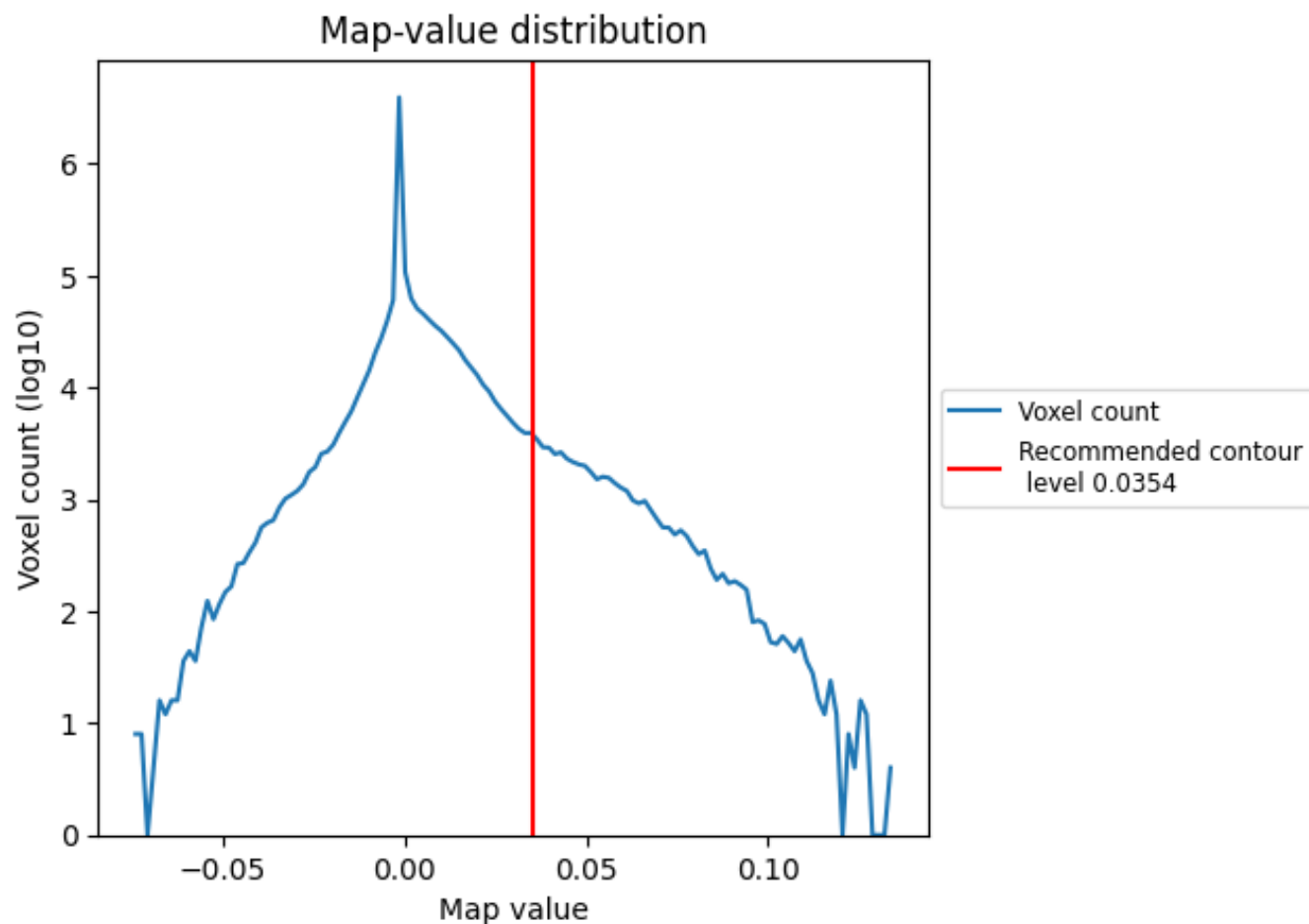
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

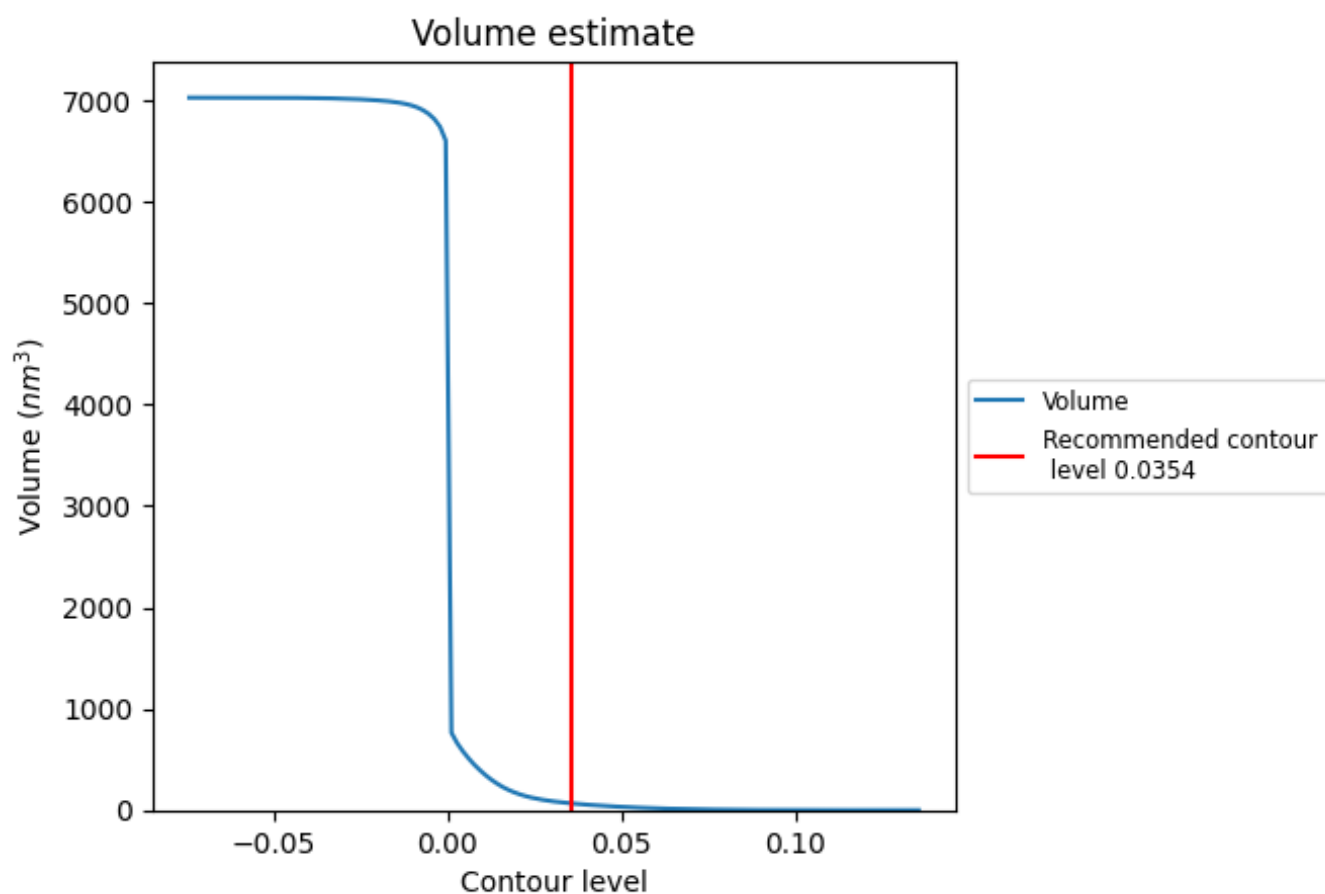
This section contains the results of statistical analysis of the map.

### 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.

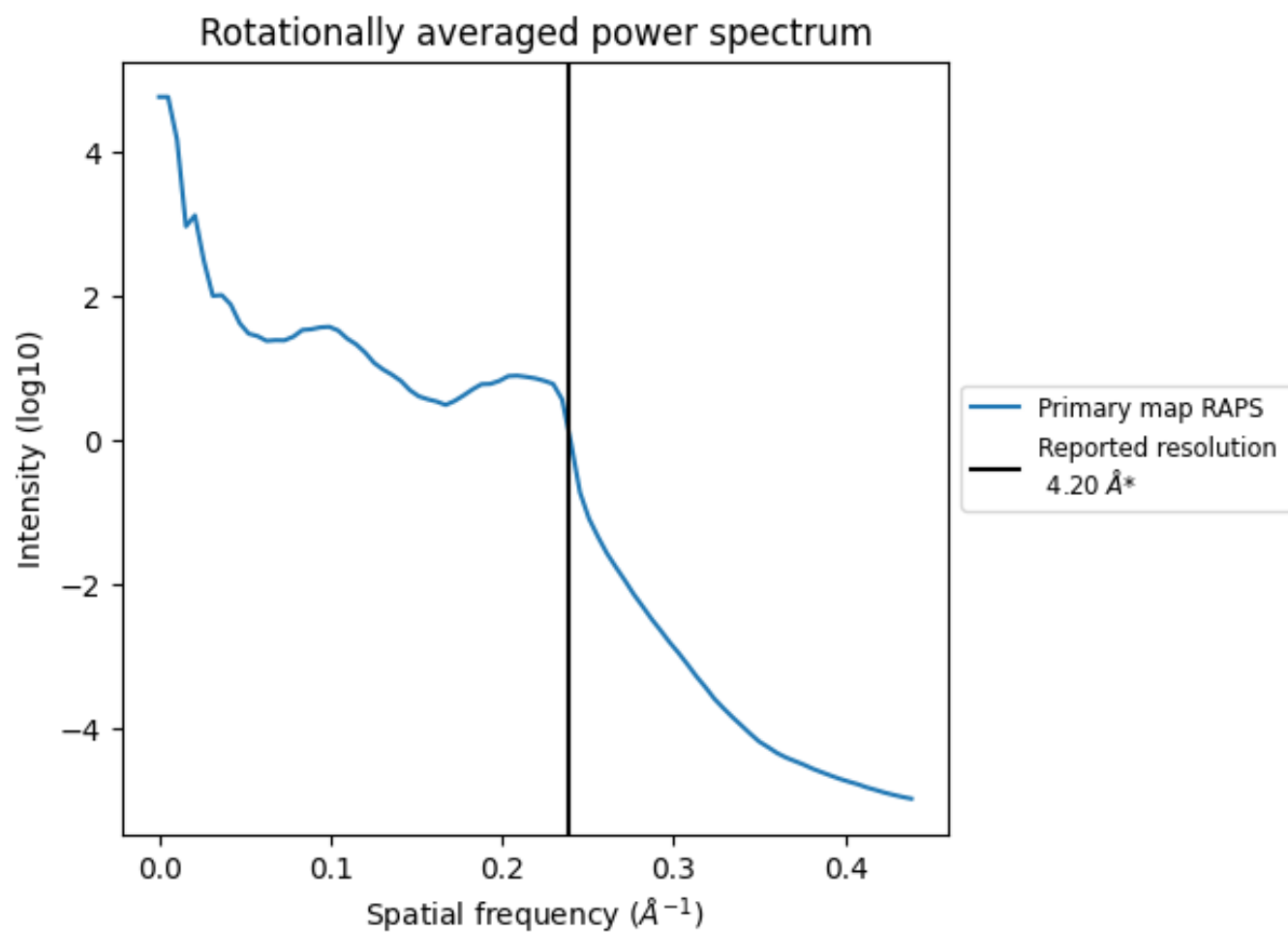
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 68  $\text{nm}^3$ ; this corresponds to an approximate mass of 61 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 ⓘ

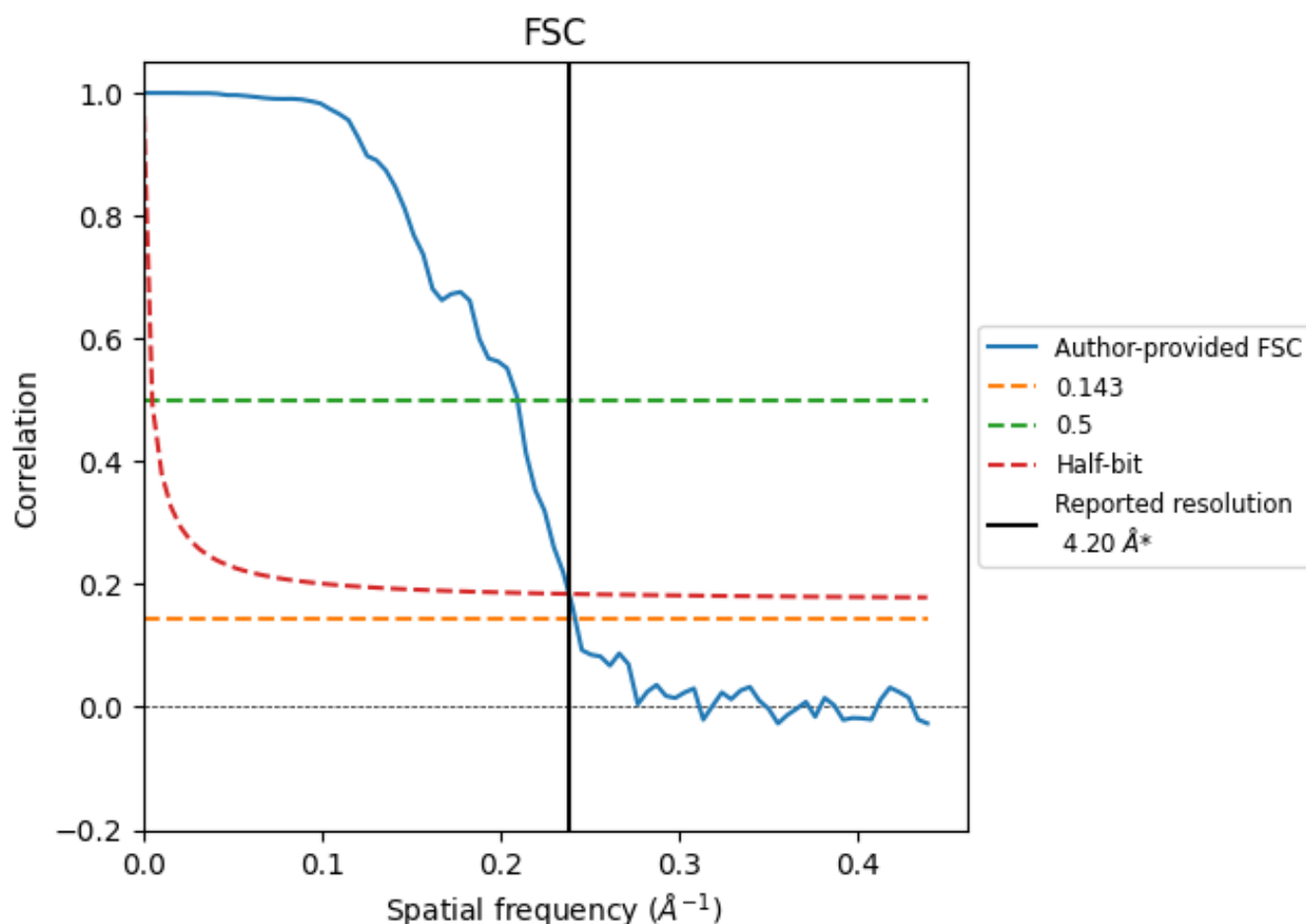


\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

## 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 0.238 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

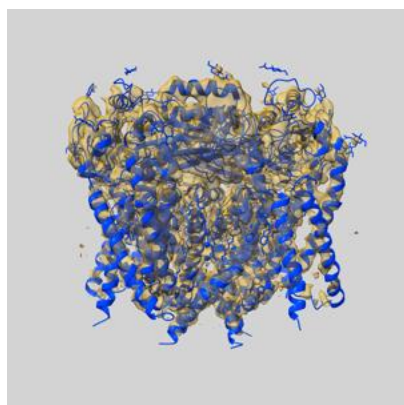
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.20                               | -    | -        |
| Author-provided FSC curve | 4.14                               | 4.78 | 4.20     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

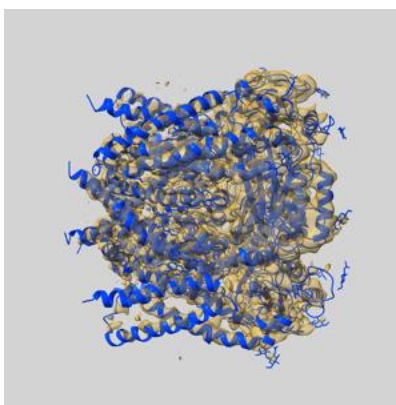
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3524 and PDB model 5MKF. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

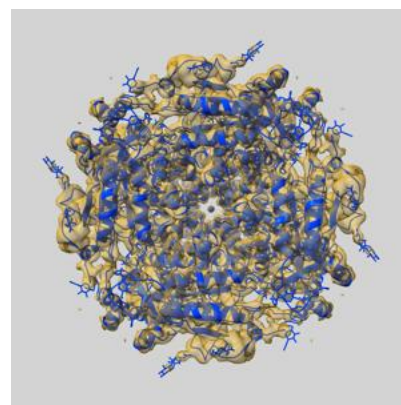
### 9.1 Map-model overlay [i](#)



X



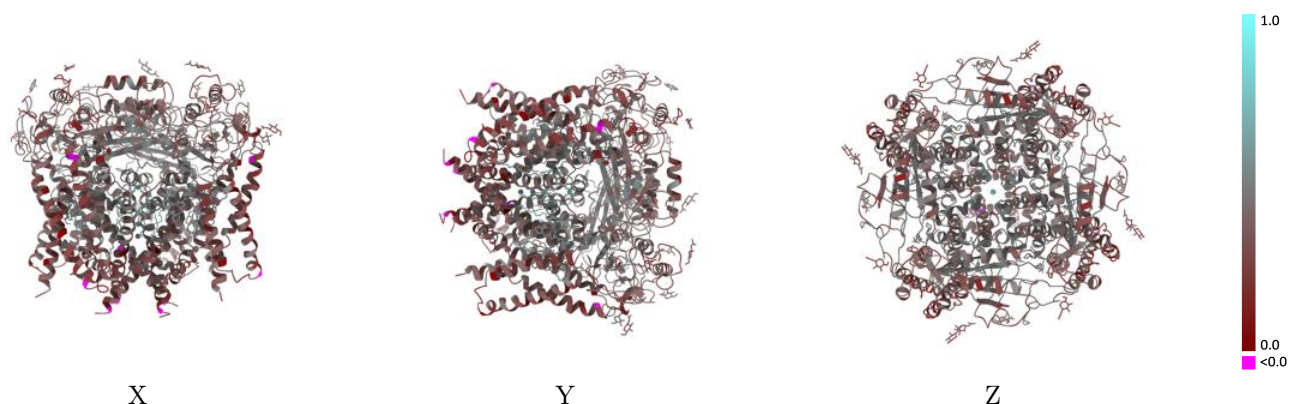
Y



Z

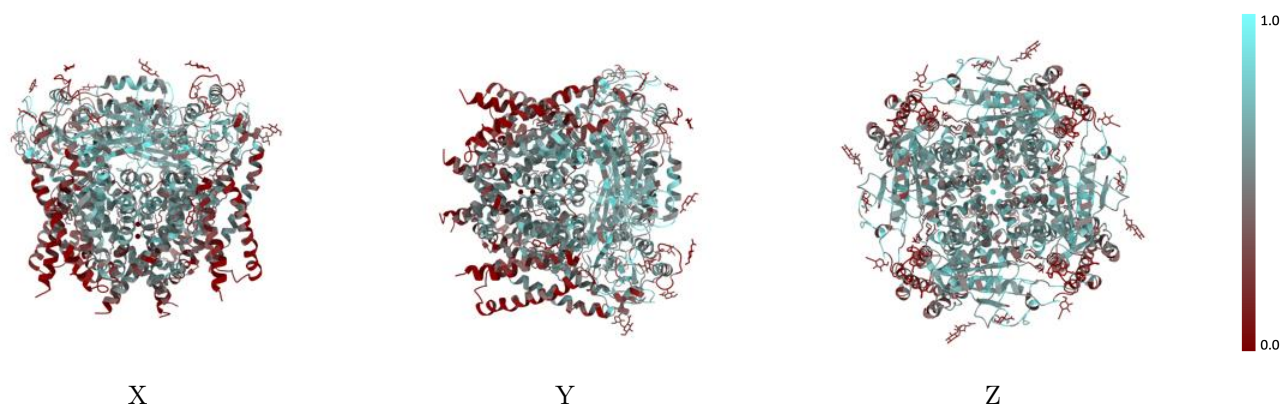
The images above show the 3D surface view of the map at the recommended contour level 0.0354 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



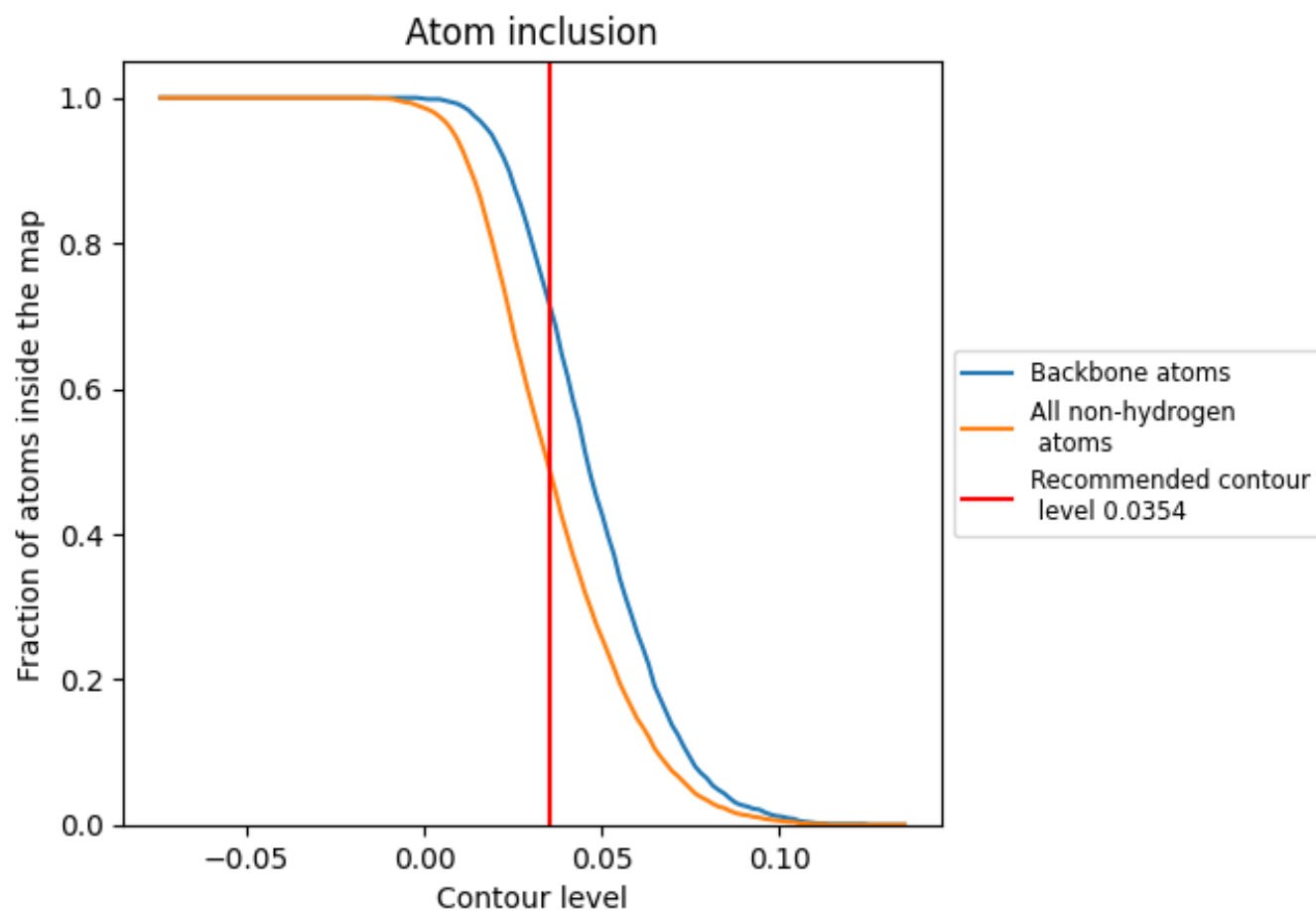
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0354).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 49% 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 (0.0354) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.4890 | <div></div> 0.3690 |
| A     | <div></div> 0.4900 | <div></div> 0.3690 |
| B     | <div></div> 0.4910 | <div></div> 0.3710 |
| C     | <div></div> 0.4910 | <div></div> 0.3680 |
| D     | <div></div> 0.4900 | <div></div> 0.3680 |
| E     | <div></div> 0.2140 | <div></div> 0.3220 |
| F     | <div></div> 0.2140 | <div></div> 0.3130 |
| G     | <div></div> 0.2140 | <div></div> 0.3010 |
| H     | <div></div> 0.2140 | <div></div> 0.3180 |

1.0

0.0

<0.0