



## Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:15 AM UTC

PDB ID : 8SS7 / pdb\_00008ss7  
EMDB ID : EMD-40746  
Title : Structure of AMPA receptor GluA2 complex with auxiliary subunits TARP gamma-5 and cornichon-2 bound to competitive antagonist ZK, channel blocker spermidine and antiepileptic drug perampanel (closed state)  
Authors : Gangwar, S.P.; Yen, L.Y.; Yelshanskaya, M.V.; Sobolevsky, A.I.  
Deposited on : 2023-05-08  
Resolution : 2.76 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

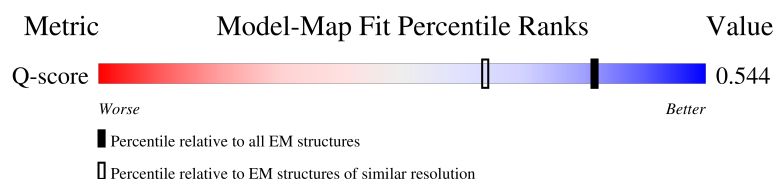
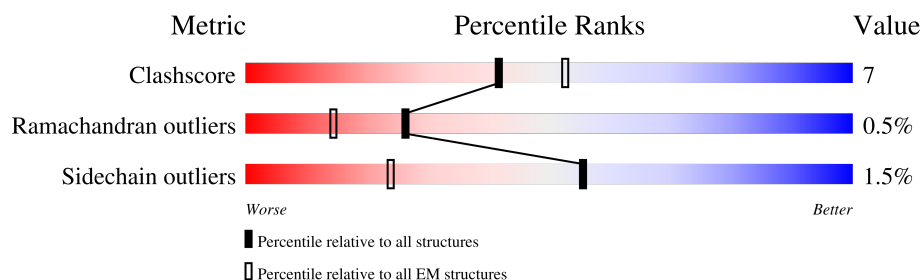
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.76 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                       | 10642 ( 2.26 - 3.26 )                                    |

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     | 1026   |                  |
| 1   | B     | 1026   |                  |
| 1   | C     | 1026   |                  |
| 1   | D     | 1026   |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | E     | 160    |                  |
| 2   | F     | 160    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 6   | CLR  | A     | 1107 | X         | -        | -       | -                |
| 6   | CLR  | A     | 1108 | X         | -        | -       | -                |
| 6   | CLR  | B     | 1107 | X         | -        | -       | -                |
| 6   | CLR  | B     | 1108 | X         | -        | -       | -                |
| 6   | CLR  | C     | 1107 | X         | -        | -       | -                |
| 6   | CLR  | C     | 1108 | X         | -        | -       | -                |
| 6   | CLR  | D     | 1108 | X         | -        | -       | -                |
| 6   | CLR  | D     | 1109 | X         | -        | -       | -                |

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19437 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 Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 592      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4639  | 3030 | 748 | 830 | 31 |         |       |
| 1   | B     | 401      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3134  | 2036 | 505 | 572 | 21 |         |       |
| 1   | C     | 592      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4639  | 3030 | 748 | 830 | 31 |         |       |
| 1   | D     | 401      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3134  | 2036 | 505 | 572 | 21 |         |       |

There are 72 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 241     | GLU      | ASN    | conflict | UNP P19491 |
| A     | 382     | LEU      | VAL    | conflict | UNP P19491 |
| A     | ?       | -        | LEU    | deletion | UNP P19491 |
| A     | ?       | -        | THR    | deletion | UNP P19491 |
| A     | ?       | -        | GLU    | deletion | UNP P19491 |
| A     | ?       | -        | LEU    | deletion | UNP P19491 |
| A     | ?       | -        | PRO    | deletion | UNP P19491 |
| A     | ?       | -        | SER    | deletion | UNP P19491 |
| A     | 384     | GLU      | GLY    | conflict | UNP P19491 |
| A     | 385     | ASP      | ASN    | conflict | UNP P19491 |
| A     | 392     | GLN      | ASN    | conflict | UNP P19491 |
| A     | 754     | SER      | ASN    | conflict | UNP P19491 |
| A     | 758     | VAL      | LEU    | conflict | UNP P19491 |
| A     | 827     | GLY      | -      | linker   | UNP P19491 |
| A     | 828     | THR      | -      | linker   | UNP P19491 |
| A     | 829     | GLY      | -      | linker   | UNP P19491 |
| A     | 830     | SER      | -      | linker   | UNP P19491 |
| A     | 831     | ALA      | -      | linker   | UNP P19491 |
| B     | 241     | GLU      | ASN    | conflict | UNP P19491 |
| B     | 382     | LEU      | VAL    | conflict | UNP P19491 |
| B     | ?       | -        | LEU    | deletion | UNP P19491 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | ?       | -        | THR    | deletion | UNP P19491 |
| B     | ?       | -        | GLU    | deletion | UNP P19491 |
| B     | ?       | -        | LEU    | deletion | UNP P19491 |
| B     | ?       | -        | PRO    | deletion | UNP P19491 |
| B     | ?       | -        | SER    | deletion | UNP P19491 |
| B     | 384     | GLU      | GLY    | conflict | UNP P19491 |
| B     | 385     | ASP      | ASN    | conflict | UNP P19491 |
| B     | 392     | GLN      | ASN    | conflict | UNP P19491 |
| B     | 754     | SER      | ASN    | conflict | UNP P19491 |
| B     | 758     | VAL      | LEU    | conflict | UNP P19491 |
| B     | 827     | GLY      | -      | linker   | UNP P19491 |
| B     | 828     | THR      | -      | linker   | UNP P19491 |
| B     | 829     | GLY      | -      | linker   | UNP P19491 |
| B     | 830     | SER      | -      | linker   | UNP P19491 |
| B     | 831     | ALA      | -      | linker   | UNP P19491 |
| C     | 241     | GLU      | ASN    | conflict | UNP P19491 |
| C     | 382     | LEU      | VAL    | conflict | UNP P19491 |
| C     | ?       | -        | LEU    | deletion | UNP P19491 |
| C     | ?       | -        | THR    | deletion | UNP P19491 |
| C     | ?       | -        | GLU    | deletion | UNP P19491 |
| C     | ?       | -        | LEU    | deletion | UNP P19491 |
| C     | ?       | -        | PRO    | deletion | UNP P19491 |
| C     | ?       | -        | SER    | deletion | UNP P19491 |
| C     | 384     | GLU      | GLY    | conflict | UNP P19491 |
| C     | 385     | ASP      | ASN    | conflict | UNP P19491 |
| C     | 392     | GLN      | ASN    | conflict | UNP P19491 |
| C     | 754     | SER      | ASN    | conflict | UNP P19491 |
| C     | 758     | VAL      | LEU    | conflict | UNP P19491 |
| C     | 827     | GLY      | -      | linker   | UNP P19491 |
| C     | 828     | THR      | -      | linker   | UNP P19491 |
| C     | 829     | GLY      | -      | linker   | UNP P19491 |
| C     | 830     | SER      | -      | linker   | UNP P19491 |
| C     | 831     | ALA      | -      | linker   | UNP P19491 |
| D     | 241     | GLU      | ASN    | conflict | UNP P19491 |
| D     | 382     | LEU      | VAL    | conflict | UNP P19491 |
| D     | ?       | -        | LEU    | deletion | UNP P19491 |
| D     | ?       | -        | THR    | deletion | UNP P19491 |
| D     | ?       | -        | GLU    | deletion | UNP P19491 |
| D     | ?       | -        | LEU    | deletion | UNP P19491 |
| D     | ?       | -        | PRO    | deletion | UNP P19491 |
| D     | ?       | -        | SER    | deletion | UNP P19491 |
| D     | 384     | GLU      | GLY    | conflict | UNP P19491 |

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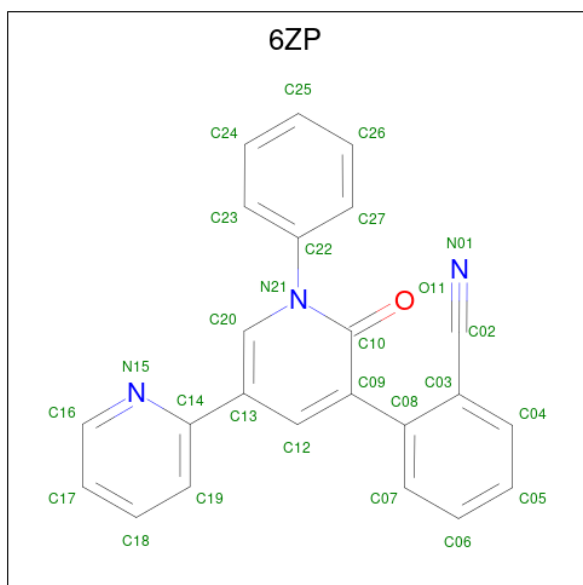
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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 385     | ASP      | ASN    | conflict | UNP P19491 |
| D     | 392     | GLN      | ASN    | conflict | UNP P19491 |
| D     | 754     | SER      | ASN    | conflict | UNP P19491 |
| D     | 758     | VAL      | LEU    | conflict | UNP P19491 |
| D     | 827     | GLY      | -      | linker   | UNP P19491 |
| D     | 828     | THR      | -      | linker   | UNP P19491 |
| D     | 829     | GLY      | -      | linker   | UNP P19491 |
| D     | 830     | SER      | -      | linker   | UNP P19491 |
| D     | 831     | ALA      | -      | linker   | UNP P19491 |

- Molecule 2 is a protein called Protein cornichon homolog 2.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | E     | 140      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1166  | 787 | 175 | 191 | 13 |         |       |
| 2   | F     | 140      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1166  | 787 | 175 | 191 | 13 |         |       |

- Molecule 3 is 2-(6'-oxo-1'-phenyl[1',6'-dihydro[2,3'-bipyridine]]-5'-yl)benzonitrile (CCD ID: 6ZP) (formula: C<sub>23</sub>H<sub>15</sub>N<sub>3</sub>O) (labeled as "Ligand of Interest" by depositor).



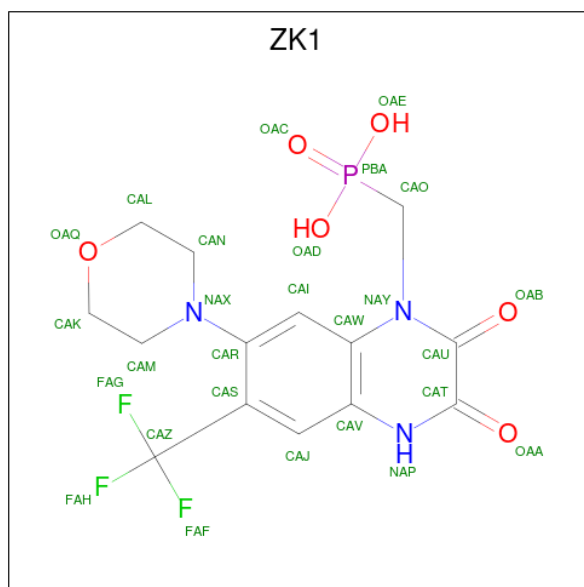
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 3   | A     | 1        | Total | C  | N | O | 0       |
|     |       |          | 27    | 23 | 3 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | 0       |
|     |       |          | 27    | 23 | 3 | 1 |         |

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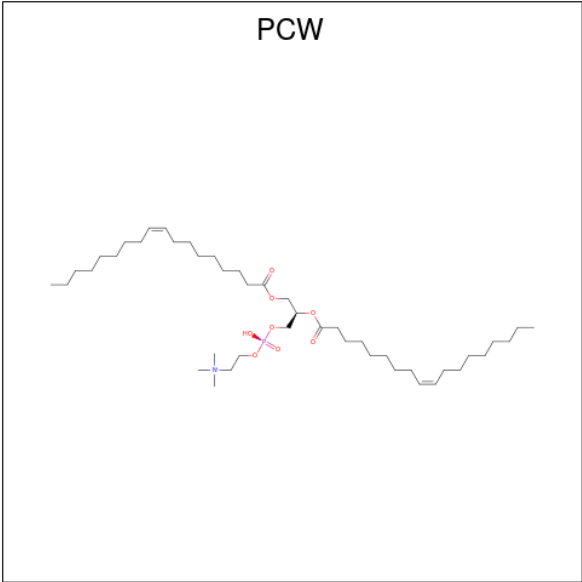
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 3   | C     | 1        | Total | C  | N | O | 0       |
|     |       |          | 27    | 23 | 3 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | 0       |
|     |       |          | 27    | 23 | 3 | 1 |         |

- Molecule 4 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (CCD ID: ZK1) (formula: C<sub>14</sub>H<sub>15</sub>F<sub>3</sub>N<sub>3</sub>O<sub>6</sub>P) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| 4   | A     | 1        | Total | C  | F | N | O | P | 0       |
|     |       |          | 27    | 14 | 3 | 3 | 6 | 1 |         |
| 4   | B     | 1        | Total | C  | F | N | O | P | 0       |
|     |       |          | 27    | 14 | 3 | 3 | 6 | 1 |         |
| 4   | C     | 1        | Total | C  | F | N | O | P | 0       |
|     |       |          | 27    | 14 | 3 | 3 | 6 | 1 |         |
| 4   | D     | 1        | Total | C  | F | N | O | P | 0       |
|     |       |          | 27    | 14 | 3 | 3 | 6 | 1 |         |

- Molecule 5 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 5   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | A     | 1        | Total | C  |   |   |   | 0       |
|     |       |          | 11    | 11 |   |   |   |         |
| 5   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | B     | 1        | Total | C  |   |   |   | 0       |
|     |       |          | 11    | 11 |   |   |   |         |
| 5   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |

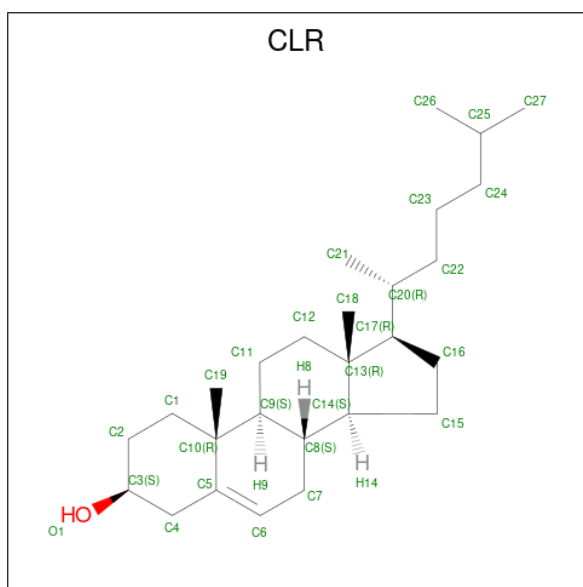
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| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 5   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | C     | 1        | Total | C  |   |   |   | 0       |
|     |       |          | 11    | 11 |   |   |   |         |
| 5   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | D     | 1        | Total | C  |   |   |   | 0       |
|     |       |          | 11    | 11 |   |   |   |         |
| 5   | E     | 1        | Total | C  |   |   |   | 0       |
|     |       |          | 11    | 11 |   |   |   |         |
| 5   | E     | 1        | Total | C  |   |   |   | 0       |
|     |       |          | 11    | 11 |   |   |   |         |
| 5   | E     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | F     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 5   | F     | 1        | Total | C  |   |   |   | 0       |
|     |       |          | 11    | 11 |   |   |   |         |
| 5   | F     | 1        | Total | C  |   |   |   | 0       |
|     |       |          | 11    | 11 |   |   |   |         |

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).

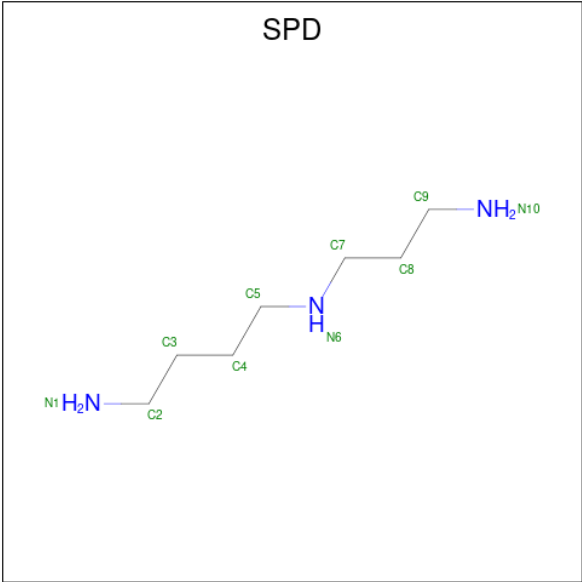


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 6   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 27 | 1 |         |
| 6   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 27 | 1 |         |
| 6   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 27 | 1 |         |
| 6   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 27 | 1 |         |
| 6   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 27 | 1 |         |
| 6   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 27 | 1 |         |
| 6   | D     | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 27 | 1 |         |
| 6   | D     | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 27 | 1 |         |

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 7   | A     | 1        | Total | Na | 0       |
|     |       |          | 1     | 1  |         |

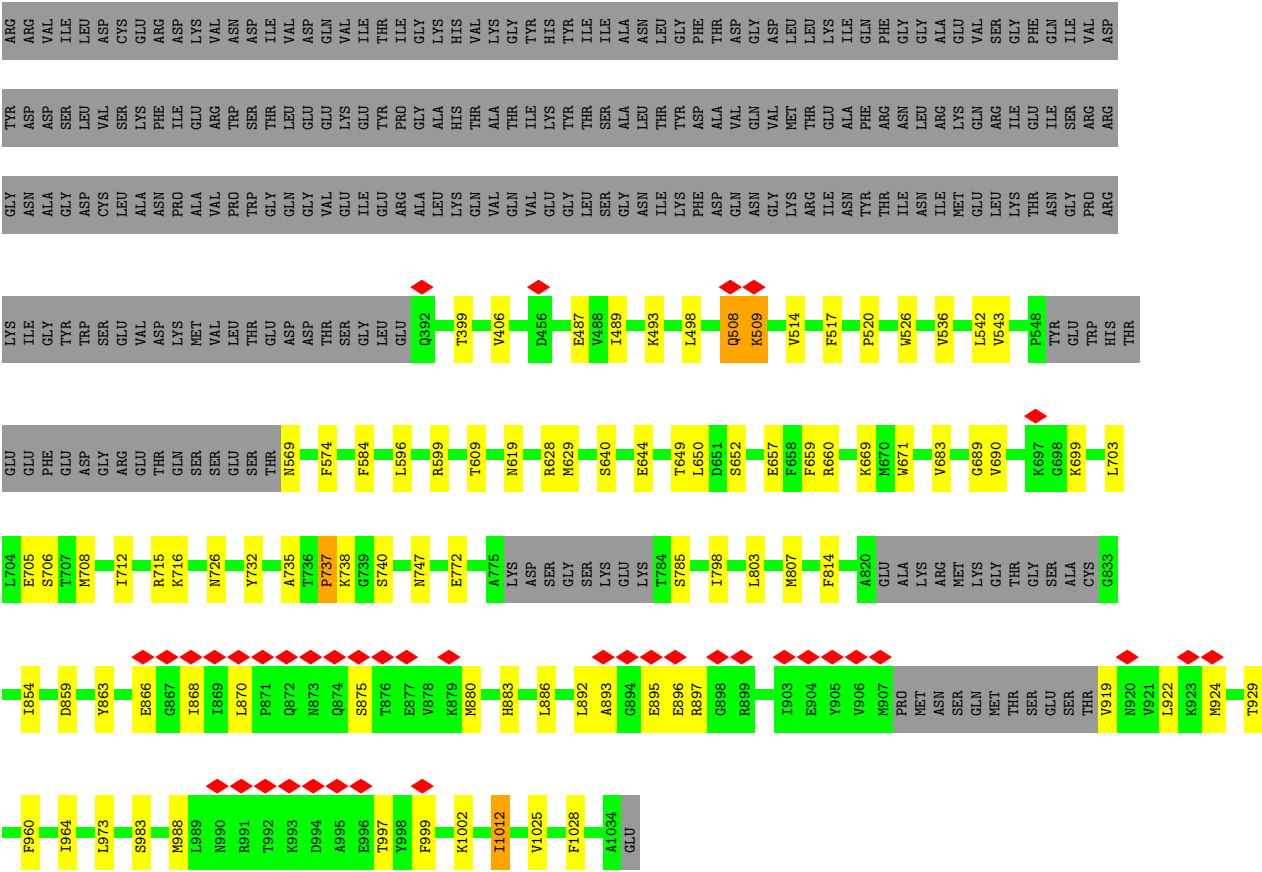
- Molecule 8 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 8   | A     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

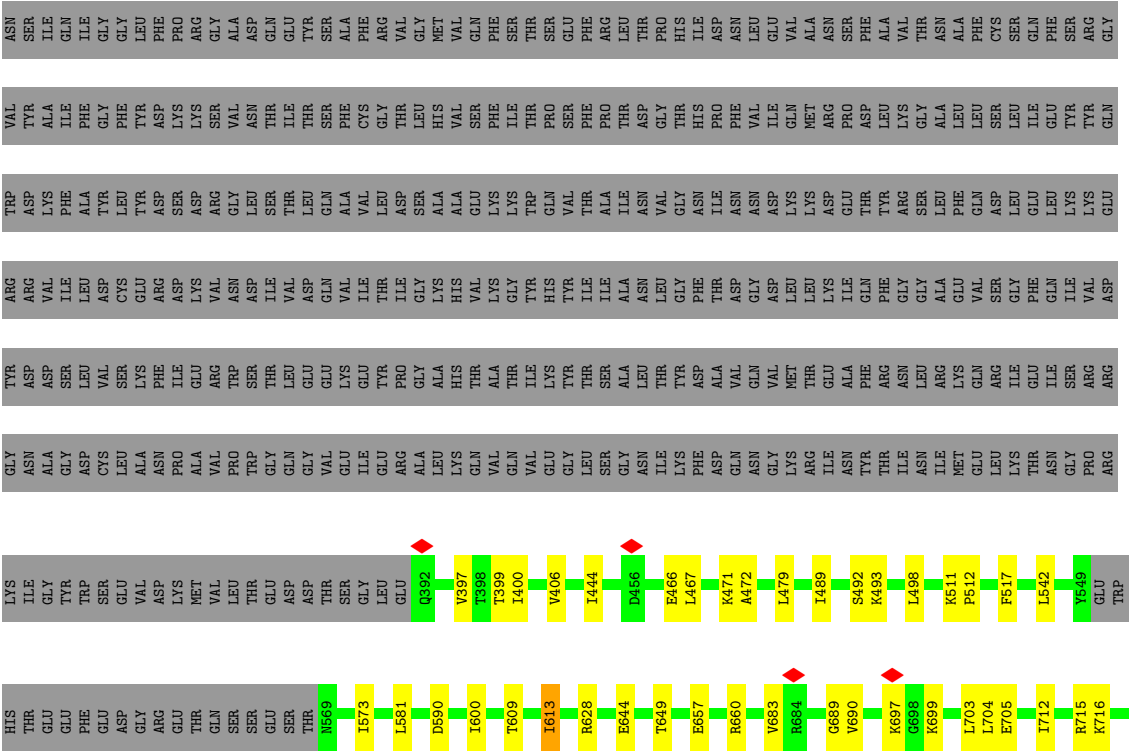


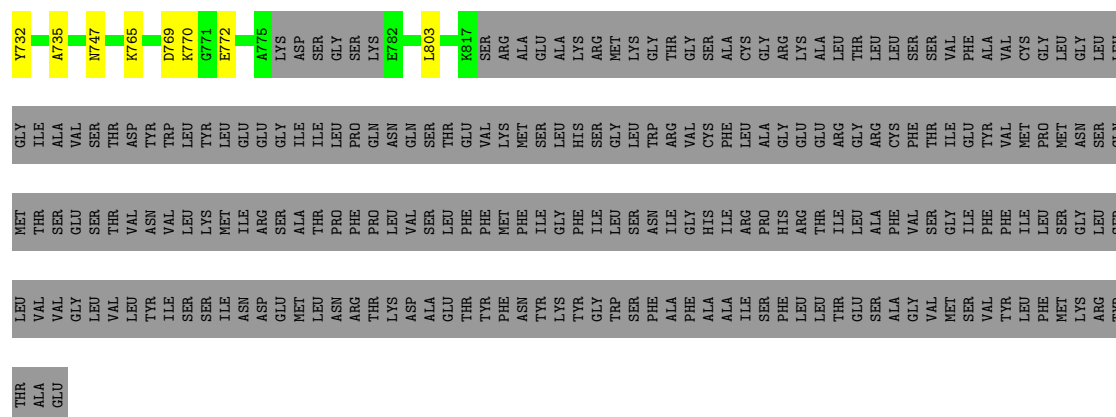
- [illegible]



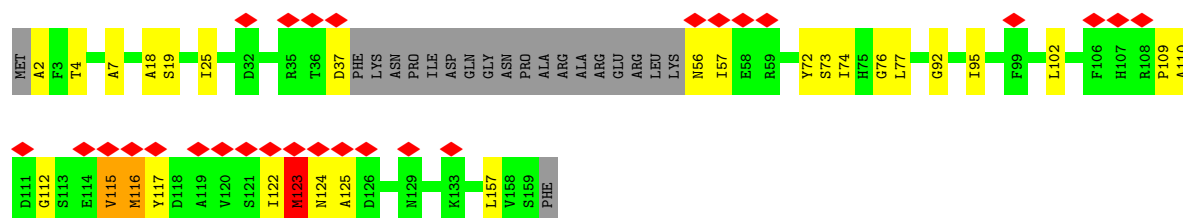
● Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

Chain D: 34% 5% 61%

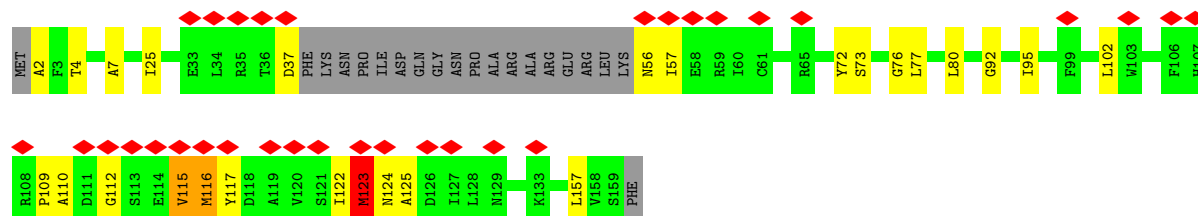
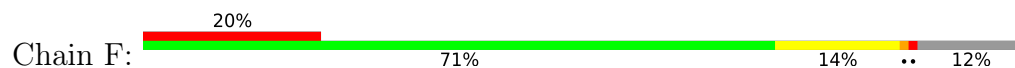




• Molecule 2: Protein cornichon homolog 2



• Molecule 2: Protein cornichon homolog 2



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C2                               | Depositor |
| Number of particles used             | 126263                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 10.298                                  | Depositor |
| Minimum map value                    | -6.046                                  | Depositor |
| Average map value                    | 0.007                                   | Depositor |
| Map value standard deviation         | 0.172                                   | Depositor |
| Recommended contour level            | 1                                       | Depositor |
| Map size (Å)                         | 384.80002, 384.80002, 384.80002         | wwPDB     |
| Map dimensions                       | 416, 416, 416                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.9250001, 0.9250001, 0.9250001         | Depositor |



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCW, SPD, ZK1, NA, CLR, 6ZP

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     | 0.35         | 0/4742  | 0.66        | 2/6404 (0.0%)  |
| 1   | B     | 0.37         | 0/3202  | 0.65        | 0/4321         |
| 1   | C     | 0.35         | 0/4742  | 0.66        | 2/6404 (0.0%)  |
| 1   | D     | 0.37         | 0/3202  | 0.65        | 0/4321         |
| 2   | E     | 0.34         | 0/1203  | 0.82        | 2/1636 (0.1%)  |
| 2   | F     | 0.34         | 0/1203  | 0.82        | 2/1636 (0.1%)  |
| All | All   | 0.36         | 0/18294 | 0.68        | 8/24722 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | C     | 0                   | 2                   |
| 2   | E     | 0                   | 4                   |
| 2   | F     | 0                   | 4                   |
| All | All   | 0                   | 12                  |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | F     | 115 | VAL  | CA-C-N | 5.78 | 132.57      | 121.54   |
| 2   | F     | 115 | VAL  | C-N-CA | 5.78 | 132.57      | 121.54   |
| 2   | E     | 115 | VAL  | CA-C-N | 5.74 | 132.50      | 121.54   |
| 2   | E     | 115 | VAL  | C-N-CA | 5.74 | 132.50      | 121.54   |
| 1   | A     | 508 | GLN  | CA-C-N | 5.10 | 131.28      | 121.54   |
| 1   | A     | 508 | GLN  | C-N-CA | 5.10 | 131.28      | 121.54   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | C     | 508 | GLN  | CA-C-N | 5.09 | 131.25      | 121.54   |
| 1   | C     | 508 | GLN  | C-N-CA | 5.09 | 131.25      | 121.54   |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 508 | GLN  | Peptide |
| 1   | A     | 509 | LYS  | Peptide |
| 1   | C     | 508 | GLN  | Peptide |
| 1   | C     | 509 | LYS  | Peptide |
| 2   | E     | 110 | ALA  | Peptide |
| 2   | E     | 115 | VAL  | Peptide |
| 2   | E     | 123 | MET  | Peptide |
| 2   | E     | 124 | ASN  | Peptide |
| 2   | F     | 110 | ALA  | Peptide |
| 2   | F     | 115 | VAL  | Peptide |
| 2   | F     | 123 | MET  | Peptide |
| 2   | F     | 124 | ASN  | 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     | 4639  | 0        | 4714     | 52      | 0            |
| 1   | B     | 3134  | 0        | 3177     | 32      | 0            |
| 1   | C     | 4639  | 0        | 4714     | 53      | 0            |
| 1   | D     | 3134  | 0        | 3177     | 26      | 0            |
| 2   | E     | 1166  | 0        | 1152     | 14      | 0            |
| 2   | F     | 1166  | 0        | 1152     | 11      | 0            |
| 3   | A     | 27    | 0        | 0        | 1       | 0            |
| 3   | B     | 27    | 0        | 0        | 1       | 0            |
| 3   | C     | 27    | 0        | 0        | 2       | 0            |
| 3   | D     | 27    | 0        | 0        | 1       | 0            |
| 4   | A     | 27    | 0        | 13       | 1       | 0            |
| 4   | B     | 27    | 0        | 13       | 0       | 0            |
| 4   | C     | 27    | 0        | 13       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | D     | 27    | 0        | 13       | 0       | 0            |
| 5   | A     | 266   | 0        | 391      | 19      | 0            |
| 5   | B     | 215   | 0        | 316      | 26      | 0            |
| 5   | C     | 266   | 0        | 391      | 20      | 0            |
| 5   | D     | 215   | 0        | 316      | 26      | 0            |
| 5   | E     | 73    | 0        | 107      | 8       | 0            |
| 5   | F     | 73    | 0        | 107      | 8       | 0            |
| 6   | A     | 56    | 0        | 76       | 8       | 0            |
| 6   | B     | 56    | 0        | 75       | 14      | 0            |
| 6   | C     | 56    | 0        | 76       | 11      | 0            |
| 6   | D     | 56    | 0        | 75       | 13      | 0            |
| 7   | A     | 1     | 0        | 0        | 0       | 0            |
| 8   | A     | 10    | 0        | 19       | 0       | 0            |
| All | All   | 19437 | 0        | 20087    | 268     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (268) 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) |
|------------------|------------------|--------------------------|-------------------|
| 6:D:1109:CLR:C14 | 6:D:1109:CLR:C8  | 1.85                     | 1.54              |
| 6:A:1108:CLR:C14 | 6:A:1108:CLR:C8  | 1.85                     | 1.54              |
| 6:B:1108:CLR:C14 | 6:B:1108:CLR:C8  | 1.85                     | 1.53              |
| 6:D:1108:CLR:C14 | 6:D:1108:CLR:C8  | 1.87                     | 1.52              |
| 6:B:1107:CLR:C14 | 6:B:1107:CLR:C8  | 1.87                     | 1.52              |
| 6:C:1107:CLR:C14 | 6:C:1107:CLR:C8  | 1.85                     | 1.52              |
| 6:A:1107:CLR:C14 | 6:A:1107:CLR:C8  | 1.85                     | 1.51              |
| 6:C:1108:CLR:C14 | 6:C:1108:CLR:C8  | 1.85                     | 1.50              |
| 6:C:1108:CLR:C14 | 6:C:1108:CLR:C7  | 2.60                     | 0.79              |
| 6:A:1107:CLR:C14 | 6:A:1107:CLR:C7  | 2.60                     | 0.79              |
| 6:A:1108:CLR:C14 | 6:A:1108:CLR:C7  | 2.60                     | 0.79              |
| 6:B:1107:CLR:C8  | 6:B:1107:CLR:H14 | 2.10                     | 0.79              |
| 6:B:1107:CLR:C14 | 6:B:1107:CLR:C7  | 2.60                     | 0.78              |
| 6:D:1108:CLR:C14 | 6:D:1108:CLR:C7  | 2.60                     | 0.78              |
| 6:C:1107:CLR:C14 | 6:C:1107:CLR:C7  | 2.61                     | 0.77              |
| 1:A:493:LYS:HG2  | 1:A:747:ASN:HD21 | 1.52                     | 0.74              |
| 1:C:493:LYS:HG2  | 1:C:747:ASN:HD21 | 1.52                     | 0.72              |
| 6:D:1108:CLR:C8  | 6:D:1108:CLR:H14 | 2.11                     | 0.71              |
| 6:D:1109:CLR:C14 | 6:D:1109:CLR:C7  | 2.65                     | 0.70              |
| 6:B:1108:CLR:C14 | 6:B:1108:CLR:C7  | 2.66                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:B:1108:CLR:C14  | 6:B:1108:CLR:C9   | 2.64                     | 0.68              |
| 6:D:1109:CLR:C14  | 6:D:1109:CLR:C9   | 2.64                     | 0.66              |
| 1:D:517:PHE:HA    | 3:D:1102:6ZP:C07  | 2.26                     | 0.65              |
| 5:D:1106:PCW:H11  | 5:E:203:PCW:H122  | 1.81                     | 0.63              |
| 5:B:1109:PCW:H40  | 5:C:1105:PCW:H161 | 1.81                     | 0.62              |
| 5:B:1109:PCW:H281 | 1:C:798:ILE:HD13  | 1.82                     | 0.62              |
| 1:B:547:SER:HB2   | 1:C:814:PHE:HB2   | 1.80                     | 0.61              |
| 1:C:924:MET:HB3   | 1:C:983:SER:HB2   | 1.82                     | 0.61              |
| 5:A:1103:PCW:H172 | 6:A:1107:CLR:H181 | 1.82                     | 0.61              |
| 1:A:924:MET:HB3   | 1:A:983:SER:HB2   | 1.82                     | 0.61              |
| 2:F:80:LEU:HD22   | 5:F:201:PCW:H40   | 1.81                     | 0.60              |
| 5:B:1105:PCW:H52  | 5:F:201:PCW:H31   | 1.84                     | 0.60              |
| 5:D:1106:PCW:H32  | 5:E:203:PCW:H142  | 1.83                     | 0.60              |
| 5:B:1105:PCW:H11  | 5:F:201:PCW:H122  | 1.84                     | 0.60              |
| 2:E:57:ILE:HG23   | 2:E:122:ILE:HD12  | 1.83                     | 0.59              |
| 1:A:708:MET:HG3   | 4:A:1102:ZK1:HAK  | 1.84                     | 0.59              |
| 1:B:628:ARG:NH1   | 1:C:785:SER:OG    | 2.35                     | 0.59              |
| 1:A:798:ILE:HD13  | 5:D:1101:PCW:H281 | 1.85                     | 0.59              |
| 2:F:57:ILE:HG23   | 2:F:122:ILE:HD12  | 1.83                     | 0.59              |
| 1:B:517:PHE:HA    | 3:B:1101:6ZP:C07  | 2.33                     | 0.58              |
| 1:A:706:SER:OG    | 1:A:726:ASN:ND2   | 2.36                     | 0.58              |
| 5:D:1104:PCW:H171 | 6:D:1108:CLR:H152 | 1.85                     | 0.58              |
| 6:D:1109:CLR:C8   | 6:D:1109:CLR:H14  | 2.21                     | 0.58              |
| 1:C:706:SER:OG    | 1:C:726:ASN:ND2   | 2.37                     | 0.58              |
| 1:A:866:GLU:HB3   | 1:A:880:MET:HB3   | 1.86                     | 0.58              |
| 1:B:493:LYS:HG2   | 1:B:747:ASN:HD21  | 1.69                     | 0.57              |
| 1:D:493:LYS:HG2   | 1:D:747:ASN:HD21  | 1.69                     | 0.57              |
| 1:C:866:GLU:HB3   | 1:C:880:MET:HB3   | 1.86                     | 0.57              |
| 1:A:863:TYR:HB2   | 1:A:1002:LYS:HB2  | 1.87                     | 0.57              |
| 5:B:1105:PCW:H32  | 5:F:201:PCW:H142  | 1.85                     | 0.57              |
| 5:C:1103:PCW:H172 | 6:C:1107:CLR:H181 | 1.86                     | 0.56              |
| 5:D:1106:PCW:H52  | 5:E:203:PCW:H31   | 1.88                     | 0.56              |
| 1:D:542:LEU:HD21  | 2:E:74:ILE:HD11   | 1.88                     | 0.56              |
| 1:C:863:TYR:HB2   | 1:C:1002:LYS:HB2  | 1.87                     | 0.56              |
| 1:A:596:LEU:HB2   | 5:A:1109:PCW:H31  | 1.87                     | 0.56              |
| 1:B:657:GLU:OE1   | 1:B:660:ARG:NH2   | 2.39                     | 0.56              |
| 1:C:487:GLU:O     | 1:C:738:LYS:NZ    | 2.39                     | 0.55              |
| 6:C:1107:CLR:H193 | 2:F:157:LEU:HD13  | 1.89                     | 0.55              |
| 1:A:487:GLU:O     | 1:A:738:LYS:NZ    | 2.39                     | 0.55              |
| 1:D:657:GLU:OE1   | 1:D:660:ARG:NH2   | 2.40                     | 0.55              |
| 1:A:964:ILE:HD13  | 5:B:1106:PCW:H182 | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:708:MET:HG3   | 4:C:1102:ZK1:HAK  | 1.88                     | 0.54              |
| 1:C:964:ILE:HD13  | 5:D:1107:PCW:H182 | 1.88                     | 0.54              |
| 5:D:1104:PCW:H361 | 5:D:1104:PCW:H142 | 1.88                     | 0.54              |
| 2:E:2:ALA:N       | 2:E:157:LEU:O     | 2.40                     | 0.54              |
| 2:F:2:ALA:N       | 2:F:157:LEU:O     | 2.40                     | 0.54              |
| 6:B:1107:CLR:H14  | 6:B:1107:CLR:C7   | 2.36                     | 0.54              |
| 5:C:1109:PCW:H381 | 6:D:1109:CLR:H151 | 1.89                     | 0.54              |
| 1:A:868:ILE:HG22  | 1:A:997:THR:HG22  | 1.91                     | 0.53              |
| 1:C:690:VAL:HG21  | 1:C:712:ILE:HD13  | 1.91                     | 0.53              |
| 1:A:895:GLU:HG2   | 1:A:897:ARG:HH21  | 1.73                     | 0.53              |
| 1:C:886:LEU:HD23  | 1:C:929:THR:HG23  | 1.91                     | 0.53              |
| 1:A:690:VAL:HG21  | 1:A:712:ILE:HD13  | 1.91                     | 0.53              |
| 1:A:886:LEU:HD23  | 1:A:929:THR:HG23  | 1.91                     | 0.53              |
| 1:B:406:VAL:HG11  | 1:B:444:ILE:HD11  | 1.91                     | 0.53              |
| 1:C:868:ILE:HG22  | 1:C:997:THR:HG22  | 1.91                     | 0.53              |
| 1:C:536:VAL:HG22  | 1:D:803:LEU:HD21  | 1.90                     | 0.53              |
| 5:A:1109:PCW:H361 | 6:B:1108:CLR:H72  | 1.91                     | 0.52              |
| 6:B:1108:CLR:C8   | 6:B:1108:CLR:H14  | 2.22                     | 0.52              |
| 1:A:399:THR:HB    | 1:A:406:VAL:HG21  | 1.91                     | 0.52              |
| 1:A:883:HIS:HD2   | 1:A:892:LEU:HD23  | 1.74                     | 0.52              |
| 1:C:883:HIS:HD2   | 1:C:892:LEU:HD23  | 1.74                     | 0.52              |
| 6:C:1107:CLR:C8   | 6:C:1107:CLR:H14  | 2.21                     | 0.52              |
| 1:A:644:GLU:OE1   | 1:A:699:LYS:NZ    | 2.40                     | 0.52              |
| 1:C:705:GLU:OE1   | 1:C:732:TYR:OH    | 2.28                     | 0.52              |
| 5:D:1106:PCW:H262 | 5:D:1106:PCW:H351 | 1.91                     | 0.52              |
| 1:C:644:GLU:OE1   | 1:C:699:LYS:NZ    | 2.40                     | 0.52              |
| 1:A:649:THR:HG22  | 1:A:703:LEU:HB2   | 1.91                     | 0.52              |
| 2:F:37:ASP:O      | 2:F:56:ASN:ND2    | 2.43                     | 0.52              |
| 1:A:650:LEU:HD23  | 1:A:652:SER:H     | 1.74                     | 0.51              |
| 1:C:399:THR:HB    | 1:C:406:VAL:HG21  | 1.91                     | 0.51              |
| 1:C:649:THR:HG22  | 1:C:703:LEU:HB2   | 1.91                     | 0.51              |
| 1:C:895:GLU:HG2   | 1:C:897:ARG:HH21  | 1.73                     | 0.51              |
| 2:E:92:GLY:HA2    | 2:E:95:ILE:HD12   | 1.92                     | 0.51              |
| 1:D:406:VAL:HG11  | 1:D:444:ILE:HD11  | 1.91                     | 0.51              |
| 2:E:37:ASP:O      | 2:E:56:ASN:ND2    | 2.43                     | 0.51              |
| 2:F:112:GLY:HA3   | 2:F:116:MET:HG2   | 1.93                     | 0.51              |
| 1:A:514:VAL:HG21  | 5:A:1103:PCW:H122 | 1.92                     | 0.51              |
| 1:C:650:LEU:HD23  | 1:C:652:SER:H     | 1.74                     | 0.51              |
| 1:A:705:GLU:OE1   | 1:A:732:TYR:OH    | 2.28                     | 0.51              |
| 2:F:92:GLY:HA2    | 2:F:95:ILE:HD12   | 1.92                     | 0.51              |
| 6:A:1107:CLR:C7   | 6:A:1107:CLR:H14  | 2.41                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:1107:CLR:H193 | 2:E:157:LEU:HD13  | 1.93                     | 0.51              |
| 5:B:1109:PCW:H412 | 5:C:1105:PCW:H231 | 1.92                     | 0.51              |
| 1:A:785:SER:OG    | 1:D:628:ARG:NH1   | 2.45                     | 0.50              |
| 5:A:1105:PCW:H161 | 5:D:1101:PCW:H40  | 1.93                     | 0.50              |
| 5:B:1105:PCW:H351 | 5:B:1105:PCW:H241 | 1.94                     | 0.50              |
| 1:C:640:SER:HB2   | 1:C:669:LYS:HD2   | 1.94                     | 0.50              |
| 1:C:659:PHE:HB3   | 1:C:671:TRP:HB2   | 1.94                     | 0.50              |
| 5:B:1103:PCW:H171 | 6:B:1107:CLR:H152 | 1.94                     | 0.50              |
| 1:D:715:ARG:NH2   | 1:D:770:LYS:O     | 2.44                     | 0.50              |
| 2:E:112:GLY:HA3   | 2:E:116:MET:HG2   | 1.93                     | 0.50              |
| 1:A:606:TRP:CG    | 1:B:587:GLN:HG3   | 2.47                     | 0.49              |
| 1:A:659:PHE:HB3   | 1:A:671:TRP:HB2   | 1.94                     | 0.49              |
| 1:B:715:ARG:NH2   | 1:B:770:LYS:O     | 2.44                     | 0.49              |
| 1:A:640:SER:HB2   | 1:A:669:LYS:HD2   | 1.94                     | 0.48              |
| 1:A:574:PHE:HE2   | 5:A:1105:PCW:H2   | 1.78                     | 0.48              |
| 5:D:1105:PCW:H352 | 5:D:1105:PCW:H321 | 1.69                     | 0.48              |
| 1:C:517:PHE:HA    | 3:C:1101:6ZP:C07  | 2.43                     | 0.48              |
| 6:D:1108:CLR:C7   | 6:D:1108:CLR:H14  | 2.40                     | 0.48              |
| 5:A:1109:PCW:H172 | 1:B:581:LEU:HD22  | 1.95                     | 0.48              |
| 6:C:1107:CLR:C7   | 6:C:1107:CLR:H14  | 2.43                     | 0.48              |
| 1:D:466:GLU:HG2   | 1:D:471:LYS:HE2   | 1.96                     | 0.48              |
| 5:C:1110:PCW:H162 | 5:D:1107:PCW:H172 | 1.95                     | 0.47              |
| 1:A:584:PHE:HA    | 1:A:609:THR:HG21  | 1.96                     | 0.47              |
| 5:D:1104:PCW:H151 | 5:D:1104:PCW:H181 | 1.63                     | 0.47              |
| 2:F:72:TYR:O      | 2:F:76:GLY:N      | 2.44                     | 0.47              |
| 5:B:1106:PCW:H19  | 5:B:1106:PCW:H162 | 1.69                     | 0.47              |
| 1:A:716:LYS:HG3   | 1:A:772:GLU:HB3   | 1.96                     | 0.47              |
| 1:B:466:GLU:HG2   | 1:B:471:LYS:HE2   | 1.96                     | 0.47              |
| 5:B:1105:PCW:H132 | 5:B:1105:PCW:H2   | 1.95                     | 0.47              |
| 1:C:584:PHE:HA    | 1:C:609:THR:HG21  | 1.96                     | 0.47              |
| 1:A:807:MET:HB3   | 5:E:201:PCW:H182  | 1.95                     | 0.47              |
| 1:C:574:PHE:HE2   | 5:C:1105:PCW:H2   | 1.79                     | 0.47              |
| 5:D:1106:PCW:H121 | 5:D:1106:PCW:H151 | 1.55                     | 0.47              |
| 1:A:629:MET:HE2   | 1:C:629:MET:HE2   | 1.96                     | 0.47              |
| 1:A:657:GLU:OE2   | 1:A:660:ARG:NH1   | 2.49                     | 0.46              |
| 1:C:716:LYS:HG3   | 1:C:772:GLU:HB3   | 1.96                     | 0.46              |
| 5:A:1105:PCW:H231 | 5:D:1101:PCW:H412 | 1.97                     | 0.46              |
| 1:B:765:LYS:HA    | 1:B:769:ASP:HB2   | 1.97                     | 0.46              |
| 1:C:514:VAL:HG21  | 5:C:1103:PCW:H122 | 1.96                     | 0.46              |
| 1:D:765:LYS:HA    | 1:D:769:ASP:HB2   | 1.97                     | 0.46              |
| 5:B:1105:PCW:H151 | 5:B:1105:PCW:H121 | 1.68                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:609:THR:HG23  | 1:D:613:ILE:HD13  | 1.98                     | 0.46              |
| 1:A:628:ARG:HH12  | 1:A:785:SER:HB3   | 1.81                     | 0.46              |
| 1:A:979:LEU:HD21  | 6:B:1107:CLR:H3   | 1.98                     | 0.46              |
| 1:A:989:LEU:HD11  | 1:B:509:LYS:HG2   | 1.96                     | 0.46              |
| 1:C:526:TRP:HB3   | 5:C:1106:PCW:H362 | 1.98                     | 0.46              |
| 5:E:203:PCW:H132  | 5:E:203:PCW:H321  | 1.97                     | 0.46              |
| 1:D:644:GLU:OE2   | 1:D:699:LYS:NZ    | 2.48                     | 0.46              |
| 1:C:657:GLU:OE2   | 1:C:660:ARG:NH1   | 2.49                     | 0.46              |
| 5:F:201:PCW:H321  | 5:F:201:PCW:H351  | 1.76                     | 0.46              |
| 1:A:807:MET:HE1   | 2:E:19:SER:HB3    | 1.98                     | 0.45              |
| 1:D:716:LYS:HG3   | 1:D:772:GLU:HB3   | 1.97                     | 0.45              |
| 2:E:123:MET:HA    | 2:E:125:ALA:H     | 1.82                     | 0.45              |
| 1:B:644:GLU:OE2   | 1:B:699:LYS:NZ    | 2.48                     | 0.45              |
| 2:F:123:MET:HA    | 2:F:125:ALA:H     | 1.81                     | 0.45              |
| 1:A:517:PHE:HA    | 3:A:1101:6ZP:C07  | 2.46                     | 0.45              |
| 1:B:573:ILE:HG21  | 5:B:1104:PCW:H322 | 1.99                     | 0.45              |
| 1:B:716:LYS:HG3   | 1:B:772:GLU:HB3   | 1.97                     | 0.45              |
| 1:C:807:MET:HE2   | 5:F:202:PCW:H182  | 1.98                     | 0.45              |
| 1:B:705:GLU:OE1   | 1:B:732:TYR:OH    | 2.35                     | 0.45              |
| 1:C:628:ARG:HH12  | 1:C:785:SER:HB3   | 1.81                     | 0.45              |
| 1:D:573:ILE:HG21  | 5:D:1105:PCW:H322 | 1.98                     | 0.45              |
| 1:A:606:TRP:CD2   | 1:B:587:GLN:HG3   | 2.52                     | 0.45              |
| 1:B:590:ASP:OD1   | 1:B:590:ASP:N     | 2.47                     | 0.45              |
| 1:D:705:GLU:OE1   | 1:D:732:TYR:OH    | 2.35                     | 0.45              |
| 5:A:1103:PCW:H232 | 5:A:1103:PCW:H20  | 1.66                     | 0.45              |
| 5:B:1104:PCW:H281 | 5:F:201:PCW:H20   | 1.97                     | 0.45              |
| 5:E:203:PCW:H321  | 5:E:203:PCW:H351  | 1.67                     | 0.45              |
| 1:D:690:VAL:HG21  | 1:D:712:ILE:HD13  | 1.98                     | 0.45              |
| 1:D:649:THR:HG22  | 1:D:703:LEU:HB2   | 1.98                     | 0.45              |
| 1:B:609:THR:HG23  | 1:B:613:ILE:HD13  | 1.98                     | 0.44              |
| 1:B:649:THR:HG22  | 1:B:703:LEU:HB2   | 1.98                     | 0.44              |
| 1:A:870:LEU:HB2   | 1:A:875:SER:HB2   | 1.99                     | 0.44              |
| 5:D:1105:PCW:H142 | 5:D:1105:PCW:H172 | 1.91                     | 0.44              |
| 1:C:599:ARG:HD2   | 5:C:1109:PCW:H131 | 1.99                     | 0.44              |
| 2:E:72:TYR:O      | 2:E:76:GLY:N      | 2.44                     | 0.44              |
| 1:C:517:PHE:HA    | 3:C:1101:6ZP:C06  | 2.48                     | 0.44              |
| 1:D:600:ILE:HA    | 5:D:1101:PCW:H19  | 1.98                     | 0.44              |
| 6:D:1108:CLR:H25  | 6:D:1108:CLR:H222 | 1.55                     | 0.44              |
| 5:B:1103:PCW:H182 | 5:B:1103:PCW:H211 | 1.73                     | 0.44              |
| 1:A:520:PRO:O     | 1:A:619:ASN:ND2   | 2.48                     | 0.43              |
| 1:A:805:LEU:HD23  | 5:A:1103:PCW:H261 | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:A:1106:PCW:H62  | 5:A:1106:PCW:H41  | 1.84                     | 0.43              |
| 1:B:536:VAL:HG12  | 1:C:803:LEU:HD11  | 2.00                     | 0.43              |
| 5:C:1109:PCW:H212 | 5:D:1104:PCW:H262 | 1.98                     | 0.43              |
| 1:B:536:VAL:HG12  | 1:C:803:LEU:HD21  | 1.99                     | 0.43              |
| 1:B:690:VAL:HG21  | 1:B:712:ILE:HD13  | 1.98                     | 0.43              |
| 2:F:73:SER:O      | 2:F:77:LEU:N      | 2.50                     | 0.43              |
| 5:C:1109:PCW:H172 | 1:D:581:LEU:HD22  | 1.99                     | 0.43              |
| 5:A:1105:PCW:H251 | 5:D:1101:PCW:H441 | 1.99                     | 0.43              |
| 1:C:988:MET:HE1   | 1:C:999:PHE:HB3   | 2.00                     | 0.43              |
| 5:D:1106:PCW:H351 | 5:D:1106:PCW:H241 | 1.99                     | 0.43              |
| 1:A:542:LEU:HD12  | 1:A:1025:VAL:HG21 | 2.00                     | 0.43              |
| 5:B:1105:PCW:H351 | 5:B:1105:PCW:H262 | 2.01                     | 0.43              |
| 1:D:683:VAL:HG11  | 1:D:689:GLY:HA2   | 2.01                     | 0.43              |
| 5:A:1109:PCW:H141 | 1:B:574:PHE:HD1   | 1.83                     | 0.43              |
| 1:C:870:LEU:HB2   | 1:C:875:SER:HB2   | 1.99                     | 0.43              |
| 1:A:859:ASP:OD1   | 1:A:859:ASP:N     | 2.50                     | 0.43              |
| 5:A:1109:PCW:H262 | 5:A:1109:PCW:H232 | 1.64                     | 0.43              |
| 5:C:1106:PCW:H331 | 5:C:1106:PCW:H361 | 1.77                     | 0.43              |
| 1:A:683:VAL:HG11  | 1:A:689:GLY:HA2   | 2.01                     | 0.43              |
| 6:D:1109:CLR:H122 | 6:D:1109:CLR:H20  | 1.87                     | 0.43              |
| 1:A:988:MET:HE1   | 1:A:999:PHE:HB3   | 2.00                     | 0.43              |
| 1:B:596:LEU:HD22  | 5:B:1109:PCW:H342 | 2.01                     | 0.43              |
| 1:B:683:VAL:HG11  | 1:B:689:GLY:HA2   | 2.01                     | 0.43              |
| 5:B:1103:PCW:H151 | 5:B:1103:PCW:H181 | 1.61                     | 0.43              |
| 1:C:1012:ILE:HD11 | 5:C:1104:PCW:H382 | 2.00                     | 0.43              |
| 5:B:1104:PCW:H322 | 5:B:1104:PCW:H2   | 1.92                     | 0.42              |
| 1:C:683:VAL:HG11  | 1:C:689:GLY:HA2   | 2.01                     | 0.42              |
| 5:C:1109:PCW:H41  | 5:C:1109:PCW:H83  | 1.82                     | 0.42              |
| 1:D:399:THR:HG22  | 1:D:400:ILE:H     | 1.84                     | 0.42              |
| 1:B:798:ILE:HA    | 5:B:1103:PCW:H212 | 2.01                     | 0.42              |
| 1:D:467:LEU:HD12  | 1:D:472:ALA:HB3   | 2.02                     | 0.42              |
| 1:A:493:LYS:NZ    | 1:D:492:SER:O     | 2.51                     | 0.42              |
| 1:B:600:ILE:HG12  | 5:B:1109:PCW:H19  | 2.01                     | 0.42              |
| 1:C:520:PRO:O     | 1:C:619:ASN:ND2   | 2.48                     | 0.42              |
| 1:C:715:ARG:HA    | 1:C:715:ARG:HD3   | 1.88                     | 0.42              |
| 2:E:73:SER:O      | 2:E:77:LEU:N      | 2.50                     | 0.42              |
| 1:B:399:THR:HG22  | 1:B:400:ILE:H     | 1.84                     | 0.42              |
| 1:B:492:SER:O     | 1:C:493:LYS:NZ    | 2.52                     | 0.42              |
| 2:E:18:ALA:HB1    | 5:E:201:PCW:H162  | 2.00                     | 0.42              |
| 1:C:859:ASP:OD1   | 1:C:859:ASP:N     | 2.50                     | 0.42              |
| 5:C:1103:PCW:H19  | 5:C:1103:PCW:H162 | 1.79                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:511:LYS:HA    | 1:D:512:PRO:HD3   | 1.87                     | 0.42              |
| 1:C:737:PRO:HD2   | 1:C:740:SER:HB2   | 2.01                     | 0.42              |
| 1:A:801:GLY:HA3   | 5:A:1103:PCW:H212 | 2.02                     | 0.42              |
| 6:C:1108:CLR:H211 | 6:C:1108:CLR:H232 | 1.82                     | 0.42              |
| 1:D:489:ILE:HD12  | 1:D:735:ALA:HB1   | 2.01                     | 0.41              |
| 1:B:467:LEU:HD12  | 1:B:472:ALA:HB3   | 2.02                     | 0.41              |
| 1:C:542:LEU:HD12  | 1:C:1025:VAL:HG21 | 2.00                     | 0.41              |
| 1:B:489:ILE:HD12  | 1:B:735:ALA:HB1   | 2.01                     | 0.41              |
| 5:C:1106:PCW:H282 | 5:C:1106:PCW:H251 | 1.88                     | 0.41              |
| 1:A:596:LEU:HD21  | 6:B:1108:CLR:H152 | 2.03                     | 0.41              |
| 1:A:715:ARG:HA    | 1:A:715:ARG:HD3   | 1.88                     | 0.41              |
| 6:C:1108:CLR:C8   | 6:C:1108:CLR:C15  | 2.89                     | 0.41              |
| 5:D:1104:PCW:H412 | 5:D:1104:PCW:H382 | 1.85                     | 0.41              |
| 5:D:1104:PCW:H421 | 5:D:1104:PCW:H221 | 2.02                     | 0.41              |
| 5:A:1110:PCW:H162 | 5:B:1106:PCW:H172 | 2.03                     | 0.41              |
| 6:C:1107:CLR:H25  | 6:C:1107:CLR:H221 | 1.71                     | 0.41              |
| 5:C:1109:PCW:H372 | 5:D:1105:PCW:H342 | 2.01                     | 0.41              |
| 2:F:4:THR:HG23    | 2:F:7:ALA:H       | 1.85                     | 0.41              |
| 5:B:1105:PCW:H62  | 5:B:1105:PCW:H41  | 1.83                     | 0.41              |
| 1:C:489:ILE:HD12  | 1:C:735:ALA:HB1   | 2.03                     | 0.41              |
| 5:B:1109:PCW:H252 | 5:B:1109:PCW:H283 | 1.80                     | 0.41              |
| 1:C:919:VAL:HB    | 1:C:922:LEU:HD13  | 2.03                     | 0.41              |
| 5:C:1109:PCW:H282 | 5:D:1106:PCW:H39  | 2.03                     | 0.41              |
| 1:D:590:ASP:OD1   | 1:D:590:ASP:N     | 2.47                     | 0.41              |
| 6:D:1108:CLR:H162 | 6:D:1108:CLR:H231 | 2.03                     | 0.41              |
| 1:A:737:PRO:HD2   | 1:A:740:SER:HB2   | 2.01                     | 0.41              |
| 5:A:1109:PCW:H381 | 6:B:1108:CLR:H151 | 2.02                     | 0.40              |
| 1:C:596:LEU:HB2   | 5:C:1109:PCW:H31  | 2.03                     | 0.40              |
| 5:D:1105:PCW:H281 | 5:E:203:PCW:H20   | 2.03                     | 0.40              |
| 2:E:37:ASP:HB3    | 2:E:56:ASN:HD22   | 1.86                     | 0.40              |
| 5:A:1109:PCW:H282 | 5:B:1105:PCW:H39  | 2.03                     | 0.40              |
| 5:B:1103:PCW:H361 | 5:B:1103:PCW:H142 | 2.02                     | 0.40              |
| 1:C:960:PHE:HB2   | 1:C:1028:PHE:CG   | 2.56                     | 0.40              |
| 1:A:981:ILE:HD11  | 1:A:1007:PHE:HZ   | 1.87                     | 0.40              |
| 6:A:1107:CLR:H221 | 6:A:1107:CLR:H25  | 1.91                     | 0.40              |
| 6:B:1107:CLR:H222 | 6:B:1107:CLR:H25  | 1.61                     | 0.40              |
| 2:E:4:THR:HG23    | 2:E:7:ALA:H       | 1.85                     | 0.40              |
| 1:A:919:VAL:HB    | 1:A:922:LEU:HD13  | 2.03                     | 0.40              |
| 1:A:960:PHE:HB2   | 1:A:1028:PHE:CG   | 2.56                     | 0.40              |
| 5:A:1106:PCW:H331 | 5:A:1106:PCW:H361 | 1.78                     | 0.40              |
| 1:C:893:ALA:H     | 1:C:896:GLU:HG3   | 1.87                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:1109:PCW:H281 | 5:D:1106:PCW:H271 | 2.03                     | 0.40              |
| 5:F:201:PCW:H351  | 5:F:201:PCW:H132  | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 582/1026 (57%)  | 551 (95%)  | 29 (5%)  | 2 (0%)   | 36          | 56  |
| 1   | B     | 395/1026 (38%)  | 372 (94%)  | 23 (6%)  | 0        | 100         | 100 |
| 1   | C     | 582/1026 (57%)  | 551 (95%)  | 29 (5%)  | 2 (0%)   | 36          | 56  |
| 1   | D     | 395/1026 (38%)  | 372 (94%)  | 23 (6%)  | 0        | 100         | 100 |
| 2   | E     | 136/160 (85%)   | 121 (89%)  | 11 (8%)  | 4 (3%)   | 3           | 6   |
| 2   | F     | 136/160 (85%)   | 121 (89%)  | 11 (8%)  | 4 (3%)   | 3           | 6   |
| All | All   | 2226/4424 (50%) | 2088 (94%) | 126 (6%) | 12 (0%)  | 26          | 43  |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 123 | MET  |
| 2   | F     | 123 | MET  |
| 2   | E     | 116 | MET  |
| 2   | F     | 116 | MET  |
| 1   | A     | 509 | LYS  |
| 1   | C     | 509 | LYS  |
| 2   | E     | 117 | TYR  |
| 2   | F     | 117 | TYR  |
| 2   | E     | 109 | PRO  |
| 2   | F     | 109 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 737 | PRO  |
| 1   | C     | 737 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 501/877 (57%)   | 495 (99%)  | 6 (1%)   | 63          | 78 |
| 1   | B     | 338/877 (38%)   | 332 (98%)  | 6 (2%)   | 51          | 71 |
| 1   | C     | 501/877 (57%)   | 495 (99%)  | 6 (1%)   | 63          | 78 |
| 1   | D     | 338/877 (38%)   | 332 (98%)  | 6 (2%)   | 51          | 71 |
| 2   | E     | 126/143 (88%)   | 124 (98%)  | 2 (2%)   | 55          | 73 |
| 2   | F     | 126/143 (88%)   | 124 (98%)  | 2 (2%)   | 55          | 73 |
| All | All   | 1930/3794 (51%) | 1902 (98%) | 28 (2%)  | 55          | 74 |

All (28) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 498  | LEU  |
| 1   | A     | 543  | VAL  |
| 1   | A     | 569  | ASN  |
| 1   | A     | 854  | ILE  |
| 1   | A     | 973  | LEU  |
| 1   | A     | 1012 | ILE  |
| 1   | B     | 397  | VAL  |
| 1   | B     | 479  | LEU  |
| 1   | B     | 498  | LEU  |
| 1   | B     | 613  | ILE  |
| 1   | B     | 697  | LYS  |
| 1   | B     | 704  | LEU  |
| 1   | C     | 498  | LEU  |
| 1   | C     | 543  | VAL  |
| 1   | C     | 569  | ASN  |
| 1   | C     | 854  | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 973  | LEU  |
| 1   | C     | 1012 | ILE  |
| 1   | D     | 397  | VAL  |
| 1   | D     | 479  | LEU  |
| 1   | D     | 498  | LEU  |
| 1   | D     | 613  | ILE  |
| 1   | D     | 697  | LYS  |
| 1   | D     | 704  | LEU  |
| 2   | E     | 25   | ILE  |
| 2   | E     | 102  | LEU  |
| 2   | F     | 25   | ILE  |
| 2   | F     | 102  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 569 | ASN  |
| 1   | A     | 726 | ASN  |
| 1   | A     | 747 | ASN  |
| 1   | A     | 764 | ASN  |
| 1   | A     | 985 | ASN  |
| 1   | B     | 587 | GLN  |
| 1   | B     | 747 | ASN  |
| 1   | C     | 508 | GLN  |
| 1   | C     | 569 | ASN  |
| 1   | C     | 726 | ASN  |
| 1   | C     | 747 | ASN  |
| 1   | C     | 764 | ASN  |
| 1   | C     | 985 | ASN  |
| 1   | C     | 990 | ASN  |
| 1   | D     | 747 | ASN  |
| 2   | E     | 75  | HIS  |
| 2   | E     | 94  | ASN  |
| 2   | E     | 101 | HIS  |
| 2   | F     | 56  | ASN  |
| 2   | F     | 75  | HIS  |
| 2   | F     | 94  | ASN  |
| 2   | F     | 101 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 46 ligands modelled in this entry, 1 is monoatomic - leaving 45 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   | PCW  | B     | 1106 | -    | 10,10,53     | 0.80 | 0           | 9,9,61      | 0.37 | 0           |
| 5   | PCW  | C     | 1103 | -    | 50,50,53     | 1.16 | 5 (10%)     | 56,58,61    | 0.94 | 3 (5%)      |
| 6   | CLR  | C     | 1107 | -    | 31,31,31     | 8.55 | 17 (54%)    | 48,48,48    | 3.16 | 21 (43%)    |
| 5   | PCW  | A     | 1104 | -    | 50,50,53     | 1.15 | 3 (6%)      | 56,58,61    | 1.07 | 4 (7%)      |
| 3   | 6ZP  | B     | 1101 | -    | 30,30,30     | 0.99 | 1 (3%)      | 37,41,41    | 0.86 | 1 (2%)      |
| 5   | PCW  | A     | 1106 | -    | 50,50,53     | 1.13 | 4 (8%)      | 56,58,61    | 0.98 | 3 (5%)      |
| 5   | PCW  | D     | 1104 | -    | 50,50,53     | 1.15 | 5 (10%)     | 56,58,61    | 0.95 | 3 (5%)      |
| 6   | CLR  | A     | 1107 | -    | 31,31,31     | 8.56 | 17 (54%)    | 48,48,48    | 3.21 | 21 (43%)    |
| 6   | CLR  | B     | 1108 | -    | 31,31,31     | 8.58 | 17 (54%)    | 48,48,48    | 3.09 | 25 (52%)    |
| 5   | PCW  | C     | 1104 | -    | 50,50,53     | 1.15 | 3 (6%)      | 56,58,61    | 1.08 | 4 (7%)      |
| 6   | CLR  | A     | 1108 | -    | 31,31,31     | 8.52 | 17 (54%)    | 48,48,48    | 3.56 | 25 (52%)    |
| 5   | PCW  | D     | 1101 | -    | 50,50,53     | 1.10 | 4 (8%)      | 56,58,61    | 0.94 | 4 (7%)      |
| 4   | ZK1  | A     | 1102 | -    | 29,29,29     | 3.41 | 8 (27%)     | 45,45,45    | 1.64 | 7 (15%)     |
| 5   | PCW  | A     | 1110 | -    | 10,10,53     | 0.82 | 0           | 9,9,61      | 0.38 | 0           |
| 6   | CLR  | C     | 1108 | -    | 31,31,31     | 8.52 | 17 (54%)    | 48,48,48    | 3.45 | 25 (52%)    |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | ZK1  | C     | 1102 | -    | 29,29,29     | 3.38 | 8 (27%)  | 45,45,45    | 1.62 | 7 (15%)  |
| 5   | PCW  | C     | 1109 | -    | 50,50,53     | 1.13 | 3 (6%)   | 56,58,61    | 0.99 | 3 (5%)   |
| 5   | PCW  | B     | 1103 | -    | 50,50,53     | 1.14 | 5 (10%)  | 56,58,61    | 0.96 | 3 (5%)   |
| 5   | PCW  | C     | 1110 | -    | 10,10,53     | 0.82 | 0        | 9,9,61      | 0.38 | 0        |
| 5   | PCW  | D     | 1106 | -    | 50,50,53     | 1.13 | 5 (10%)  | 56,58,61    | 0.87 | 3 (5%)   |
| 6   | CLR  | D     | 1108 | -    | 31,31,31     | 8.62 | 19 (61%) | 48,48,48    | 5.17 | 26 (54%) |
| 6   | CLR  | D     | 1109 | -    | 31,31,31     | 8.57 | 17 (54%) | 48,48,48    | 3.10 | 24 (50%) |
| 8   | SPD  | A     | 1112 | -    | 9,9,9        | 0.37 | 0        | 8,8,8       | 0.72 | 0        |
| 5   | PCW  | E     | 202  | -    | 10,10,53     | 0.84 | 0        | 9,9,61      | 0.26 | 0        |
| 4   | ZK1  | D     | 1103 | -    | 29,29,29     | 3.35 | 9 (31%)  | 45,45,45    | 1.73 | 7 (15%)  |
| 5   | PCW  | F     | 201  | -    | 50,50,53     | 1.16 | 4 (8%)   | 56,58,61    | 0.95 | 3 (5%)   |
| 5   | PCW  | C     | 1105 | -    | 50,50,53     | 1.16 | 4 (8%)   | 56,58,61    | 0.98 | 3 (5%)   |
| 5   | PCW  | F     | 203  | -    | 10,10,53     | 0.84 | 0        | 9,9,61      | 0.26 | 0        |
| 5   | PCW  | D     | 1105 | -    | 50,50,53     | 1.13 | 3 (6%)   | 56,58,61    | 0.99 | 3 (5%)   |
| 4   | ZK1  | B     | 1102 | -    | 29,29,29     | 3.35 | 9 (31%)  | 45,45,45    | 1.71 | 7 (15%)  |
| 5   | PCW  | B     | 1104 | -    | 50,50,53     | 1.13 | 3 (6%)   | 56,58,61    | 1.00 | 4 (7%)   |
| 3   | 6ZP  | D     | 1102 | -    | 30,30,30     | 0.99 | 1 (3%)   | 37,41,41    | 0.86 | 1 (2%)   |
| 5   | PCW  | A     | 1103 | -    | 50,50,53     | 1.16 | 5 (10%)  | 56,58,61    | 0.93 | 3 (5%)   |
| 5   | PCW  | A     | 1109 | -    | 50,50,53     | 1.13 | 5 (10%)  | 56,58,61    | 0.94 | 3 (5%)   |
| 3   | 6ZP  | C     | 1101 | -    | 30,30,30     | 1.12 | 1 (3%)   | 37,41,41    | 0.94 | 1 (2%)   |
| 5   | PCW  | B     | 1105 | -    | 50,50,53     | 1.13 | 5 (10%)  | 56,58,61    | 0.86 | 3 (5%)   |
| 3   | 6ZP  | A     | 1101 | -    | 30,30,30     | 1.12 | 1 (3%)   | 37,41,41    | 0.93 | 1 (2%)   |
| 5   | PCW  | C     | 1106 | -    | 50,50,53     | 1.13 | 4 (8%)   | 56,58,61    | 0.99 | 3 (5%)   |
| 5   | PCW  | A     | 1105 | -    | 50,50,53     | 1.16 | 4 (8%)   | 56,58,61    | 1.00 | 3 (5%)   |
| 5   | PCW  | E     | 203  | -    | 50,50,53     | 1.15 | 4 (8%)   | 56,58,61    | 0.95 | 3 (5%)   |
| 5   | PCW  | B     | 1109 | -    | 50,50,53     | 1.09 | 4 (8%)   | 56,58,61    | 0.96 | 4 (7%)   |
| 5   | PCW  | F     | 202  | -    | 10,10,53     | 0.83 | 0        | 9,9,61      | 0.36 | 0        |
| 5   | PCW  | D     | 1107 | -    | 10,10,53     | 0.78 | 0        | 9,9,61      | 0.39 | 0        |
| 6   | CLR  | B     | 1107 | -    | 31,31,31     | 8.63 | 20 (64%) | 48,48,48    | 5.13 | 25 (52%) |
| 5   | PCW  | E     | 201  | -    | 10,10,53     | 0.82 | 0        | 9,9,61      | 0.30 | 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   | PCW  | B     | 1106 | -    | -         | 3/8/8/57    | -       |
| 5   | PCW  | C     | 1103 | -    | -         | 27/54/54/57 | -       |
| 6   | CLR  | C     | 1107 | -    | 2/2/10/11 | 8/10/68/68  | 0/4/4/4 |
| 5   | PCW  | A     | 1104 | -    | -         | 27/54/54/57 | -       |
| 3   | 6ZP  | B     | 1101 | -    | -         | 1/13/14/14  | 0/4/4/4 |
| 5   | PCW  | A     | 1106 | -    | -         | 25/54/54/57 | -       |
| 5   | PCW  | D     | 1104 | -    | -         | 24/54/54/57 | -       |
| 6   | CLR  | A     | 1107 | -    | 2/2/10/11 | 8/10/68/68  | 0/4/4/4 |
| 6   | CLR  | B     | 1108 | -    | 2/2/10/11 | 9/10/68/68  | 0/4/4/4 |
| 5   | PCW  | C     | 1104 | -    | -         | 24/54/54/57 | -       |
| 6   | CLR  | A     | 1108 | -    | 2/2/10/11 | 8/10/68/68  | 0/4/4/4 |
| 5   | PCW  | D     | 1101 | -    | -         | 24/54/54/57 | -       |
| 6   | CLR  | C     | 1108 | -    | 2/2/10/11 | 8/10/68/68  | 0/4/4/4 |
| 4   | ZK1  | A     | 1102 | -    | -         | 5/13/23/23  | 0/3/3/3 |
| 5   | PCW  | A     | 1110 | -    | -         | 2/8/8/57    | -       |
| 4   | ZK1  | C     | 1102 | -    | -         | 5/13/23/23  | 0/3/3/3 |
| 5   | PCW  | C     | 1109 | -    | -         | 23/54/54/57 | -       |
| 6   | CLR  | D     | 1108 | -    | 2/2/10/11 | 9/10/68/68  | 0/4/4/4 |
| 6   | CLR  | D     | 1109 | -    | 2/2/10/11 | 9/10/68/68  | 0/4/4/4 |
| 5   | PCW  | B     | 1103 | -    | -         | 21/54/54/57 | -       |
| 5   | PCW  | C     | 1110 | -    | -         | 2/8/8/57    | -       |
| 5   | PCW  | D     | 1106 | -    | -         | 31/54/54/57 | -       |
| 8   | SPD  | A     | 1112 | -    | -         | 0/7/7/7     | -       |
| 5   | PCW  | E     | 202  | -    | -         | 4/8/8/57    | -       |
| 4   | ZK1  | D     | 1103 | -    | -         | 5/13/23/23  | 0/3/3/3 |
| 5   | PCW  | F     | 201  | -    | -         | 24/54/54/57 | -       |
| 5   | PCW  | C     | 1105 | -    | -         | 33/54/54/57 | -       |
| 5   | PCW  | F     | 203  | -    | -         | 3/8/8/57    | -       |
| 5   | PCW  | D     | 1105 | -    | -         | 25/54/54/57 | -       |
| 4   | ZK1  | B     | 1102 | -    | -         | 5/13/23/23  | 0/3/3/3 |
| 5   | PCW  | B     | 1104 | -    | -         | 25/54/54/57 | -       |
| 3   | 6ZP  | D     | 1102 | -    | -         | 1/13/14/14  | 0/4/4/4 |
| 5   | PCW  | A     | 1103 | -    | -         | 26/54/54/57 | -       |
| 5   | PCW  | A     | 1109 | -    | -         | 20/54/54/57 | -       |
| 3   | 6ZP  | C     | 1101 | -    | -         | 1/13/14/14  | 0/4/4/4 |
| 5   | PCW  | B     | 1105 | -    | -         | 33/54/54/57 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions    | Rings   |
|-----|------|-------|------|------|-----------|-------------|---------|
| 3   | 6ZP  | A     | 1101 | -    | -         | 1/13/14/14  | 0/4/4/4 |
| 5   | PCW  | C     | 1106 | -    | -         | 27/54/54/57 | -       |
| 5   | PCW  | A     | 1105 | -    | -         | 33/54/54/57 | -       |
| 5   | PCW  | E     | 203  | -    | -         | 27/54/54/57 | -       |
| 5   | PCW  | B     | 1109 | -    | -         | 24/54/54/57 | -       |
| 5   | PCW  | F     | 202  | -    | -         | 6/8/8/57    | -       |
| 5   | PCW  | D     | 1107 | -    | -         | 3/8/8/57    | -       |
| 6   | CLR  | B     | 1107 | -    | 2/2/10/11 | 9/10/68/68  | 0/4/4/4 |
| 5   | PCW  | E     | 201  | -    | -         | 4/8/8/57    | -       |

All (261) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 6   | D     | 1109 | CLR  | C4-C5  | -25.34 | 1.01        | 1.51     |
| 6   | D     | 1108 | CLR  | C4-C5  | -25.28 | 1.01        | 1.51     |
| 6   | A     | 1107 | CLR  | C4-C5  | -25.27 | 1.01        | 1.51     |
| 6   | C     | 1107 | CLR  | C4-C5  | -25.25 | 1.01        | 1.51     |
| 6   | B     | 1108 | CLR  | C4-C5  | -25.24 | 1.01        | 1.51     |
| 6   | A     | 1108 | CLR  | C4-C5  | -25.23 | 1.01        | 1.51     |
| 6   | B     | 1107 | CLR  | C4-C5  | -25.21 | 1.01        | 1.51     |
| 6   | C     | 1108 | CLR  | C4-C5  | -25.14 | 1.01        | 1.51     |
| 6   | A     | 1108 | CLR  | C1-C2  | -21.15 | 1.11        | 1.53     |
| 6   | C     | 1108 | CLR  | C1-C2  | -21.13 | 1.11        | 1.53     |
| 6   | A     | 1107 | CLR  | C1-C2  | -21.12 | 1.11        | 1.53     |
| 6   | C     | 1107 | CLR  | C1-C2  | -21.12 | 1.11        | 1.53     |
| 6   | D     | 1108 | CLR  | C1-C2  | -21.02 | 1.11        | 1.53     |
| 6   | B     | 1107 | CLR  | C1-C2  | -21.02 | 1.11        | 1.53     |
| 6   | B     | 1108 | CLR  | C1-C2  | -20.98 | 1.11        | 1.53     |
| 6   | D     | 1109 | CLR  | C1-C2  | -20.96 | 1.11        | 1.53     |
| 6   | B     | 1107 | CLR  | C8-C14 | 17.88  | 1.87        | 1.53     |
| 6   | D     | 1108 | CLR  | C8-C14 | 17.84  | 1.87        | 1.53     |
| 6   | A     | 1107 | CLR  | C8-C14 | 17.21  | 1.85        | 1.53     |
| 6   | C     | 1107 | CLR  | C8-C14 | 17.19  | 1.85        | 1.53     |
| 6   | C     | 1108 | CLR  | C8-C14 | 17.05  | 1.85        | 1.53     |
| 6   | A     | 1108 | CLR  | C8-C14 | 16.96  | 1.85        | 1.53     |
| 6   | B     | 1108 | CLR  | C8-C14 | 16.92  | 1.85        | 1.53     |
| 6   | D     | 1109 | CLR  | C8-C14 | 16.90  | 1.85        | 1.53     |
| 6   | B     | 1108 | CLR  | C8-C9  | -14.46 | 1.26        | 1.53     |
| 6   | D     | 1109 | CLR  | C8-C9  | -14.42 | 1.26        | 1.53     |
| 6   | C     | 1107 | CLR  | C8-C9  | -13.77 | 1.27        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 6   | A     | 1108 | CLR  | C8-C9   | -13.75 | 1.27        | 1.53     |
| 6   | A     | 1107 | CLR  | C8-C9   | -13.72 | 1.27        | 1.53     |
| 6   | C     | 1108 | CLR  | C8-C9   | -13.72 | 1.27        | 1.53     |
| 6   | B     | 1107 | CLR  | C8-C9   | -13.21 | 1.28        | 1.53     |
| 6   | D     | 1108 | CLR  | C8-C9   | -13.04 | 1.29        | 1.53     |
| 6   | B     | 1108 | CLR  | C7-C6   | 10.91  | 1.72        | 1.50     |
| 6   | D     | 1109 | CLR  | C7-C6   | 10.83  | 1.72        | 1.50     |
| 4   | A     | 1102 | ZK1  | CAU-CAT | -10.80 | 1.38        | 1.53     |
| 4   | C     | 1102 | ZK1  | CAU-CAT | -10.71 | 1.38        | 1.53     |
| 6   | D     | 1108 | CLR  | C7-C6   | 10.69  | 1.72        | 1.50     |
| 6   | B     | 1107 | CLR  | C7-C6   | 10.69  | 1.72        | 1.50     |
| 6   | C     | 1107 | CLR  | C7-C6   | 10.67  | 1.72        | 1.50     |
| 6   | C     | 1108 | CLR  | C7-C6   | 10.64  | 1.71        | 1.50     |
| 6   | A     | 1108 | CLR  | C7-C6   | 10.64  | 1.71        | 1.50     |
| 4   | D     | 1103 | ZK1  | CAU-CAT | -10.58 | 1.38        | 1.53     |
| 6   | A     | 1107 | CLR  | C7-C6   | 10.55  | 1.71        | 1.50     |
| 4   | B     | 1102 | ZK1  | CAU-CAT | -10.53 | 1.38        | 1.53     |
| 6   | D     | 1109 | CLR  | C7-C8   | -10.04 | 1.36        | 1.53     |
| 6   | B     | 1108 | CLR  | C7-C8   | -10.04 | 1.36        | 1.53     |
| 6   | B     | 1107 | CLR  | C7-C8   | -9.83  | 1.37        | 1.53     |
| 6   | C     | 1108 | CLR  | C6-C5   | -9.78  | 1.12        | 1.33     |
| 6   | D     | 1108 | CLR  | C7-C8   | -9.73  | 1.37        | 1.53     |
| 6   | A     | 1108 | CLR  | C6-C5   | -9.67  | 1.13        | 1.33     |
| 6   | A     | 1107 | CLR  | C6-C5   | -9.63  | 1.13        | 1.33     |
| 6   | C     | 1107 | CLR  | C6-C5   | -9.58  | 1.13        | 1.33     |
| 6   | A     | 1107 | CLR  | C7-C8   | -9.57  | 1.37        | 1.53     |
| 6   | C     | 1107 | CLR  | C7-C8   | -9.56  | 1.37        | 1.53     |
| 6   | D     | 1108 | CLR  | C6-C5   | -9.45  | 1.13        | 1.33     |
| 6   | B     | 1107 | CLR  | C6-C5   | -9.42  | 1.13        | 1.33     |
| 6   | C     | 1108 | CLR  | C7-C8   | -9.31  | 1.38        | 1.53     |
| 6   | A     | 1108 | CLR  | C7-C8   | -9.29  | 1.38        | 1.53     |
| 6   | B     | 1108 | CLR  | C6-C5   | -9.29  | 1.13        | 1.33     |
| 6   | B     | 1107 | CLR  | C4-C3   | 9.29   | 1.68        | 1.52     |
| 6   | B     | 1108 | CLR  | C4-C3   | 9.28   | 1.68        | 1.52     |
| 6   | D     | 1109 | CLR  | C6-C5   | -9.27  | 1.13        | 1.33     |
| 6   | D     | 1108 | CLR  | C4-C3   | 9.26   | 1.68        | 1.52     |
| 6   | C     | 1108 | CLR  | C4-C3   | 9.23   | 1.68        | 1.52     |
| 6   | A     | 1108 | CLR  | C4-C3   | 9.21   | 1.68        | 1.52     |
| 6   | D     | 1109 | CLR  | C4-C3   | 9.16   | 1.68        | 1.52     |
| 6   | A     | 1107 | CLR  | C4-C3   | 9.11   | 1.68        | 1.52     |
| 6   | C     | 1107 | CLR  | C4-C3   | 9.11   | 1.68        | 1.52     |
| 4   | D     | 1103 | ZK1  | OAB-CAU | 8.41   | 1.40        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | B     | 1102 | ZK1  | OAB-CAU | 8.41  | 1.40        | 1.23     |
| 4   | A     | 1102 | ZK1  | OAA-CAT | 8.39  | 1.39        | 1.23     |
| 4   | D     | 1103 | ZK1  | OAA-CAT | 8.39  | 1.39        | 1.23     |
| 4   | A     | 1102 | ZK1  | OAB-CAU | 8.36  | 1.40        | 1.23     |
| 4   | B     | 1102 | ZK1  | OAA-CAT | 8.36  | 1.39        | 1.23     |
| 4   | C     | 1102 | ZK1  | OAA-CAT | 8.35  | 1.39        | 1.23     |
| 4   | C     | 1102 | ZK1  | OAB-CAU | 8.31  | 1.40        | 1.23     |
| 6   | D     | 1108 | CLR  | C13-C14 | -8.18 | 1.39        | 1.55     |
| 6   | B     | 1107 | CLR  | C13-C14 | -8.14 | 1.40        | 1.55     |
| 6   | B     | 1108 | CLR  | C13-C14 | -7.67 | 1.40        | 1.55     |
| 6   | D     | 1109 | CLR  | C13-C14 | -7.54 | 1.41        | 1.55     |
| 6   | A     | 1107 | CLR  | C13-C14 | -7.49 | 1.41        | 1.55     |
| 6   | C     | 1107 | CLR  | C13-C14 | -7.43 | 1.41        | 1.55     |
| 6   | A     | 1108 | CLR  | C13-C14 | -7.35 | 1.41        | 1.55     |
| 6   | D     | 1108 | CLR  | C11-C9  | 7.31  | 1.65        | 1.53     |
| 6   | B     | 1107 | CLR  | C11-C9  | 7.28  | 1.65        | 1.53     |
| 6   | C     | 1108 | CLR  | C13-C14 | -7.28 | 1.41        | 1.55     |
| 6   | A     | 1108 | CLR  | C11-C9  | 6.66  | 1.64        | 1.53     |
| 6   | C     | 1108 | CLR  | C11-C9  | 6.63  | 1.64        | 1.53     |
| 6   | D     | 1109 | CLR  | C10-C9  | 6.54  | 1.66        | 1.56     |
| 6   | D     | 1108 | CLR  | C12-C13 | -6.53 | 1.42        | 1.54     |
| 6   | B     | 1107 | CLR  | C12-C13 | -6.49 | 1.42        | 1.54     |
| 6   | B     | 1108 | CLR  | C10-C9  | 6.48  | 1.66        | 1.56     |
| 6   | A     | 1107 | CLR  | C10-C9  | 6.48  | 1.66        | 1.56     |
| 6   | C     | 1107 | CLR  | C10-C9  | 6.41  | 1.66        | 1.56     |
| 6   | A     | 1107 | CLR  | C11-C9  | 6.34  | 1.64        | 1.53     |
| 6   | C     | 1107 | CLR  | C11-C9  | 6.34  | 1.64        | 1.53     |
| 6   | A     | 1107 | CLR  | C12-C13 | -6.33 | 1.43        | 1.54     |
| 6   | C     | 1107 | CLR  | C12-C13 | -6.26 | 1.43        | 1.54     |
| 6   | B     | 1107 | CLR  | C13-C17 | 6.09  | 1.66        | 1.55     |
| 6   | A     | 1107 | CLR  | C13-C17 | 6.08  | 1.66        | 1.55     |
| 6   | B     | 1108 | CLR  | C11-C9  | 6.06  | 1.63        | 1.53     |
| 6   | A     | 1108 | CLR  | C12-C13 | -6.05 | 1.43        | 1.54     |
| 6   | C     | 1108 | CLR  | C10-C9  | 6.05  | 1.65        | 1.56     |
| 6   | C     | 1108 | CLR  | C12-C13 | -6.02 | 1.43        | 1.54     |
| 6   | D     | 1109 | CLR  | C11-C9  | 6.01  | 1.63        | 1.53     |
| 6   | B     | 1108 | CLR  | C12-C13 | -6.00 | 1.43        | 1.54     |
| 6   | D     | 1109 | CLR  | C12-C13 | -5.99 | 1.43        | 1.54     |
| 6   | D     | 1108 | CLR  | C13-C17 | 5.98  | 1.66        | 1.55     |
| 6   | A     | 1108 | CLR  | C10-C9  | 5.96  | 1.65        | 1.56     |
| 6   | C     | 1107 | CLR  | C13-C17 | 5.94  | 1.65        | 1.55     |
| 6   | A     | 1108 | CLR  | C16-C17 | -5.93 | 1.42        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6   | D     | 1109 | CLR  | C13-C17 | 5.85  | 1.65        | 1.55     |
| 6   | B     | 1108 | CLR  | C13-C17 | 5.80  | 1.65        | 1.55     |
| 6   | C     | 1108 | CLR  | C16-C17 | -5.79 | 1.42        | 1.54     |
| 6   | C     | 1108 | CLR  | C13-C17 | 5.75  | 1.65        | 1.55     |
| 6   | D     | 1109 | CLR  | C16-C17 | -5.66 | 1.42        | 1.54     |
| 6   | A     | 1108 | CLR  | C13-C17 | 5.65  | 1.65        | 1.55     |
| 6   | B     | 1108 | CLR  | C16-C17 | -5.64 | 1.42        | 1.54     |
| 6   | A     | 1108 | CLR  | C2-C3   | -5.63 | 1.38        | 1.51     |
| 6   | C     | 1108 | CLR  | C2-C3   | -5.62 | 1.38        | 1.51     |
| 6   | C     | 1107 | CLR  | C16-C17 | -5.62 | 1.42        | 1.54     |
| 6   | B     | 1107 | CLR  | C10-C9  | 5.57  | 1.64        | 1.56     |
| 6   | A     | 1107 | CLR  | C16-C17 | -5.54 | 1.43        | 1.54     |
| 6   | A     | 1107 | CLR  | C2-C3   | -5.50 | 1.39        | 1.51     |
| 6   | D     | 1108 | CLR  | C10-C9  | 5.49  | 1.64        | 1.56     |
| 6   | C     | 1107 | CLR  | C2-C3   | -5.46 | 1.39        | 1.51     |
| 6   | D     | 1109 | CLR  | C2-C3   | -5.46 | 1.39        | 1.51     |
| 6   | B     | 1108 | CLR  | C2-C3   | -5.45 | 1.39        | 1.51     |
| 6   | D     | 1108 | CLR  | C2-C3   | -5.44 | 1.39        | 1.51     |
| 6   | B     | 1107 | CLR  | C2-C3   | -5.32 | 1.39        | 1.51     |
| 3   | C     | 1101 | 6ZP  | C09-C10 | -5.15 | 1.38        | 1.46     |
| 3   | A     | 1101 | 6ZP  | C09-C10 | -5.15 | 1.38        | 1.46     |
| 3   | B     | 1101 | 6ZP  | C09-C10 | -4.64 | 1.39        | 1.46     |
| 3   | D     | 1102 | 6ZP  | C09-C10 | -4.63 | 1.39        | 1.46     |
| 6   | D     | 1109 | CLR  | C1-C10  | 4.35  | 1.62        | 1.54     |
| 6   | B     | 1108 | CLR  | C1-C10  | 4.30  | 1.62        | 1.54     |
| 6   | A     | 1107 | CLR  | C1-C10  | 4.26  | 1.62        | 1.54     |
| 6   | D     | 1108 | CLR  | C16-C17 | -4.26 | 1.45        | 1.54     |
| 6   | C     | 1107 | CLR  | C1-C10  | 4.24  | 1.62        | 1.54     |
| 6   | B     | 1107 | CLR  | C16-C17 | -4.23 | 1.45        | 1.54     |
| 6   | D     | 1108 | CLR  | C15-C14 | 4.20  | 1.63        | 1.54     |
| 6   | B     | 1107 | CLR  | C15-C14 | 4.17  | 1.62        | 1.54     |
| 6   | A     | 1108 | CLR  | C1-C10  | 4.12  | 1.61        | 1.54     |
| 6   | C     | 1108 | CLR  | C1-C10  | 4.11  | 1.61        | 1.54     |
| 6   | D     | 1108 | CLR  | C1-C10  | 4.09  | 1.61        | 1.54     |
| 6   | B     | 1107 | CLR  | C1-C10  | 4.07  | 1.61        | 1.54     |
| 4   | B     | 1102 | ZK1  | CAW-NAY | -3.70 | 1.34        | 1.41     |
| 4   | A     | 1102 | ZK1  | CAW-NAY | -3.66 | 1.34        | 1.41     |
| 4   | C     | 1102 | ZK1  | CAW-NAY | -3.66 | 1.34        | 1.41     |
| 4   | D     | 1103 | ZK1  | CAW-NAY | -3.64 | 1.34        | 1.41     |
| 4   | A     | 1102 | ZK1  | CAU-NAY | -3.47 | 1.32        | 1.38     |
| 4   | C     | 1102 | ZK1  | CAU-NAY | -3.44 | 1.32        | 1.38     |
| 6   | A     | 1107 | CLR  | C15-C14 | 3.42  | 1.61        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | A     | 1102 | ZK1  | CAV-CAW | -3.42 | 1.36        | 1.40     |
| 6   | B     | 1107 | CLR  | C18-C13 | 3.39  | 1.59        | 1.54     |
| 6   | C     | 1107 | CLR  | C15-C14 | 3.39  | 1.61        | 1.54     |
| 4   | D     | 1103 | ZK1  | CAU-NAY | -3.39 | 1.32        | 1.38     |
| 4   | A     | 1102 | ZK1  | CAV-NAP | -3.38 | 1.34        | 1.39     |
| 4   | C     | 1102 | ZK1  | CAV-NAP | -3.37 | 1.34        | 1.39     |
| 4   | B     | 1102 | ZK1  | CAU-NAY | -3.36 | 1.32        | 1.38     |
| 6   | B     | 1108 | CLR  | C15-C14 | 3.36  | 1.61        | 1.54     |
| 6   | D     | 1108 | CLR  | C18-C13 | 3.32  | 1.59        | 1.54     |
| 4   | C     | 1102 | ZK1  | CAV-CAW | -3.32 | 1.36        | 1.40     |
| 6   | D     | 1109 | CLR  | C15-C14 | 3.24  | 1.61        | 1.54     |
| 6   | C     | 1108 | CLR  | C15-C14 | 3.15  | 1.60        | 1.54     |
| 4   | B     | 1102 | ZK1  | CAV-NAP | -3.12 | 1.34        | 1.39     |
| 5   | A     | 1105 | PCW  | O2-C31  | 3.11  | 1.43        | 1.34     |
| 4   | D     | 1103 | ZK1  | CAV-NAP | -3.11 | 1.34        | 1.39     |
| 5   | A     | 1106 | PCW  | O3-C11  | 3.11  | 1.42        | 1.33     |
| 5   | C     | 1106 | PCW  | O3-C11  | 3.09  | 1.42        | 1.33     |
| 6   | A     | 1108 | CLR  | C15-C14 | 3.09  | 1.60        | 1.54     |
| 5   | C     | 1105 | PCW  | O3-C11  | 3.05  | 1.42        | 1.33     |
| 5   | C     | 1104 | PCW  | O2-C31  | 3.05  | 1.42        | 1.34     |
| 5   | C     | 1105 | PCW  | O2-C31  | 3.04  | 1.42        | 1.34     |
| 5   | C     | 1109 | PCW  | O2-C31  | 3.04  | 1.42        | 1.34     |
| 5   | D     | 1106 | PCW  | O2-C31  | 3.03  | 1.42        | 1.34     |
| 5   | B     | 1105 | PCW  | O3-C11  | 3.03  | 1.42        | 1.33     |
| 5   | D     | 1104 | PCW  | O3-C11  | 3.00  | 1.42        | 1.33     |
| 5   | F     | 201  | PCW  | O3-C11  | 3.00  | 1.42        | 1.33     |
| 5   | A     | 1109 | PCW  | O2-C31  | 2.99  | 1.42        | 1.34     |
| 5   | A     | 1105 | PCW  | O3-C11  | 2.99  | 1.42        | 1.33     |
| 5   | D     | 1106 | PCW  | O3-C11  | 2.98  | 1.42        | 1.33     |
| 5   | E     | 203  | PCW  | O3-C11  | 2.98  | 1.42        | 1.33     |
| 5   | A     | 1104 | PCW  | O2-C31  | 2.98  | 1.42        | 1.34     |
| 5   | C     | 1103 | PCW  | O2-C31  | 2.97  | 1.42        | 1.34     |
| 5   | A     | 1103 | PCW  | O2-C31  | 2.96  | 1.42        | 1.34     |
| 5   | B     | 1105 | PCW  | O2-C31  | 2.93  | 1.42        | 1.34     |
| 5   | B     | 1103 | PCW  | O3-C11  | 2.92  | 1.41        | 1.33     |
| 5   | B     | 1104 | PCW  | O2-C31  | 2.89  | 1.42        | 1.34     |
| 5   | C     | 1104 | PCW  | O3-C11  | 2.89  | 1.41        | 1.33     |
| 5   | D     | 1104 | PCW  | O2-C31  | 2.89  | 1.42        | 1.34     |
| 5   | C     | 1103 | PCW  | O3-C11  | 2.89  | 1.41        | 1.33     |
| 5   | D     | 1105 | PCW  | O2-C31  | 2.88  | 1.42        | 1.34     |
| 5   | D     | 1101 | PCW  | O2-C31  | 2.88  | 1.42        | 1.34     |
| 4   | B     | 1102 | ZK1  | CAV-CAW | -2.87 | 1.37        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5   | A     | 1103 | PCW  | O3-C11  | 2.87  | 1.41        | 1.33     |
| 5   | A     | 1104 | PCW  | O3-C11  | 2.87  | 1.41        | 1.33     |
| 5   | B     | 1103 | PCW  | O2-C31  | 2.85  | 1.42        | 1.34     |
| 4   | D     | 1103 | ZK1  | CAV-CAW | -2.85 | 1.37        | 1.40     |
| 5   | B     | 1109 | PCW  | O2-C31  | 2.84  | 1.42        | 1.34     |
| 4   | A     | 1102 | ZK1  | CAT-NAP | -2.82 | 1.31        | 1.35     |
| 5   | C     | 1109 | PCW  | O3-C11  | 2.81  | 1.41        | 1.33     |
| 5   | C     | 1106 | PCW  | O2-C31  | 2.79  | 1.42        | 1.34     |
| 5   | B     | 1104 | PCW  | O3-C11  | 2.79  | 1.41        | 1.33     |
| 5   | A     | 1106 | PCW  | O2-C31  | 2.79  | 1.42        | 1.34     |
| 5   | A     | 1109 | PCW  | O3-C11  | 2.78  | 1.41        | 1.33     |
| 6   | D     | 1108 | CLR  | C16-C15 | 2.77  | 1.61        | 1.54     |
| 5   | E     | 203  | PCW  | O2-C31  | 2.77  | 1.42        | 1.34     |
| 5   | D     | 1105 | PCW  | O3-C11  | 2.76  | 1.41        | 1.33     |
| 6   | B     | 1107 | CLR  | C16-C15 | 2.73  | 1.61        | 1.54     |
| 5   | F     | 201  | PCW  | O2-C31  | 2.73  | 1.42        | 1.34     |
| 5   | B     | 1109 | PCW  | O2-C2   | -2.72 | 1.40        | 1.46     |
| 5   | D     | 1105 | PCW  | O2-C2   | -2.72 | 1.40        | 1.46     |
| 5   | B     | 1104 | PCW  | O2-C2   | -2.71 | 1.40        | 1.46     |
| 5   | F     | 201  | PCW  | O2-C2   | -2.71 | 1.40        | 1.46     |
| 4   | C     | 1102 | ZK1  | CAT-NAP | -2.70 | 1.32        | 1.35     |
| 5   | E     | 203  | PCW  | O2-C2   | -2.68 | 1.40        | 1.46     |
| 5   | D     | 1101 | PCW  | O2-C2   | -2.68 | 1.40        | 1.46     |
| 5   | A     | 1106 | PCW  | O2-C2   | -2.67 | 1.40        | 1.46     |
| 5   | C     | 1106 | PCW  | O2-C2   | -2.65 | 1.40        | 1.46     |
| 4   | D     | 1103 | ZK1  | CAT-NAP | -2.58 | 1.32        | 1.35     |
| 4   | B     | 1102 | ZK1  | CAT-NAP | -2.52 | 1.32        | 1.35     |
| 5   | D     | 1101 | PCW  | O3-C11  | 2.51  | 1.40        | 1.33     |
| 5   | A     | 1103 | PCW  | O2-C2   | -2.49 | 1.40        | 1.46     |
| 5   | C     | 1105 | PCW  | O2-C2   | -2.48 | 1.40        | 1.46     |
| 5   | B     | 1103 | PCW  | O2-C2   | -2.48 | 1.40        | 1.46     |
| 5   | C     | 1103 | PCW  | O2-C2   | -2.47 | 1.40        | 1.46     |
| 5   | D     | 1104 | PCW  | O2-C2   | -2.46 | 1.40        | 1.46     |
| 5   | B     | 1109 | PCW  | O3-C11  | 2.44  | 1.40        | 1.33     |
| 5   | A     | 1104 | PCW  | O2-C2   | -2.43 | 1.40        | 1.46     |
| 5   | A     | 1109 | PCW  | O2-C2   | -2.43 | 1.40        | 1.46     |
| 5   | A     | 1105 | PCW  | O2-C2   | -2.38 | 1.41        | 1.46     |
| 5   | C     | 1109 | PCW  | O2-C2   | -2.34 | 1.41        | 1.46     |
| 5   | C     | 1104 | PCW  | O2-C2   | -2.32 | 1.41        | 1.46     |
| 5   | B     | 1105 | PCW  | O2-C2   | -2.30 | 1.41        | 1.46     |
| 4   | B     | 1102 | ZK1  | PBA-CAO | 2.28  | 1.86        | 1.81     |
| 5   | D     | 1106 | PCW  | O2-C2   | -2.25 | 1.41        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 4   | D     | 1103 | ZK1  | PBA-CAO | 2.22 | 1.86        | 1.81     |
| 5   | D     | 1101 | PCW  | P-O4P   | 2.15 | 1.67        | 1.59     |
| 5   | C     | 1103 | PCW  | P-O4P   | 2.11 | 1.67        | 1.59     |
| 5   | B     | 1109 | PCW  | P-O4P   | 2.10 | 1.67        | 1.59     |
| 5   | A     | 1103 | PCW  | P-O4P   | 2.10 | 1.67        | 1.59     |
| 5   | F     | 201  | PCW  | P-O4P   | 2.09 | 1.67        | 1.59     |
| 5   | C     | 1103 | PCW  | P-O3P   | 2.08 | 1.67        | 1.59     |
| 5   | E     | 203  | PCW  | P-O4P   | 2.08 | 1.67        | 1.59     |
| 5   | B     | 1105 | PCW  | P-O4P   | 2.07 | 1.67        | 1.59     |
| 5   | D     | 1106 | PCW  | P-O4P   | 2.07 | 1.67        | 1.59     |
| 5   | A     | 1103 | PCW  | P-O3P   | 2.06 | 1.67        | 1.59     |
| 5   | C     | 1106 | PCW  | P-O4P   | 2.05 | 1.67        | 1.59     |
| 5   | D     | 1104 | PCW  | P-O4P   | 2.04 | 1.67        | 1.59     |
| 5   | A     | 1105 | PCW  | P-O3P   | 2.04 | 1.67        | 1.59     |
| 5   | D     | 1104 | PCW  | P-O3P   | 2.04 | 1.67        | 1.59     |
| 5   | A     | 1109 | PCW  | P-O3P   | 2.04 | 1.67        | 1.59     |
| 5   | C     | 1105 | PCW  | P-O3P   | 2.04 | 1.67        | 1.59     |
| 5   | B     | 1103 | PCW  | P-O4P   | 2.03 | 1.67        | 1.59     |
| 5   | A     | 1106 | PCW  | P-O4P   | 2.03 | 1.67        | 1.59     |
| 5   | B     | 1103 | PCW  | P-O3P   | 2.02 | 1.67        | 1.59     |
| 5   | B     | 1105 | PCW  | P-O3P   | 2.02 | 1.67        | 1.59     |
| 5   | A     | 1109 | PCW  | P-O4P   | 2.01 | 1.67        | 1.59     |
| 5   | D     | 1106 | PCW  | P-O3P   | 2.01 | 1.67        | 1.59     |
| 6   | B     | 1107 | CLR  | C22-C20 | 2.01 | 1.59        | 1.54     |

All (289) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 6   | D     | 1108 | CLR  | C18-C13-C12 | -18.93 | 82.70       | 110.61   |
| 6   | B     | 1107 | CLR  | C18-C13-C12 | -18.85 | 82.82       | 110.61   |
| 6   | D     | 1108 | CLR  | C12-C13-C14 | 10.38  | 122.78      | 107.25   |
| 6   | D     | 1108 | CLR  | C18-C13-C17 | -10.38 | 92.85       | 111.68   |
| 6   | B     | 1107 | CLR  | C18-C13-C17 | -10.35 | 92.91       | 111.68   |
| 6   | B     | 1107 | CLR  | C12-C13-C14 | 10.33  | 122.70      | 107.25   |
| 6   | D     | 1108 | CLR  | C22-C20-C17 | 9.37   | 129.76      | 110.33   |
| 6   | B     | 1107 | CLR  | C22-C20-C17 | 9.18   | 129.37      | 110.33   |
| 6   | B     | 1107 | CLR  | C19-C10-C9  | -9.06  | 101.49      | 111.66   |
| 6   | A     | 1107 | CLR  | C4-C5-C6    | -8.90  | 108.50      | 120.57   |
| 6   | B     | 1107 | CLR  | C12-C13-C17 | 8.83   | 129.61      | 116.60   |
| 6   | C     | 1107 | CLR  | C4-C5-C6    | -8.80  | 108.64      | 120.57   |
| 6   | B     | 1108 | CLR  | C19-C10-C9  | -8.70  | 101.89      | 111.66   |
| 6   | D     | 1108 | CLR  | C12-C13-C17 | 8.66   | 129.35      | 116.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | D     | 1108 | CLR  | C19-C10-C9  | -8.57 | 102.04      | 111.66   |
| 6   | D     | 1109 | CLR  | C4-C5-C6    | -8.55 | 108.98      | 120.57   |
| 6   | C     | 1108 | CLR  | C4-C5-C6    | -8.55 | 108.98      | 120.57   |
| 6   | B     | 1107 | CLR  | C4-C5-C6    | -8.51 | 109.04      | 120.57   |
| 6   | D     | 1108 | CLR  | C4-C5-C6    | -8.45 | 109.12      | 120.57   |
| 6   | A     | 1108 | CLR  | C4-C5-C6    | -8.34 | 109.27      | 120.57   |
| 6   | B     | 1108 | CLR  | C4-C5-C6    | -8.32 | 109.29      | 120.57   |
| 6   | A     | 1108 | CLR  | C7-C8-C9    | 8.04  | 119.01      | 109.72   |
| 6   | D     | 1109 | CLR  | C19-C10-C9  | -7.99 | 102.69      | 111.66   |
| 6   | C     | 1108 | CLR  | C7-C8-C9    | 7.95  | 118.91      | 109.72   |
| 6   | D     | 1109 | CLR  | C12-C13-C17 | -7.95 | 104.90      | 116.60   |
| 6   | B     | 1108 | CLR  | C12-C13-C17 | -7.82 | 105.09      | 116.60   |
| 6   | A     | 1108 | CLR  | C19-C10-C9  | -7.61 | 103.11      | 111.66   |
| 6   | A     | 1108 | CLR  | C21-C20-C17 | -7.60 | 101.48      | 112.88   |
| 6   | C     | 1108 | CLR  | C19-C10-C9  | -7.30 | 103.47      | 111.66   |
| 6   | A     | 1107 | CLR  | C12-C13-C17 | -7.17 | 106.04      | 116.60   |
| 6   | C     | 1107 | CLR  | C19-C10-C9  | -7.00 | 103.81      | 111.66   |
| 6   | C     | 1107 | CLR  | C12-C13-C17 | -6.94 | 106.38      | 116.60   |
| 6   | C     | 1108 | CLR  | C12-C13-C17 | -6.93 | 106.39      | 116.60   |
| 6   | A     | 1108 | CLR  | C1-C2-C3    | 6.88  | 119.59      | 110.48   |
| 6   | A     | 1107 | CLR  | C19-C10-C9  | -6.86 | 103.96      | 111.66   |
| 6   | A     | 1108 | CLR  | C12-C13-C17 | -6.68 | 106.76      | 116.60   |
| 6   | B     | 1108 | CLR  | C1-C2-C3    | 6.65  | 119.30      | 110.48   |
| 6   | D     | 1109 | CLR  | C1-C2-C3    | 6.64  | 119.28      | 110.48   |
| 6   | D     | 1108 | CLR  | C16-C17-C20 | 6.51  | 122.03      | 112.18   |
| 6   | D     | 1108 | CLR  | C17-C13-C14 | 6.49  | 107.55      | 100.10   |
| 6   | A     | 1107 | CLR  | C7-C8-C9    | 6.44  | 117.17      | 109.72   |
| 6   | D     | 1108 | CLR  | C1-C2-C3    | 6.40  | 118.96      | 110.48   |
| 6   | C     | 1108 | CLR  | C21-C20-C17 | -6.34 | 103.36      | 112.88   |
| 6   | B     | 1107 | CLR  | C16-C17-C20 | 6.34  | 121.77      | 112.18   |
| 6   | B     | 1107 | CLR  | C1-C2-C3    | 6.33  | 118.87      | 110.48   |
| 6   | B     | 1107 | CLR  | C17-C13-C14 | 6.28  | 107.31      | 100.10   |
| 6   | C     | 1108 | CLR  | C1-C2-C3    | 6.25  | 118.75      | 110.48   |
| 6   | C     | 1107 | CLR  | C7-C8-C9    | 6.23  | 116.92      | 109.72   |
| 6   | C     | 1107 | CLR  | C1-C2-C3    | 6.01  | 118.44      | 110.48   |
| 6   | A     | 1107 | CLR  | C1-C2-C3    | 5.94  | 118.34      | 110.48   |
| 6   | D     | 1108 | CLR  | C21-C20-C17 | -5.80 | 104.18      | 112.88   |
| 6   | A     | 1107 | CLR  | C14-C8-C9   | 5.73  | 116.57      | 109.09   |
| 6   | C     | 1107 | CLR  | C14-C8-C9   | 5.67  | 116.49      | 109.09   |
| 6   | D     | 1108 | CLR  | C7-C8-C9    | 5.50  | 116.08      | 109.72   |
| 6   | B     | 1107 | CLR  | C21-C20-C17 | -5.49 | 104.65      | 112.88   |
| 6   | A     | 1108 | CLR  | C15-C16-C17 | -5.38 | 94.61       | 105.14   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | D     | 1108 | CLR  | C18-C13-C14 | -5.28 | 102.09      | 111.68   |
| 6   | B     | 1107 | CLR  | C18-C13-C14 | -5.10 | 102.42      | 111.68   |
| 6   | B     | 1107 | CLR  | C14-C8-C9   | 5.06  | 115.69      | 109.09   |
| 4   | A     | 1102 | ZK1  | CAI-CAR-NAX | -5.02 | 115.28      | 122.59   |
| 6   | A     | 1108 | CLR  | C14-C8-C9   | 4.96  | 115.56      | 109.09   |
| 5   | A     | 1104 | PCW  | O2-C31-C32  | 4.94  | 122.18      | 111.48   |
| 5   | C     | 1104 | PCW  | O2-C31-C32  | 4.94  | 122.17      | 111.48   |
| 6   | C     | 1108 | CLR  | C7-C6-C5    | -4.91 | 116.73      | 125.02   |
| 6   | A     | 1108 | CLR  | C12-C13-C14 | 4.89  | 114.57      | 107.25   |
| 5   | B     | 1104 | PCW  | O2-C31-C32  | 4.89  | 122.06      | 111.48   |
| 4   | D     | 1103 | ZK1  | CAN-NAX-CAM | 4.88  | 122.54      | 111.57   |
| 4   | B     | 1102 | ZK1  | CAN-NAX-CAM | 4.86  | 122.51      | 111.57   |
| 6   | C     | 1108 | CLR  | C12-C13-C14 | 4.86  | 114.52      | 107.25   |
| 5   | D     | 1105 | PCW  | O2-C31-C32  | 4.84  | 121.96      | 111.48   |
| 6   | C     | 1108 | CLR  | C14-C8-C9   | 4.82  | 115.38      | 109.09   |
| 6   | D     | 1108 | CLR  | C14-C8-C9   | 4.80  | 115.36      | 109.09   |
| 4   | C     | 1102 | ZK1  | CAI-CAR-NAX | -4.80 | 115.60      | 122.59   |
| 6   | A     | 1108 | CLR  | C7-C6-C5    | -4.80 | 116.92      | 125.02   |
| 6   | B     | 1107 | CLR  | C7-C8-C9    | 4.70  | 115.16      | 109.72   |
| 6   | A     | 1107 | CLR  | C7-C6-C5    | -4.62 | 117.21      | 125.02   |
| 6   | C     | 1107 | CLR  | C7-C6-C5    | -4.57 | 117.30      | 125.02   |
| 4   | D     | 1103 | ZK1  | CAI-CAR-NAX | -4.54 | 115.97      | 122.59   |
| 4   | B     | 1102 | ZK1  | CAI-CAR-NAX | -4.53 | 115.99      | 122.59   |
| 6   | D     | 1108 | CLR  | C10-C9-C8   | 4.49  | 119.27      | 112.71   |
| 6   | D     | 1109 | CLR  | C14-C8-C9   | 4.45  | 114.90      | 109.09   |
| 6   | C     | 1108 | CLR  | C15-C16-C17 | -4.43 | 96.48       | 105.14   |
| 6   | B     | 1107 | CLR  | C10-C9-C8   | 4.40  | 119.14      | 112.71   |
| 4   | A     | 1102 | ZK1  | CAN-NAX-CAM | 4.37  | 121.40      | 111.57   |
| 6   | D     | 1109 | CLR  | C12-C13-C14 | 4.35  | 113.76      | 107.25   |
| 4   | C     | 1102 | ZK1  | CAN-NAX-CAM | 4.29  | 121.23      | 111.57   |
| 5   | C     | 1109 | PCW  | O2-C31-C32  | 4.29  | 120.75      | 111.48   |
| 5   | A     | 1105 | PCW  | O2-C31-C32  | 4.25  | 120.68      | 111.48   |
| 6   | A     | 1107 | CLR  | C17-C13-C14 | 4.25  | 104.97      | 100.10   |
| 4   | A     | 1102 | ZK1  | CAS-CAR-NAX | 4.24  | 124.78      | 119.92   |
| 6   | D     | 1109 | CLR  | C7-C6-C5    | -4.24 | 117.87      | 125.02   |
| 6   | B     | 1108 | CLR  | C14-C8-C9   | 4.23  | 114.61      | 109.09   |
| 6   | C     | 1108 | CLR  | C3-C4-C5    | 4.22  | 118.78      | 112.05   |
| 4   | D     | 1103 | ZK1  | CAV-NAP-CAT | -4.19 | 118.96      | 124.82   |
| 5   | C     | 1105 | PCW  | O2-C31-C32  | 4.17  | 120.49      | 111.48   |
| 4   | B     | 1102 | ZK1  | CAV-NAP-CAT | -4.14 | 119.02      | 124.82   |
| 5   | A     | 1109 | PCW  | O2-C31-C32  | 4.12  | 120.39      | 111.48   |
| 6   | A     | 1108 | CLR  | C3-C4-C5    | 4.09  | 118.56      | 112.05   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | A     | 1108 | CLR  | C15-C14-C8  | -4.07 | 112.60      | 119.10   |
| 6   | B     | 1108 | CLR  | C12-C13-C14 | 4.06  | 113.32      | 107.25   |
| 6   | D     | 1108 | CLR  | C7-C6-C5    | -4.06 | 118.17      | 125.02   |
| 4   | C     | 1102 | ZK1  | CAS-CAR-NAX | 4.05  | 124.56      | 119.92   |
| 5   | D     | 1104 | PCW  | O2-C31-C32  | 4.04  | 120.22      | 111.48   |
| 5   | C     | 1103 | PCW  | O2-C31-C32  | 4.03  | 120.21      | 111.48   |
| 5   | B     | 1103 | PCW  | O2-C31-C32  | 4.02  | 120.17      | 111.48   |
| 6   | C     | 1107 | CLR  | C17-C13-C14 | 4.01  | 104.70      | 100.10   |
| 6   | B     | 1107 | CLR  | C7-C6-C5    | -3.98 | 118.29      | 125.02   |
| 5   | C     | 1106 | PCW  | O2-C31-C32  | 3.96  | 120.05      | 111.48   |
| 5   | E     | 203  | PCW  | O2-C31-C32  | 3.96  | 120.04      | 111.48   |
| 6   | B     | 1108 | CLR  | C7-C6-C5    | -3.95 | 118.36      | 125.02   |
| 6   | A     | 1107 | CLR  | C21-C20-C22 | -3.93 | 104.25      | 110.34   |
| 6   | A     | 1108 | CLR  | C11-C9-C8   | 3.93  | 117.26      | 111.78   |
| 6   | C     | 1108 | CLR  | C11-C9-C8   | 3.92  | 117.25      | 111.78   |
| 6   | D     | 1108 | CLR  | C23-C22-C20 | 3.90  | 125.99      | 115.08   |
| 5   | A     | 1103 | PCW  | O2-C31-C32  | 3.89  | 119.90      | 111.48   |
| 5   | A     | 1106 | PCW  | O2-C31-C32  | 3.89  | 119.89      | 111.48   |
| 6   | B     | 1108 | CLR  | C3-C4-C5    | 3.87  | 118.21      | 112.05   |
| 6   | D     | 1108 | CLR  | C21-C20-C22 | -3.86 | 104.37      | 110.34   |
| 5   | F     | 201  | PCW  | O2-C31-C32  | 3.84  | 119.78      | 111.48   |
| 6   | C     | 1107 | CLR  | C12-C13-C14 | 3.83  | 112.98      | 107.25   |
| 6   | A     | 1107 | CLR  | C12-C13-C14 | 3.78  | 112.90      | 107.25   |
| 4   | D     | 1103 | ZK1  | CAS-CAR-NAX | 3.77  | 124.25      | 119.92   |
| 6   | A     | 1107 | CLR  | C9-C10-C5   | 3.75  | 115.14      | 109.65   |
| 6   | B     | 1107 | CLR  | C15-C14-C8  | 3.74  | 125.07      | 119.10   |
| 6   | A     | 1107 | CLR  | C3-C4-C5    | 3.73  | 118.00      | 112.05   |
| 4   | B     | 1102 | ZK1  | CAS-CAR-NAX | 3.73  | 124.19      | 119.92   |
| 6   | D     | 1108 | CLR  | C15-C14-C8  | 3.72  | 125.03      | 119.10   |
| 5   | B     | 1109 | PCW  | O2-C31-C32  | 3.70  | 119.47      | 111.48   |
| 6   | C     | 1107 | CLR  | C9-C10-C5   | 3.69  | 115.06      | 109.65   |
| 6   | C     | 1107 | CLR  | C21-C20-C22 | -3.67 | 104.66      | 110.34   |
| 5   | D     | 1101 | PCW  | O2-C31-C32  | 3.66  | 119.40      | 111.48   |
| 6   | B     | 1107 | CLR  | C3-C4-C5    | 3.66  | 117.88      | 112.05   |
| 6   | B     | 1108 | CLR  | C9-C10-C5   | 3.64  | 114.99      | 109.65   |
| 6   | C     | 1108 | CLR  | C15-C14-C8  | -3.62 | 113.33      | 119.10   |
| 4   | C     | 1102 | ZK1  | CAV-NAP-CAT | -3.61 | 119.76      | 124.82   |
| 6   | C     | 1107 | CLR  | C3-C4-C5    | 3.60  | 117.79      | 112.05   |
| 6   | D     | 1109 | CLR  | C3-C4-C5    | 3.59  | 117.78      | 112.05   |
| 6   | B     | 1107 | CLR  | C23-C22-C20 | 3.59  | 125.10      | 115.08   |
| 6   | D     | 1108 | CLR  | C3-C4-C5    | 3.58  | 117.75      | 112.05   |
| 6   | A     | 1108 | CLR  | C9-C10-C5   | 3.53  | 114.83      | 109.65   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | B     | 1107 | CLR  | C7-C8-C14   | -3.53 | 105.93      | 110.93   |
| 6   | A     | 1107 | CLR  | C11-C9-C8   | 3.51  | 116.68      | 111.78   |
| 6   | D     | 1109 | CLR  | C9-C10-C5   | 3.51  | 114.80      | 109.65   |
| 6   | C     | 1108 | CLR  | C9-C10-C5   | 3.48  | 114.74      | 109.65   |
| 6   | B     | 1108 | CLR  | C7-C8-C9    | 3.48  | 113.74      | 109.72   |
| 6   | B     | 1108 | CLR  | C2-C1-C10   | 3.44  | 120.11      | 112.78   |
| 6   | D     | 1109 | CLR  | C2-C1-C10   | 3.42  | 120.07      | 112.78   |
| 4   | A     | 1102 | ZK1  | CAV-NAP-CAT | -3.41 | 120.05      | 124.82   |
| 6   | D     | 1109 | CLR  | C17-C13-C14 | 3.41  | 104.01      | 100.10   |
| 5   | D     | 1106 | PCW  | O2-C31-C32  | 3.41  | 118.85      | 111.48   |
| 6   | D     | 1108 | CLR  | C7-C8-C14   | -3.38 | 106.15      | 110.93   |
| 6   | C     | 1107 | CLR  | C11-C9-C8   | 3.35  | 116.45      | 111.78   |
| 6   | A     | 1107 | CLR  | C7-C8-C14   | -3.33 | 106.22      | 110.93   |
| 6   | B     | 1107 | CLR  | C21-C20-C22 | -3.31 | 105.22      | 110.34   |
| 6   | B     | 1108 | CLR  | C17-C13-C14 | 3.30  | 103.89      | 100.10   |
| 6   | B     | 1107 | CLR  | C9-C10-C5   | 3.26  | 114.42      | 109.65   |
| 5   | B     | 1105 | PCW  | O2-C31-C32  | 3.25  | 118.52      | 111.48   |
| 4   | D     | 1103 | ZK1  | CAU-CAT-NAP | 3.25  | 120.78      | 117.46   |
| 6   | C     | 1108 | CLR  | C7-C8-C14   | -3.25 | 106.33      | 110.93   |
| 6   | A     | 1108 | CLR  | C7-C8-C14   | -3.25 | 106.33      | 110.93   |
| 6   | D     | 1109 | CLR  | C21-C20-C17 | -3.19 | 108.09      | 112.88   |
| 6   | A     | 1107 | CLR  | C15-C14-C13 | 3.19  | 107.59      | 103.84   |
| 6   | C     | 1108 | CLR  | C10-C9-C8   | 3.19  | 117.38      | 112.71   |
| 6   | D     | 1108 | CLR  | C9-C10-C5   | 3.18  | 114.31      | 109.65   |
| 6   | C     | 1108 | CLR  | C17-C13-C14 | 3.15  | 103.72      | 100.10   |
| 6   | D     | 1109 | CLR  | C7-C8-C9    | 3.14  | 113.36      | 109.72   |
| 4   | B     | 1102 | ZK1  | CAU-CAT-NAP | 3.14  | 120.67      | 117.46   |
| 5   | C     | 1106 | PCW  | O3-C11-C12  | 3.13  | 121.37      | 111.83   |
| 5   | A     | 1106 | PCW  | O3-C11-C12  | 3.11  | 121.31      | 111.83   |
| 6   | A     | 1108 | CLR  | C10-C9-C8   | 3.06  | 117.19      | 112.71   |
| 6   | A     | 1108 | CLR  | C16-C17-C20 | 3.04  | 116.77      | 112.18   |
| 5   | C     | 1105 | PCW  | O3-C11-C12  | 3.03  | 121.07      | 111.83   |
| 6   | B     | 1108 | CLR  | C21-C20-C17 | -3.00 | 108.37      | 112.88   |
| 6   | C     | 1107 | CLR  | C15-C14-C13 | 2.99  | 107.36      | 103.84   |
| 6   | D     | 1108 | CLR  | C11-C9-C8   | 2.97  | 115.93      | 111.78   |
| 6   | D     | 1109 | CLR  | C8-C7-C6    | -2.95 | 108.67      | 112.76   |
| 5   | A     | 1105 | PCW  | O3-C11-C12  | 2.93  | 120.76      | 111.83   |
| 6   | B     | 1108 | CLR  | C8-C7-C6    | -2.90 | 108.74      | 112.76   |
| 6   | C     | 1107 | CLR  | C10-C9-C8   | 2.89  | 116.94      | 112.71   |
| 6   | A     | 1107 | CLR  | C10-C9-C8   | 2.89  | 116.93      | 112.71   |
| 6   | A     | 1107 | CLR  | C2-C1-C10   | 2.87  | 118.90      | 112.78   |
| 6   | C     | 1107 | CLR  | C2-C1-C10   | 2.86  | 118.87      | 112.78   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | C     | 1108 | CLR  | C4-C5-C10   | 2.84  | 120.06      | 116.42   |
| 6   | D     | 1109 | CLR  | C15-C16-C17 | -2.80 | 99.66       | 105.14   |
| 6   | C     | 1108 | CLR  | C1-C10-C5   | 2.80  | 113.57      | 108.74   |
| 4   | C     | 1102 | ZK1  | CAU-CAT-NAP | 2.78  | 120.30      | 117.46   |
| 6   | A     | 1108 | CLR  | C1-C10-C5   | 2.78  | 113.53      | 108.74   |
| 6   | B     | 1108 | CLR  | C13-C17-C20 | -2.76 | 115.23      | 119.50   |
| 6   | C     | 1108 | CLR  | C16-C17-C20 | 2.76  | 116.35      | 112.18   |
| 6   | D     | 1108 | CLR  | C2-C1-C10   | 2.76  | 118.65      | 112.78   |
| 6   | C     | 1107 | CLR  | C7-C8-C14   | -2.75 | 107.04      | 110.93   |
| 6   | D     | 1108 | CLR  | C1-C10-C5   | 2.73  | 113.45      | 108.74   |
| 6   | B     | 1107 | CLR  | C11-C9-C8   | 2.73  | 115.59      | 111.78   |
| 6   | A     | 1107 | CLR  | C4-C5-C10   | 2.73  | 119.92      | 116.42   |
| 6   | B     | 1107 | CLR  | C2-C1-C10   | 2.73  | 118.59      | 112.78   |
| 6   | A     | 1108 | CLR  | C2-C1-C10   | 2.72  | 118.58      | 112.78   |
| 5   | F     | 201  | PCW  | C7-N-C5     | 2.72  | 120.72      | 109.91   |
| 5   | F     | 201  | PCW  | O3-C11-C12  | 2.72  | 120.12      | 111.83   |
| 6   | A     | 1108 | CLR  | C22-C20-C17 | 2.71  | 115.96      | 110.33   |
| 5   | C     | 1104 | PCW  | O3-C11-C12  | 2.71  | 120.11      | 111.83   |
| 5   | B     | 1105 | PCW  | O3-C11-C12  | 2.70  | 120.08      | 111.83   |
| 5   | A     | 1103 | PCW  | O3-C11-C12  | 2.68  | 120.02      | 111.83   |
| 5   | E     | 203  | PCW  | C7-N-C5     | 2.68  | 120.58      | 109.91   |
| 5   | A     | 1104 | PCW  | O3-C11-C12  | 2.68  | 120.00      | 111.83   |
| 4   | A     | 1102 | ZK1  | CAU-CAT-NAP | 2.67  | 120.19      | 117.46   |
| 6   | D     | 1109 | CLR  | C13-C17-C20 | -2.65 | 115.40      | 119.50   |
| 5   | C     | 1103 | PCW  | O3-C11-C12  | 2.63  | 119.86      | 111.83   |
| 5   | E     | 203  | PCW  | O3-C11-C12  | 2.62  | 119.82      | 111.83   |
| 6   | A     | 1108 | CLR  | C4-C5-C10   | 2.61  | 119.77      | 116.42   |
| 6   | B     | 1107 | CLR  | C1-C10-C5   | 2.58  | 113.19      | 108.74   |
| 6   | C     | 1107 | CLR  | C4-C5-C10   | 2.57  | 119.71      | 116.42   |
| 6   | D     | 1109 | CLR  | C12-C11-C9  | -2.56 | 108.78      | 113.14   |
| 6   | C     | 1108 | CLR  | C2-C1-C10   | 2.56  | 118.23      | 112.78   |
| 3   | C     | 1101 | 6ZP  | C20-C13-C12 | 2.55  | 120.34      | 117.65   |
| 3   | A     | 1101 | 6ZP  | C20-C13-C12 | 2.54  | 120.33      | 117.65   |
| 5   | D     | 1106 | PCW  | O3-C11-C12  | 2.53  | 119.56      | 111.83   |
| 6   | A     | 1107 | CLR  | C18-C13-C14 | -2.53 | 107.08      | 111.68   |
| 6   | A     | 1107 | CLR  | C1-C10-C5   | 2.51  | 113.07      | 108.74   |
| 6   | C     | 1107 | CLR  | C1-C10-C5   | 2.51  | 113.07      | 108.74   |
| 6   | B     | 1108 | CLR  | C22-C20-C17 | 2.49  | 115.49      | 110.33   |
| 6   | D     | 1109 | CLR  | C16-C17-C20 | 2.47  | 115.92      | 112.18   |
| 5   | D     | 1104 | PCW  | O3-C11-C12  | 2.47  | 119.35      | 111.83   |
| 5   | C     | 1103 | PCW  | C7-N-C5     | 2.46  | 119.70      | 109.91   |
| 5   | B     | 1104 | PCW  | O3-C11-C12  | 2.44  | 119.28      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | B     | 1103 | PCW  | C7-N-C5     | 2.43  | 119.59      | 109.91   |
| 5   | A     | 1103 | PCW  | C7-N-C5     | 2.43  | 119.58      | 109.91   |
| 5   | D     | 1104 | PCW  | C7-N-C5     | 2.43  | 119.58      | 109.91   |
| 6   | D     | 1109 | CLR  | C15-C14-C13 | 2.41  | 106.68      | 103.84   |
| 6   | D     | 1109 | CLR  | C22-C20-C17 | 2.41  | 115.33      | 110.33   |
| 5   | B     | 1109 | PCW  | C3-C2-C1    | -2.41 | 106.18      | 111.78   |
| 6   | B     | 1108 | CLR  | C15-C14-C13 | 2.40  | 106.67      | 103.84   |
| 6   | B     | 1108 | CLR  | C15-C16-C17 | -2.40 | 100.45      | 105.14   |
| 6   | C     | 1108 | CLR  | C22-C20-C17 | 2.40  | 115.30      | 110.33   |
| 6   | C     | 1107 | CLR  | C21-C20-C17 | -2.39 | 109.30      | 112.88   |
| 5   | D     | 1101 | PCW  | C3-C2-C1    | -2.38 | 106.23      | 111.78   |
| 6   | B     | 1108 | CLR  | C12-C11-C9  | -2.38 | 109.09      | 113.14   |
| 5   | B     | 1103 | PCW  | O3-C11-C12  | 2.38  | 119.09      | 111.83   |
| 6   | D     | 1109 | CLR  | C15-C14-C8  | -2.36 | 115.33      | 119.10   |
| 6   | B     | 1108 | CLR  | C16-C17-C20 | 2.36  | 115.75      | 112.18   |
| 5   | A     | 1105 | PCW  | C7-N-C5     | 2.35  | 119.24      | 109.91   |
| 5   | D     | 1106 | PCW  | C7-N-C5     | 2.34  | 119.22      | 109.91   |
| 5   | C     | 1106 | PCW  | C7-N-C5     | 2.33  | 119.16      | 109.91   |
| 5   | D     | 1105 | PCW  | C7-N-C5     | 2.33  | 119.16      | 109.91   |
| 6   | A     | 1108 | CLR  | C13-C14-C8  | 2.33  | 117.72      | 114.41   |
| 5   | A     | 1106 | PCW  | C7-N-C5     | 2.33  | 119.16      | 109.91   |
| 5   | A     | 1109 | PCW  | C7-N-C5     | 2.31  | 119.08      | 109.91   |
| 5   | A     | 1104 | PCW  | C7-N-C5     | 2.31  | 119.08      | 109.91   |
| 5   | B     | 1109 | PCW  | C7-N-C5     | 2.30  | 119.07      | 109.91   |
| 5   | B     | 1105 | PCW  | C7-N-C5     | 2.30  | 119.05      | 109.91   |
| 5   | D     | 1101 | PCW  | C7-N-C5     | 2.29  | 119.03      | 109.91   |
| 5   | B     | 1104 | PCW  | C7-N-C5     | 2.29  | 119.02      | 109.91   |
| 4   | D     | 1103 | ZK1  | CAO-NAY-CAU | 2.28  | 118.88      | 116.55   |
| 6   | B     | 1108 | CLR  | C2-C3-C4    | 2.28  | 113.50      | 110.29   |
| 5   | C     | 1104 | PCW  | C7-N-C5     | 2.28  | 118.96      | 109.91   |
| 6   | C     | 1108 | CLR  | C16-C15-C14 | -2.27 | 100.71      | 105.14   |
| 3   | B     | 1101 | 6ZP  | C20-C13-C12 | 2.26  | 120.04      | 117.65   |
| 6   | D     | 1109 | CLR  | C1-C10-C5   | 2.25  | 112.62      | 108.74   |
| 3   | D     | 1102 | 6ZP  | C20-C13-C12 | 2.24  | 120.02      | 117.65   |
| 5   | D     | 1101 | PCW  | O3-C11-C12  | 2.24  | 118.66      | 111.83   |
| 5   | C     | 1109 | PCW  | C7-N-C5     | 2.24  | 118.81      | 109.91   |
| 5   | C     | 1105 | PCW  | C7-N-C5     | 2.24  | 118.80      | 109.91   |
| 6   | B     | 1108 | CLR  | C10-C5-C6   | -2.23 | 119.67      | 122.93   |
| 6   | A     | 1108 | CLR  | C16-C15-C14 | -2.22 | 100.79      | 105.14   |
| 5   | D     | 1105 | PCW  | O3-C11-C12  | 2.22  | 118.60      | 111.83   |
| 4   | B     | 1102 | ZK1  | CAO-NAY-CAU | 2.22  | 118.81      | 116.55   |
| 5   | B     | 1109 | PCW  | O3-C11-C12  | 2.21  | 118.59      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | A     | 1102 | ZK1  | CAO-NAY-CAU | 2.20  | 118.79      | 116.55   |
| 5   | C     | 1109 | PCW  | O3-C11-C12  | 2.19  | 118.53      | 111.83   |
| 6   | C     | 1108 | CLR  | C11-C9-C10  | -2.18 | 110.39      | 113.08   |
| 5   | C     | 1104 | PCW  | O2-C31-O31  | -2.18 | 118.60      | 123.70   |
| 6   | C     | 1107 | CLR  | C15-C14-C8  | -2.16 | 115.65      | 119.10   |
| 4   | B     | 1102 | ZK1  | CAT-CAU-NAY | 2.15  | 119.75      | 117.41   |
| 5   | A     | 1109 | PCW  | O3-C11-C12  | 2.15  | 118.39      | 111.83   |
| 5   | A     | 1104 | PCW  | O2-C31-O31  | -2.14 | 118.70      | 123.70   |
| 6   | B     | 1108 | CLR  | C15-C14-C8  | -2.13 | 115.69      | 119.10   |
| 6   | A     | 1108 | CLR  | C17-C13-C14 | 2.13  | 102.55      | 100.10   |
| 6   | C     | 1108 | CLR  | C13-C14-C8  | 2.13  | 117.44      | 114.41   |
| 4   | D     | 1103 | ZK1  | CAT-CAU-NAY | 2.12  | 119.72      | 117.41   |
| 4   | C     | 1102 | ZK1  | CAO-NAY-CAU | 2.12  | 118.71      | 116.55   |
| 6   | B     | 1108 | CLR  | C1-C10-C5   | 2.11  | 112.39      | 108.74   |
| 6   | B     | 1108 | CLR  | C4-C5-C10   | 2.10  | 119.11      | 116.42   |
| 6   | D     | 1109 | CLR  | C4-C5-C10   | 2.10  | 119.11      | 116.42   |
| 6   | A     | 1108 | CLR  | C21-C20-C22 | -2.08 | 107.11      | 110.34   |
| 6   | D     | 1109 | CLR  | C2-C3-C4    | 2.07  | 113.20      | 110.29   |
| 6   | A     | 1107 | CLR  | C15-C14-C8  | -2.06 | 115.82      | 119.10   |
| 4   | A     | 1102 | ZK1  | FAG-CAZ-CAS | -2.06 | 109.00      | 112.65   |
| 6   | D     | 1108 | CLR  | C16-C17-C13 | 2.04  | 106.24      | 103.84   |
| 5   | B     | 1104 | PCW  | O2-C31-O31  | -2.02 | 118.98      | 123.70   |
| 4   | C     | 1102 | ZK1  | CAT-CAU-NAY | 2.01  | 119.59      | 117.41   |

All (16) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 6   | A     | 1107 | CLR  | C13  |
| 6   | A     | 1107 | CLR  | C9   |
| 6   | A     | 1108 | CLR  | C13  |
| 6   | A     | 1108 | CLR  | C9   |
| 6   | B     | 1107 | CLR  | C9   |
| 6   | B     | 1107 | CLR  | C13  |
| 6   | B     | 1108 | CLR  | C13  |
| 6   | B     | 1108 | CLR  | C9   |
| 6   | C     | 1107 | CLR  | C13  |
| 6   | C     | 1107 | CLR  | C9   |
| 6   | C     | 1108 | CLR  | C13  |
| 6   | C     | 1108 | CLR  | C9   |
| 6   | D     | 1108 | CLR  | C9   |
| 6   | D     | 1108 | CLR  | C13  |
| 6   | D     | 1109 | CLR  | C13  |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 6   | D     | 1109 | CLR  | C9   |

All (642) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 5   | A     | 1103 | PCW  | O4P-C4-C5-N   |
| 5   | A     | 1103 | PCW  | C32-C31-O2-C2 |
| 5   | A     | 1103 | PCW  | C1-O3P-P-O1P  |
| 5   | A     | 1103 | PCW  | C1-O3P-P-O2P  |
| 5   | A     | 1103 | PCW  | C1-O3P-P-O4P  |
| 5   | A     | 1104 | PCW  | O4P-C4-C5-N   |
| 5   | A     | 1104 | PCW  | O11-C11-O3-C3 |
| 5   | A     | 1104 | PCW  | O31-C31-O2-C2 |
| 5   | A     | 1104 | PCW  | C1-O3P-P-O2P  |
| 5   | A     | 1104 | PCW  | C4-O4P-P-O2P  |
| 5   | A     | 1105 | PCW  | O4P-C4-C5-N   |
| 5   | A     | 1105 | PCW  | C1-O3P-P-O1P  |
| 5   | A     | 1105 | PCW  | C1-O3P-P-O4P  |
| 5   | A     | 1105 | PCW  | C4-O4P-P-O1P  |
| 5   | A     | 1105 | PCW  | C4-O4P-P-O3P  |
| 5   | A     | 1106 | PCW  | O4P-C4-C5-N   |
| 5   | A     | 1106 | PCW  | O31-C31-O2-C2 |
| 5   | A     | 1106 | PCW  | C1-O3P-P-O1P  |
| 5   | A     | 1106 | PCW  | C1-O3P-P-O2P  |
| 5   | A     | 1106 | PCW  | C1-O3P-P-O4P  |
| 5   | A     | 1106 | PCW  | C4-O4P-P-O3P  |
| 5   | A     | 1109 | PCW  | C32-C31-O2-C2 |
| 5   | A     | 1109 | PCW  | C1-O3P-P-O2P  |
| 5   | A     | 1109 | PCW  | C4-O4P-P-O2P  |
| 5   | A     | 1109 | PCW  | C4-O4P-P-O3P  |
| 5   | B     | 1103 | PCW  | O4P-C4-C5-N   |
| 5   | B     | 1103 | PCW  | C32-C31-O2-C2 |
| 5   | B     | 1103 | PCW  | C4-O4P-P-O1P  |
| 5   | B     | 1103 | PCW  | C4-O4P-P-O3P  |
| 5   | B     | 1104 | PCW  | O4P-C4-C5-N   |
| 5   | B     | 1104 | PCW  | C32-C31-O2-C2 |
| 5   | B     | 1104 | PCW  | O31-C31-O2-C2 |
| 5   | B     | 1104 | PCW  | C1-O3P-P-O1P  |
| 5   | B     | 1104 | PCW  | C1-O3P-P-O4P  |
| 5   | B     | 1104 | PCW  | C4-O4P-P-O2P  |
| 5   | B     | 1105 | PCW  | O4P-C4-C5-N   |
| 5   | B     | 1105 | PCW  | C1-O3P-P-O1P  |

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| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 5   | B     | 1105 | PCW  | C1-O3P-P-O2P  |
| 5   | B     | 1105 | PCW  | C1-O3P-P-O4P  |
| 5   | B     | 1105 | PCW  | C4-O4P-P-O2P  |
| 5   | B     | 1109 | PCW  | O4P-C4-C5-N   |
| 5   | B     | 1109 | PCW  | C5-C4-O4P-P   |
| 5   | B     | 1109 | PCW  | C1-O3P-P-O2P  |
| 5   | B     | 1109 | PCW  | C1-O3P-P-O4P  |
| 5   | B     | 1109 | PCW  | C4-O4P-P-O3P  |
| 5   | C     | 1103 | PCW  | C32-C31-O2-C2 |
| 5   | C     | 1103 | PCW  | C1-O3P-P-O1P  |
| 5   | C     | 1103 | PCW  | C1-O3P-P-O2P  |
| 5   | C     | 1103 | PCW  | C1-O3P-P-O4P  |
| 5   | C     | 1103 | PCW  | C4-O4P-P-O1P  |
| 5   | C     | 1104 | PCW  | O4P-C4-C5-N   |
| 5   | C     | 1104 | PCW  | C32-C31-O2-C2 |
| 5   | C     | 1104 | PCW  | O31-C31-O2-C2 |
| 5   | C     | 1104 | PCW  | C1-O3P-P-O2P  |
| 5   | C     | 1104 | PCW  | C4-O4P-P-O2P  |
| 5   | C     | 1105 | PCW  | O4P-C4-C5-N   |
| 5   | C     | 1105 | PCW  | C12-C11-O3-C3 |
| 5   | C     | 1105 | PCW  | O11-C11-O3-C3 |
| 5   | C     | 1105 | PCW  | C1-O3P-P-O1P  |
| 5   | C     | 1105 | PCW  | C1-O3P-P-O4P  |
| 5   | C     | 1105 | PCW  | C4-O4P-P-O3P  |
| 5   | C     | 1106 | PCW  | O4P-C4-C5-N   |
| 5   | C     | 1106 | PCW  | O31-C31-O2-C2 |
| 5   | C     | 1106 | PCW  | C1-O3P-P-O1P  |
| 5   | C     | 1106 | PCW  | C1-O3P-P-O2P  |
| 5   | C     | 1106 | PCW  | C1-O3P-P-O4P  |
| 5   | C     | 1106 | PCW  | C4-O4P-P-O3P  |
| 5   | C     | 1109 | PCW  | C32-C31-O2-C2 |
| 5   | C     | 1109 | PCW  | O31-C31-O2-C2 |
| 5   | C     | 1109 | PCW  | C1-O3P-P-O2P  |
| 5   | C     | 1109 | PCW  | C4-O4P-P-O3P  |
| 5   | D     | 1101 | PCW  | O4P-C4-C5-N   |
| 5   | D     | 1101 | PCW  | C5-C4-O4P-P   |
| 5   | D     | 1101 | PCW  | C1-O3P-P-O2P  |
| 5   | D     | 1101 | PCW  | C4-O4P-P-O3P  |
| 5   | D     | 1104 | PCW  | C32-C31-O2-C2 |
| 5   | D     | 1104 | PCW  | C4-O4P-P-O1P  |
| 5   | D     | 1104 | PCW  | C4-O4P-P-O3P  |
| 5   | D     | 1105 | PCW  | O4P-C4-C5-N   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | D     | 1105 | PCW  | C32-C31-O2-C2   |
| 5   | D     | 1105 | PCW  | O31-C31-O2-C2   |
| 5   | D     | 1105 | PCW  | C1-O3P-P-O1P    |
| 5   | D     | 1105 | PCW  | C4-O4P-P-O2P    |
| 5   | D     | 1106 | PCW  | C1-O3P-P-O1P    |
| 5   | D     | 1106 | PCW  | C1-O3P-P-O2P    |
| 5   | D     | 1106 | PCW  | C1-O3P-P-O4P    |
| 5   | D     | 1106 | PCW  | C4-O4P-P-O2P    |
| 5   | E     | 203  | PCW  | O4P-C4-C5-N     |
| 5   | E     | 203  | PCW  | O31-C31-O2-C2   |
| 5   | E     | 203  | PCW  | C4-O4P-P-O1P    |
| 5   | E     | 203  | PCW  | C4-O4P-P-O2P    |
| 5   | E     | 203  | PCW  | C4-O4P-P-O3P    |
| 5   | F     | 201  | PCW  | O3P-C1-C2-O2    |
| 5   | F     | 201  | PCW  | O4P-C4-C5-N     |
| 5   | F     | 201  | PCW  | O31-C31-O2-C2   |
| 5   | F     | 201  | PCW  | C4-O4P-P-O1P    |
| 5   | F     | 201  | PCW  | C4-O4P-P-O2P    |
| 5   | F     | 201  | PCW  | C4-O4P-P-O3P    |
| 5   | F     | 202  | PCW  | C20-C21-C22-C23 |
| 6   | A     | 1108 | CLR  | C13-C17-C20-C21 |
| 6   | A     | 1108 | CLR  | C16-C17-C20-C21 |
| 6   | A     | 1108 | CLR  | C16-C17-C20-C22 |
| 6   | B     | 1107 | CLR  | C17-C20-C22-C23 |
| 6   | B     | 1108 | CLR  | C13-C17-C20-C21 |
| 6   | C     | 1108 | CLR  | C13-C17-C20-C21 |
| 6   | C     | 1108 | CLR  | C16-C17-C20-C22 |
| 6   | D     | 1108 | CLR  | C17-C20-C22-C23 |
| 6   | D     | 1109 | CLR  | C13-C17-C20-C21 |
| 5   | A     | 1105 | PCW  | O11-C11-O3-C3   |
| 5   | A     | 1109 | PCW  | O11-C11-O3-C3   |
| 5   | C     | 1109 | PCW  | O11-C11-O3-C3   |
| 5   | A     | 1105 | PCW  | C12-C11-O3-C3   |
| 5   | A     | 1109 | PCW  | C12-C11-O3-C3   |
| 5   | C     | 1109 | PCW  | C12-C11-O3-C3   |
| 5   | C     | 1104 | PCW  | O11-C11-O3-C3   |
| 5   | E     | 203  | PCW  | O11-C11-O3-C3   |
| 5   | F     | 201  | PCW  | O11-C11-O3-C3   |
| 6   | C     | 1108 | CLR  | C16-C17-C20-C21 |
| 6   | D     | 1109 | CLR  | C16-C17-C20-C21 |
| 6   | C     | 1107 | CLR  | C13-C17-C20-C21 |
| 6   | A     | 1108 | CLR  | C13-C17-C20-C22 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | A     | 1103 | PCW  | O31-C31-O2-C2   |
| 5   | A     | 1109 | PCW  | O31-C31-O2-C2   |
| 5   | B     | 1103 | PCW  | O31-C31-O2-C2   |
| 5   | C     | 1103 | PCW  | O31-C31-O2-C2   |
| 5   | D     | 1104 | PCW  | O31-C31-O2-C2   |
| 5   | A     | 1104 | PCW  | C12-C11-O3-C3   |
| 5   | C     | 1104 | PCW  | C12-C11-O3-C3   |
| 5   | E     | 203  | PCW  | C12-C11-O3-C3   |
| 5   | A     | 1104 | PCW  | C32-C31-O2-C2   |
| 5   | A     | 1106 | PCW  | C32-C31-O2-C2   |
| 5   | C     | 1106 | PCW  | C32-C31-O2-C2   |
| 5   | E     | 203  | PCW  | C32-C31-O2-C2   |
| 5   | F     | 201  | PCW  | C32-C31-O2-C2   |
| 6   | B     | 1108 | CLR  | C16-C17-C20-C21 |
| 6   | C     | 1107 | CLR  | C16-C17-C20-C21 |
| 6   | B     | 1108 | CLR  | C16-C17-C20-C22 |
| 6   | D     | 1109 | CLR  | C16-C17-C20-C22 |
| 6   | B     | 1108 | CLR  | C13-C17-C20-C22 |
| 6   | C     | 1108 | CLR  | C13-C17-C20-C22 |
| 6   | D     | 1109 | CLR  | C13-C17-C20-C22 |
| 5   | F     | 201  | PCW  | C12-C11-O3-C3   |
| 5   | B     | 1105 | PCW  | O31-C31-O2-C2   |
| 5   | B     | 1105 | PCW  | C32-C31-O2-C2   |
| 5   | D     | 1106 | PCW  | C32-C31-O2-C2   |
| 6   | D     | 1108 | CLR  | C21-C20-C22-C23 |
| 5   | A     | 1109 | PCW  | C32-C33-C34-C35 |
| 6   | D     | 1109 | CLR  | C17-C20-C22-C23 |
| 6   | C     | 1107 | CLR  | C22-C23-C24-C25 |
| 5   | C     | 1109 | PCW  | C32-C33-C34-C35 |
| 5   | D     | 1106 | PCW  | C12-C13-C14-C15 |
| 6   | A     | 1107 | CLR  | C22-C23-C24-C25 |
| 5   | D     | 1106 | PCW  | O31-C31-O2-C2   |
| 5   | A     | 1106 | PCW  | C12-C11-O3-C3   |
| 5   | C     | 1106 | PCW  | C12-C11-O3-C3   |
| 5   | C     | 1103 | PCW  | C24-C25-C26-C27 |
| 6   | C     | 1107 | CLR  | C13-C17-C20-C22 |
| 5   | B     | 1104 | PCW  | C32-C33-C34-C35 |
| 6   | B     | 1108 | CLR  | C17-C20-C22-C23 |
| 5   | B     | 1109 | PCW  | C11-C12-C13-C14 |
| 5   | A     | 1106 | PCW  | O11-C11-O3-C3   |
| 5   | D     | 1105 | PCW  | C32-C33-C34-C35 |
| 5   | E     | 203  | PCW  | C32-C33-C34-C35 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 6   | D     | 1108 | CLR  | C22-C23-C24-C25 |
| 6   | D     | 1109 | CLR  | C21-C20-C22-C23 |
| 5   | C     | 1106 | PCW  | O11-C11-O3-C3   |
| 5   | F     | 201  | PCW  | C32-C33-C34-C35 |
| 5   | A     | 1109 | PCW  | C31-C32-C33-C34 |
| 5   | B     | 1105 | PCW  | C11-C12-C13-C14 |
| 5   | B     | 1103 | PCW  | C15-C16-C17-C18 |
| 5   | D     | 1104 | PCW  | C15-C16-C17-C18 |
| 5   | F     | 201  | PCW  | C4-C5-N-C7      |
| 5   | C     | 1109 | PCW  | C31-C32-C33-C34 |
| 6   | B     | 1108 | CLR  | C20-C22-C23-C24 |
| 6   | B     | 1107 | CLR  | C13-C17-C20-C22 |
| 6   | D     | 1108 | CLR  | C13-C17-C20-C22 |
| 5   | D     | 1101 | PCW  | C11-C12-C13-C14 |
| 6   | A     | 1108 | CLR  | C22-C23-C24-C25 |
| 6   | D     | 1109 | CLR  | C20-C22-C23-C24 |
| 6   | A     | 1108 | CLR  | C20-C22-C23-C24 |
| 6   | C     | 1107 | CLR  | C20-C22-C23-C24 |
| 6   | C     | 1108 | CLR  | C22-C23-C24-C25 |
| 5   | C     | 1103 | PCW  | C16-C17-C18-C19 |
| 5   | D     | 1105 | PCW  | C31-C32-C33-C34 |
| 6   | B     | 1107 | CLR  | C16-C17-C20-C21 |
| 5   | B     | 1104 | PCW  | C31-C32-C33-C34 |
| 5   | C     | 1106 | PCW  | C31-C32-C33-C34 |
| 6   | C     | 1108 | CLR  | C20-C22-C23-C24 |
| 5   | F     | 201  | PCW  | C4-C5-N-C8      |
| 6   | B     | 1108 | CLR  | C21-C20-C22-C23 |
| 5   | A     | 1106 | PCW  | C31-C32-C33-C34 |
| 6   | D     | 1108 | CLR  | C20-C22-C23-C24 |
| 6   | D     | 1108 | CLR  | C16-C17-C20-C21 |
| 6   | B     | 1107 | CLR  | C13-C17-C20-C21 |
| 6   | D     | 1108 | CLR  | C13-C17-C20-C21 |
| 5   | A     | 1103 | PCW  | C11-C12-C13-C14 |
| 5   | B     | 1105 | PCW  | C12-C13-C14-C15 |
| 5   | E     | 203  | PCW  | C15-C16-C17-C18 |
| 5   | A     | 1103 | PCW  | C16-C17-C18-C19 |
| 6   | A     | 1108 | CLR  | C23-C24-C25-C26 |
| 6   | D     | 1108 | CLR  | C23-C24-C25-C26 |
| 5   | A     | 1109 | PCW  | C23-C24-C25-C26 |
| 5   | F     | 201  | PCW  | C15-C16-C17-C18 |
| 6   | A     | 1107 | CLR  | C23-C24-C25-C26 |
| 5   | A     | 1103 | PCW  | C22-C23-C24-C25 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | A     | 1109 | PCW  | C35-C36-C37-C38 |
| 5   | B     | 1109 | PCW  | C35-C36-C37-C38 |
| 5   | C     | 1105 | PCW  | C14-C15-C16-C17 |
| 5   | D     | 1105 | PCW  | C15-C16-C17-C18 |
| 5   | D     | 1106 | PCW  | C14-C15-C16-C17 |
| 5   | E     | 203  | PCW  | C35-C36-C37-C38 |
| 5   | F     | 203  | PCW  | C15-C16-C17-C18 |
| 5   | A     | 1109 | PCW  | C11-C12-C13-C14 |
| 5   | A     | 1103 | PCW  | C32-C33-C34-C35 |
| 5   | D     | 1106 | PCW  | C13-C14-C15-C16 |
| 5   | B     | 1105 | PCW  | C12-C11-O3-C3   |
| 5   | A     | 1106 | PCW  | C32-C33-C34-C35 |
| 5   | A     | 1109 | PCW  | C22-C23-C24-C25 |
| 5   | B     | 1104 | PCW  | C15-C16-C17-C18 |
| 5   | B     | 1109 | PCW  | C14-C15-C16-C17 |
| 5   | C     | 1105 | PCW  | C22-C23-C24-C25 |
| 5   | D     | 1101 | PCW  | C35-C36-C37-C38 |
| 5   | D     | 1106 | PCW  | C23-C24-C25-C26 |
| 5   | B     | 1104 | PCW  | C24-C25-C26-C27 |
| 5   | B     | 1105 | PCW  | C23-C24-C25-C26 |
| 5   | C     | 1106 | PCW  | C12-C13-C14-C15 |
| 5   | A     | 1106 | PCW  | C12-C13-C14-C15 |
| 5   | D     | 1101 | PCW  | C14-C15-C16-C17 |
| 6   | A     | 1107 | CLR  | C23-C24-C25-C27 |
| 6   | D     | 1108 | CLR  | C23-C24-C25-C27 |
| 5   | B     | 1104 | PCW  | C21-C22-C23-C24 |
| 5   | C     | 1103 | PCW  | C32-C33-C34-C35 |
| 5   | D     | 1106 | PCW  | C34-C35-C36-C37 |
| 5   | C     | 1106 | PCW  | C32-C33-C34-C35 |
| 5   | D     | 1105 | PCW  | C21-C22-C23-C24 |
| 5   | A     | 1104 | PCW  | C33-C34-C35-C36 |
| 5   | A     | 1109 | PCW  | C12-C13-C14-C15 |
| 5   | B     | 1105 | PCW  | C34-C35-C36-C37 |
| 5   | D     | 1104 | PCW  | C32-C33-C34-C35 |
| 5   | D     | 1104 | PCW  | C34-C35-C36-C37 |
| 6   | A     | 1107 | CLR  | C13-C17-C20-C21 |
| 5   | A     | 1105 | PCW  | C12-C13-C14-C15 |
| 5   | A     | 1105 | PCW  | C22-C23-C24-C25 |
| 5   | B     | 1103 | PCW  | C32-C33-C34-C35 |
| 5   | B     | 1105 | PCW  | C14-C15-C16-C17 |
| 5   | E     | 203  | PCW  | C21-C22-C23-C24 |
| 5   | F     | 201  | PCW  | C21-C22-C23-C24 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | A     | 1105 | PCW  | C31-C32-C33-C34 |
| 5   | D     | 1104 | PCW  | C11-C12-C13-C14 |
| 5   | A     | 1105 | PCW  | C15-C16-C17-C18 |
| 5   | A     | 1109 | PCW  | C13-C14-C15-C16 |
| 5   | C     | 1103 | PCW  | C23-C24-C25-C26 |
| 5   | C     | 1104 | PCW  | C24-C25-C26-C27 |
| 5   | C     | 1104 | PCW  | C33-C34-C35-C36 |
| 5   | B     | 1104 | PCW  | C35-C36-C37-C38 |
| 5   | D     | 1101 | PCW  | C15-C16-C17-C18 |
| 5   | C     | 1109 | PCW  | C35-C36-C37-C38 |
| 5   | F     | 201  | PCW  | C35-C36-C37-C38 |
| 5   | F     | 201  | PCW  | C4-C5-N-C6      |
| 5   | A     | 1105 | PCW  | C14-C15-C16-C17 |
| 5   | C     | 1105 | PCW  | C12-C13-C14-C15 |
| 5   | C     | 1105 | PCW  | C15-C16-C17-C18 |
| 5   | D     | 1101 | PCW  | C12-C13-C14-C15 |
| 5   | D     | 1105 | PCW  | C35-C36-C37-C38 |
| 6   | C     | 1107 | CLR  | C23-C24-C25-C26 |
| 5   | D     | 1106 | PCW  | C11-C12-C13-C14 |
| 5   | D     | 1106 | PCW  | C31-C32-C33-C34 |
| 5   | C     | 1105 | PCW  | C35-C36-C37-C38 |
| 5   | C     | 1109 | PCW  | C13-C14-C15-C16 |
| 5   | D     | 1106 | PCW  | C37-C38-C39-C40 |
| 5   | D     | 1101 | PCW  | C40-C41-C42-C43 |
| 5   | D     | 1106 | PCW  | C36-C37-C38-C39 |
| 5   | D     | 1105 | PCW  | C12-C11-O3-C3   |
| 5   | C     | 1109 | PCW  | C12-C13-C14-C15 |
| 5   | D     | 1105 | PCW  | C14-C15-C16-C17 |
| 5   | A     | 1104 | PCW  | C13-C14-C15-C16 |
| 5   | B     | 1109 | PCW  | C12-C13-C14-C15 |
| 5   | B     | 1105 | PCW  | O11-C11-O3-C3   |
| 5   | A     | 1105 | PCW  | C33-C34-C35-C36 |
| 5   | C     | 1104 | PCW  | C13-C14-C15-C16 |
| 5   | D     | 1104 | PCW  | C21-C22-C23-C24 |
| 6   | C     | 1108 | CLR  | C23-C24-C25-C26 |
| 5   | C     | 1109 | PCW  | C23-C24-C25-C26 |
| 5   | D     | 1105 | PCW  | C24-C25-C26-C27 |
| 5   | E     | 201  | PCW  | C14-C15-C16-C17 |
| 5   | A     | 1103 | PCW  | C33-C34-C35-C36 |
| 5   | C     | 1105 | PCW  | C33-C34-C35-C36 |
| 6   | A     | 1108 | CLR  | C23-C24-C25-C27 |
| 5   | A     | 1105 | PCW  | C32-C31-O2-C2   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | C     | 1105 | PCW  | C32-C31-O2-C2   |
| 5   | C     | 1103 | PCW  | C11-C12-C13-C14 |
| 5   | A     | 1104 | PCW  | C12-C13-C14-C15 |
| 5   | D     | 1101 | PCW  | C23-C24-C25-C26 |
| 5   | C     | 1105 | PCW  | O31-C31-O2-C2   |
| 5   | A     | 1103 | PCW  | C40-C41-C42-C43 |
| 5   | A     | 1105 | PCW  | C16-C17-C18-C19 |
| 5   | B     | 1106 | PCW  | C16-C17-C18-C19 |
| 5   | B     | 1109 | PCW  | C40-C41-C42-C43 |
| 5   | B     | 1109 | PCW  | C15-C16-C17-C18 |
| 5   | E     | 202  | PCW  | C15-C16-C17-C18 |
| 5   | A     | 1106 | PCW  | C35-C36-C37-C38 |
| 5   | C     | 1103 | PCW  | C33-C34-C35-C36 |
| 5   | C     | 1106 | PCW  | C24-C25-C26-C27 |
| 5   | B     | 1103 | PCW  | C11-C12-C13-C14 |
| 5   | C     | 1105 | PCW  | C31-C32-C33-C34 |
| 5   | D     | 1101 | PCW  | C24-C25-C26-C27 |
| 6   | B     | 1107 | CLR  | C23-C24-C25-C26 |
| 6   | C     | 1107 | CLR  | C23-C24-C25-C27 |
| 6   | C     | 1108 | CLR  | C23-C24-C25-C27 |
| 5   | E     | 203  | PCW  | C4-C5-N-C7      |
| 5   | A     | 1105 | PCW  | C32-C33-C34-C35 |
| 5   | A     | 1105 | PCW  | C35-C36-C37-C38 |
| 5   | D     | 1105 | PCW  | O11-C11-O3-C3   |
| 5   | B     | 1105 | PCW  | C31-C32-C33-C34 |
| 5   | B     | 1109 | PCW  | C21-C22-C23-C24 |
| 5   | A     | 1105 | PCW  | O31-C31-O2-C2   |
| 6   | A     | 1107 | CLR  | C20-C22-C23-C24 |
| 5   | A     | 1104 | PCW  | C21-C22-C23-C24 |
| 5   | A     | 1104 | PCW  | C16-C17-C18-C19 |
| 5   | A     | 1109 | PCW  | C36-C37-C38-C39 |
| 5   | D     | 1105 | PCW  | C20-C21-C22-C23 |
| 5   | F     | 201  | PCW  | C36-C37-C38-C39 |
| 5   | C     | 1105 | PCW  | C41-C42-C43-C44 |
| 5   | D     | 1104 | PCW  | C13-C14-C15-C16 |
| 5   | D     | 1104 | PCW  | C35-C36-C37-C38 |
| 5   | C     | 1104 | PCW  | C21-C22-C23-C24 |
| 5   | C     | 1106 | PCW  | C35-C36-C37-C38 |
| 6   | B     | 1107 | CLR  | C21-C20-C22-C23 |
| 6   | D     | 1109 | CLR  | C23-C24-C25-C27 |
| 5   | A     | 1106 | PCW  | C24-C25-C26-C27 |
| 5   | B     | 1109 | PCW  | C24-C25-C26-C27 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | D     | 1106 | PCW  | C12-C11-O3-C3   |
| 5   | B     | 1105 | PCW  | C37-C38-C39-C40 |
| 5   | A     | 1104 | PCW  | C40-C41-C42-C43 |
| 5   | B     | 1104 | PCW  | C20-C21-C22-C23 |
| 5   | C     | 1103 | PCW  | C40-C41-C42-C43 |
| 5   | C     | 1104 | PCW  | C16-C17-C18-C19 |
| 5   | A     | 1104 | PCW  | C35-C36-C37-C38 |
| 5   | B     | 1103 | PCW  | C14-C15-C16-C17 |
| 5   | C     | 1105 | PCW  | C32-C33-C34-C35 |
| 6   | C     | 1107 | CLR  | C16-C17-C20-C22 |
| 5   | A     | 1103 | PCW  | C12-C11-O3-C3   |
| 5   | C     | 1103 | PCW  | C12-C11-O3-C3   |
| 5   | A     | 1104 | PCW  | C1-C2-C3-O3     |
| 5   | A     | 1106 | PCW  | C1-C2-C3-O3     |
| 5   | C     | 1104 | PCW  | C1-C2-C3-O3     |
| 5   | C     | 1106 | PCW  | C1-C2-C3-O3     |
| 5   | D     | 1106 | PCW  | C1-C2-C3-O3     |
| 5   | C     | 1106 | PCW  | C33-C34-C35-C36 |
| 5   | A     | 1103 | PCW  | C20-C21-C22-C23 |
| 5   | A     | 1105 | PCW  | C40-C41-C42-C43 |
| 5   | B     | 1105 | PCW  | C36-C37-C38-C39 |
| 5   | D     | 1101 | PCW  | C36-C37-C38-C39 |
| 5   | D     | 1106 | PCW  | C16-C17-C18-C19 |
| 5   | E     | 203  | PCW  | C40-C41-C42-C43 |
| 5   | F     | 201  | PCW  | C40-C41-C42-C43 |
| 5   | D     | 1106 | PCW  | C24-C25-C26-C27 |
| 5   | C     | 1106 | PCW  | C25-C26-C27-C28 |
| 5   | F     | 202  | PCW  | C13-C14-C15-C16 |
| 5   | B     | 1103 | PCW  | C34-C35-C36-C37 |
| 5   | B     | 1105 | PCW  | C24-C25-C26-C27 |
| 5   | E     | 203  | PCW  | C4-C5-N-C8      |
| 5   | D     | 1106 | PCW  | O11-C11-O3-C3   |
| 5   | E     | 202  | PCW  | C20-C21-C22-C23 |
| 5   | A     | 1105 | PCW  | C41-C42-C43-C44 |
| 6   | A     | 1107 | CLR  | C16-C17-C20-C21 |
| 5   | A     | 1103 | PCW  | C12-C13-C14-C15 |
| 5   | C     | 1104 | PCW  | C1-C2-O2-C31    |
| 5   | E     | 203  | PCW  | C12-C13-C14-C15 |
| 5   | B     | 1109 | PCW  | C36-C37-C38-C39 |
| 5   | C     | 1104 | PCW  | C40-C41-C42-C43 |
| 5   | C     | 1105 | PCW  | C16-C17-C18-C19 |
| 5   | D     | 1107 | PCW  | C16-C17-C18-C19 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | E     | 203  | PCW  | C36-C37-C38-C39 |
| 5   | F     | 201  | PCW  | C12-C13-C14-C15 |
| 6   | B     | 1107 | CLR  | C23-C24-C25-C27 |
| 5   | E     | 203  | PCW  | O3P-C1-C2-O2    |
| 5   | A     | 1104 | PCW  | C24-C25-C26-C27 |
| 5   | E     | 203  | PCW  | C25-C26-C27-C28 |
| 5   | B     | 1105 | PCW  | C41-C42-C43-C44 |
| 5   | C     | 1109 | PCW  | C34-C35-C36-C37 |
| 5   | F     | 201  | PCW  | C25-C26-C27-C28 |
| 5   | E     | 203  | PCW  | C4-C5-N-C6      |
| 5   | D     | 1104 | PCW  | C14-C15-C16-C17 |
| 5   | B     | 1103 | PCW  | C35-C36-C37-C38 |
| 5   | B     | 1104 | PCW  | C25-C26-C27-C28 |
| 6   | B     | 1107 | CLR  | C22-C23-C24-C25 |
| 5   | B     | 1105 | PCW  | C16-C17-C18-C19 |
| 5   | F     | 202  | PCW  | C16-C17-C18-C19 |
| 5   | A     | 1106 | PCW  | C41-C42-C43-C44 |
| 5   | B     | 1104 | PCW  | C12-C11-O3-C3   |
| 6   | B     | 1108 | CLR  | C23-C24-C25-C27 |
| 5   | C     | 1103 | PCW  | O3-C11-C12-C13  |
| 5   | A     | 1105 | PCW  | C21-C22-C23-C24 |
| 5   | B     | 1103 | PCW  | C13-C14-C15-C16 |
| 5   | C     | 1103 | PCW  | O11-C11-O3-C3   |
| 5   | D     | 1105 | PCW  | C40-C41-C42-C43 |
| 6   | B     | 1107 | CLR  | C20-C22-C23-C24 |
| 5   | A     | 1106 | PCW  | C25-C26-C27-C28 |
| 5   | A     | 1103 | PCW  | O11-C11-O3-C3   |
| 5   | A     | 1103 | PCW  | C34-C35-C36-C37 |
| 5   | C     | 1105 | PCW  | C21-C22-C23-C24 |
| 5   | C     | 1109 | PCW  | C16-C17-C18-C19 |
| 5   | C     | 1103 | PCW  | C21-C22-C23-C24 |
| 5   | B     | 1103 | PCW  | C1-C2-C3-O3     |
| 5   | B     | 1105 | PCW  | C1-C2-C3-O3     |
| 5   | D     | 1105 | PCW  | C1-C2-C3-O3     |
| 5   | A     | 1103 | PCW  | C24-C25-C26-C27 |
| 5   | E     | 201  | PCW  | C13-C14-C15-C16 |
| 5   | A     | 1106 | PCW  | C15-C16-C17-C18 |
| 5   | A     | 1103 | PCW  | O3P-C1-C2-O2    |
| 5   | C     | 1103 | PCW  | O3P-C1-C2-O2    |
| 5   | B     | 1106 | PCW  | C15-C16-C17-C18 |
| 5   | C     | 1109 | PCW  | C22-C23-C24-C25 |
| 5   | B     | 1105 | PCW  | C35-C36-C37-C38 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | D     | 1107 | PCW  | C15-C16-C17-C18 |
| 5   | C     | 1103 | PCW  | C12-C13-C14-C15 |
| 6   | B     | 1108 | CLR  | C23-C24-C25-C26 |
| 5   | A     | 1106 | PCW  | O2-C2-C3-O3     |
| 5   | C     | 1104 | PCW  | O2-C2-C3-O3     |
| 5   | C     | 1105 | PCW  | O2-C2-C3-O3     |
| 5   | C     | 1106 | PCW  | O2-C2-C3-O3     |
| 5   | D     | 1106 | PCW  | C35-C36-C37-C38 |
| 5   | C     | 1109 | PCW  | C11-C12-C13-C14 |
| 5   | C     | 1110 | PCW  | C17-C18-C19-C20 |
| 5   | F     | 202  | PCW  | C19-C20-C21-C22 |
| 5   | B     | 1104 | PCW  | C14-C15-C16-C17 |
| 5   | A     | 1103 | PCW  | O3-C11-C12-C13  |
| 6   | D     | 1109 | CLR  | C23-C24-C25-C26 |
| 4   | A     | 1102 | ZK1  | NAY-CAO-PBA-OAD |
| 4   | A     | 1102 | ZK1  | NAY-CAO-PBA-OAE |
| 4   | B     | 1102 | ZK1  | NAY-CAO-PBA-OAD |
| 4   | B     | 1102 | ZK1  | NAY-CAO-PBA-OAE |
| 4   | C     | 1102 | ZK1  | NAY-CAO-PBA-OAD |
| 4   | C     | 1102 | ZK1  | NAY-CAO-PBA-OAE |
| 4   | D     | 1103 | ZK1  | NAY-CAO-PBA-OAD |
| 4   | D     | 1103 | ZK1  | NAY-CAO-PBA-OAE |
| 5   | A     | 1103 | PCW  | O3P-C1-C2-C3    |
| 5   | F     | 201  | PCW  | O3P-C1-C2-C3    |
| 5   | A     | 1110 | PCW  | C19-C20-C21-C22 |
| 5   | C     | 1110 | PCW  | C19-C20-C21-C22 |
| 5   | F     | 201  | PCW  | C41-C42-C43-C44 |
| 5   | D     | 1104 | PCW  | C42-C43-C44-C45 |
| 5   | D     | 1101 | PCW  | C41-C42-C43-C44 |
| 5   | C     | 1106 | PCW  | C14-C15-C16-C17 |
| 5   | A     | 1106 | PCW  | C33-C34-C35-C36 |
| 5   | D     | 1106 | PCW  | C41-C42-C43-C44 |
| 4   | B     | 1102 | ZK1  | CAI-CAR-NAX-CAN |
| 4   | D     | 1103 | ZK1  | CAI-CAR-NAX-CAN |
| 5   | B     | 1105 | PCW  | C1-C2-O2-C31    |
| 5   | B     | 1104 | PCW  | O11-C11-O3-C3   |
| 5   | C     | 1105 | PCW  | C13-C14-C15-C16 |
| 5   | B     | 1109 | PCW  | C23-C24-C25-C26 |
| 5   | C     | 1105 | PCW  | O3P-C1-C2-O2    |
| 5   | B     | 1109 | PCW  | C41-C42-C43-C44 |
| 6   | A     | 1107 | CLR  | C13-C17-C20-C22 |
| 5   | A     | 1104 | PCW  | O2-C2-C3-O3     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | A     | 1105 | PCW  | O2-C2-C3-O3     |
| 5   | D     | 1105 | PCW  | O2-C2-C3-O3     |
| 5   | C     | 1103 | PCW  | O4P-C4-C5-N     |
| 5   | D     | 1104 | PCW  | O4P-C4-C5-N     |
| 5   | D     | 1106 | PCW  | O4P-C4-C5-N     |
| 5   | C     | 1106 | PCW  | C42-C43-C44-C45 |
| 5   | A     | 1104 | PCW  | C23-C24-C25-C26 |
| 5   | B     | 1105 | PCW  | C15-C16-C17-C18 |
| 5   | B     | 1104 | PCW  | C37-C38-C39-C40 |
| 5   | A     | 1109 | PCW  | C16-C17-C18-C19 |
| 5   | C     | 1103 | PCW  | O3P-C1-C2-C3    |
| 5   | E     | 203  | PCW  | O3P-C1-C2-C3    |
| 5   | B     | 1103 | PCW  | C21-C22-C23-C24 |
| 5   | B     | 1103 | PCW  | C22-C23-C24-C25 |
| 5   | E     | 203  | PCW  | C33-C34-C35-C36 |
| 5   | B     | 1104 | PCW  | C23-C24-C25-C26 |
| 5   | D     | 1106 | PCW  | C2-C1-O3P-P     |
| 5   | A     | 1105 | PCW  | O3P-C1-C2-O2    |
| 5   | A     | 1110 | PCW  | C17-C18-C19-C20 |
| 5   | C     | 1106 | PCW  | C21-C22-C23-C24 |
| 5   | D     | 1101 | PCW  | C22-C23-C24-C25 |
| 5   | B     | 1105 | PCW  | C13-C14-C15-C16 |
| 5   | B     | 1103 | PCW  | O2-C2-C3-O3     |
| 5   | B     | 1104 | PCW  | O2-C2-C3-O3     |
| 5   | B     | 1105 | PCW  | O2-C2-C3-O3     |
| 5   | D     | 1106 | PCW  | O2-C2-C3-O3     |
| 5   | D     | 1105 | PCW  | C25-C26-C27-C28 |
| 5   | B     | 1109 | PCW  | C22-C23-C24-C25 |
| 5   | D     | 1104 | PCW  | C1-C2-C3-O3     |
| 5   | A     | 1104 | PCW  | C15-C16-C17-C18 |
| 5   | A     | 1103 | PCW  | C4-O4P-P-O2P    |
| 5   | A     | 1104 | PCW  | C1-O3P-P-O4P    |
| 5   | A     | 1104 | PCW  | C4-O4P-P-O1P    |
| 5   | A     | 1104 | PCW  | C4-O4P-P-O3P    |
| 5   | A     | 1105 | PCW  | C1-O3P-P-O2P    |
| 5   | A     | 1106 | PCW  | C4-O4P-P-O2P    |
| 5   | B     | 1103 | PCW  | C1-O3P-P-O2P    |
| 5   | B     | 1103 | PCW  | C4-O4P-P-O2P    |
| 5   | B     | 1109 | PCW  | C1-O3P-P-O1P    |
| 5   | B     | 1109 | PCW  | C4-O4P-P-O2P    |
| 5   | C     | 1103 | PCW  | C4-O4P-P-O2P    |
| 5   | C     | 1103 | PCW  | C4-O4P-P-O3P    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | C     | 1104 | PCW  | C4-O4P-P-O1P    |
| 5   | C     | 1104 | PCW  | C4-O4P-P-O3P    |
| 5   | C     | 1105 | PCW  | C1-O3P-P-O2P    |
| 5   | C     | 1106 | PCW  | C4-O4P-P-O2P    |
| 5   | C     | 1109 | PCW  | C4-O4P-P-O2P    |
| 5   | D     | 1101 | PCW  | C1-O3P-P-O1P    |
| 5   | D     | 1101 | PCW  | C1-O3P-P-O4P    |
| 5   | D     | 1101 | PCW  | C4-O4P-P-O2P    |
| 5   | D     | 1104 | PCW  | C1-O3P-P-O2P    |
| 5   | D     | 1104 | PCW  | C1-O3P-P-O4P    |
| 5   | D     | 1104 | PCW  | C4-O4P-P-O2P    |
| 5   | D     | 1105 | PCW  | C1-O3P-P-O2P    |
| 5   | D     | 1105 | PCW  | C1-O3P-P-O4P    |
| 5   | A     | 1106 | PCW  | C14-C15-C16-C17 |
| 5   | D     | 1105 | PCW  | C36-C37-C38-C39 |
| 5   | A     | 1109 | PCW  | C2-C1-O3P-P     |
| 5   | B     | 1105 | PCW  | C2-C1-O3P-P     |
| 5   | E     | 201  | PCW  | C20-C21-C22-C23 |
| 5   | C     | 1106 | PCW  | C15-C16-C17-C18 |
| 4   | A     | 1102 | ZK1  | CAI-CAR-NAX-CAN |
| 4   | C     | 1102 | ZK1  | CAI-CAR-NAX-CAN |
| 5   | C     | 1104 | PCW  | C12-C13-C14-C15 |
| 5   | A     | 1104 | PCW  | C1-C2-O2-C31    |
| 5   | D     | 1106 | PCW  | C1-C2-O2-C31    |
| 5   | B     | 1104 | PCW  | C11-C12-C13-C14 |
| 5   | B     | 1104 | PCW  | C36-C37-C38-C39 |
| 5   | C     | 1106 | PCW  | C40-C41-C42-C43 |
| 5   | C     | 1105 | PCW  | O3P-C1-C2-C3    |
| 5   | A     | 1105 | PCW  | C34-C35-C36-C37 |
| 5   | A     | 1103 | PCW  | C19-C20-C21-C22 |
| 5   | C     | 1109 | PCW  | C14-C15-C16-C17 |
| 5   | F     | 201  | PCW  | C23-C24-C25-C26 |
| 5   | B     | 1105 | PCW  | C42-C43-C44-C45 |
| 5   | C     | 1109 | PCW  | C2-C1-O3P-P     |
| 5   | A     | 1109 | PCW  | C34-C35-C36-C37 |
| 5   | B     | 1103 | PCW  | O3-C11-C12-C13  |
| 5   | B     | 1104 | PCW  | C40-C41-C42-C43 |
| 5   | D     | 1104 | PCW  | O3-C11-C12-C13  |
| 5   | C     | 1105 | PCW  | C40-C41-C42-C43 |
| 5   | C     | 1103 | PCW  | C34-C35-C36-C37 |
| 5   | C     | 1105 | PCW  | C34-C35-C36-C37 |
| 5   | A     | 1105 | PCW  | C19-C20-C21-C22 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | C     | 1104 | PCW  | C15-C16-C17-C18 |
| 5   | B     | 1103 | PCW  | C42-C43-C44-C45 |
| 5   | C     | 1105 | PCW  | C19-C20-C21-C22 |
| 5   | C     | 1103 | PCW  | O11-C11-C12-C13 |
| 6   | A     | 1107 | CLR  | C16-C17-C20-C22 |
| 5   | A     | 1103 | PCW  | C2-C1-O3P-P     |
| 5   | D     | 1101 | PCW  | C13-C14-C15-C16 |
| 5   | E     | 203  | PCW  | C23-C24-C25-C26 |
| 5   | B     | 1105 | PCW  | C2-C3-O3-C11    |
| 5   | D     | 1101 | PCW  | C34-C35-C36-C37 |
| 5   | F     | 202  | PCW  | C15-C16-C17-C18 |
| 5   | A     | 1103 | PCW  | C1-C2-C3-O3     |
| 5   | D     | 1105 | PCW  | C37-C38-C39-C40 |
| 5   | E     | 202  | PCW  | C13-C14-C15-C16 |
| 5   | A     | 1104 | PCW  | C20-C21-C22-C23 |
| 5   | C     | 1109 | PCW  | C36-C37-C38-C39 |
| 5   | C     | 1104 | PCW  | C35-C36-C37-C38 |
| 5   | A     | 1105 | PCW  | O3P-C1-C2-C3    |
| 5   | D     | 1104 | PCW  | O2-C2-C3-O3     |
| 5   | D     | 1101 | PCW  | C16-C17-C18-C19 |
| 5   | A     | 1105 | PCW  | C11-C12-C13-C14 |
| 5   | D     | 1106 | PCW  | C42-C43-C44-C45 |
| 5   | D     | 1104 | PCW  | C40-C41-C42-C43 |
| 5   | A     | 1105 | PCW  | C1-C2-C3-O3     |
| 5   | C     | 1103 | PCW  | C1-C2-C3-O3     |
| 5   | C     | 1105 | PCW  | C1-C2-C3-O3     |
| 5   | D     | 1106 | PCW  | C21-C22-C23-C24 |
| 4   | A     | 1102 | ZK1  | NAY-CAO-PBA-OAC |
| 4   | B     | 1102 | ZK1  | NAY-CAO-PBA-OAC |
| 4   | C     | 1102 | ZK1  | NAY-CAO-PBA-OAC |
| 4   | D     | 1103 | ZK1  | NAY-CAO-PBA-OAC |
| 5   | B     | 1106 | PCW  | C19-C20-C21-C22 |
| 5   | E     | 201  | PCW  | C17-C18-C19-C20 |
| 5   | F     | 201  | PCW  | C37-C38-C39-C40 |
| 5   | B     | 1105 | PCW  | C25-C26-C27-C28 |
| 5   | C     | 1105 | PCW  | C11-C12-C13-C14 |
| 5   | C     | 1105 | PCW  | C25-C26-C27-C28 |
| 5   | A     | 1104 | PCW  | C19-C20-C21-C22 |
| 5   | C     | 1106 | PCW  | C19-C20-C21-C22 |
| 5   | C     | 1103 | PCW  | C2-C1-O3P-P     |
| 5   | F     | 203  | PCW  | C13-C14-C15-C16 |
| 5   | A     | 1105 | PCW  | C37-C38-C39-C40 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | B     | 1105 | PCW  | C19-C20-C21-C22 |
| 5   | A     | 1103 | PCW  | O11-C11-C12-C13 |
| 5   | D     | 1104 | PCW  | C23-C24-C25-C26 |
| 5   | B     | 1109 | PCW  | C25-C26-C27-C28 |
| 5   | B     | 1109 | PCW  | C13-C14-C15-C16 |
| 5   | A     | 1106 | PCW  | C37-C38-C39-C40 |
| 5   | B     | 1109 | PCW  | C37-C38-C39-C40 |
| 5   | C     | 1105 | PCW  | C37-C38-C39-C40 |
| 5   | D     | 1107 | PCW  | C19-C20-C21-C22 |
| 5   | F     | 203  | PCW  | C19-C20-C21-C22 |
| 4   | A     | 1102 | ZK1  | CAI-CAR-NAX-CAM |
| 4   | C     | 1102 | ZK1  | CAI-CAR-NAX-CAM |
| 5   | C     | 1109 | PCW  | C20-C21-C22-C23 |
| 5   | E     | 203  | PCW  | C37-C38-C39-C40 |
| 5   | B     | 1103 | PCW  | C31-C32-C33-C34 |
| 5   | A     | 1109 | PCW  | C40-C41-C42-C43 |
| 5   | B     | 1104 | PCW  | C1-C2-C3-O3     |
| 5   | A     | 1104 | PCW  | C37-C38-C39-C40 |
| 5   | D     | 1101 | PCW  | C37-C38-C39-C40 |
| 5   | D     | 1106 | PCW  | C19-C20-C21-C22 |
| 5   | F     | 202  | PCW  | C17-C18-C19-C20 |
| 5   | D     | 1106 | PCW  | C25-C26-C27-C28 |
| 5   | A     | 1104 | PCW  | C41-C42-C43-C44 |
| 5   | C     | 1106 | PCW  | C37-C38-C39-C40 |
| 5   | D     | 1101 | PCW  | O3-C11-C12-C13  |
| 5   | A     | 1106 | PCW  | C21-C22-C23-C24 |
| 5   | B     | 1105 | PCW  | C22-C23-C24-C25 |
| 5   | C     | 1104 | PCW  | C20-C21-C22-C23 |
| 5   | C     | 1104 | PCW  | C19-C20-C21-C22 |
| 5   | E     | 202  | PCW  | C19-C20-C21-C22 |
| 5   | B     | 1109 | PCW  | O3-C11-C12-C13  |
| 5   | C     | 1104 | PCW  | C32-C33-C34-C35 |
| 5   | B     | 1105 | PCW  | C21-C22-C23-C24 |
| 5   | B     | 1104 | PCW  | C39-C40-C41-C42 |
| 5   | E     | 203  | PCW  | C31-C32-C33-C34 |
| 5   | A     | 1105 | PCW  | C25-C26-C27-C28 |
| 5   | C     | 1109 | PCW  | C24-C25-C26-C27 |
| 5   | C     | 1105 | PCW  | O2-C31-C32-C33  |
| 5   | E     | 203  | PCW  | O3-C11-C12-C13  |
| 3   | A     | 1101 | 6ZP  | C20-C13-C14-C19 |
| 3   | B     | 1101 | 6ZP  | C20-C13-C14-C19 |
| 3   | C     | 1101 | 6ZP  | C20-C13-C14-C19 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | D     | 1102 | 6ZP  | C20-C13-C14-C19 |
| 5   | D     | 1104 | PCW  | C31-C32-C33-C34 |
| 5   | A     | 1105 | PCW  | O2-C31-C32-C33  |
| 5   | D     | 1104 | PCW  | C24-C25-C26-C27 |
| 5   | D     | 1101 | PCW  | O11-C11-C12-C13 |
| 5   | D     | 1106 | PCW  | C22-C23-C24-C25 |
| 5   | E     | 203  | PCW  | O11-C11-C12-C13 |
| 5   | B     | 1109 | PCW  | O11-C11-C12-C13 |
| 5   | A     | 1106 | PCW  | C11-C12-C13-C14 |
| 5   | C     | 1105 | PCW  | O31-C31-C32-C33 |
| 5   | C     | 1109 | PCW  | C41-C42-C43-C44 |
| 4   | B     | 1102 | ZK1  | CAS-CAR-NAX-CAN |
| 4   | D     | 1103 | ZK1  | CAS-CAR-NAX-CAN |
| 5   | D     | 1105 | PCW  | C39-C40-C41-C42 |
| 5   | A     | 1105 | PCW  | O31-C31-C32-C33 |
| 5   | C     | 1106 | PCW  | C11-C12-C13-C14 |
| 5   | D     | 1105 | PCW  | C17-C18-C19-C20 |

There are no ring outliers.

39 monomers are involved in 133 short contacts:

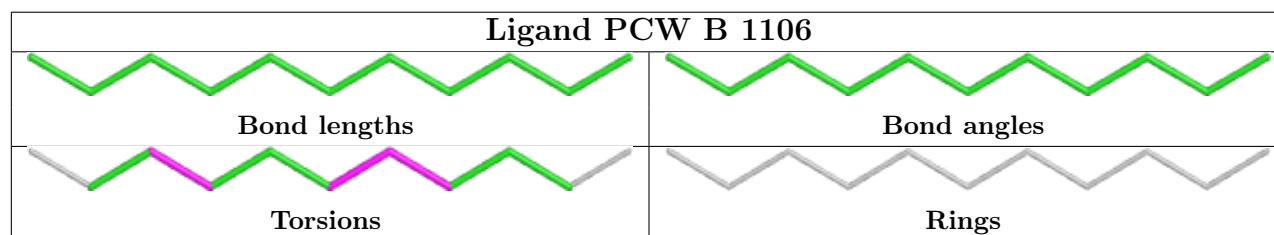
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | B     | 1106 | PCW  | 3       | 0            |
| 5   | C     | 1103 | PCW  | 3       | 0            |
| 6   | C     | 1107 | CLR  | 7       | 0            |
| 3   | B     | 1101 | 6ZP  | 1       | 0            |
| 5   | A     | 1106 | PCW  | 2       | 0            |
| 5   | D     | 1104 | PCW  | 6       | 0            |
| 6   | A     | 1107 | CLR  | 6       | 0            |
| 6   | B     | 1108 | CLR  | 7       | 0            |
| 5   | C     | 1104 | PCW  | 1       | 0            |
| 6   | A     | 1108 | CLR  | 2       | 0            |
| 5   | D     | 1101 | PCW  | 5       | 0            |
| 4   | A     | 1102 | ZK1  | 1       | 0            |
| 5   | A     | 1110 | PCW  | 1       | 0            |
| 6   | C     | 1108 | CLR  | 4       | 0            |
| 4   | C     | 1102 | ZK1  | 1       | 0            |
| 5   | C     | 1109 | PCW  | 9       | 0            |
| 5   | B     | 1103 | PCW  | 5       | 0            |
| 5   | C     | 1110 | PCW  | 1       | 0            |
| 5   | D     | 1106 | PCW  | 8       | 0            |
| 6   | D     | 1108 | CLR  | 7       | 0            |

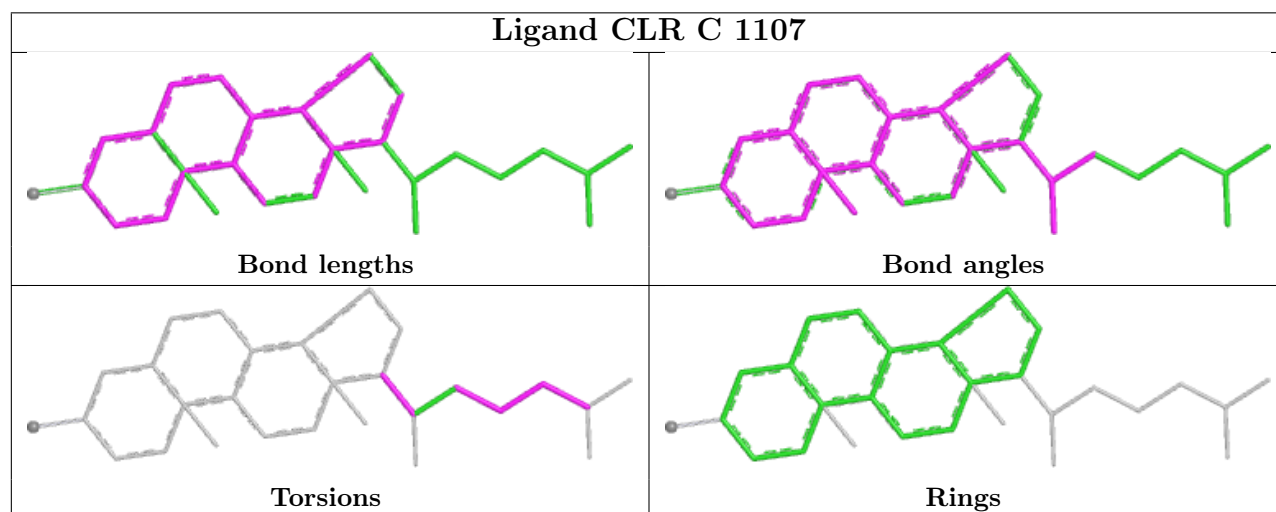
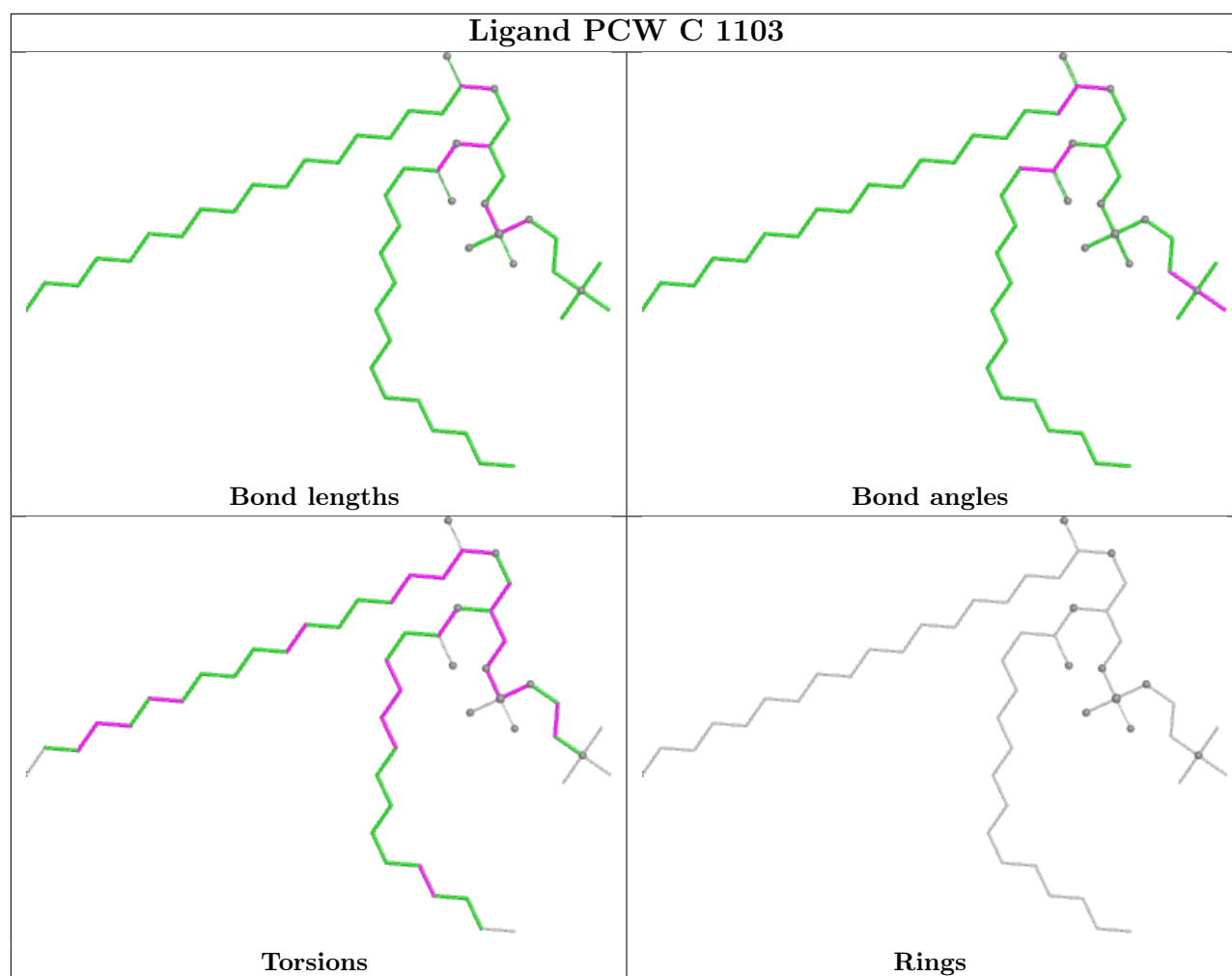
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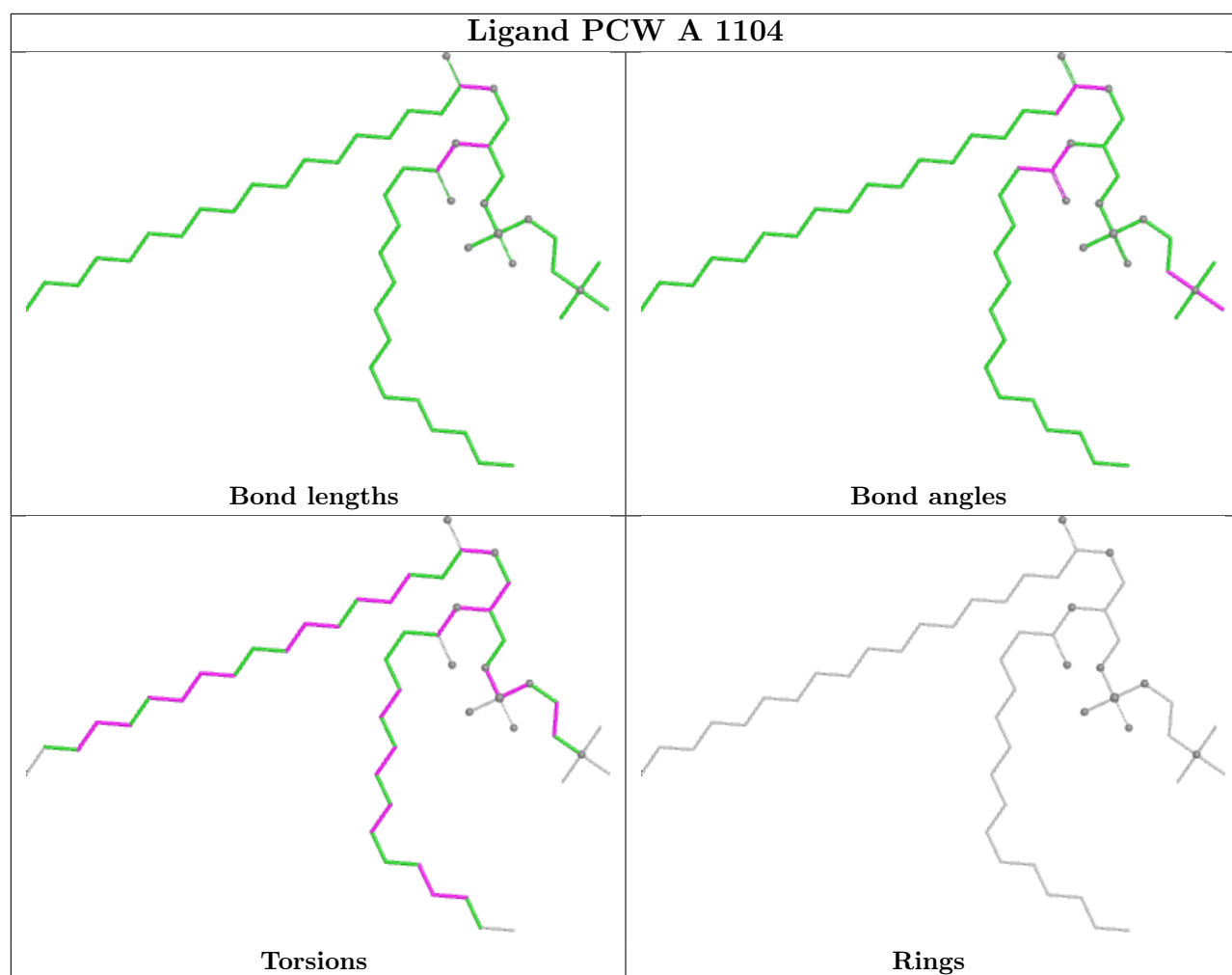
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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6   | D     | 1109 | CLR  | 6       | 0            |
| 5   | F     | 201  | PCW  | 7       | 0            |
| 5   | C     | 1105 | PCW  | 3       | 0            |
| 5   | D     | 1105 | PCW  | 5       | 0            |
| 5   | B     | 1104 | PCW  | 3       | 0            |
| 3   | D     | 1102 | 6ZP  | 1       | 0            |
| 5   | A     | 1103 | PCW  | 5       | 0            |
| 5   | A     | 1109 | PCW  | 7       | 0            |
| 3   | C     | 1101 | 6ZP  | 2       | 0            |
| 5   | B     | 1105 | PCW  | 9       | 0            |
| 3   | A     | 1101 | 6ZP  | 1       | 0            |
| 5   | C     | 1106 | PCW  | 3       | 0            |
| 5   | A     | 1105 | PCW  | 4       | 0            |
| 5   | E     | 203  | PCW  | 6       | 0            |
| 5   | B     | 1109 | PCW  | 6       | 0            |
| 5   | F     | 202  | PCW  | 1       | 0            |
| 5   | D     | 1107 | PCW  | 2       | 0            |
| 6   | B     | 1107 | CLR  | 7       | 0            |
| 5   | E     | 201  | PCW  | 2       | 0            |

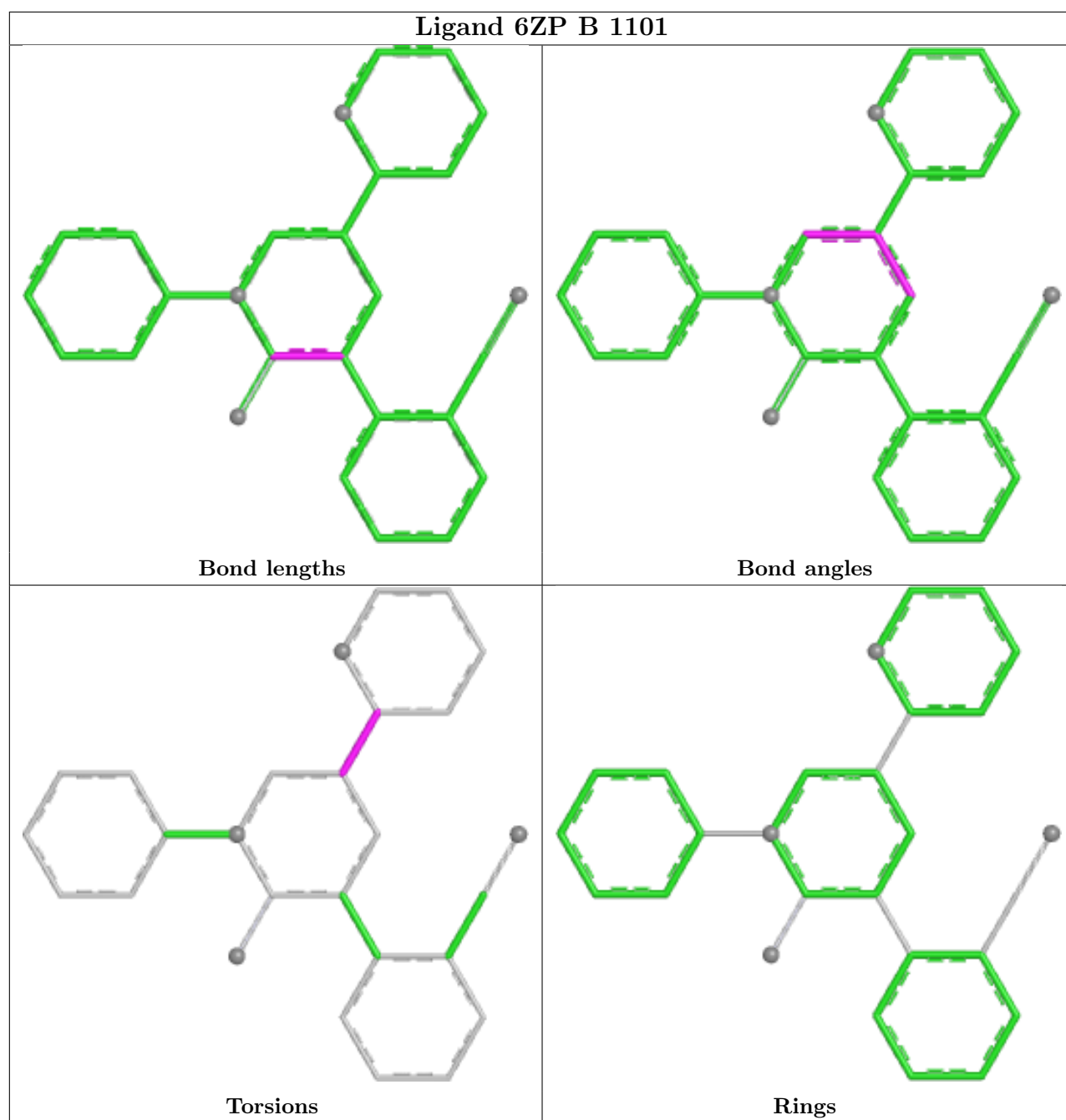
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

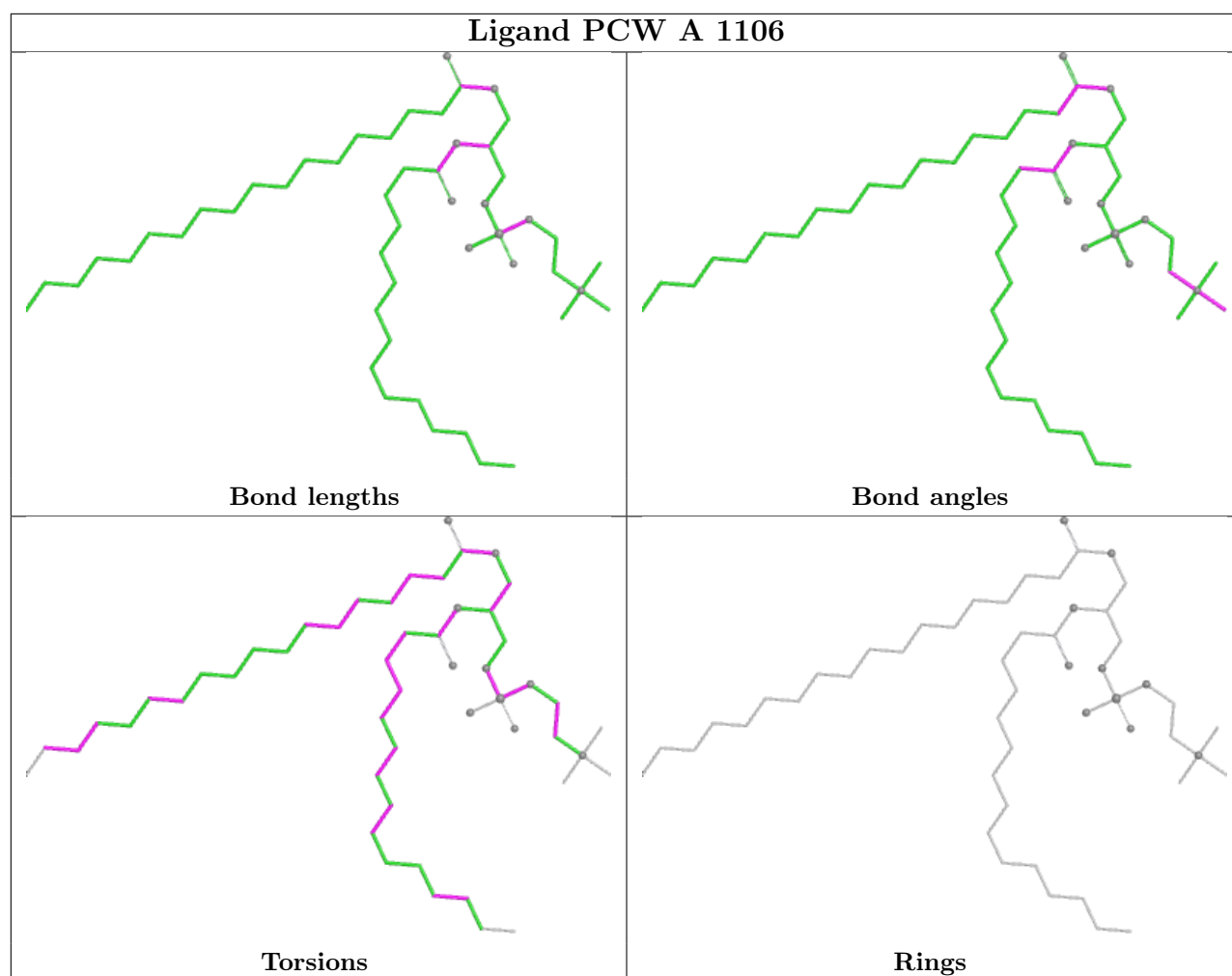


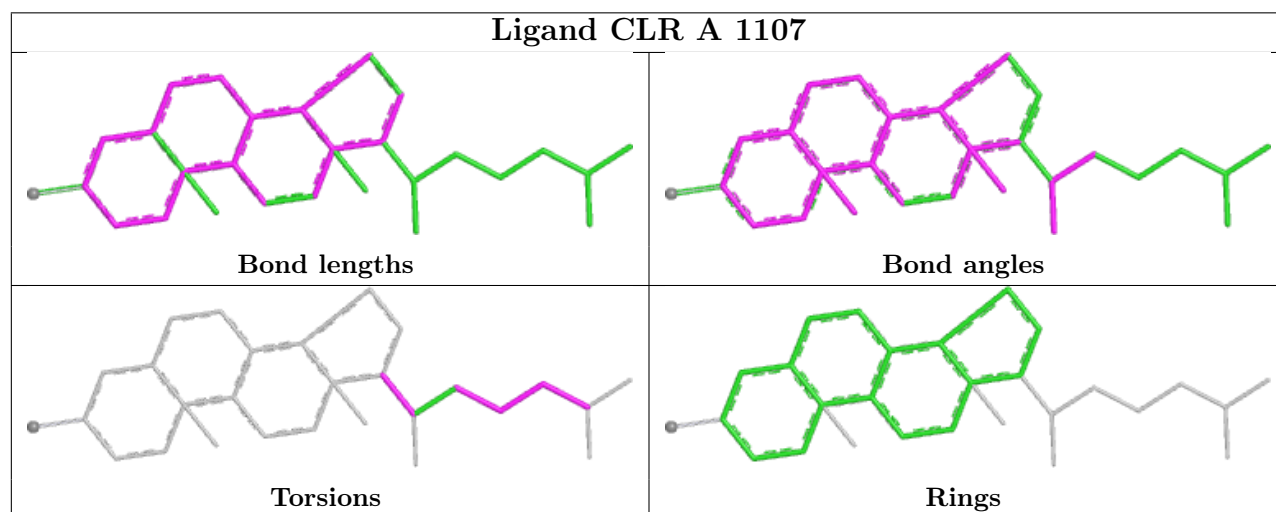
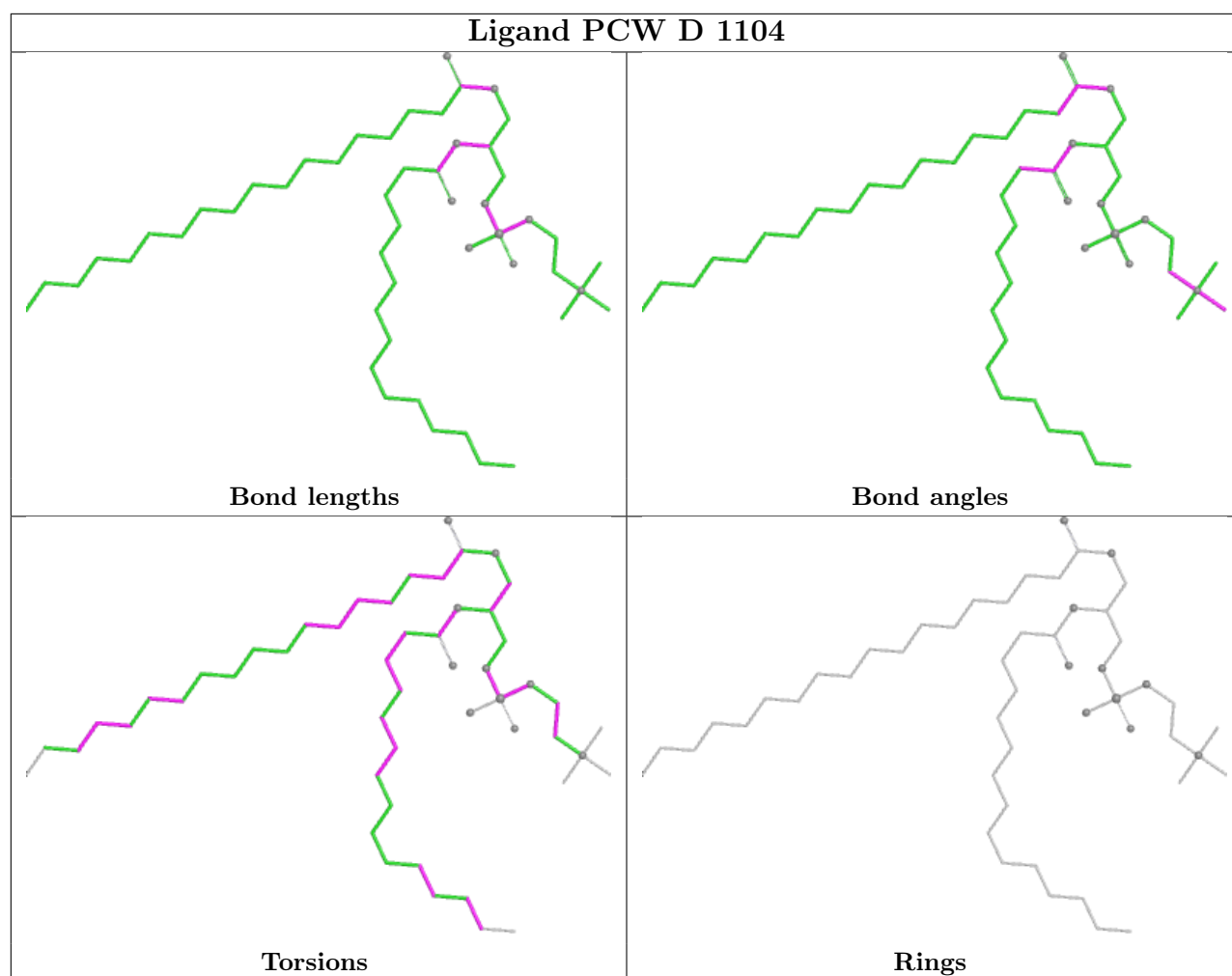


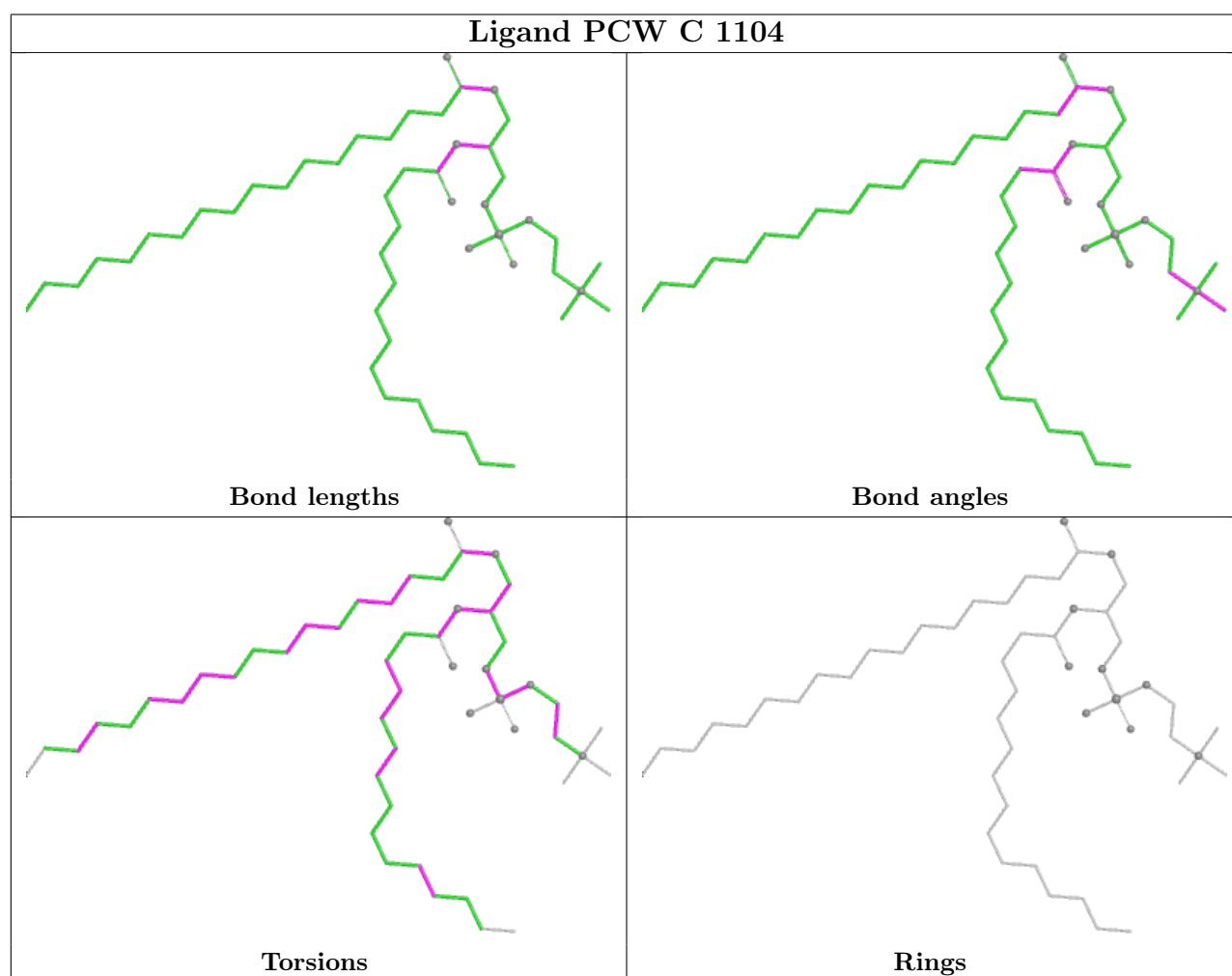
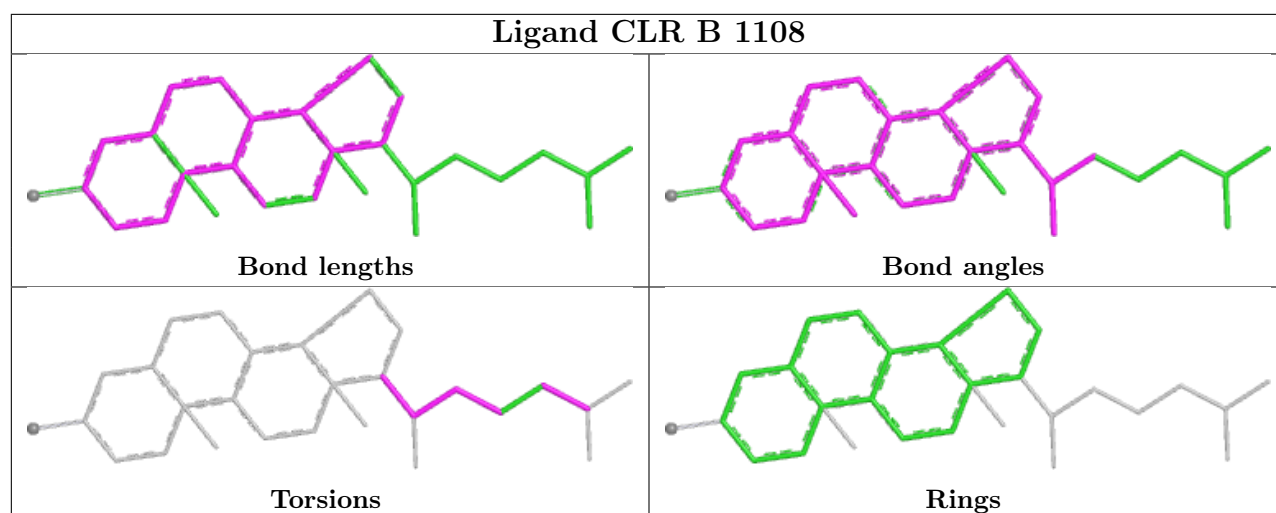


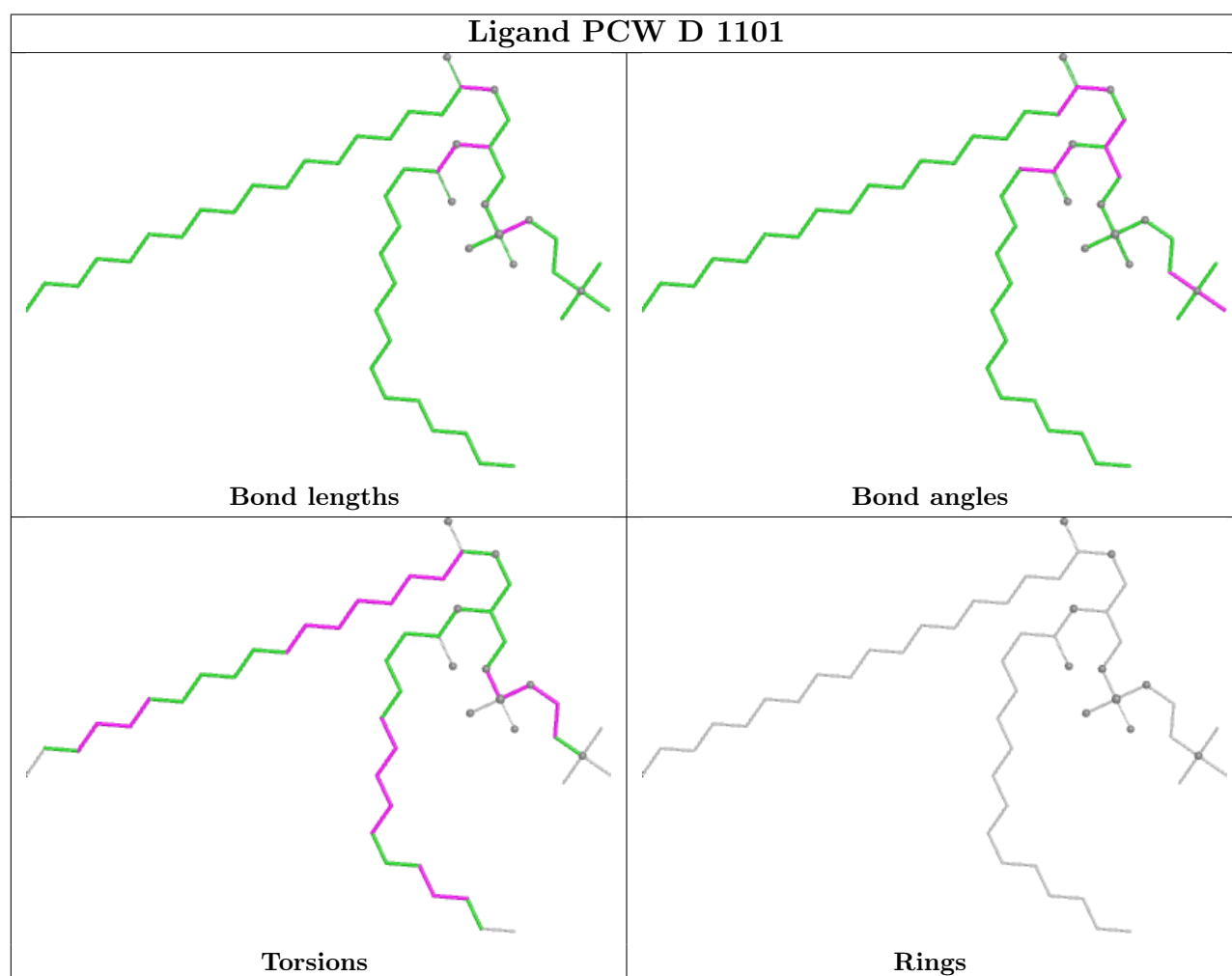
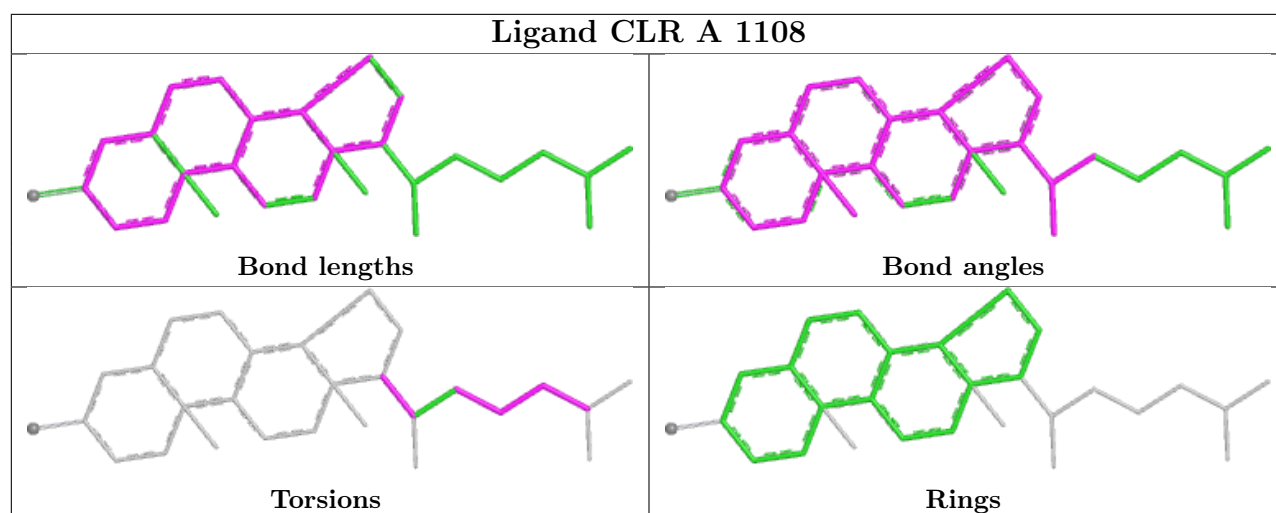


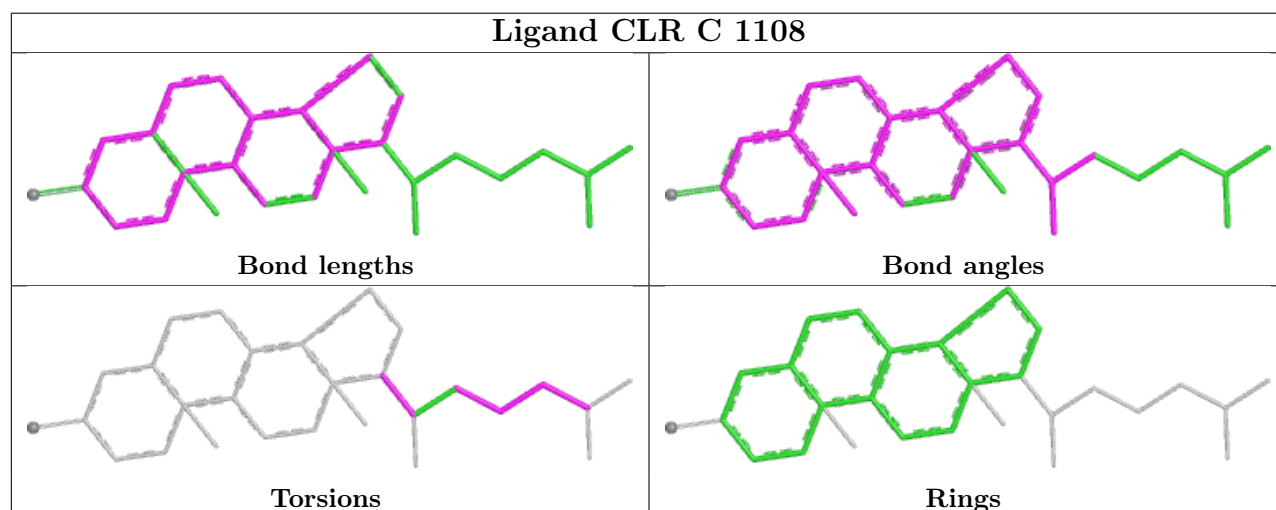
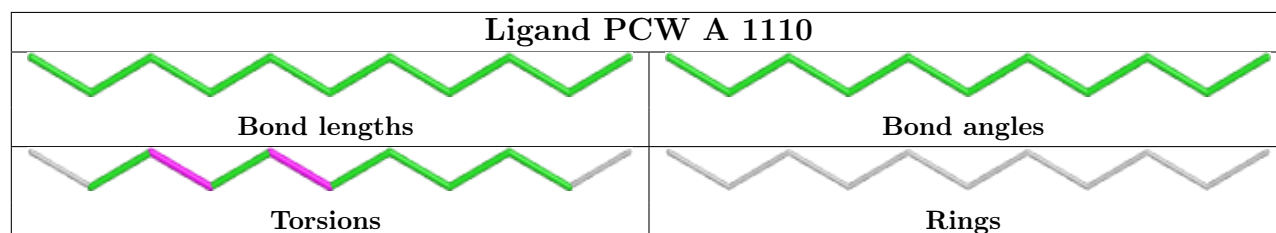
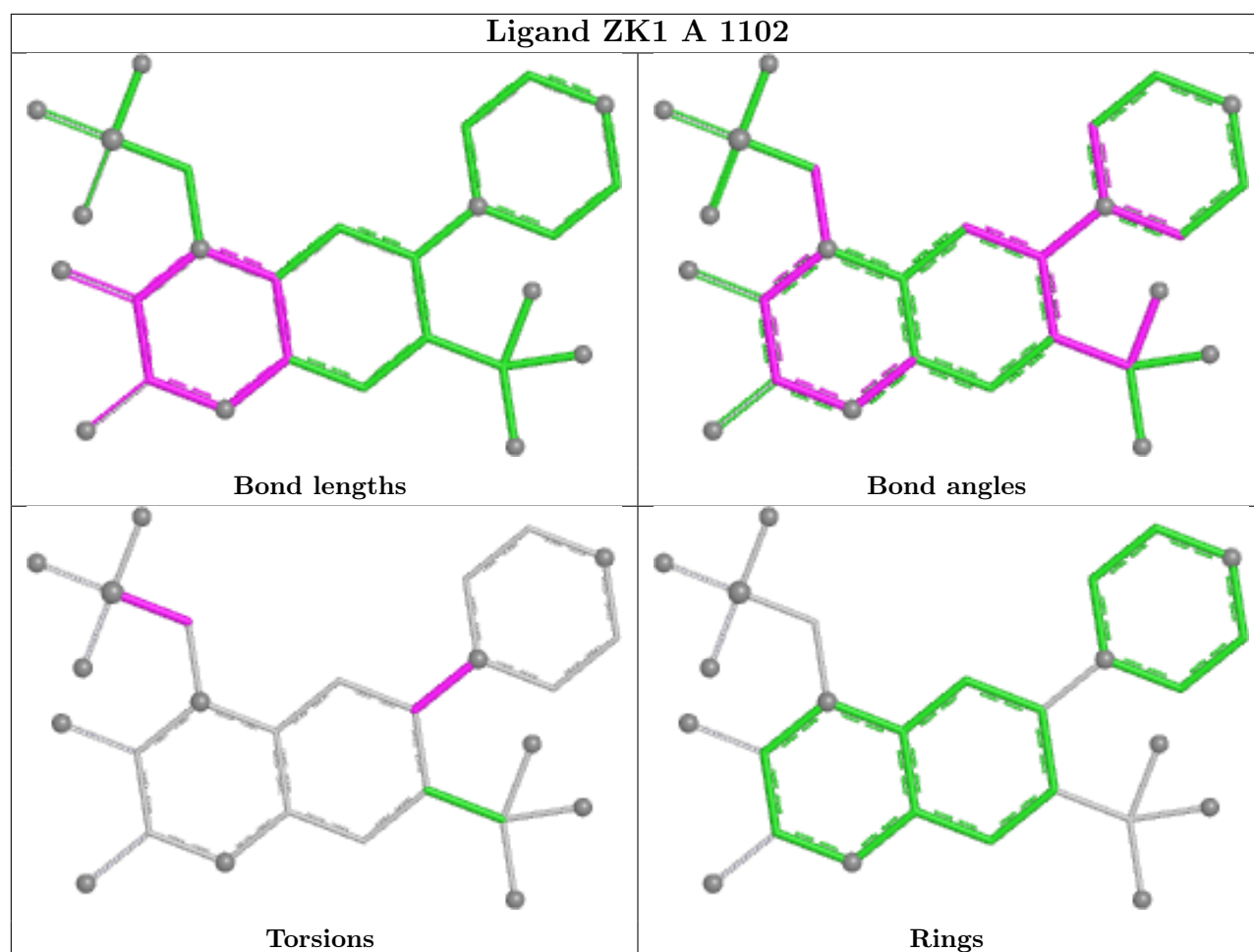


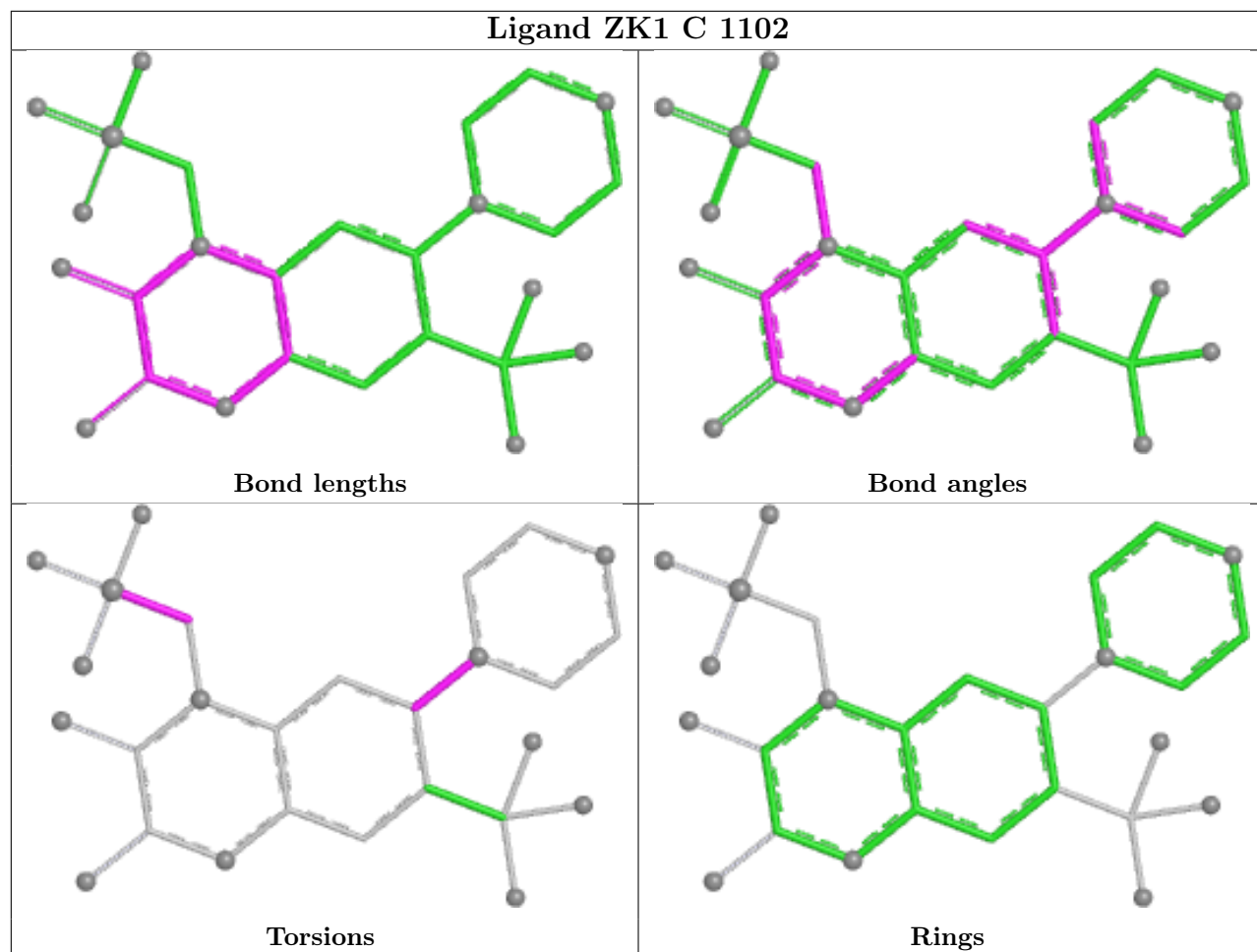


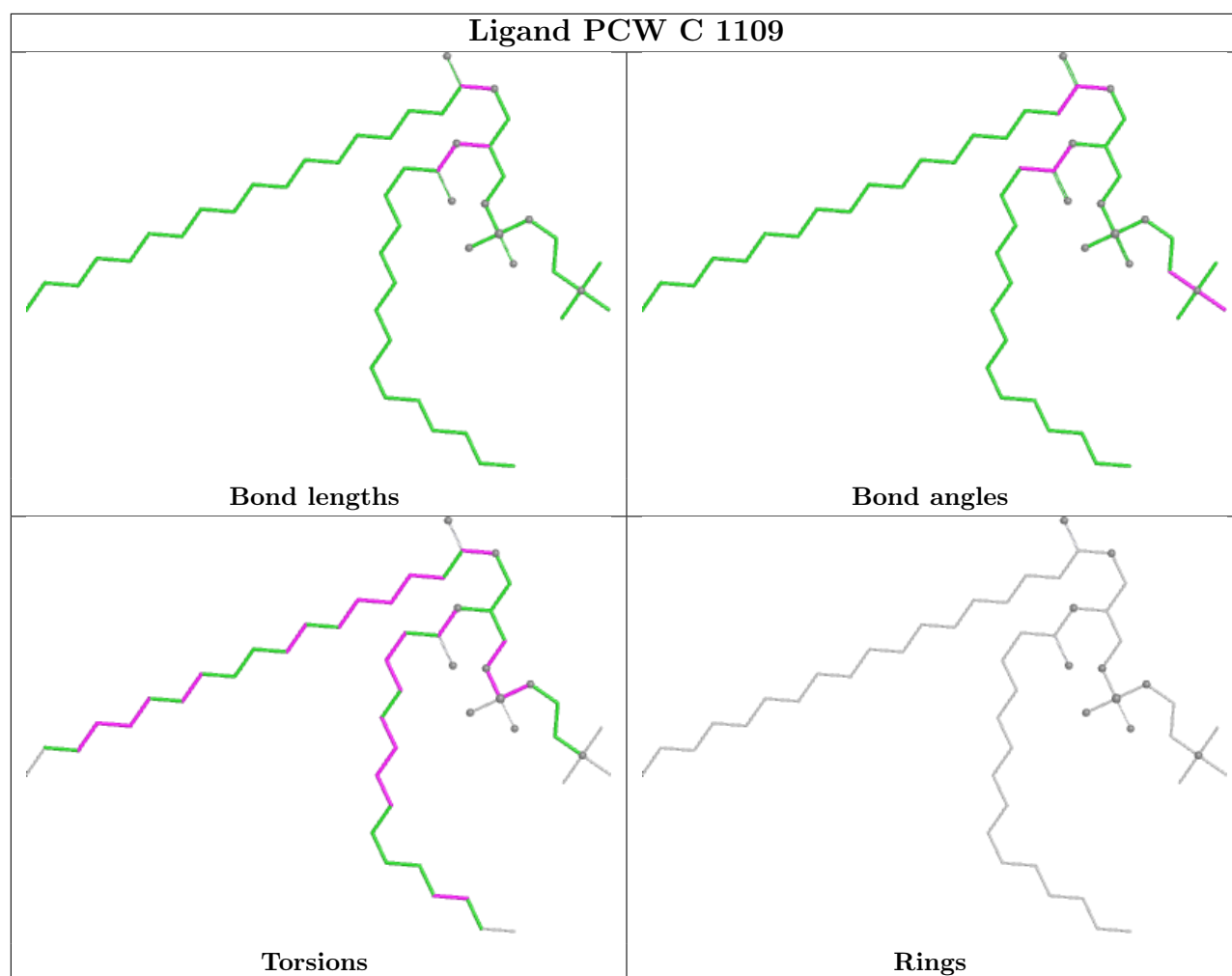




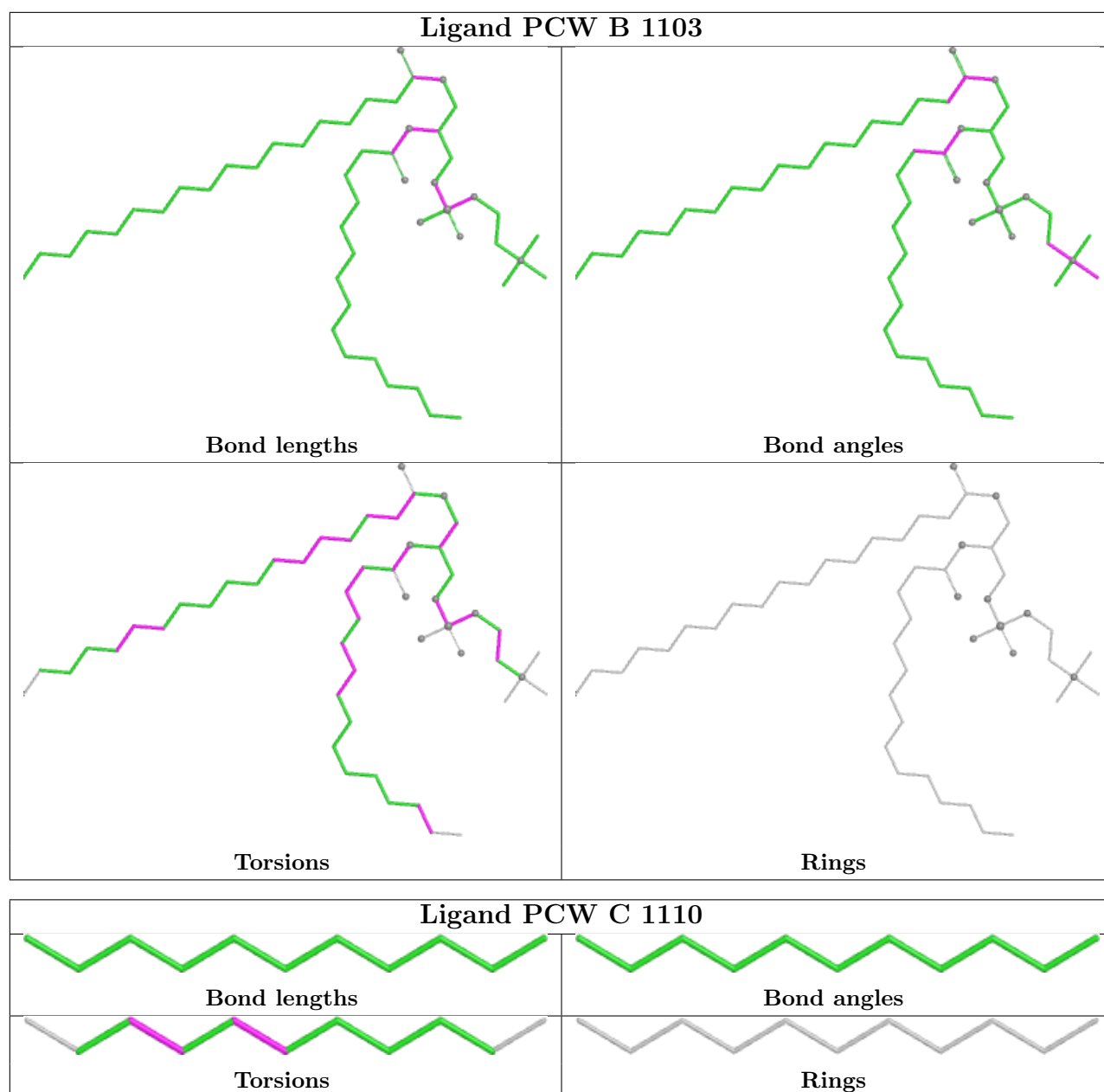


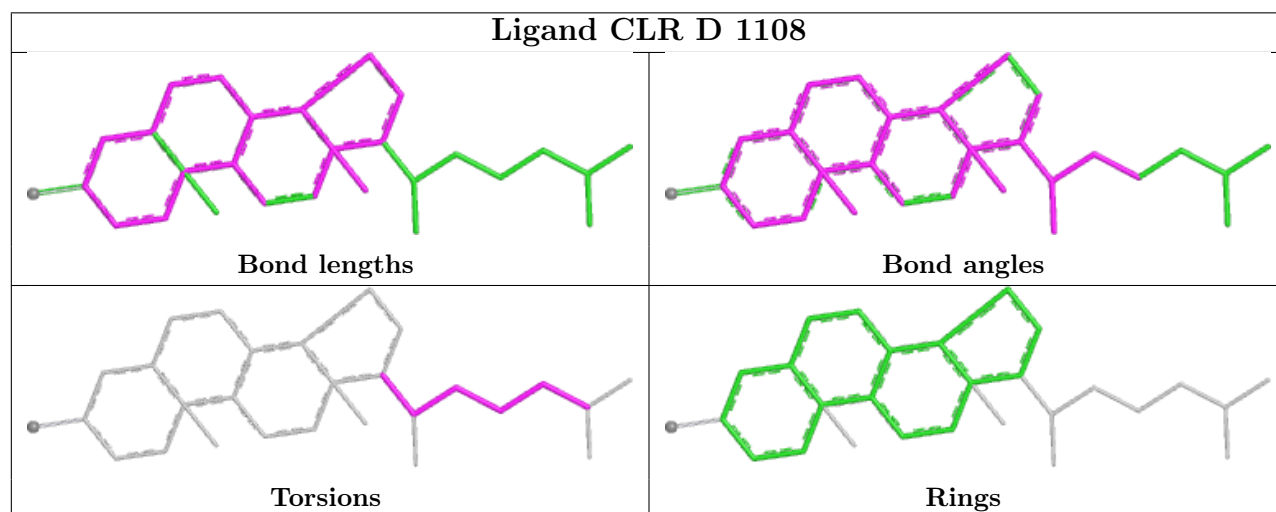
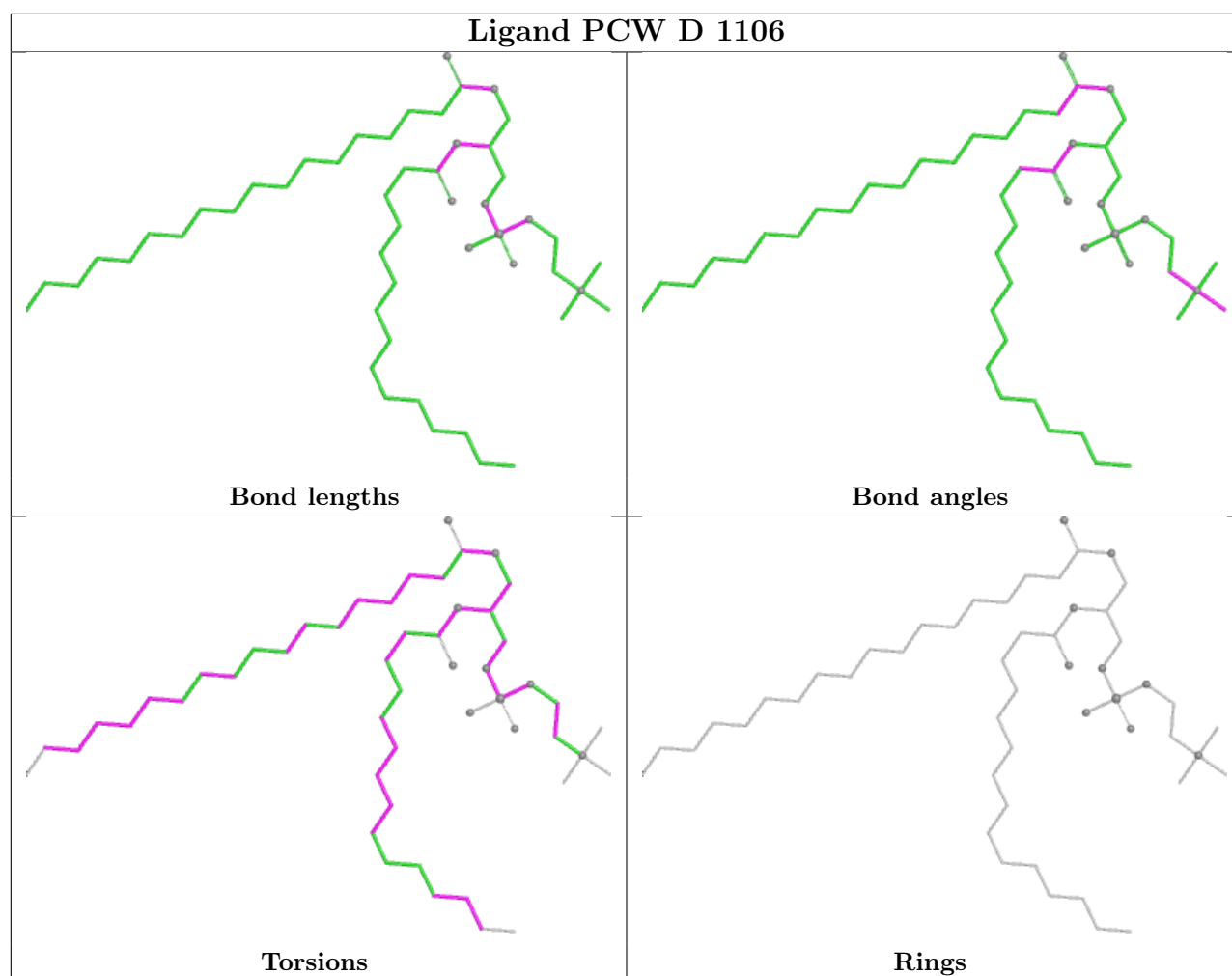


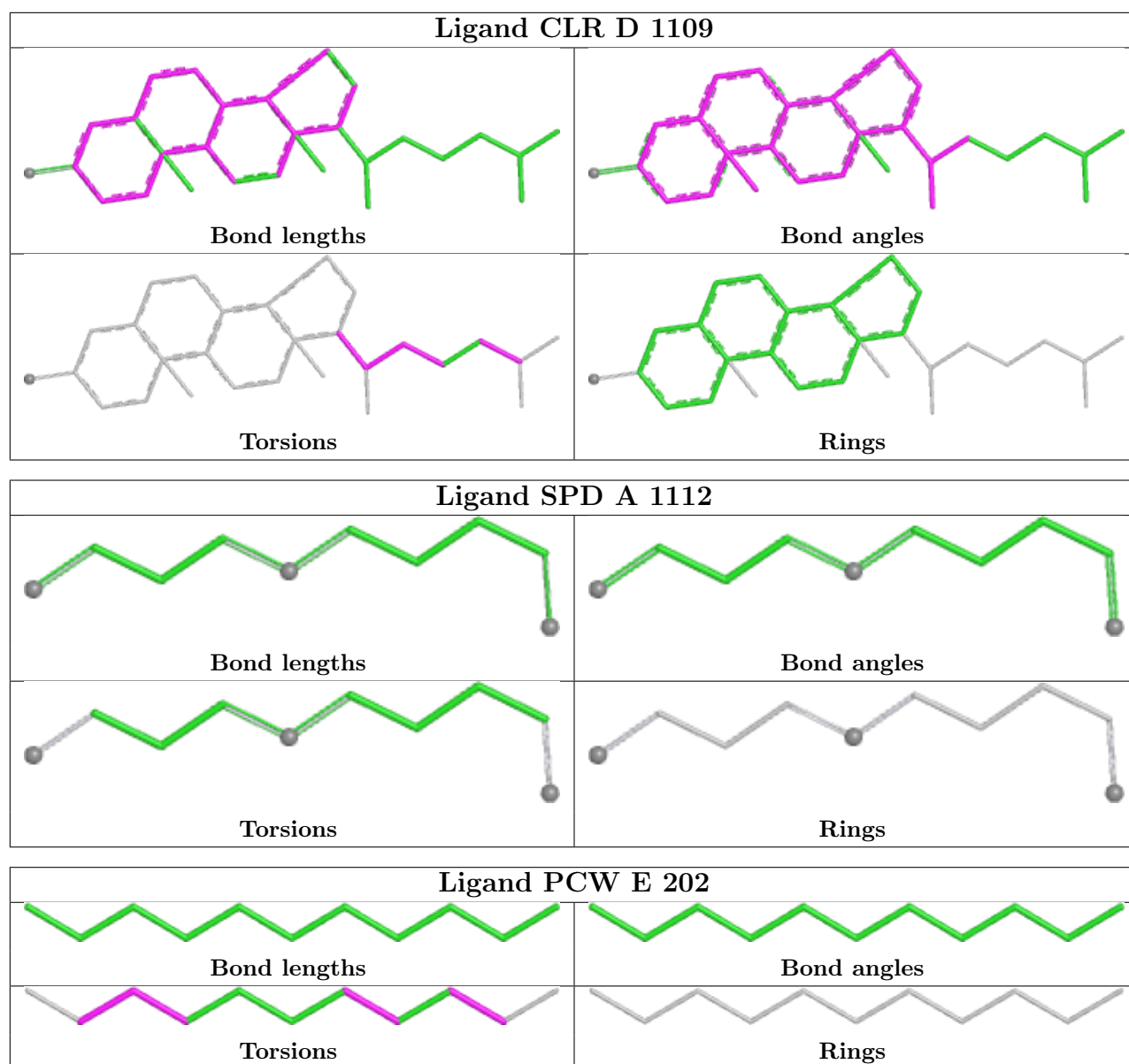


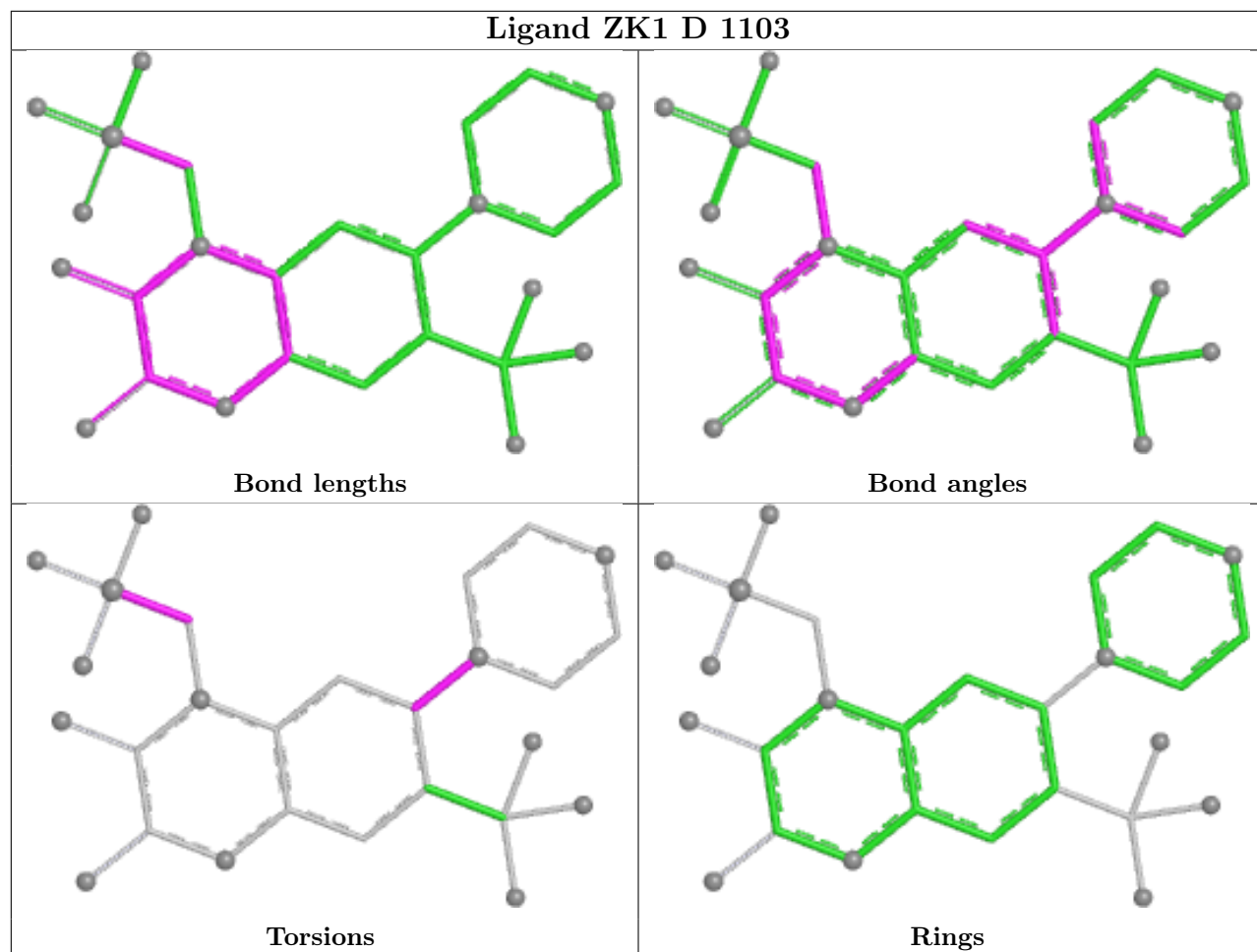


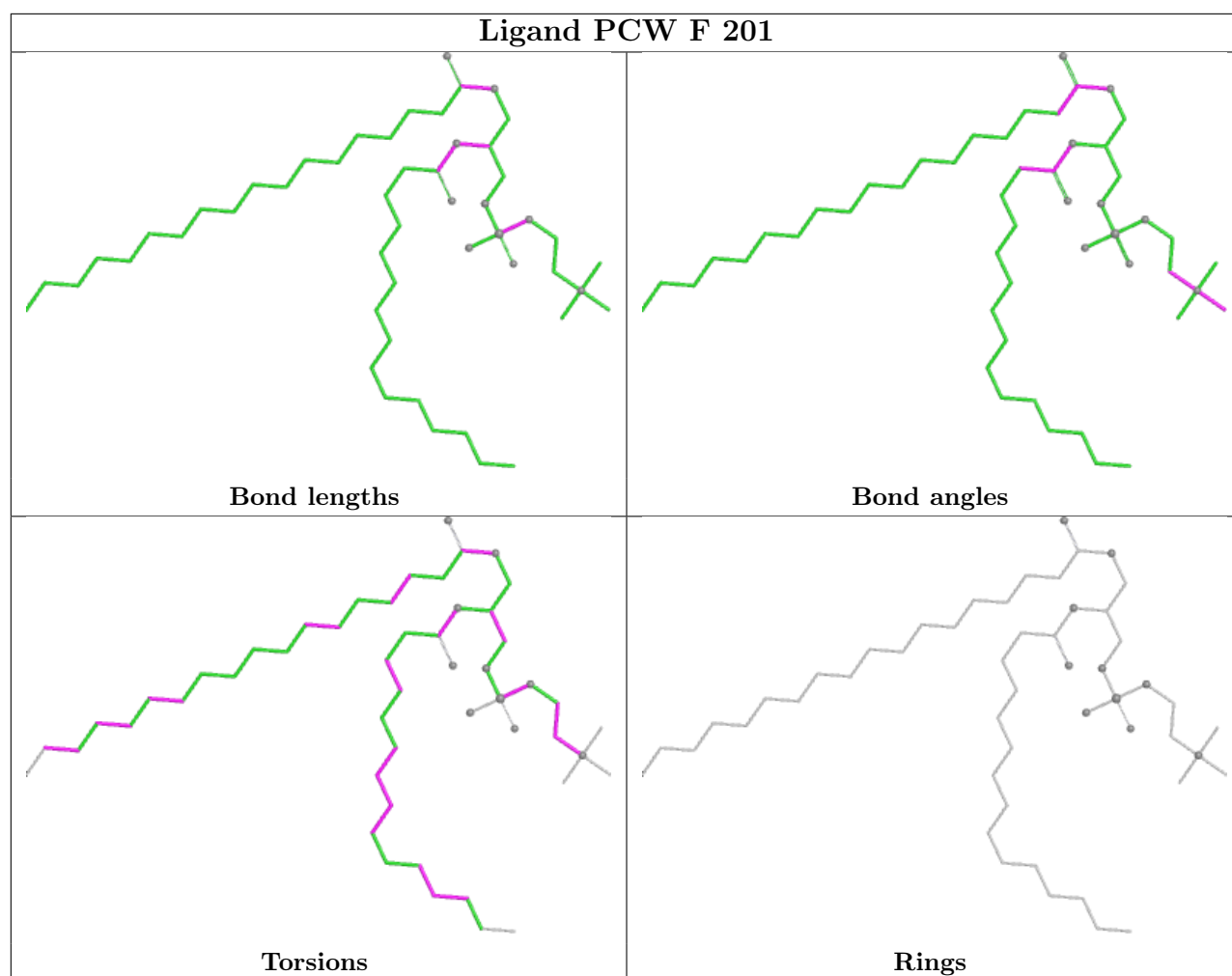


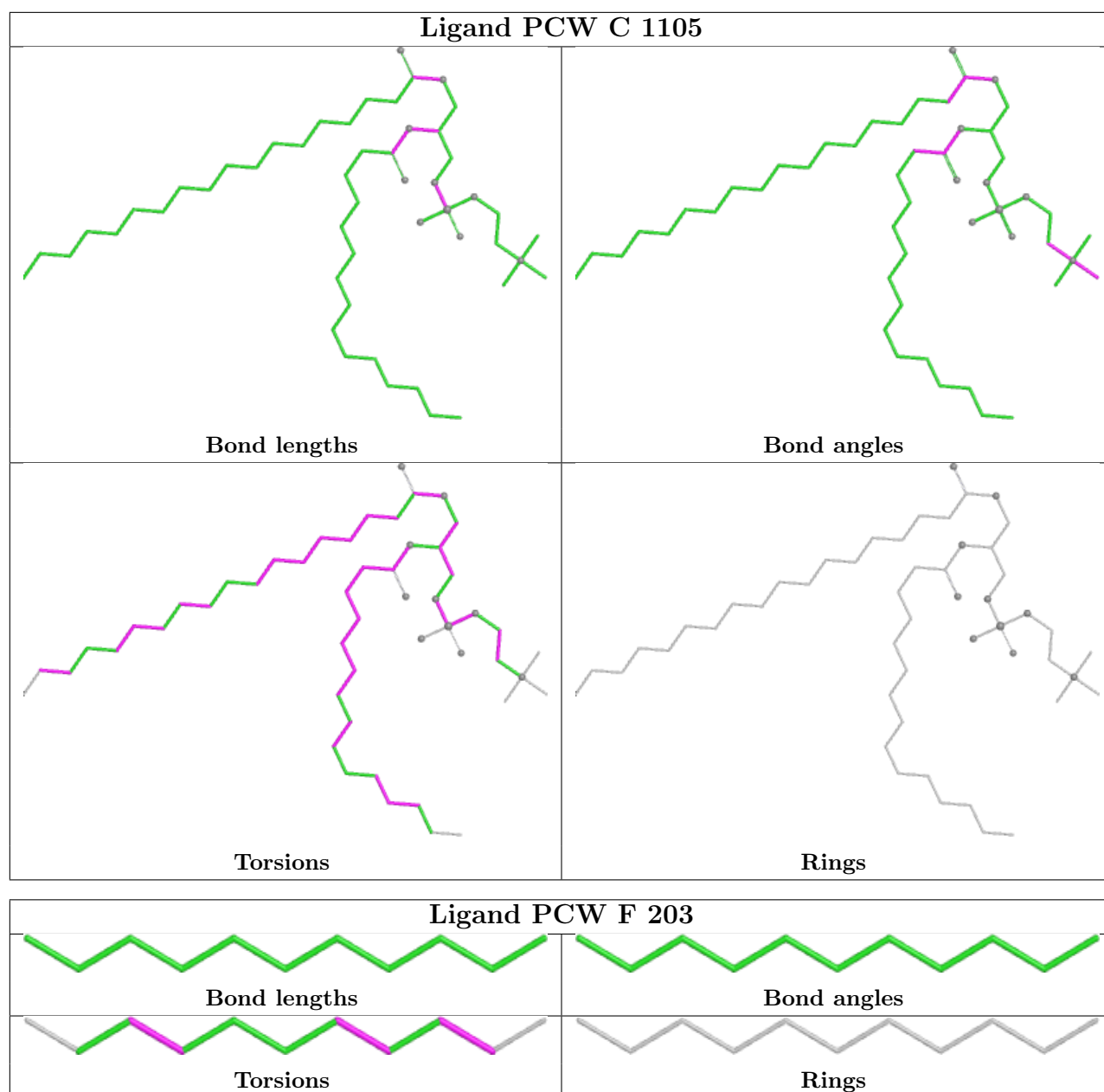


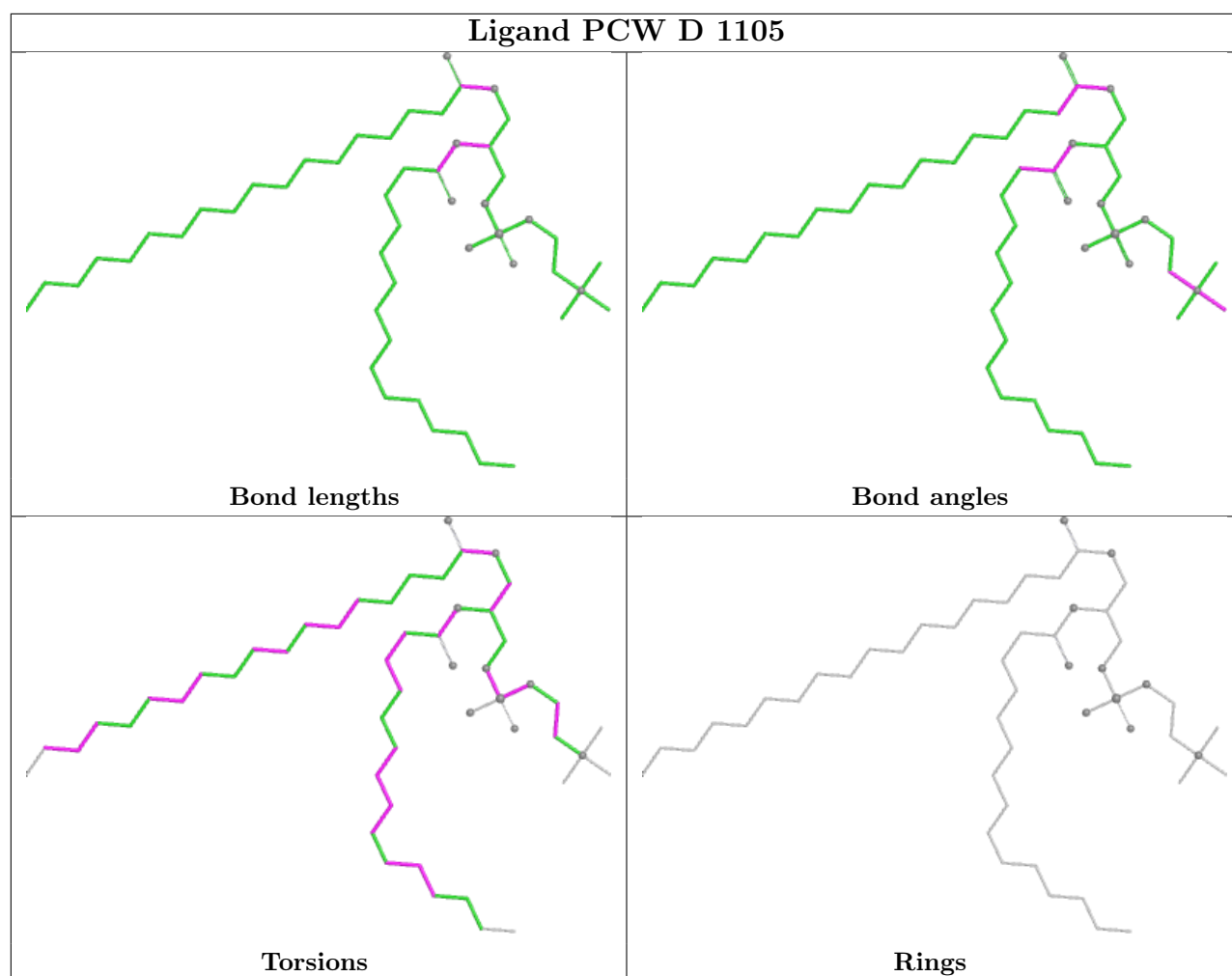


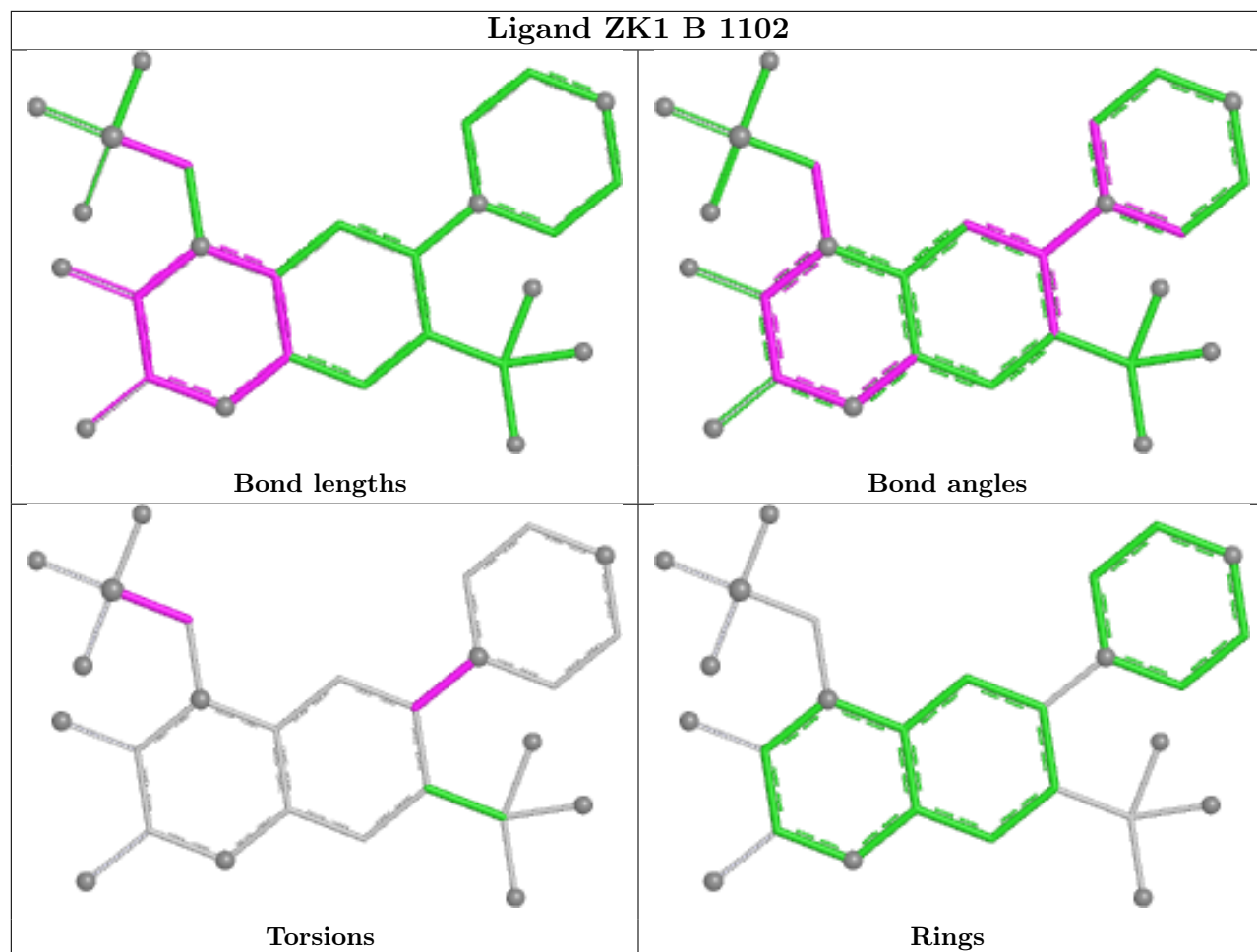




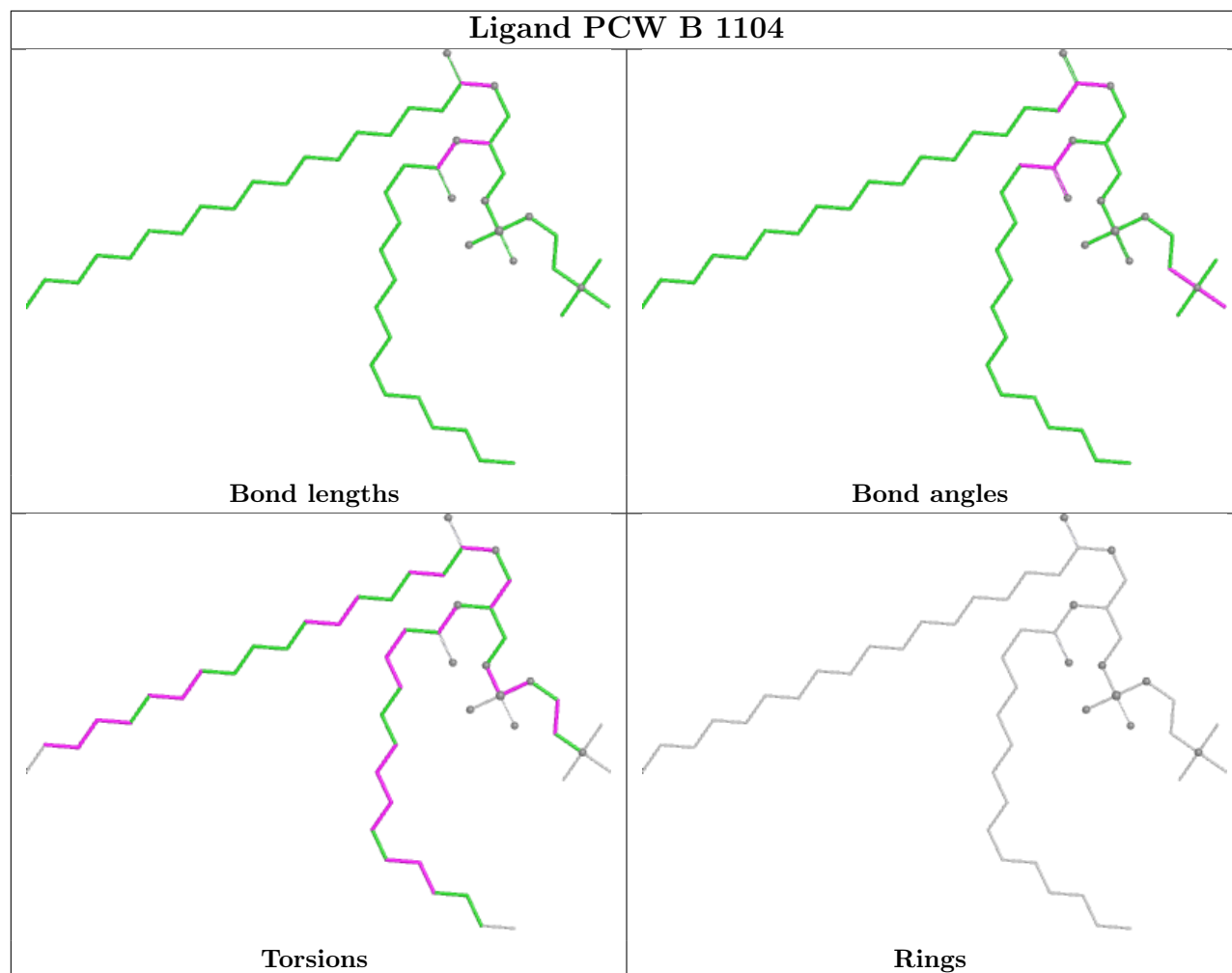


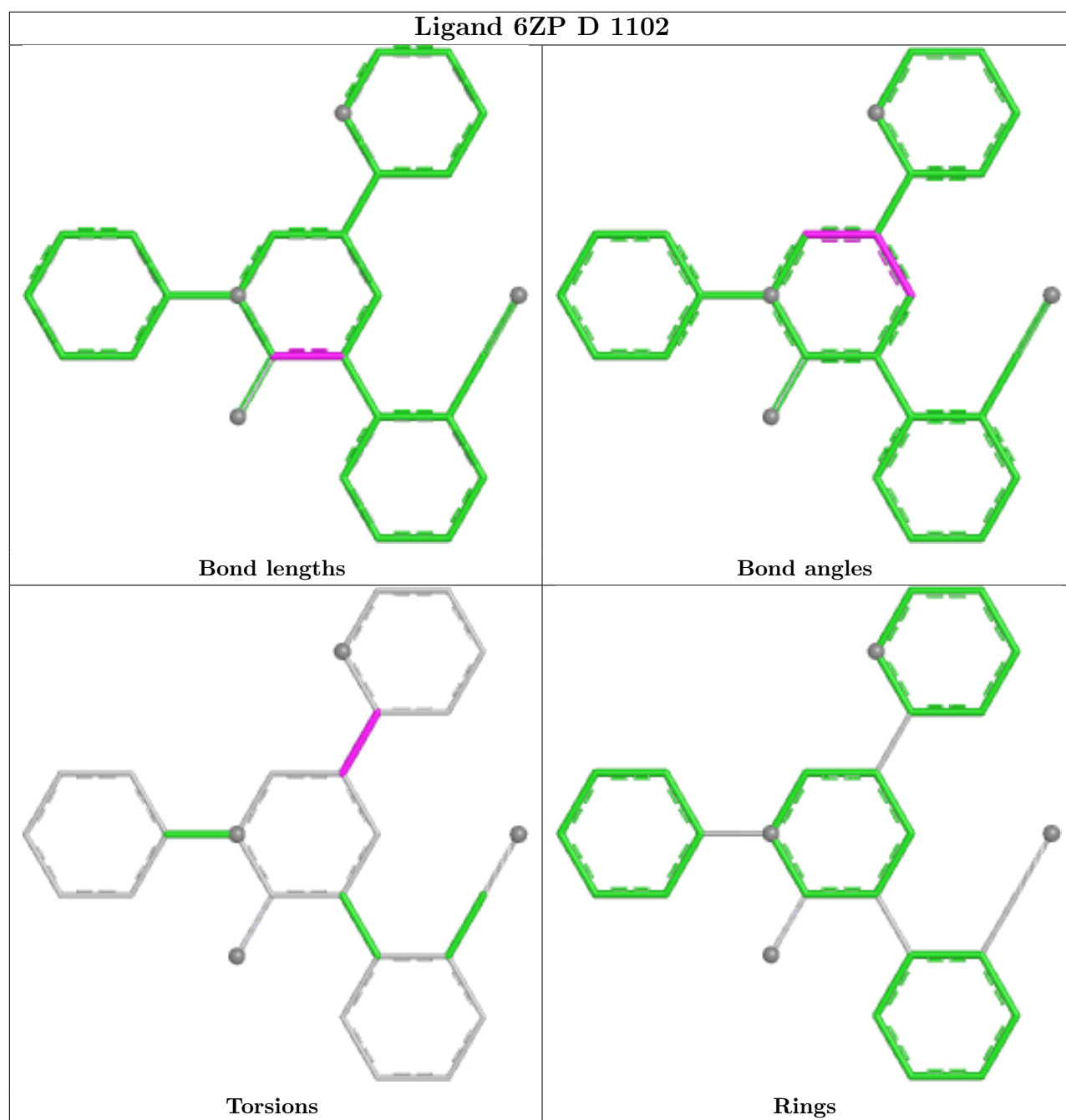


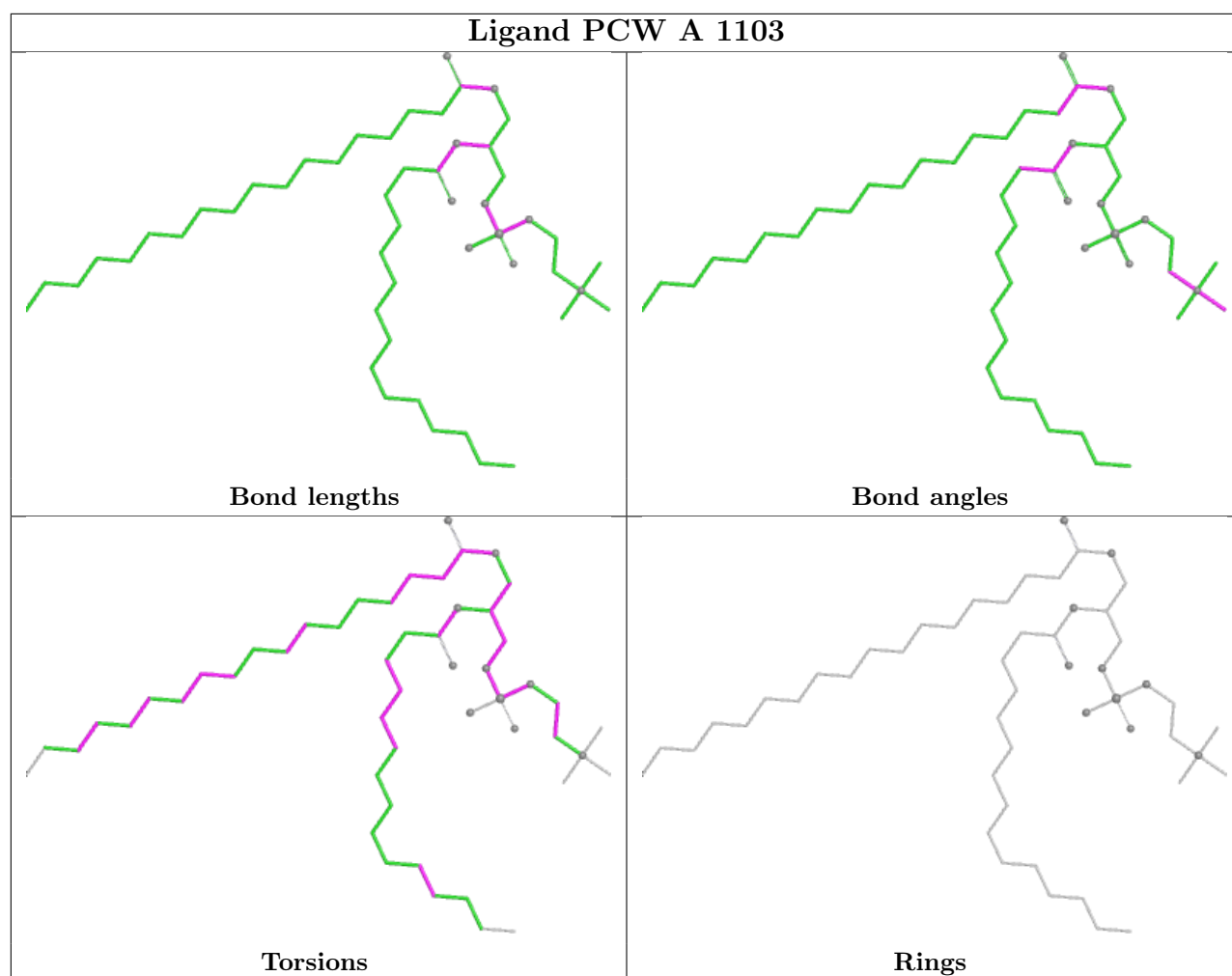


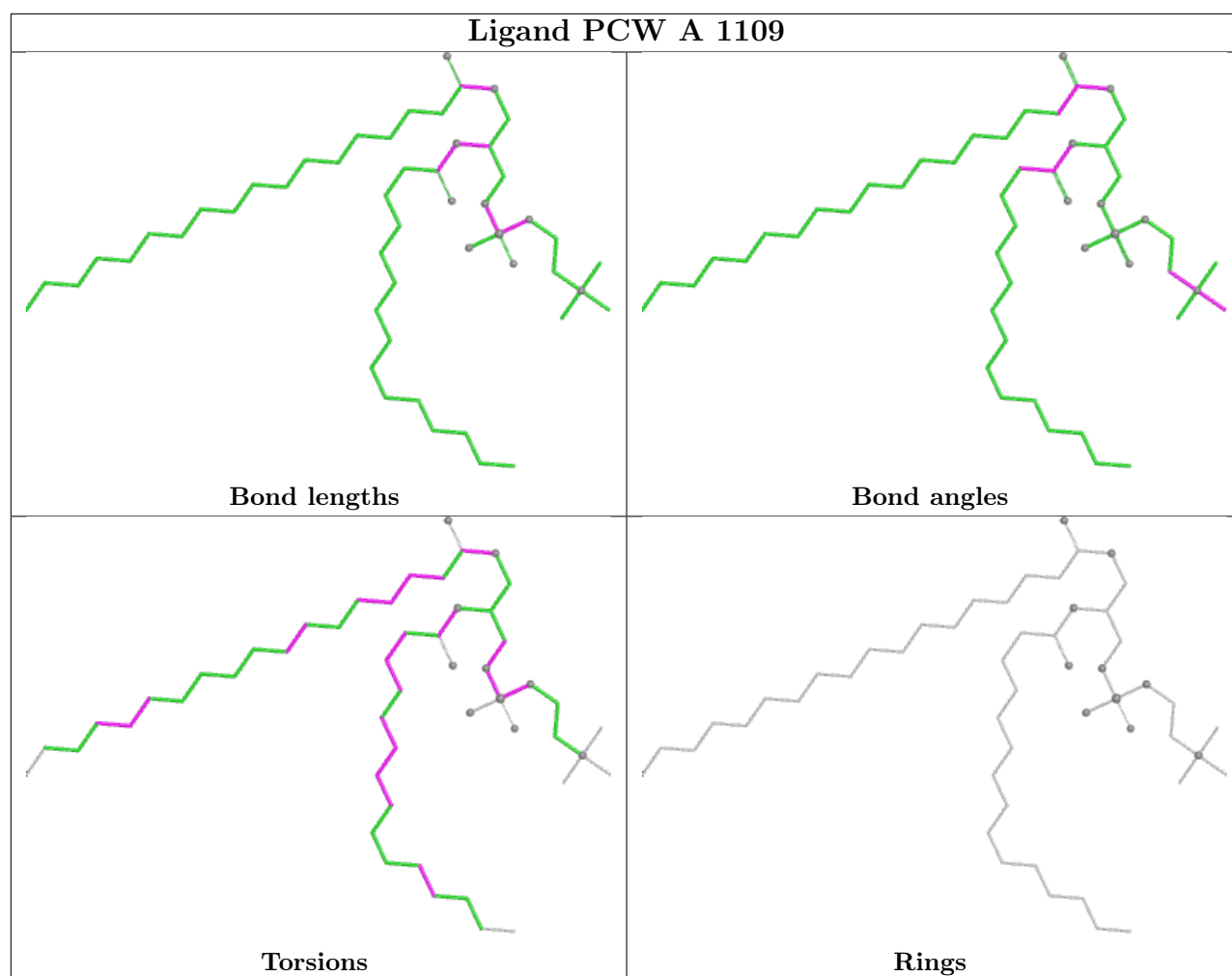


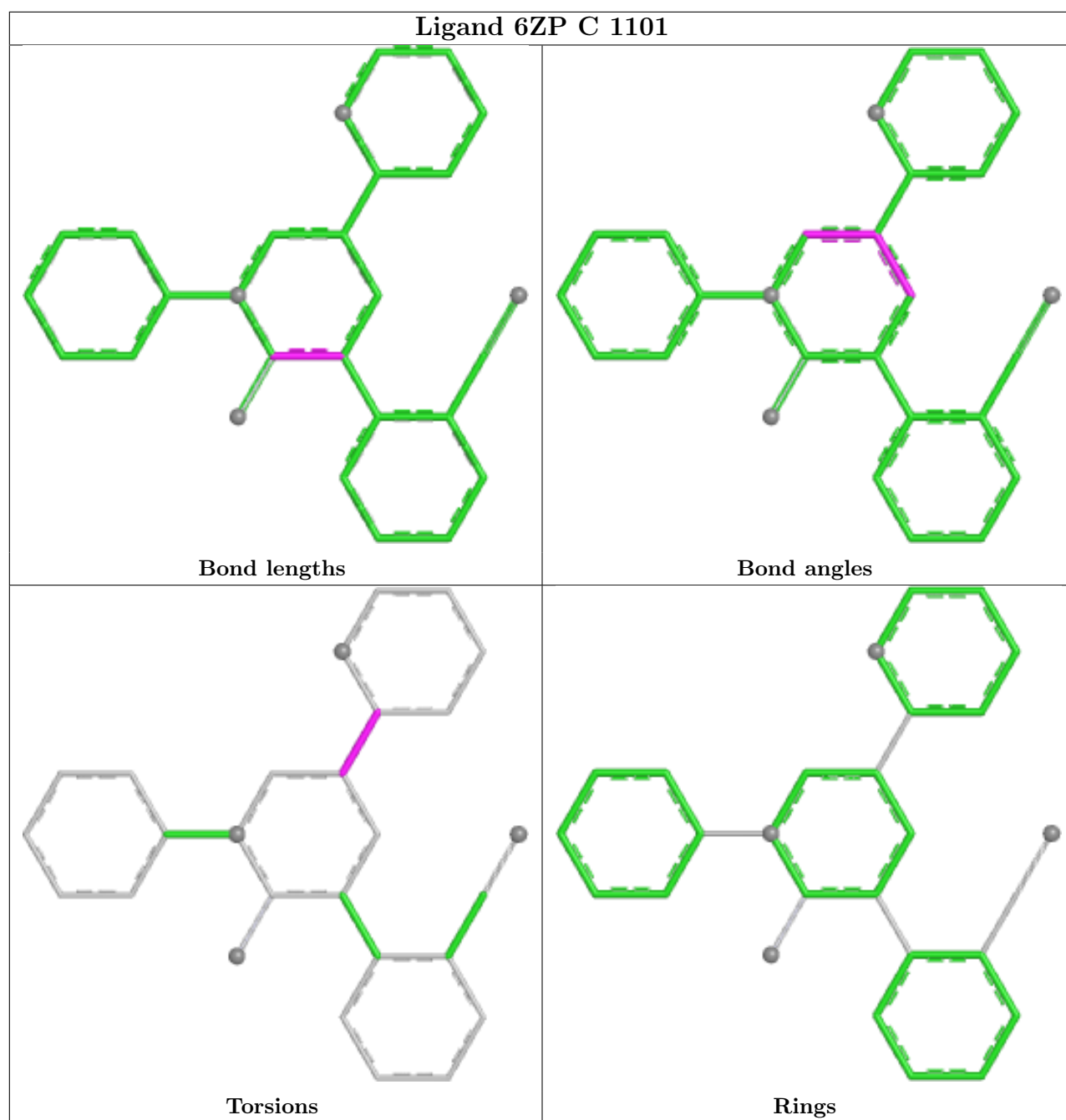


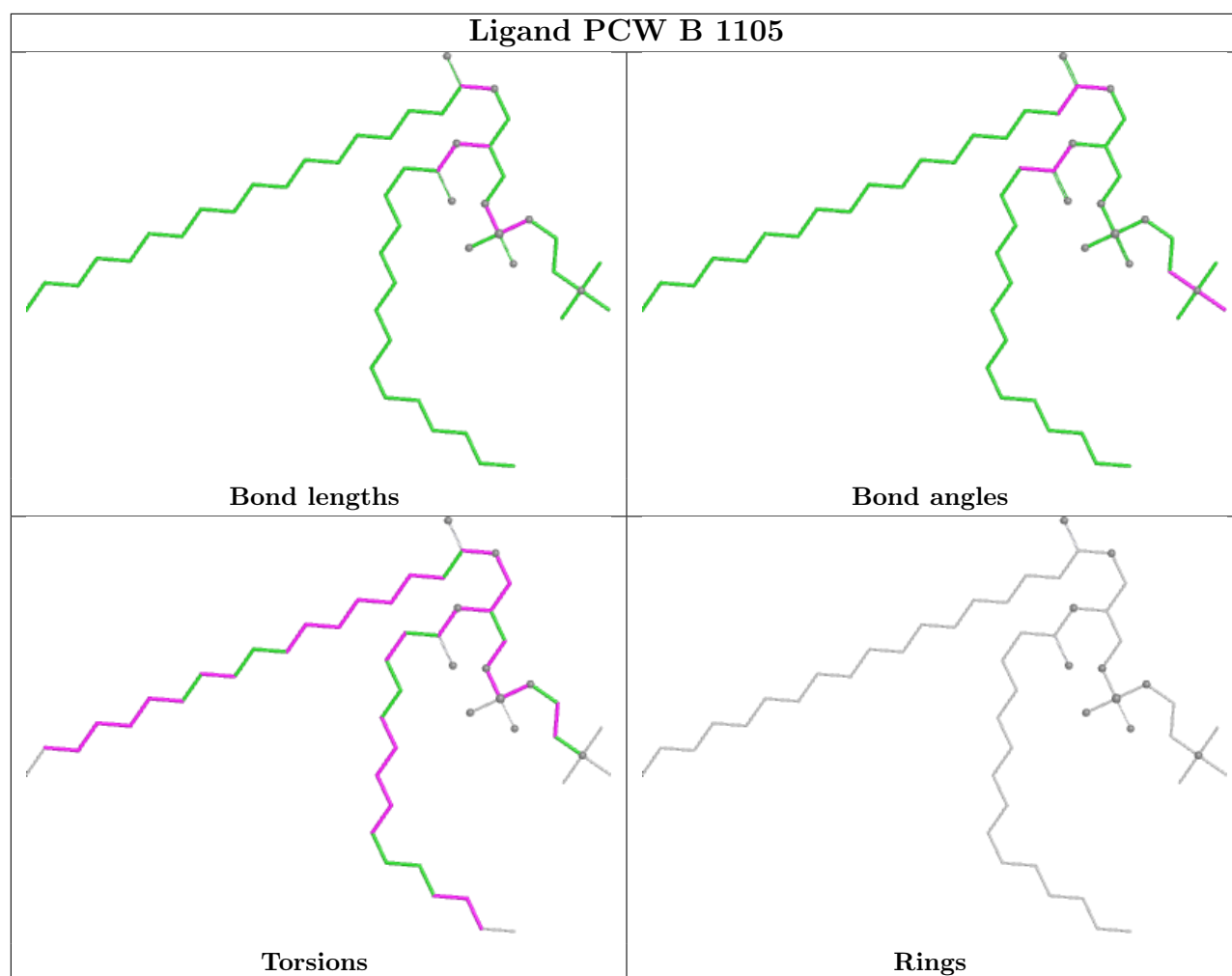


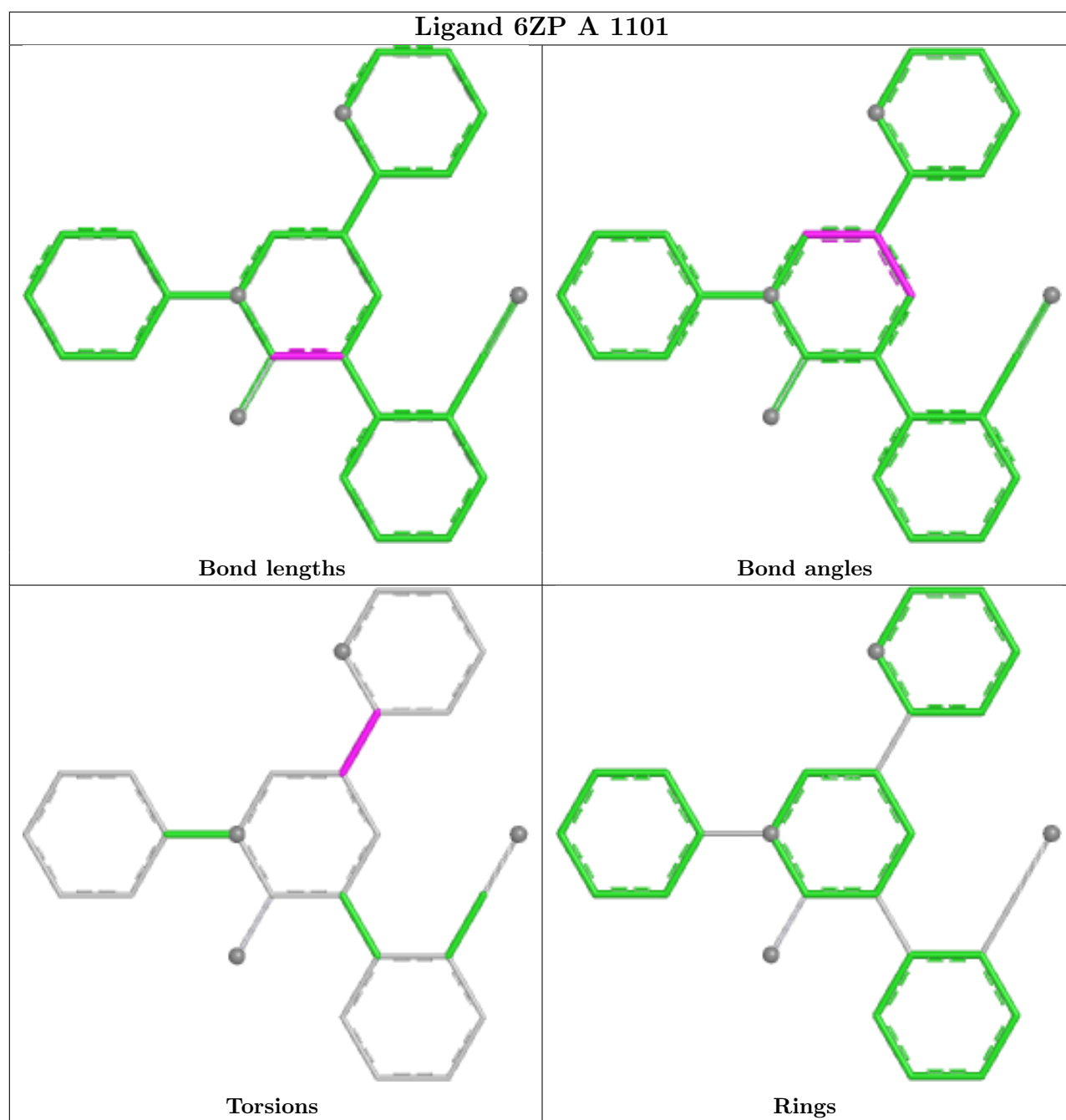


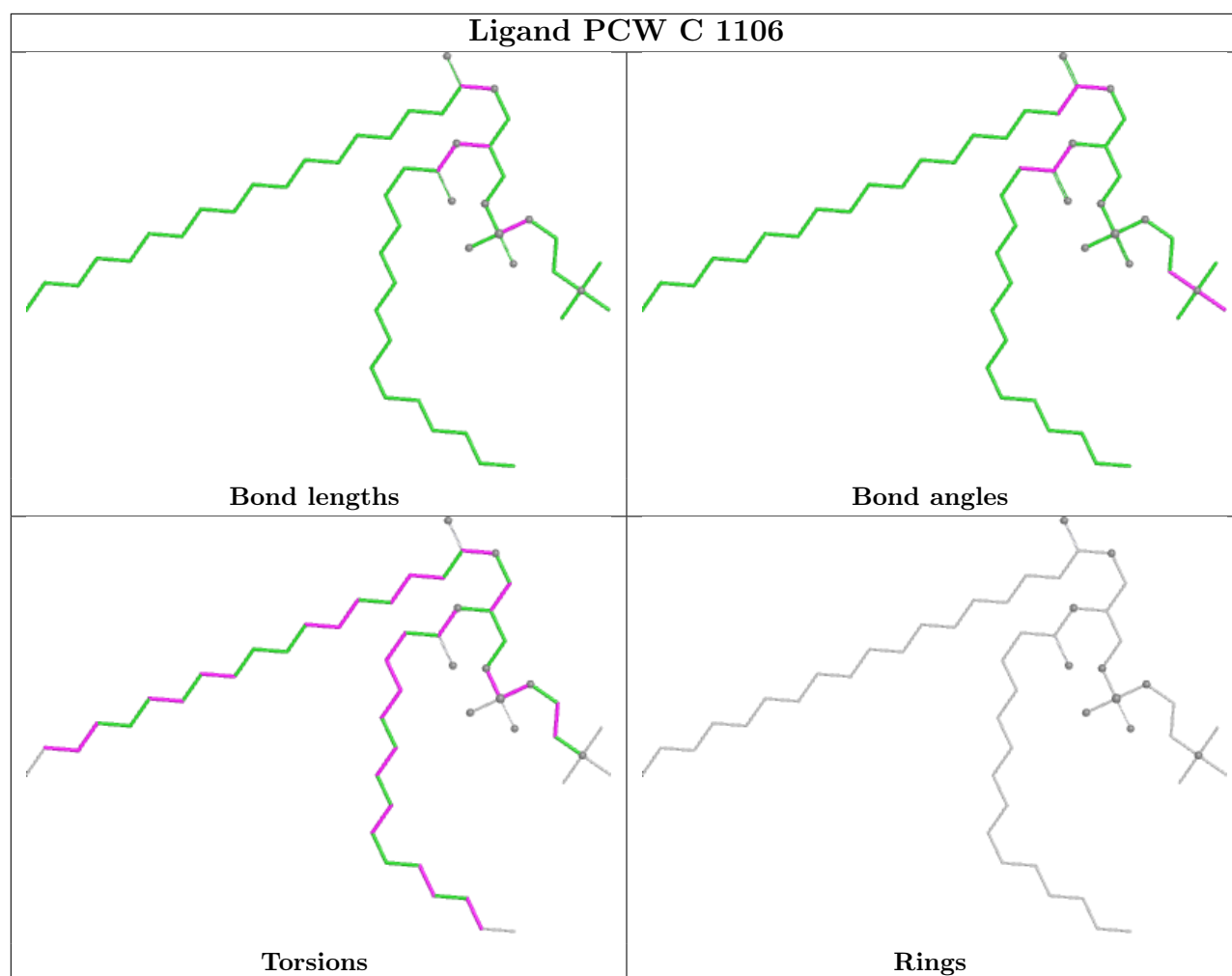




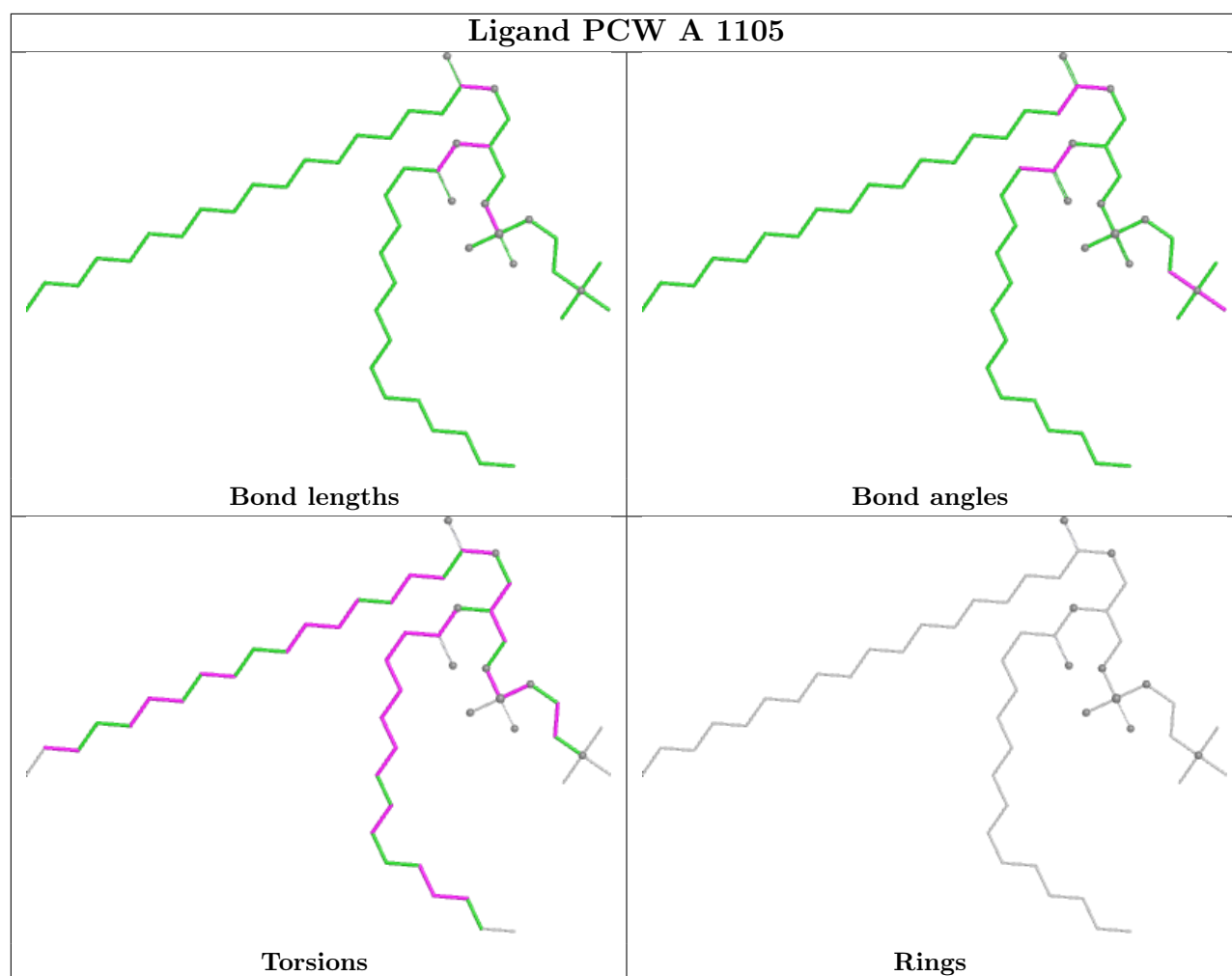


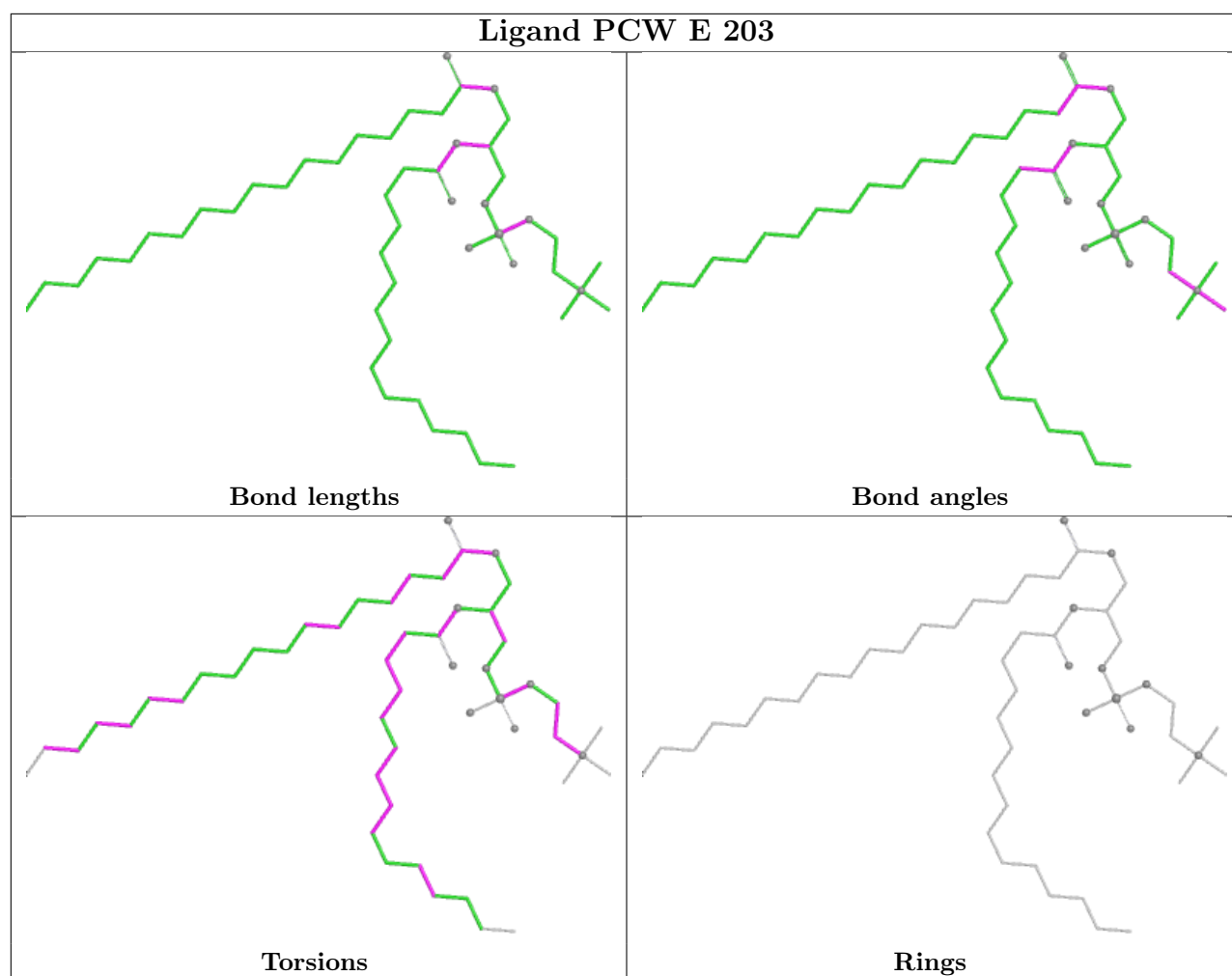


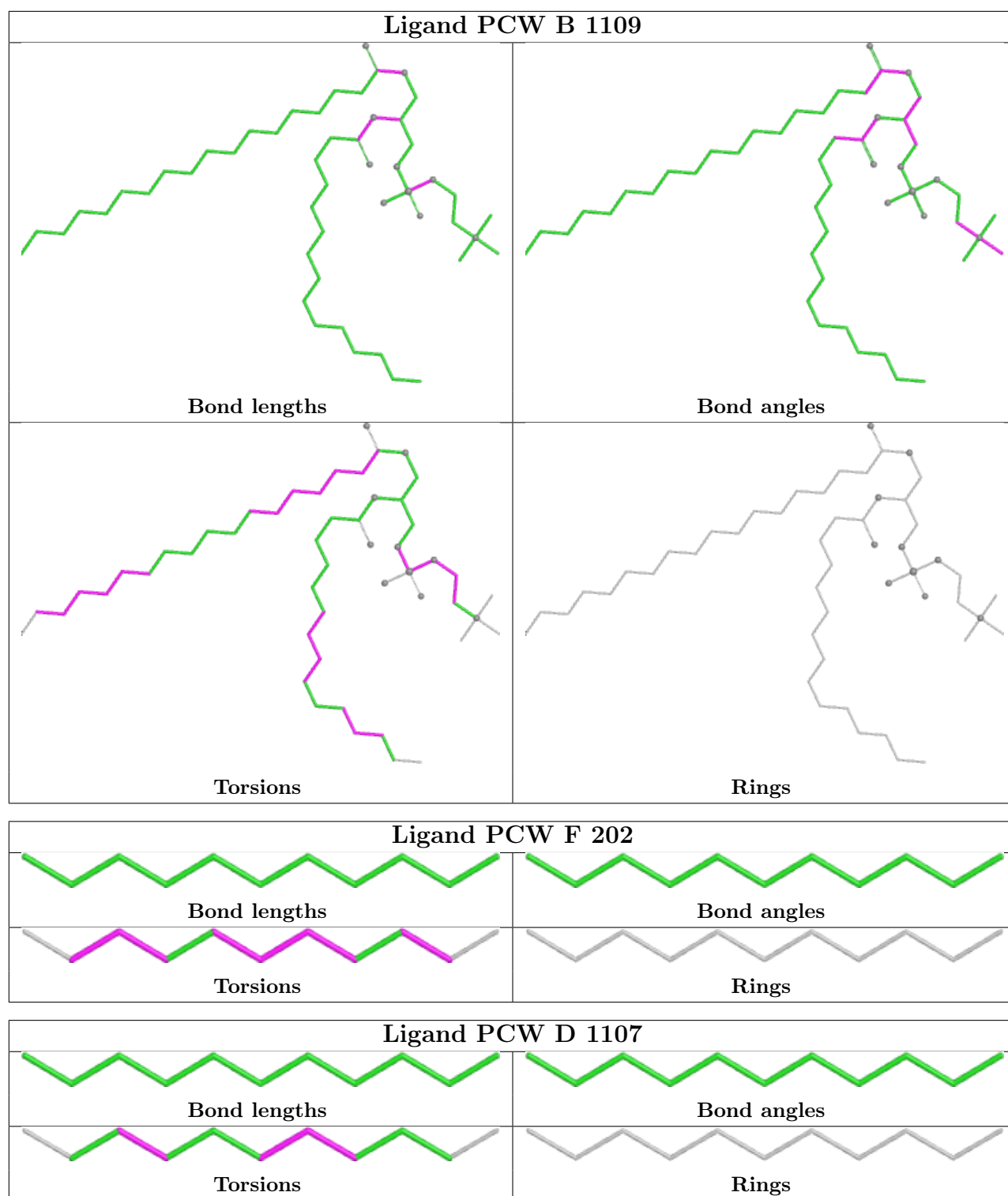


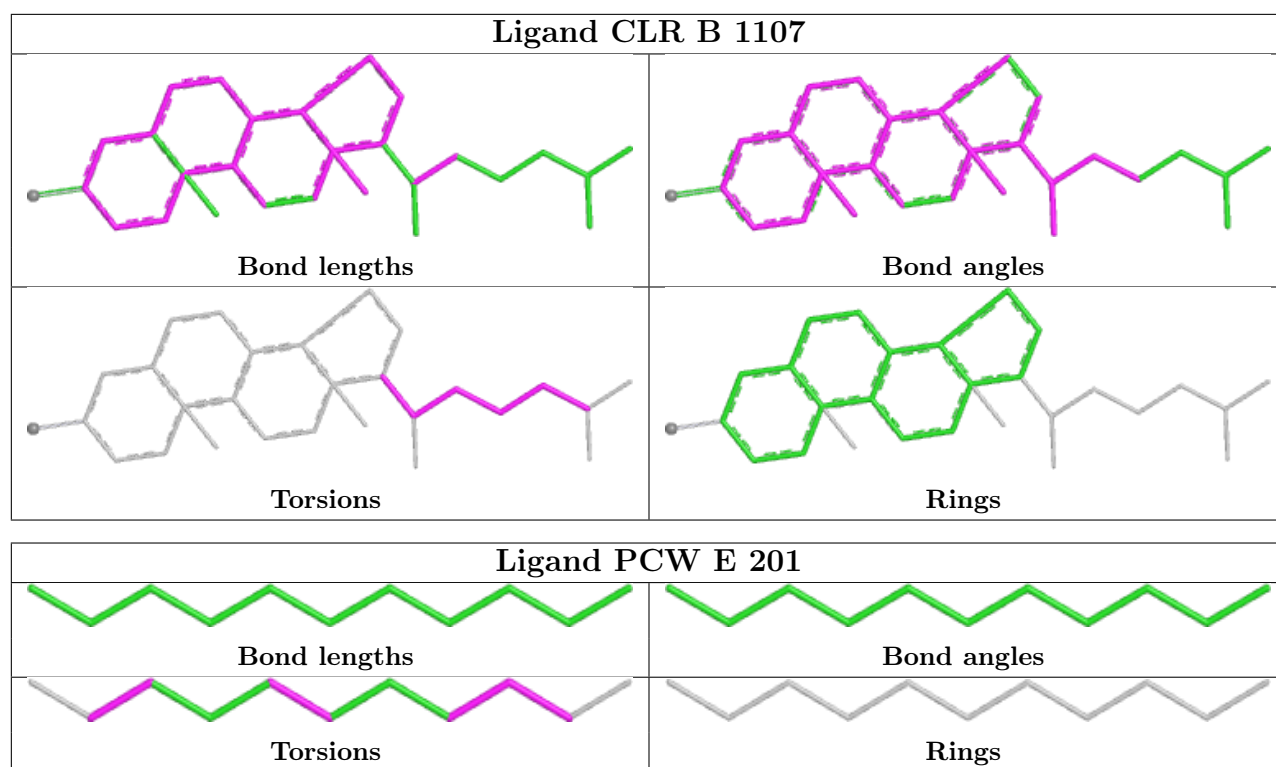












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

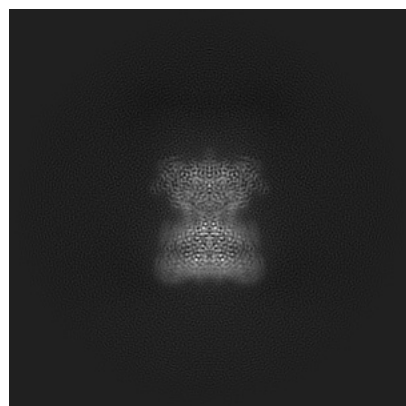
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40746. These allow visual inspection of the internal detail of the map and identification of artifacts.

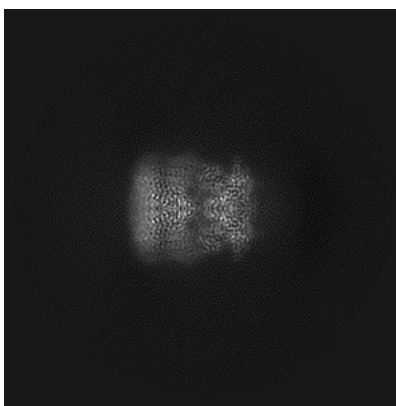
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

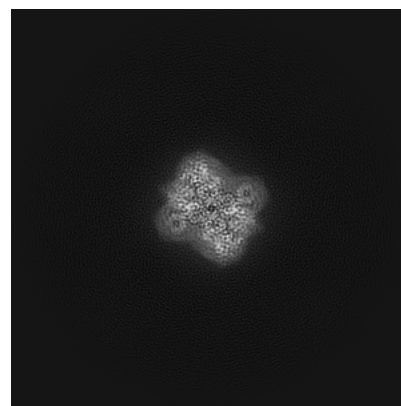
#### 6.1.1 Primary map



X

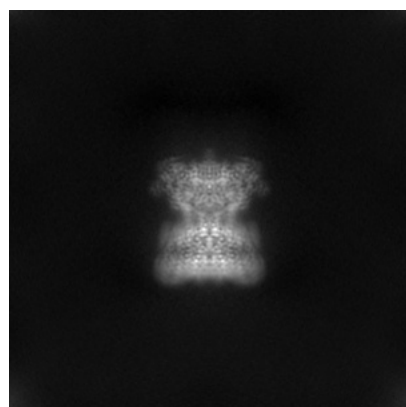


Y

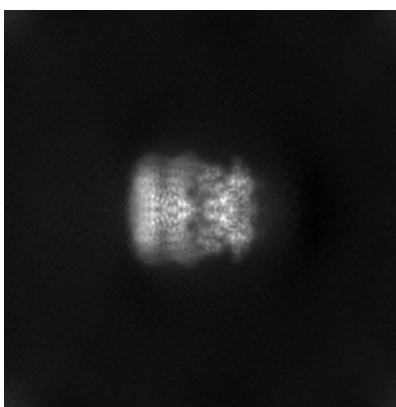


Z

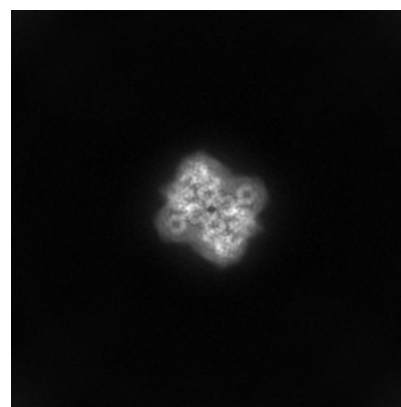
#### 6.1.2 Raw map



X



Y

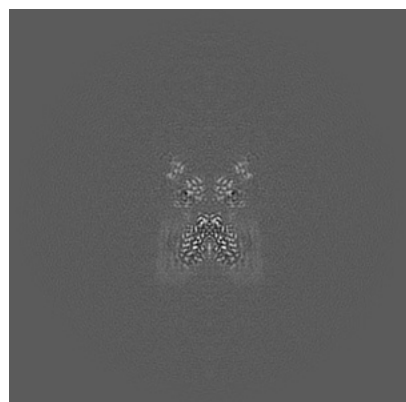


Z

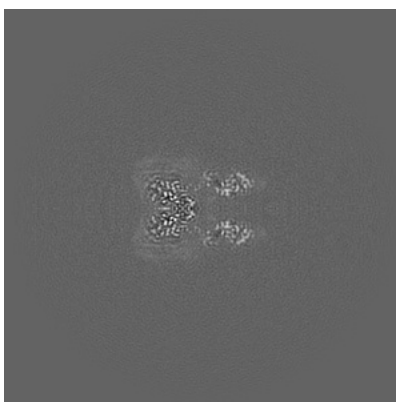
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

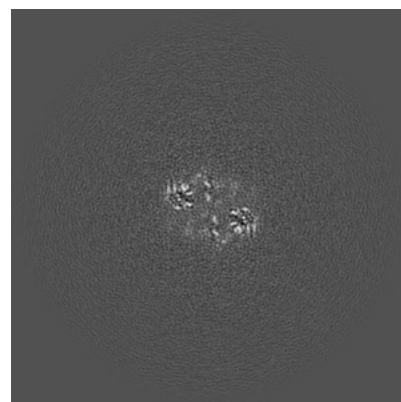
### 6.2.1 Primary map



X Index: 208

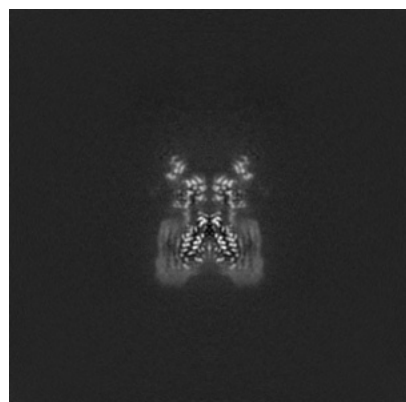


Y Index: 208

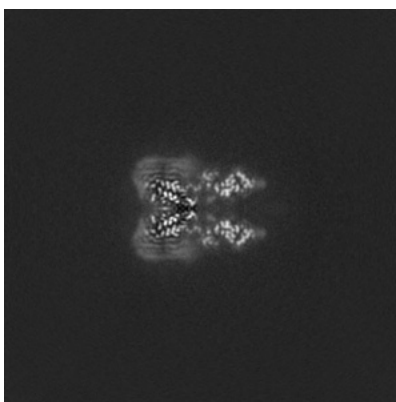


Z Index: 208

### 6.2.2 Raw map



X Index: 208



Y Index: 208

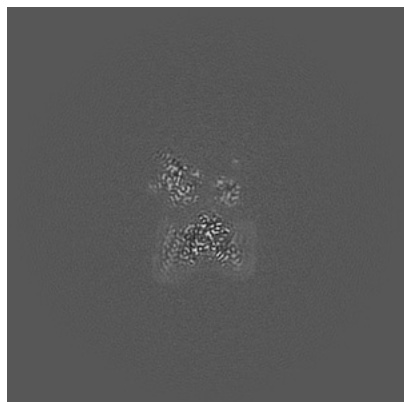


Z Index: 208

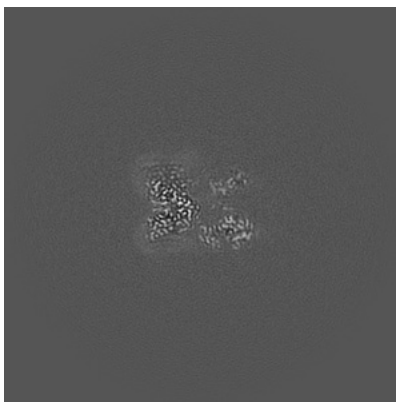
The images above show central slices of the map in three orthogonal directions.

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

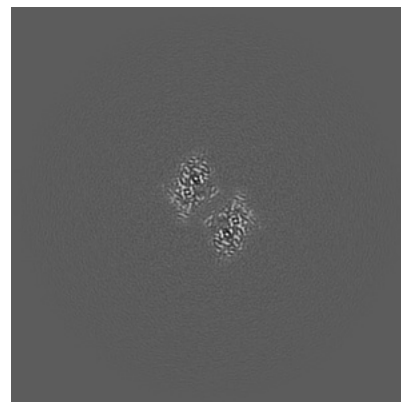
### 6.3.1 Primary map



X Index: 215

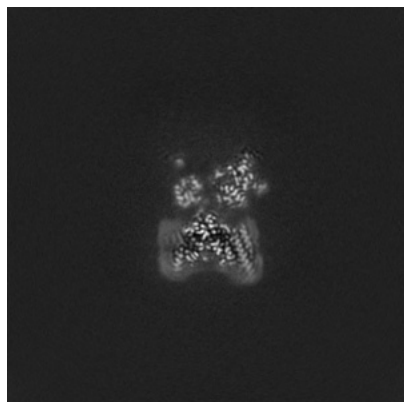


Y Index: 212

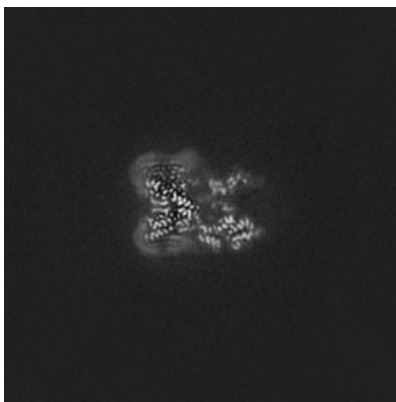


Z Index: 238

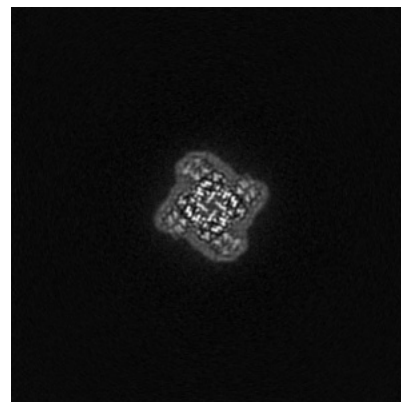
### 6.3.2 Raw map



X Index: 201



Y Index: 212

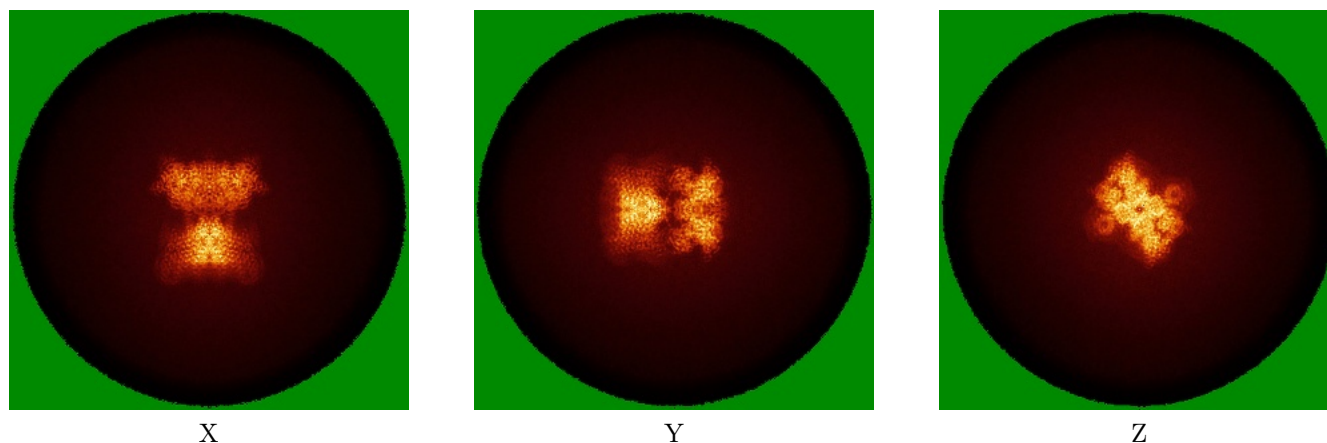


Z Index: 154

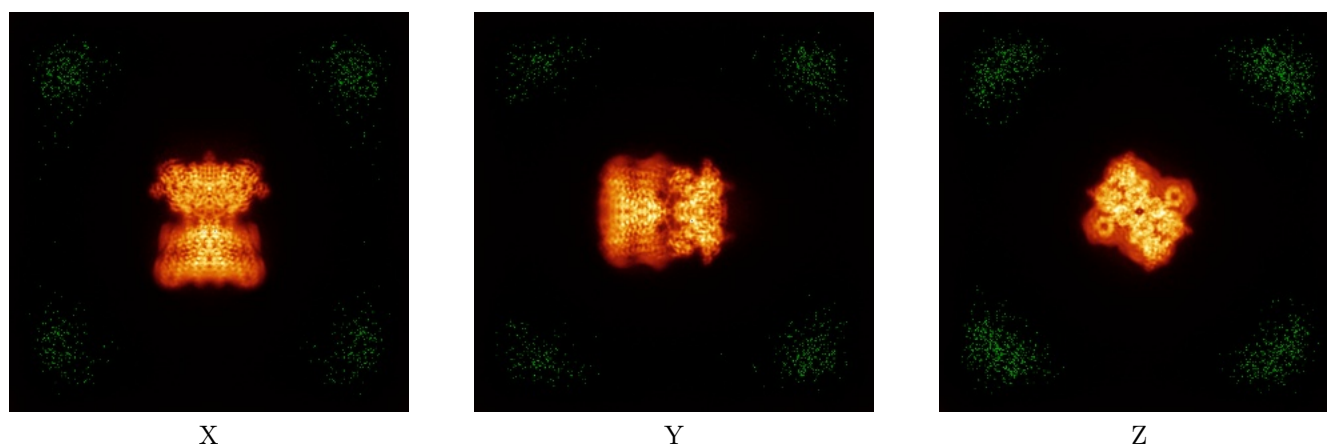
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

## 6.6 Mask visualisation [i](#)

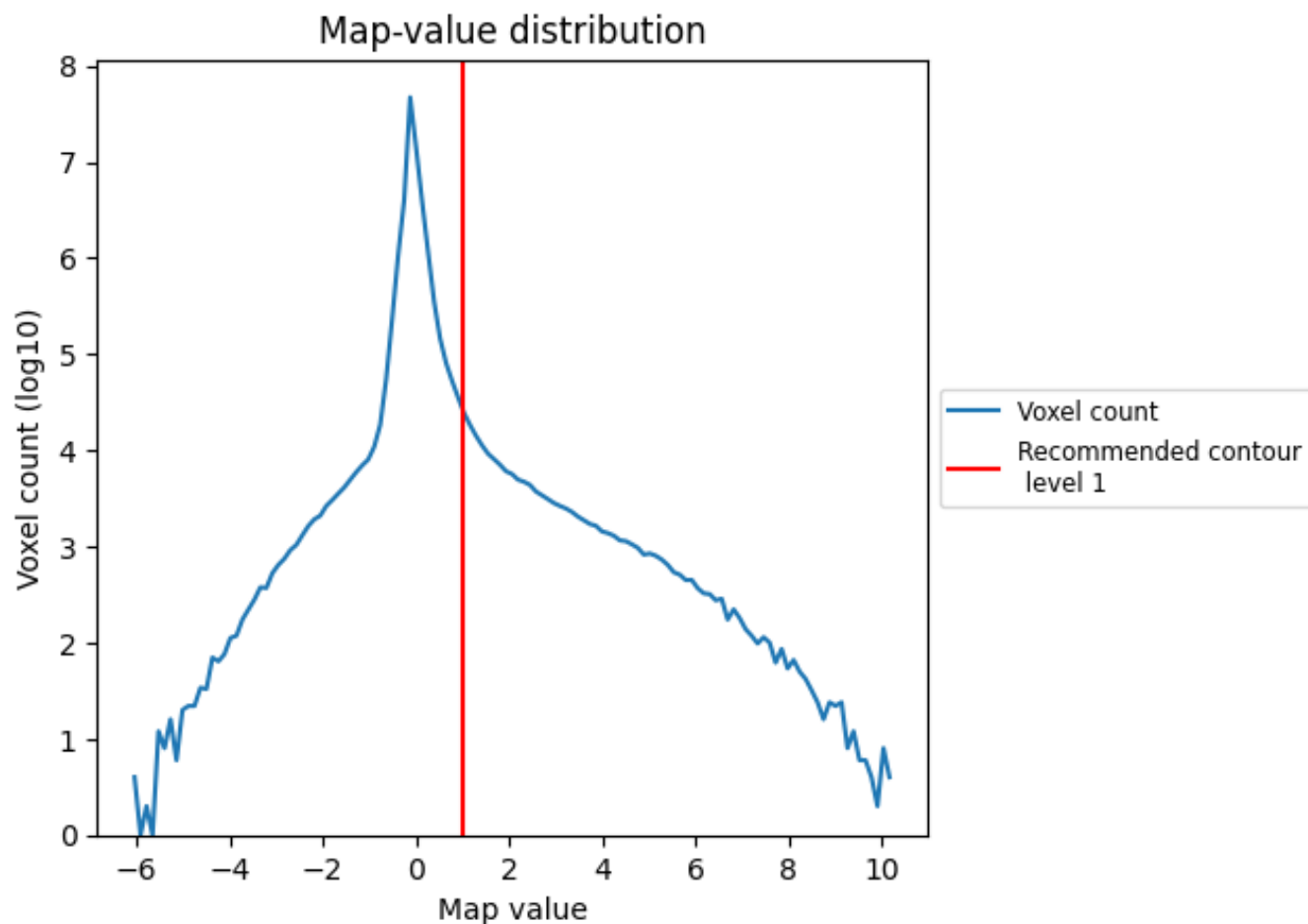
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

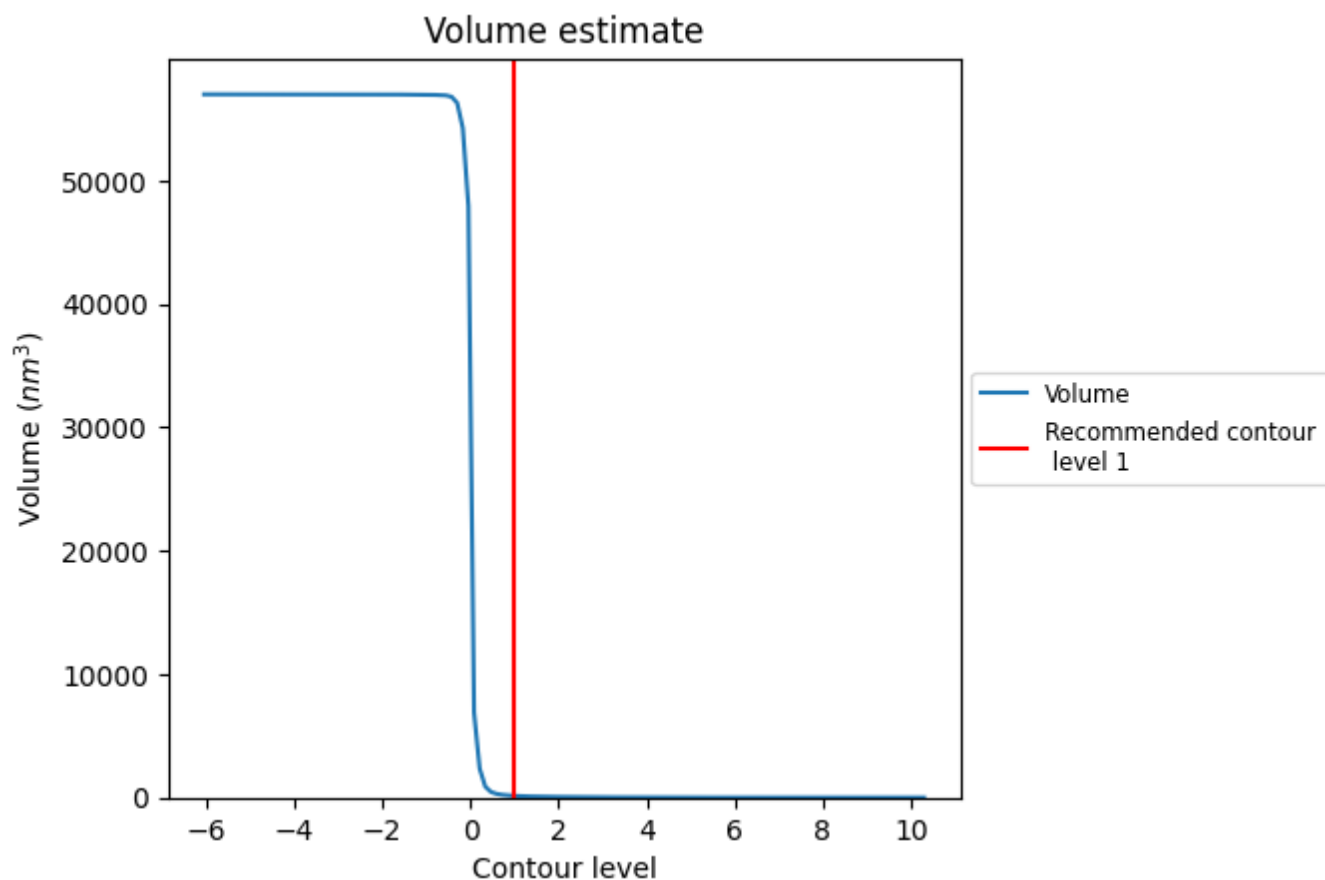
This section contains the results of statistical analysis of the map.

### 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.

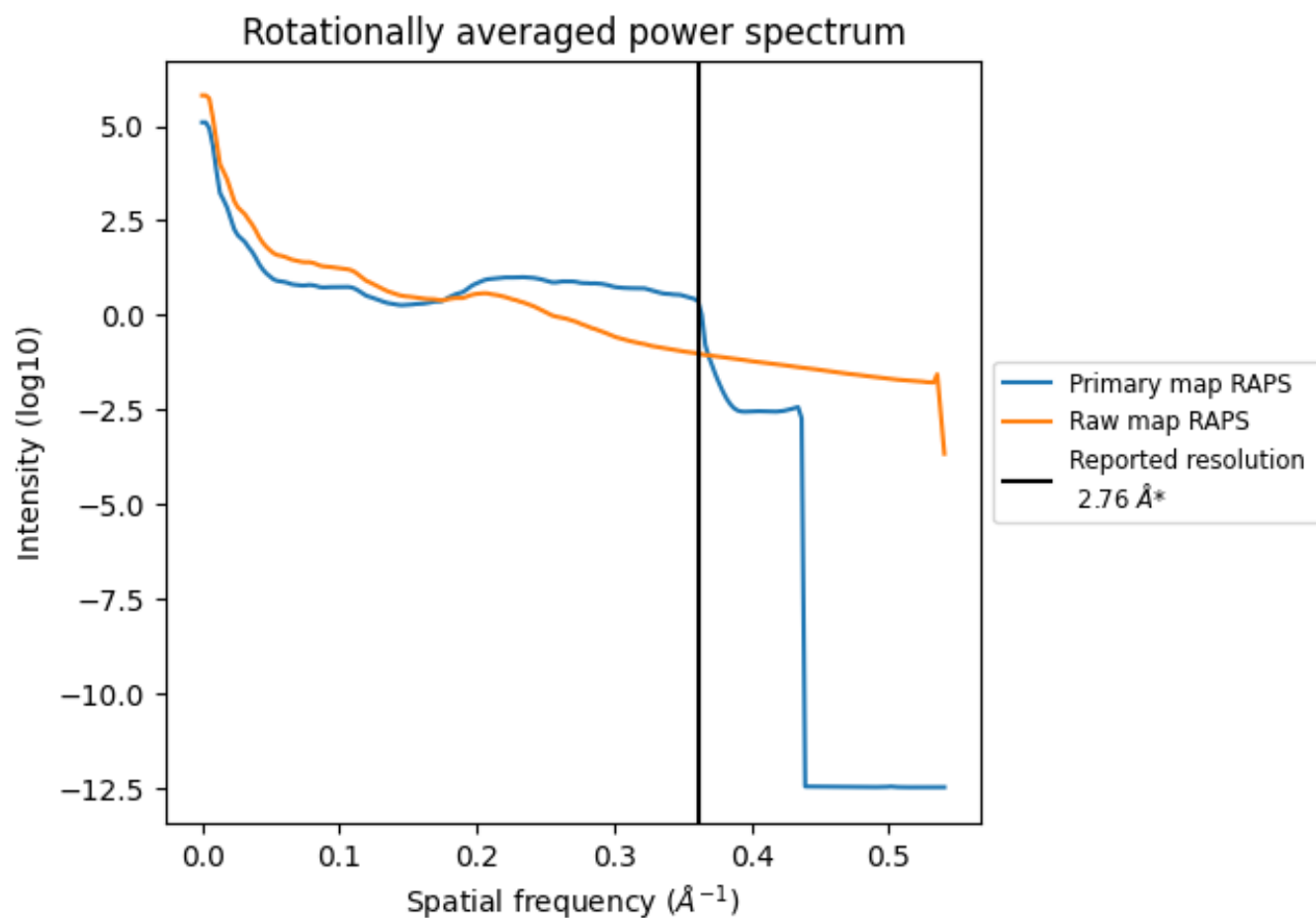
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136  $\text{nm}^3$ ; this corresponds to an approximate mass of 123 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 ⓘ

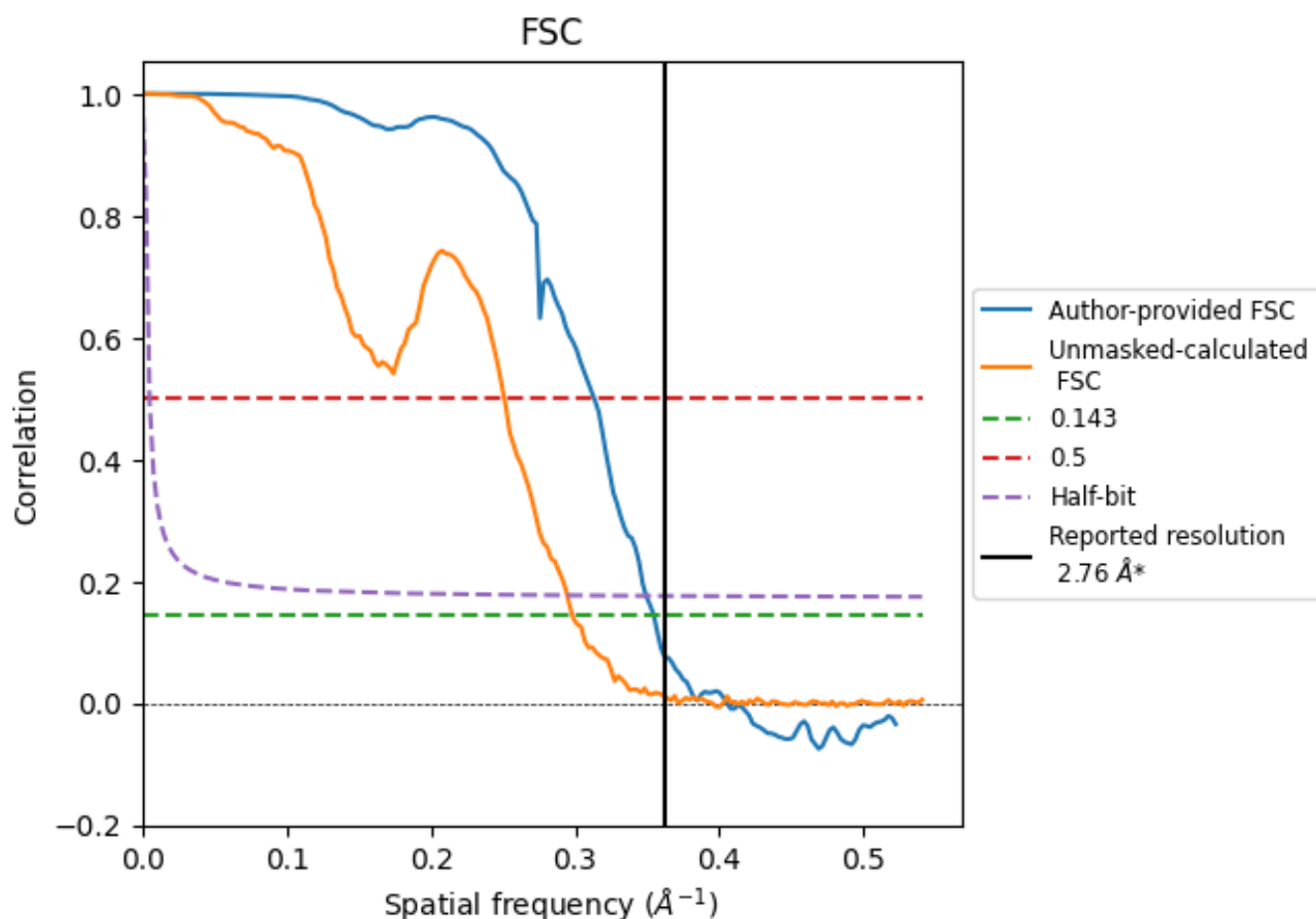


\*Reported resolution corresponds to spatial frequency of 0.362 Å<sup>-1</sup>

## 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 0.362  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.76                               | -    | -        |
| Author-provided FSC curve | 2.82                               | 3.19 | 2.86     |
| Unmasked-calculated*      | 3.35                               | 3.99 | 3.40     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.35 differs from the reported value 2.76 by more than 10 %

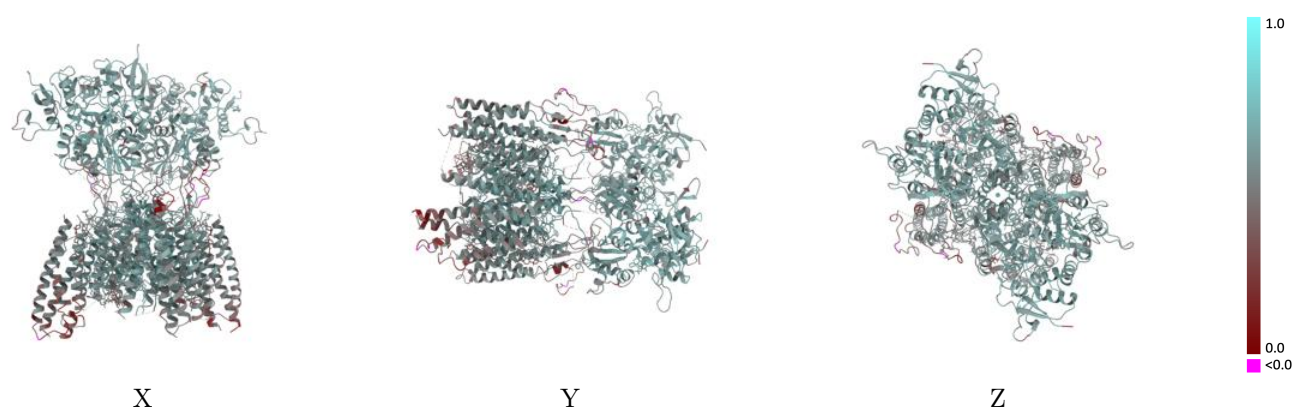
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40746 and PDB model 8SS7. Per-residue inclusion information can be found in section 3 on page 12.

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

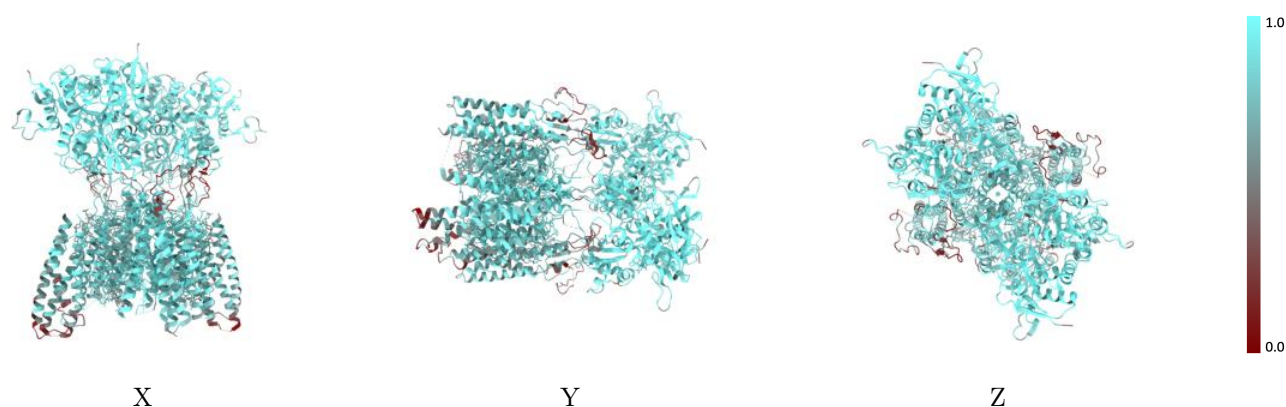
This section was not generated.

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



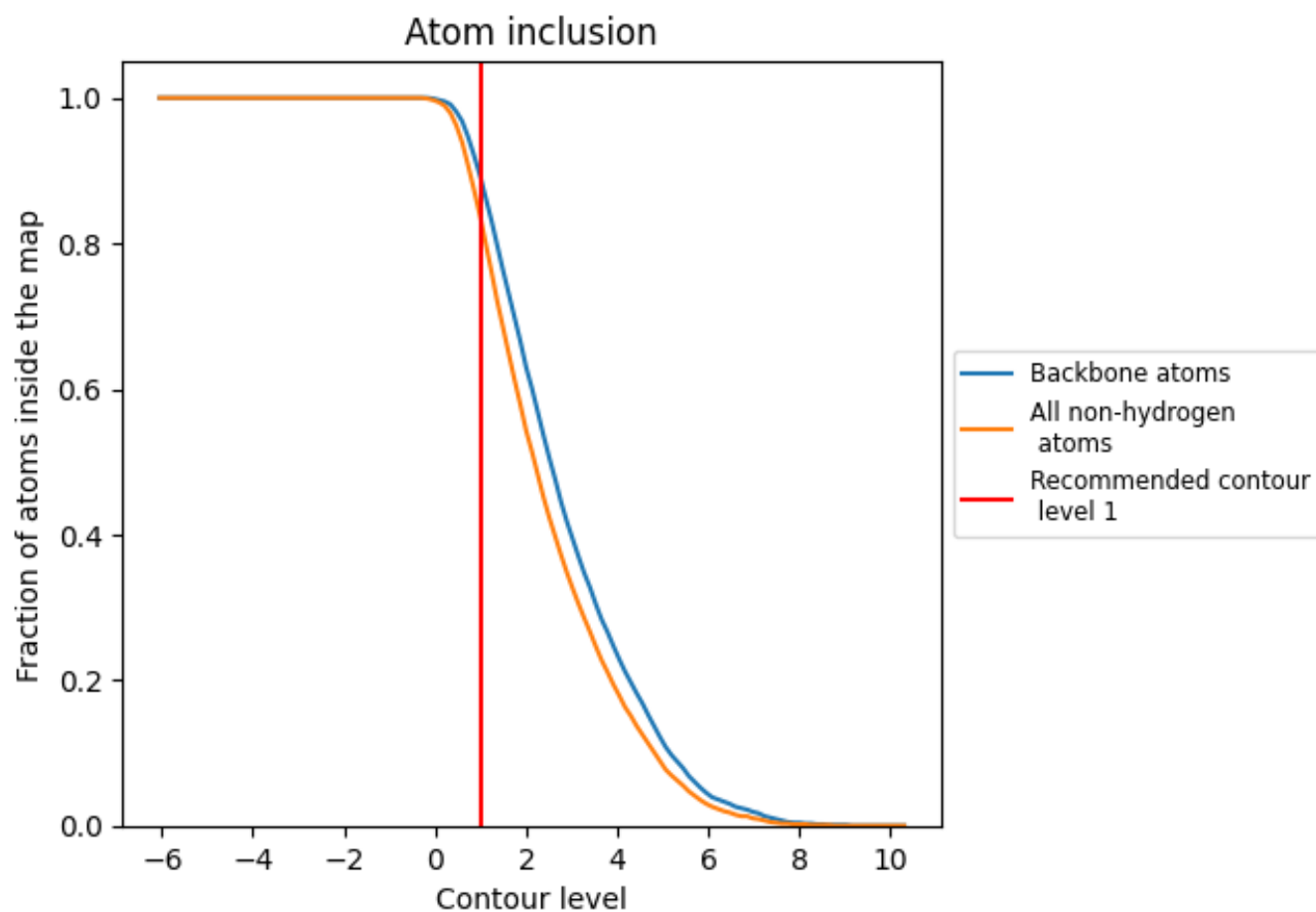
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 83% 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 (1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.8340 | <div><div></div></div> 0.5440 |
| A     | <div><div></div></div> 0.8300 | <div><div></div></div> 0.5450 |
| B     | <div><div></div></div> 0.8960 | <div><div></div></div> 0.5820 |
| C     | <div><div></div></div> 0.8310 | <div><div></div></div> 0.5440 |
| D     | <div><div></div></div> 0.8960 | <div><div></div></div> 0.5790 |
| E     | <div><div></div></div> 0.6800 | <div><div></div></div> 0.4450 |
| F     | <div><div></div></div> 0.6680 | <div><div></div></div> 0.4330 |

1.0

0.0

<0.0