



Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 03:52 PM EDT

PDB ID : 2MJS
BMRB ID : 21049
Title : Anoplin R5K T8W in DPC micelles
Authors : Uggerhoej, L.; Poulsen, T.J.; Wimmer, R.
Deposited on : 2014-01-16

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

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>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

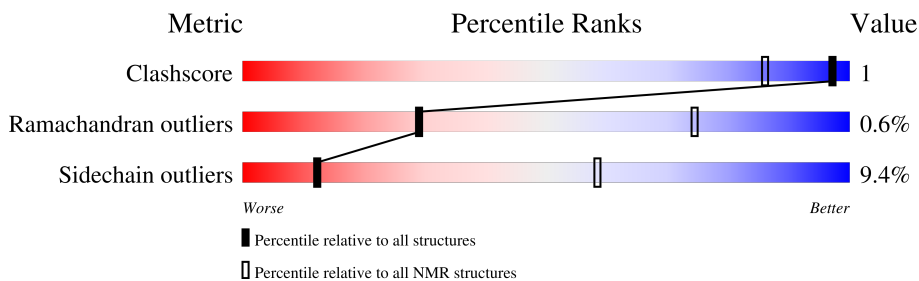
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment is 78%.

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 (#Entries) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 11 |  100% |

2 Ensemble composition and analysis

This entry contains 20 models.

Cyrange was unable to find well-defined residues.

Error message: Only domains with < 8 residues could be identified.

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

3 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 4163 atoms, of which 2581 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Anoplin.

| Mol | Chain | Residues | Atoms | | | | | Trace |
|-----|-------|----------|-------|----|-----|----|----|-------|
| | | | Total | C | H | N | O | |
| 1 | A | 11 | 197 | 61 | 111 | 15 | 10 | 1 |

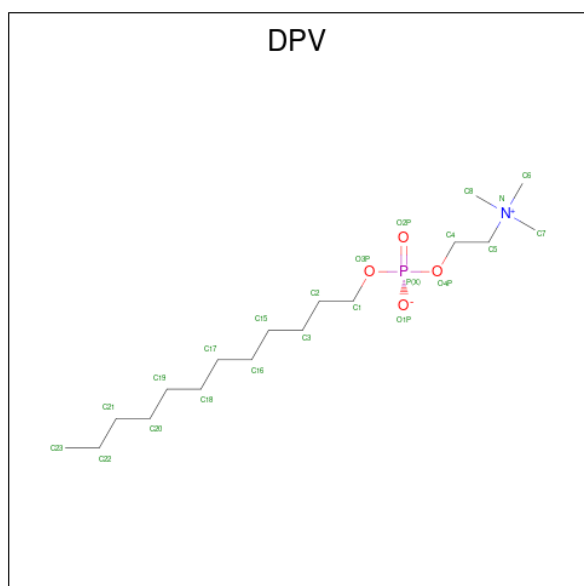
There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 5 | LYS | ARG | engineered mutation | UNP P0C005 |
| A | 8 | TRP | THR | engineered mutation | UNP P0C005 |
| A | 11 | NH2 | - | amidation | UNP P0C005 |

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

| Mol | Chain | Residues | Atoms | |
|-----|-------|----------|-------|---|
| 2 | A | 1 | Total | X |
| | | | 1 | 1 |

- Molecule 3 is dodecyl 2-(trimethylammonio)ethyl phosphate (three-letter code: DPV) (formula: $C_{17}H_{38}NO_4P$).



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| Mol | Chain | Residues | Atoms | | | | | |
|-----|-------|----------|-------|----|----|---|---|---|
| | | | Total | C | H | N | O | P |
| 3 | A | 1 | 61 | 17 | 38 | 1 | 4 | 1 |

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Anoplin

Chain A:  100%

There are no outlier residues in this chain.

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1


- Molecule 1: Anoplin

Chain A:  100%

There are no outlier residues in this chain.

4.2.2 Score per residue for model 2

- Molecule 1: Anoplin

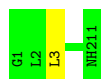
Chain A:  82% 18%



4.2.3 Score per residue for model 3

- Molecule 1: Anoplin

Chain A:  91% 9%



4.2.4 Score per residue for model 4

- Molecule 1: Anoplin

Chain A:  91% 9%



4.2.5 Score per residue for model 5

- Molecule 1: Anoplin

Chain A:  100%

There are no outlier residues in this chain.

4.2.6 Score per residue for model 6

- Molecule 1: Anoplin

Chain A:  100%

There are no outlier residues in this chain.

4.2.7 Score per residue for model 7

- Molecule 1: Anoplin

Chain A:  91% 9%



4.2.8 Score per residue for model 8

- Molecule 1: Anoplin

Chain A:  91% 9%



4.2.9 Score per residue for model 9

- Molecule 1: Anoplin

Chain A:  100%

There are no outlier residues in this chain.

4.2.10 Score per residue for model 10

- Molecule 1: Anoplin

Chain A:  100%

There are no outlier residues in this chain.

4.2.11 Score per residue for model 11

- Molecule 1: Anoplin

Chain A:  91% 9%



4.2.12 Score per residue for model 12

- Molecule 1: Anoplin

Chain A:  100%

There are no outlier residues in this chain.

4.2.13 Score per residue for model 13

- Molecule 1: Anoplin

Chain A:  91% 9%



4.2.14 Score per residue for model 14

- Molecule 1: Anoplin



4.2.15 Score per residue for model 15

- Molecule 1: Anoplin



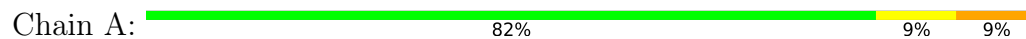
4.2.16 Score per residue for model 16

- Molecule 1: Anoplin



4.2.17 Score per residue for model 17

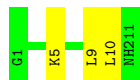
- Molecule 1: Anoplin



4.2.18 Score per residue for model 18

- Molecule 1: Anoplin

Chain A:  73% 27%



4.2.19 Score per residue for model 19


- Molecule 1: Anoplin

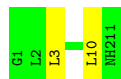
Chain A:  100%

There are no outlier residues in this chain.

4.2.20 Score per residue for model 20

- Molecule 1: Anoplin

Chain A:  82% 18%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---------------|--------------------|---------|
| CYANA | structure solution | |
| YASARA | refinement | |
| TALOS+ | structure solution | |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| Chemical shift file(s) | working_cs.cif |
|--|----------------|
| Number of chemical shift lists | 1 |
| Total number of shifts | 134 |
| Number of shifts mapped to atoms | 134 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 78% |

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, UNX, DPV

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 (average) 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 | 0.68±0.18 | 0±0/86 (0.1± 0.3%) | 0.66±0.12 | 0±0/113 (0.0± 0.2%) |
| All | All | 0.71 | 1/1720 (0.1%) | 0.67 | 1/2260 (0.0%) |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 8 | TRP | CB-CG | -8.47 | 1.34 | 1.50 | 17 | 1 |

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 8 | TRP | N-CA-CB | -5.78 | 100.19 | 110.60 | 17 | 1 |

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 3 | A | 1495 | 2470 | 2469 | 3±5 |
| All | All | 31640 | 51620 | 51568 | 54 |

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 1.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:113:DPV:C23 | 3:A:138:DPV:H23A | 1.60 | 1.25 | 19 | 1 |
| 3:A:118:DPV:H23B | 3:A:131:DPV:C23 | 1.47 | 1.35 | 19 | 1 |
| 3:A:119:DPV:H23B | 3:A:131:DPV:C23 | 1.47 | 1.35 | 20 | 1 |
| 3:A:119:DPV:C23 | 3:A:131:DPV:C23 | 1.42 | 1.95 | 20 | 1 |
| 3:A:118:DPV:C23 | 3:A:131:DPV:C23 | 1.29 | 2.11 | 19 | 2 |
| 3:A:145:DPV:H23B | 3:A:146:DPV:C23 | 1.23 | 1.63 | 16 | 1 |
| 3:A:113:DPV:C23 | 3:A:138:DPV:C23 | 1.17 | 2.21 | 19 | 2 |
| 3:A:118:DPV:H23B | 3:A:131:DPV:H23A | 1.12 | 1.17 | 19 | 1 |
| 3:A:119:DPV:H23B | 3:A:131:DPV:H23B | 1.07 | 1.08 | 20 | 1 |
| 3:A:113:DPV:H23B | 3:A:138:DPV:H23A | 1.04 | 1.23 | 19 | 1 |
| 3:A:113:DPV:H23A | 3:A:138:DPV:H23A | 1.02 | 1.19 | 19 | 1 |
| 3:A:158:DPV:C23 | 3:A:165:DPV:H23B | 1.02 | 1.84 | 16 | 1 |
| 3:A:119:DPV:C23 | 3:A:131:DPV:H23 | 1.00 | 1.84 | 20 | 1 |
| 3:A:119:DPV:C23 | 3:A:131:DPV:H23A | 0.99 | 1.88 | 20 | 1 |
| 3:A:145:DPV:H23B | 3:A:146:DPV:H23B | 0.97 | 1.35 | 16 | 1 |
| 3:A:118:DPV:H23B | 3:A:131:DPV:H23B | 0.95 | 1.32 | 19 | 1 |
| 3:A:119:DPV:H23A | 3:A:161:DPV:H23A | 0.95 | 1.36 | 20 | 1 |
| 3:A:119:DPV:H23 | 3:A:131:DPV:C23 | 0.92 | 1.93 | 20 | 1 |
| 3:A:119:DPV:H23B | 3:A:131:DPV:H23 | 0.90 | 1.31 | 20 | 1 |
| 3:A:118:DPV:C23 | 3:A:131:DPV:H23 | 0.89 | 1.94 | 19 | 1 |
| 3:A:158:DPV:H23A | 3:A:165:DPV:H23B | 0.85 | 1.46 | 16 | 1 |
| 3:A:145:DPV:C23 | 3:A:146:DPV:C23 | 0.84 | 2.53 | 16 | 1 |
| 3:A:113:DPV:C23 | 3:A:138:DPV:H23B | 0.84 | 2.02 | 7 | 1 |
| 3:A:113:DPV:H23 | 3:A:138:DPV:H23A | 0.83 | 1.48 | 19 | 1 |
| 3:A:106:DPV:C23 | 3:A:121:DPV:H23B | 0.78 | 2.09 | 8 | 1 |
| 3:A:113:DPV:H23B | 3:A:138:DPV:C23 | 0.78 | 1.94 | 19 | 1 |
| 3:A:119:DPV:H23A | 3:A:161:DPV:C23 | 0.76 | 2.09 | 20 | 1 |
| 3:A:158:DPV:H23 | 3:A:165:DPV:H23B | 0.75 | 1.58 | 16 | 1 |
| 3:A:113:DPV:C23 | 3:A:142:DPV:C23 | 0.73 | 2.66 | 7 | 1 |
| 3:A:119:DPV:H23 | 3:A:131:DPV:H23A | 0.69 | 1.57 | 20 | 1 |
| 3:A:106:DPV:H23 | 3:A:121:DPV:C23 | 0.69 | 2.18 | 8 | 1 |
| 3:A:158:DPV:C23 | 3:A:165:DPV:C23 | 0.67 | 2.70 | 16 | 1 |
| 3:A:119:DPV:C23 | 3:A:131:DPV:H23B | 0.66 | 1.88 | 20 | 1 |
| 3:A:106:DPV:H23 | 3:A:121:DPV:H23B | 0.65 | 1.66 | 8 | 1 |
| 3:A:113:DPV:H23B | 3:A:138:DPV:H23B | 0.64 | 1.66 | 7 | 1 |
| 3:A:119:DPV:C23 | 3:A:161:DPV:H23A | 0.63 | 2.21 | 20 | 1 |
| 3:A:113:DPV:H23A | 3:A:138:DPV:C23 | 0.63 | 2.05 | 19 | 1 |
| 3:A:118:DPV:H23 | 3:A:131:DPV:H23 | 0.62 | 1.69 | 19 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:119:DPV:C23 | 3:A:161:DPV:C23 | 0.61 | 2.78 | 20 | 1 |
| 3:A:118:DPV:H23A | 3:A:131:DPV:C23 | 0.61 | 2.26 | 10 | 1 |
| 3:A:145:DPV:H23B | 3:A:146:DPV:H23A | 0.60 | 1.66 | 16 | 1 |
| 3:A:118:DPV:C23 | 3:A:131:DPV:H23A | 0.60 | 1.98 | 19 | 1 |
| 3:A:113:DPV:H23 | 3:A:142:DPV:C23 | 0.59 | 2.27 | 7 | 1 |
| 3:A:113:DPV:H23 | 3:A:142:DPV:H23B | 0.55 | 1.77 | 7 | 1 |
| 3:A:158:DPV:H23 | 3:A:165:DPV:C23 | 0.51 | 2.33 | 16 | 1 |
| 3:A:145:DPV:C23 | 3:A:146:DPV:H23A | 0.49 | 2.31 | 16 | 1 |
| 3:A:118:DPV:C23 | 3:A:131:DPV:H23B | 0.49 | 2.09 | 19 | 1 |
| 3:A:113:DPV:C23 | 3:A:142:DPV:H23B | 0.46 | 2.36 | 7 | 1 |
| 3:A:113:DPV:H23A | 3:A:142:DPV:C23 | 0.46 | 2.39 | 7 | 1 |
| 3:A:119:DPV:C22 | 3:A:131:DPV:C23 | 0.44 | 2.90 | 20 | 1 |
| 3:A:158:DPV:H23A | 3:A:165:DPV:C23 | 0.43 | 2.32 | 16 | 1 |
| 3:A:113:DPV:H23B | 3:A:138:DPV:C22 | 0.42 | 2.42 | 19 | 1 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR 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 | 9/11 (82%) | 9±0 (97±5%) | 0±0 (2±4%) | 0±0 (1±2%) | 29 | 74 |
| All | All | 180/220 (82%) | 175 (97%) | 4 (2%) | 1 (1%) | 29 | 74 |

All 1 unique Ramachandran outliers are listed below.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 10 | LEU | 1 |

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR 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 | 9/9 (100%) | 8±1 (91±8%) | 1±1 (9±8%) | 12 | 58 |
| All | All | 180/180 (100%) | 163 (91%) | 17 (9%) | 12 | 58 |

All 6 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 3 | LEU | 6 |
| 1 | A | 5 | LYS | 3 |
| 1 | A | 9 | LEU | 3 |
| 1 | A | 2 | LEU | 2 |
| 1 | A | 10 | LEU | 2 |
| 1 | A | 8 | TRP | 1 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 1 is unknown - leaving 65 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | DPV | A | 134 | - | 22,22,22 | 1.04±0.02 | 0±0 (0±1%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | DPV | A | 148 | - | 22,22,22 | 1.03±0.03 | 0±1 (1±2%) |
| 3 | DPV | A | 150 | - | 22,22,22 | 1.03±0.03 | 0±0 (0±1%) |
| 3 | DPV | A | 121 | - | 22,22,22 | 1.05±0.06 | 0±0 (0±0%) |
| 3 | DPV | A | 122 | - | 22,22,22 | 1.04±0.04 | 0±0 (1±1%) |
| 3 | DPV | A | 138 | - | 22,22,22 | 1.03±0.03 | 0±0 (0±1%) |
| 3 | DPV | A | 140 | - | 22,22,22 | 1.03±0.04 | 0±0 (0±1%) |
| 3 | DPV | A | 119 | - | 22,22,22 | 1.03±0.04 | 0±0 (0±1%) |
| 3 | DPV | A | 141 | - | 22,22,22 | 1.04±0.04 | 0±1 (1±2%) |
| 3 | DPV | A | 145 | - | 22,22,22 | 1.02±0.03 | 0±0 (0±1%) |
| 3 | DPV | A | 129 | - | 22,22,22 | 1.04±0.03 | 0±1 (1±2%) |
| 3 | DPV | A | 128 | - | 22,22,22 | 1.04±0.03 | 0±0 (0±2%) |
| 3 | DPV | A | 103 | - | 22,22,22 | 1.04±0.03 | 0±1 (1±2%) |
| 3 | DPV | A | 112 | - | 22,22,22 | 1.04±0.02 | 0±0 (1±2%) |
| 3 | DPV | A | 120 | - | 22,22,22 | 1.03±0.04 | 0±0 (0±1%) |
| 3 | DPV | A | 113 | - | 22,22,22 | 1.04±0.03 | 0±0 (0±1%) |
| 3 | DPV | A | 159 | - | 22,22,22 | 1.05±0.04 | 0±1 (0±2%) |
| 3 | DPV | A | 153 | - | 22,22,22 | 1.04±0.03 | 0±1 (1±2%) |
| 3 | DPV | A | 109 | - | 22,22,22 | 1.05±0.03 | 0±0 (1±1%) |
| 3 | DPV | A | 158 | - | 22,22,22 | 1.02±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 156 | - | 22,22,22 | 1.04±0.02 | 0±0 (1±2%) |
| 3 | DPV | A | 102 | - | 22,22,22 | 1.02±0.02 | 0±1 (1±2%) |
| 3 | DPV | A | 135 | - | 22,22,22 | 1.03±0.04 | 0±1 (1±2%) |
| 3 | DPV | A | 152 | - | 22,22,22 | 1.02±0.05 | 0±0 (0±1%) |
| 3 | DPV | A | 164 | - | 22,22,22 | 1.04±0.03 | 0±0 (0±1%) |
| 3 | DPV | A | 127 | - | 22,22,22 | 1.04±0.03 | 0±1 (1±2%) |
| 3 | DPV | A | 105 | - | 22,22,22 | 1.04±0.02 | 0±1 (1±2%) |
| 3 | DPV | A | 124 | - | 22,22,22 | 1.05±0.03 | 1±1 (2±3%) |
| 3 | DPV | A | 125 | - | 22,22,22 | 1.05±0.03 | 0±0 (2±2%) |
| 3 | DPV | A | 104 | - | 22,22,22 | 1.04±0.03 | 0±0 (0±1%) |
| 3 | DPV | A | 149 | - | 22,22,22 | 1.04±0.02 | 0±1 (1±2%) |
| 3 | DPV | A | 132 | - | 22,22,22 | 1.04±0.03 | 0±1 (1±2%) |
| 3 | DPV | A | 115 | - | 22,22,22 | 1.05±0.03 | 0±0 (1±2%) |
| 3 | DPV | A | 131 | - | 22,22,22 | 1.04±0.03 | 0±0 (1±2%) |
| 3 | DPV | A | 155 | - | 22,22,22 | 1.04±0.02 | 0±0 (0±2%) |
| 3 | DPV | A | 163 | - | 22,22,22 | 1.03±0.04 | 0±1 (1±3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | DPV | A | 139 | - | 22,22,22 | 1.05±0.03 | 1±1 (2±3%) |
| 3 | DPV | A | 114 | - | 22,22,22 | 1.06±0.03 | 0±1 (2±2%) |
| 3 | DPV | A | 147 | - | 22,22,22 | 1.03±0.03 | 0±0 (1±1%) |
| 3 | DPV | A | 151 | - | 22,22,22 | 1.03±0.03 | 0±1 (1±2%) |
| 3 | DPV | A | 118 | - | 22,22,22 | 1.03±0.03 | 0±0 (1±1%) |
| 3 | DPV | A | 133 | - | 22,22,22 | 1.03±0.02 | 0±0 (0±1%) |
| 3 | DPV | A | 142 | - | 22,22,22 | 1.02±0.04 | 0±0 (0±1%) |
| 3 | DPV | A | 107 | - | 22,22,22 | 1.04±0.02 | 0±0 (0±1%) |
| 3 | DPV | A | 116 | - | 22,22,22 | 1.02±0.03 | 0±0 (1±1%) |
| 3 | DPV | A | 166 | - | 22,22,22 | 1.05±0.04 | 0±1 (1±3%) |
| 3 | DPV | A | 123 | - | 22,22,22 | 1.05±0.03 | 0±1 (2±3%) |
| 3 | DPV | A | 137 | - | 22,22,22 | 1.04±0.02 | 0±1 (2±2%) |
| 3 | DPV | A | 136 | - | 22,22,22 | 1.02±0.03 | 0±0 (0±1%) |
| 3 | DPV | A | 117 | - | 22,22,22 | 1.03±0.03 | 0±1 (0±2%) |
| 3 | DPV | A | 146 | - | 22,22,22 | 1.03±0.03 | 0±1 (1±2%) |
| 3 | DPV | A | 126 | - | 22,22,22 | 1.04±0.03 | 0±1 (0±2%) |
| 3 | DPV | A | 110 | - | 22,22,22 | 1.04±0.03 | 0±0 (0±2%) |
| 3 | DPV | A | 162 | - | 22,22,22 | 1.04±0.03 | 0±1 (1±2%) |
| 3 | DPV | A | 161 | - | 22,22,22 | 1.03±0.03 | 0±1 (1±2%) |
| 3 | DPV | A | 106 | - | 22,22,22 | 1.03±0.04 | 0±1 (0±2%) |
| 3 | DPV | A | 160 | - | 22,22,22 | 1.03±0.03 | 0±1 (2±3%) |
| 3 | DPV | A | 143 | - | 22,22,22 | 1.03±0.02 | 0±0 (0±1%) |
| 3 | DPV | A | 108 | - | 22,22,22 | 1.04±0.03 | 0±1 (1±2%) |
| 3 | DPV | A | 165 | - | 22,22,22 | 1.04±0.03 | 0±0 (0±1%) |
| 3 | DPV | A | 154 | - | 22,22,22 | 1.04±0.03 | 0±1 (1±2%) |
| 3 | DPV | A | 111 | - | 22,22,22 | 1.03±0.03 | 0±1 (0±2%) |
| 3 | DPV | A | 157 | - | 22,22,22 | 1.05±0.02 | 0±0 (1±1%) |
| 3 | DPV | A | 144 | - | 22,22,22 | 1.03±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 130 | - | 22,22,22 | 1.03±0.03 | 0±0 (1±1%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of

the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | DPV | A | 134 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 148 | - | 26,27,27 | 0.61±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 150 | - | 26,27,27 | 0.62±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 121 | - | 26,27,27 | 0.62±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 122 | - | 26,27,27 | 0.62±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 138 | - | 26,27,27 | 0.62±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 140 | - | 26,27,27 | 0.60±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 119 | - | 26,27,27 | 0.62±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 141 | - | 26,27,27 | 0.59±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 145 | - | 26,27,27 | 0.63±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 129 | - | 26,27,27 | 0.61±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 128 | - | 26,27,27 | 0.60±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 103 | - | 26,27,27 | 0.61±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 112 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 120 | - | 26,27,27 | 0.61±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 113 | - | 26,27,27 | 0.60±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 159 | - | 26,27,27 | 0.60±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 153 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 109 | - | 26,27,27 | 0.60±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 158 | - | 26,27,27 | 0.62±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 156 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 102 | - | 26,27,27 | 0.61±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 135 | - | 26,27,27 | 0.61±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 152 | - | 26,27,27 | 0.63±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 164 | - | 26,27,27 | 0.61±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 127 | - | 26,27,27 | 0.61±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 105 | - | 26,27,27 | 0.61±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 124 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 125 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 104 | - | 26,27,27 | 0.60±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 149 | - | 26,27,27 | 0.61±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 132 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 115 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 131 | - | 26,27,27 | 0.62±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 155 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 163 | - | 26,27,27 | 0.62±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 139 | - | 26,27,27 | 0.60±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 114 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 147 | - | 26,27,27 | 0.60±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 151 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 118 | - | 26,27,27 | 0.61±0.03 | 0±0 (0±0%) |

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | DPV | A | 133 | - | 26,27,27 | 0.61±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 142 | - | 26,27,27 | 0.62±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 107 | - | 26,27,27 | 0.60±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 116 | - | 26,27,27 | 0.61±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 166 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 123 | - | 26,27,27 | 0.59±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 137 | - | 26,27,27 | 0.60±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 136 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 117 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 146 | - | 26,27,27 | 0.61±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 126 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 110 | - | 26,27,27 | 0.59±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 162 | - | 26,27,27 | 0.61±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 161 | - | 26,27,27 | 0.62±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 106 | - | 26,27,27 | 0.61±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 160 | - | 26,27,27 | 0.60±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 143 | - | 26,27,27 | 0.61±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 108 | - | 26,27,27 | 0.60±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 165 | - | 26,27,27 | 0.59±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 154 | - | 26,27,27 | 0.60±0.03 | 0±0 (0±0%) |
| 3 | DPV | A | 111 | - | 26,27,27 | 0.61±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 157 | - | 26,27,27 | 0.60±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 144 | - | 26,27,27 | 0.61±0.02 | 0±0 (0±0%) |
| 3 | DPV | A | 130 | - | 26,27,27 | 0.62±0.02 | 0±0 (0±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 |
|-----|------|-------|-----|------|---------|--------------|-------|
| 3 | DPV | A | 134 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 128 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 150 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 156 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 164 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 104 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 102 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 105 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 158 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 112 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 155 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 123 | - | - | 0±0,22,22,22 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|-------|
| 3 | DPV | A | 152 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 122 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 151 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 143 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 111 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 127 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 115 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 110 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 137 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 135 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 142 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 148 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 132 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 153 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 120 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 109 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 106 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 146 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 159 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 162 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 166 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 136 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 113 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 138 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 118 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 139 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 130 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 125 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 163 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 133 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 157 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 124 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 114 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 141 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 144 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 126 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 129 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 165 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 103 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 117 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 161 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 147 | - | - | 0±0,22,22,22 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|-------|
| 3 | DPV | A | 160 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 119 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 149 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 107 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 140 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 145 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 121 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 154 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 108 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 116 | - | - | 0±0,22,22,22 | - |
| 3 | DPV | A | 131 | - | - | 0±0,22,22,22 | - |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 109 | DPV | C5-C4 | 2.38 | 1.58 | 1.51 | 19 | 3 |
| 3 | A | 139 | DPV | C5-C4 | 2.36 | 1.58 | 1.51 | 3 | 8 |
| 3 | A | 119 | DPV | C23-C22 | 2.29 | 1.68 | 1.49 | 20 | 1 |
| 3 | A | 127 | DPV | C5-C4 | 2.29 | 1.58 | 1.51 | 9 | 3 |
| 3 | A | 148 | DPV | C5-C4 | 2.29 | 1.58 | 1.51 | 15 | 5 |
| 3 | A | 131 | DPV | C5-C4 | 2.28 | 1.58 | 1.51 | 13 | 5 |
| 3 | A | 157 | DPV | C5-C4 | 2.28 | 1.58 | 1.51 | 1 | 5 |
| 3 | A | 122 | DPV | C5-C4 | 2.27 | 1.58 | 1.51 | 15 | 4 |
| 3 | A | 129 | DPV | C5-C4 | 2.26 | 1.58 | 1.51 | 20 | 5 |
| 3 | A | 120 | DPV | C5-N | 2.23 | 1.58 | 1.51 | 20 | 2 |
| 3 | A | 123 | DPV | C5-C4 | 2.22 | 1.58 | 1.51 | 8 | 6 |
| 3 | A | 126 | DPV | C5-C4 | 2.21 | 1.58 | 1.51 | 12 | 3 |
| 3 | A | 113 | DPV | C5-C4 | 2.21 | 1.58 | 1.51 | 5 | 2 |
| 3 | A | 162 | DPV | C5-C4 | 2.21 | 1.58 | 1.51 | 18 | 3 |
| 3 | A | 102 | DPV | C5-C4 | 2.21 | 1.58 | 1.51 | 13 | 4 |
| 3 | A | 163 | DPV | C5-C4 | 2.20 | 1.58 | 1.51 | 8 | 6 |
| 3 | A | 151 | DPV | C5-C4 | 2.20 | 1.58 | 1.51 | 5 | 4 |
| 3 | A | 139 | DPV | C5-N | 2.19 | 1.58 | 1.51 | 11 | 4 |
| 3 | A | 143 | DPV | C5-C4 | 2.18 | 1.58 | 1.51 | 18 | 3 |
| 3 | A | 146 | DPV | C5-C4 | 2.18 | 1.58 | 1.51 | 17 | 6 |
| 3 | A | 141 | DPV | C5-C4 | 2.18 | 1.58 | 1.51 | 2 | 3 |
| 3 | A | 159 | DPV | C5-C4 | 2.18 | 1.58 | 1.51 | 14 | 3 |
| 3 | A | 166 | DPV | C5-N | 2.18 | 1.58 | 1.51 | 8 | 2 |
| 3 | A | 104 | DPV | C5-C4 | 2.18 | 1.58 | 1.51 | 14 | 3 |
| 3 | A | 111 | DPV | C5-N | 2.18 | 1.58 | 1.51 | 20 | 2 |
| 3 | A | 108 | DPV | C5-C4 | 2.16 | 1.58 | 1.51 | 18 | 5 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 115 | DPV | C5-C4 | 2.16 | 1.58 | 1.51 | 7 | 4 |
| 3 | A | 141 | DPV | C5-N | 2.16 | 1.58 | 1.51 | 3 | 2 |
| 3 | A | 148 | DPV | C5-N | 2.16 | 1.58 | 1.51 | 13 | 2 |
| 3 | A | 105 | DPV | C5-N | 2.16 | 1.58 | 1.51 | 1 | 4 |
| 3 | A | 105 | DPV | C5-C4 | 2.16 | 1.58 | 1.51 | 7 | 3 |
| 3 | A | 121 | DPV | C5-C4 | 2.16 | 1.58 | 1.51 | 8 | 1 |
| 3 | A | 161 | DPV | C5-C4 | 2.16 | 1.58 | 1.51 | 17 | 2 |
| 3 | A | 140 | DPV | C5-N | 2.15 | 1.58 | 1.51 | 1 | 1 |
| 3 | A | 128 | DPV | C5-C4 | 2.15 | 1.58 | 1.51 | 16 | 2 |
| 3 | A | 103 | DPV | C5-C4 | 2.15 | 1.58 | 1.51 | 12 | 6 |
| 3 | A | 106 | DPV | C5-C4 | 2.15 | 1.58 | 1.51 | 9 | 2 |
| 3 | A | 135 | DPV | C5-C4 | 2.15 | 1.58 | 1.51 | 5 | 3 |
| 3 | A | 132 | DPV | C5-C4 | 2.14 | 1.58 | 1.51 | 2 | 4 |
| 3 | A | 160 | DPV | C5-C4 | 2.14 | 1.58 | 1.51 | 17 | 5 |
| 3 | A | 104 | DPV | C5-N | 2.14 | 1.58 | 1.51 | 5 | 1 |
| 3 | A | 154 | DPV | C5-C4 | 2.14 | 1.58 | 1.51 | 7 | 5 |
| 3 | A | 138 | DPV | C5-C4 | 2.14 | 1.58 | 1.51 | 15 | 3 |
| 3 | A | 137 | DPV | C5-N | 2.13 | 1.58 | 1.51 | 13 | 4 |
| 3 | A | 155 | DPV | C5-C4 | 2.13 | 1.58 | 1.51 | 7 | 2 |
| 3 | A | 112 | DPV | C5-N | 2.13 | 1.58 | 1.51 | 6 | 1 |
| 3 | A | 116 | DPV | C5-N | 2.13 | 1.58 | 1.51 | 14 | 1 |
| 3 | A | 166 | DPV | C5-C4 | 2.12 | 1.58 | 1.51 | 12 | 6 |
| 3 | A | 124 | DPV | C5-N | 2.12 | 1.58 | 1.51 | 3 | 5 |
| 3 | A | 156 | DPV | C5-C4 | 2.12 | 1.58 | 1.51 | 16 | 5 |
| 3 | A | 122 | DPV | C5-N | 2.12 | 1.58 | 1.51 | 20 | 1 |
| 3 | A | 136 | DPV | C5-C4 | 2.11 | 1.57 | 1.51 | 10 | 2 |
| 3 | A | 106 | DPV | C5-N | 2.11 | 1.58 | 1.51 | 1 | 2 |
| 3 | A | 125 | DPV | C5-C4 | 2.11 | 1.57 | 1.51 | 7 | 7 |
| 3 | A | 159 | DPV | C5-N | 2.11 | 1.58 | 1.51 | 17 | 1 |
| 3 | A | 116 | DPV | C5-C4 | 2.11 | 1.57 | 1.51 | 12 | 4 |
| 3 | A | 130 | DPV | C5-N | 2.11 | 1.58 | 1.51 | 10 | 3 |
| 3 | A | 137 | DPV | C5-C4 | 2.10 | 1.57 | 1.51 | 14 | 5 |
| 3 | A | 114 | DPV | C5-C4 | 2.10 | 1.57 | 1.51 | 12 | 5 |
| 3 | A | 130 | DPV | C5-C4 | 2.10 | 1.57 | 1.51 | 8 | 2 |
| 3 | A | 114 | DPV | C5-N | 2.10 | 1.58 | 1.51 | 20 | 4 |
| 3 | A | 162 | DPV | C5-N | 2.10 | 1.58 | 1.51 | 15 | 3 |
| 3 | A | 118 | DPV | C5-C4 | 2.10 | 1.57 | 1.51 | 11 | 3 |
| 3 | A | 147 | DPV | C5-C4 | 2.10 | 1.57 | 1.51 | 6 | 4 |
| 3 | A | 111 | DPV | C5-C4 | 2.09 | 1.57 | 1.51 | 2 | 2 |
| 3 | A | 127 | DPV | C5-N | 2.09 | 1.58 | 1.51 | 5 | 2 |
| 3 | A | 124 | DPV | C5-C4 | 2.09 | 1.57 | 1.51 | 18 | 6 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 153 | DPV | C5-N | 2.09 | 1.58 | 1.51 | 13 | 1 |
| 3 | A | 160 | DPV | C5-N | 2.09 | 1.58 | 1.51 | 12 | 4 |
| 3 | A | 133 | DPV | C5-C4 | 2.09 | 1.57 | 1.51 | 17 | 3 |
| 3 | A | 112 | DPV | C5-C4 | 2.09 | 1.57 | 1.51 | 1 | 5 |
| 3 | A | 153 | DPV | C5-C4 | 2.09 | 1.57 | 1.51 | 19 | 4 |
| 3 | A | 129 | DPV | C5-N | 2.09 | 1.58 | 1.51 | 10 | 1 |
| 3 | A | 126 | DPV | C5-N | 2.08 | 1.58 | 1.51 | 14 | 1 |
| 3 | A | 110 | DPV | C5-N | 2.08 | 1.58 | 1.51 | 8 | 2 |
| 3 | A | 123 | DPV | C5-N | 2.08 | 1.58 | 1.51 | 9 | 4 |
| 3 | A | 158 | DPV | C5-C4 | 2.08 | 1.57 | 1.51 | 3 | 1 |
| 3 | A | 164 | DPV | C5-N | 2.08 | 1.58 | 1.51 | 20 | 3 |
| 3 | A | 109 | DPV | C5-N | 2.08 | 1.58 | 1.51 | 17 | 2 |
| 3 | A | 134 | DPV | C5-N | 2.08 | 1.58 | 1.51 | 14 | 2 |
| 3 | A | 152 | DPV | C5-N | 2.08 | 1.58 | 1.51 | 8 | 2 |
| 3 | A | 107 | DPV | C5-C4 | 2.07 | 1.57 | 1.51 | 18 | 3 |
| 3 | A | 161 | DPV | C5-N | 2.07 | 1.58 | 1.51 | 17 | 3 |
| 3 | A | 163 | DPV | C5-N | 2.07 | 1.58 | 1.51 | 3 | 2 |
| 3 | A | 142 | DPV | C5-C4 | 2.06 | 1.57 | 1.51 | 16 | 4 |
| 3 | A | 140 | DPV | C5-C4 | 2.06 | 1.57 | 1.51 | 1 | 1 |
| 3 | A | 132 | DPV | C5-N | 2.06 | 1.58 | 1.51 | 10 | 3 |
| 3 | A | 113 | DPV | C5-N | 2.05 | 1.58 | 1.51 | 4 | 2 |
| 3 | A | 120 | DPV | C5-C4 | 2.05 | 1.57 | 1.51 | 2 | 2 |
| 3 | A | 135 | DPV | C5-N | 2.05 | 1.58 | 1.51 | 1 | 3 |
| 3 | A | 117 | DPV | C5-N | 2.05 | 1.58 | 1.51 | 5 | 2 |
| 3 | A | 154 | DPV | C5-N | 2.05 | 1.58 | 1.51 | 12 | 1 |
| 3 | A | 156 | DPV | C5-N | 2.05 | 1.58 | 1.51 | 1 | 2 |
| 3 | A | 102 | DPV | C5-N | 2.04 | 1.58 | 1.51 | 13 | 4 |
| 3 | A | 143 | DPV | C5-N | 2.05 | 1.58 | 1.51 | 6 | 1 |
| 3 | A | 149 | DPV | C5-N | 2.05 | 1.58 | 1.51 | 6 | 2 |
| 3 | A | 149 | DPV | C5-C4 | 2.05 | 1.57 | 1.51 | 7 | 3 |
| 3 | A | 115 | DPV | C5-N | 2.04 | 1.58 | 1.51 | 13 | 2 |
| 3 | A | 164 | DPV | C5-C4 | 2.04 | 1.57 | 1.51 | 12 | 1 |
| 3 | A | 131 | DPV | C5-N | 2.04 | 1.58 | 1.51 | 3 | 3 |
| 3 | A | 103 | DPV | C5-N | 2.04 | 1.58 | 1.51 | 12 | 2 |
| 3 | A | 118 | DPV | C5-N | 2.04 | 1.58 | 1.51 | 14 | 2 |
| 3 | A | 119 | DPV | C5-N | 2.04 | 1.58 | 1.51 | 14 | 1 |
| 3 | A | 165 | DPV | C5-C4 | 2.04 | 1.57 | 1.51 | 16 | 3 |
| 3 | A | 125 | DPV | C5-N | 2.04 | 1.58 | 1.51 | 20 | 2 |
| 3 | A | 150 | DPV | C5-N | 2.04 | 1.58 | 1.51 | 6 | 2 |
| 3 | A | 145 | DPV | C5-C4 | 2.03 | 1.57 | 1.51 | 16 | 3 |
| 3 | A | 108 | DPV | C5-N | 2.03 | 1.58 | 1.51 | 16 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 134 | DPV | C5-C4 | 2.03 | 1.57 | 1.51 | 1 | 2 |
| 3 | A | 128 | DPV | C5-N | 2.02 | 1.58 | 1.51 | 20 | 1 |
| 3 | A | 110 | DPV | C5-C4 | 2.02 | 1.57 | 1.51 | 8 | 1 |
| 3 | A | 138 | DPV | C5-N | 2.02 | 1.58 | 1.51 | 11 | 1 |
| 3 | A | 150 | DPV | C5-C4 | 2.02 | 1.57 | 1.51 | 11 | 2 |
| 3 | A | 117 | DPV | C5-C4 | 2.02 | 1.57 | 1.51 | 5 | 2 |
| 3 | A | 147 | DPV | C5-N | 2.02 | 1.58 | 1.51 | 11 | 1 |
| 3 | A | 119 | DPV | C5-C4 | 2.01 | 1.57 | 1.51 | 2 | 1 |
| 3 | A | 136 | DPV | C5-N | 2.01 | 1.58 | 1.51 | 6 | 1 |
| 3 | A | 151 | DPV | C5-N | 2.02 | 1.58 | 1.51 | 5 | 1 |
| 3 | A | 155 | DPV | C5-N | 2.01 | 1.58 | 1.51 | 7 | 1 |
| 3 | A | 107 | DPV | C5-N | 2.01 | 1.58 | 1.51 | 5 | 1 |
| 3 | A | 144 | DPV | C5-C4 | 2.01 | 1.57 | 1.51 | 12 | 1 |
| 3 | A | 146 | DPV | C5-N | 2.01 | 1.58 | 1.51 | 14 | 1 |
| 3 | A | 152 | DPV | C5-C4 | 2.00 | 1.57 | 1.51 | 3 | 1 |

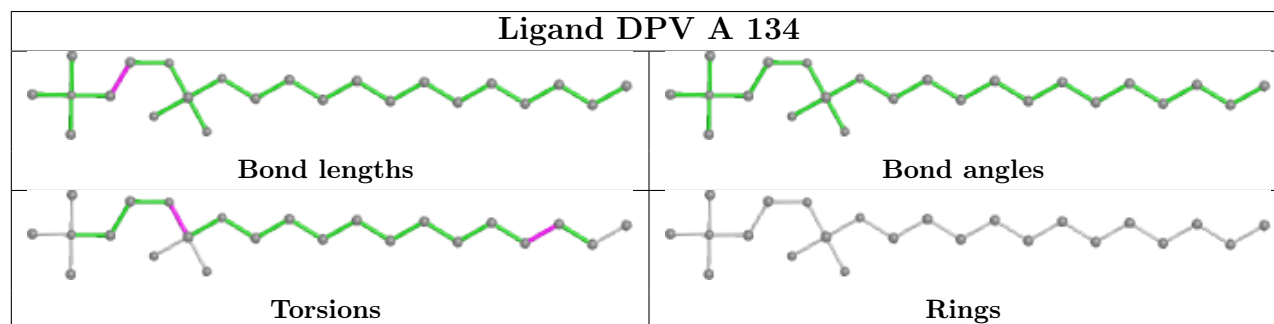
There are no bond-angle outliers.

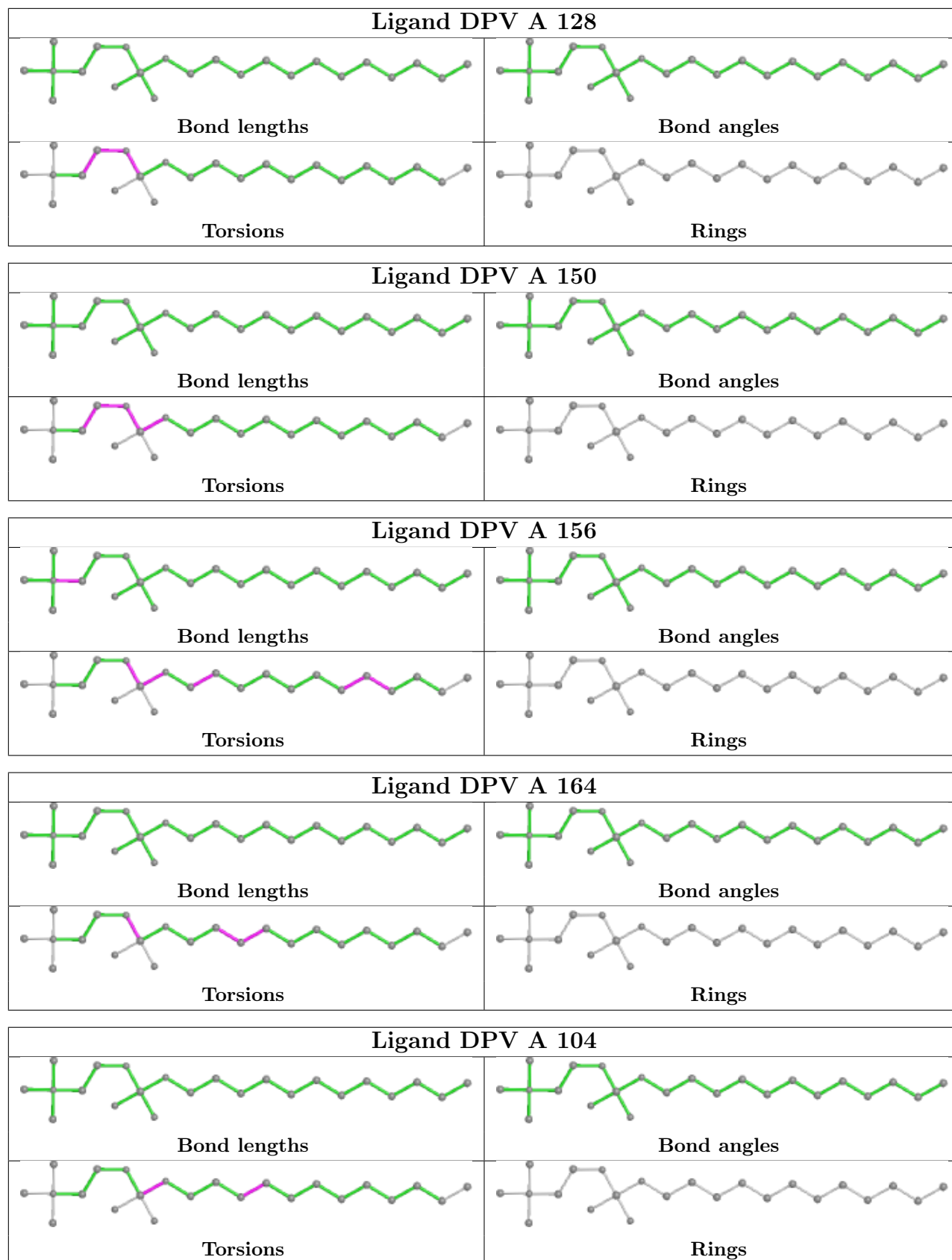
There are no chirality outliers.

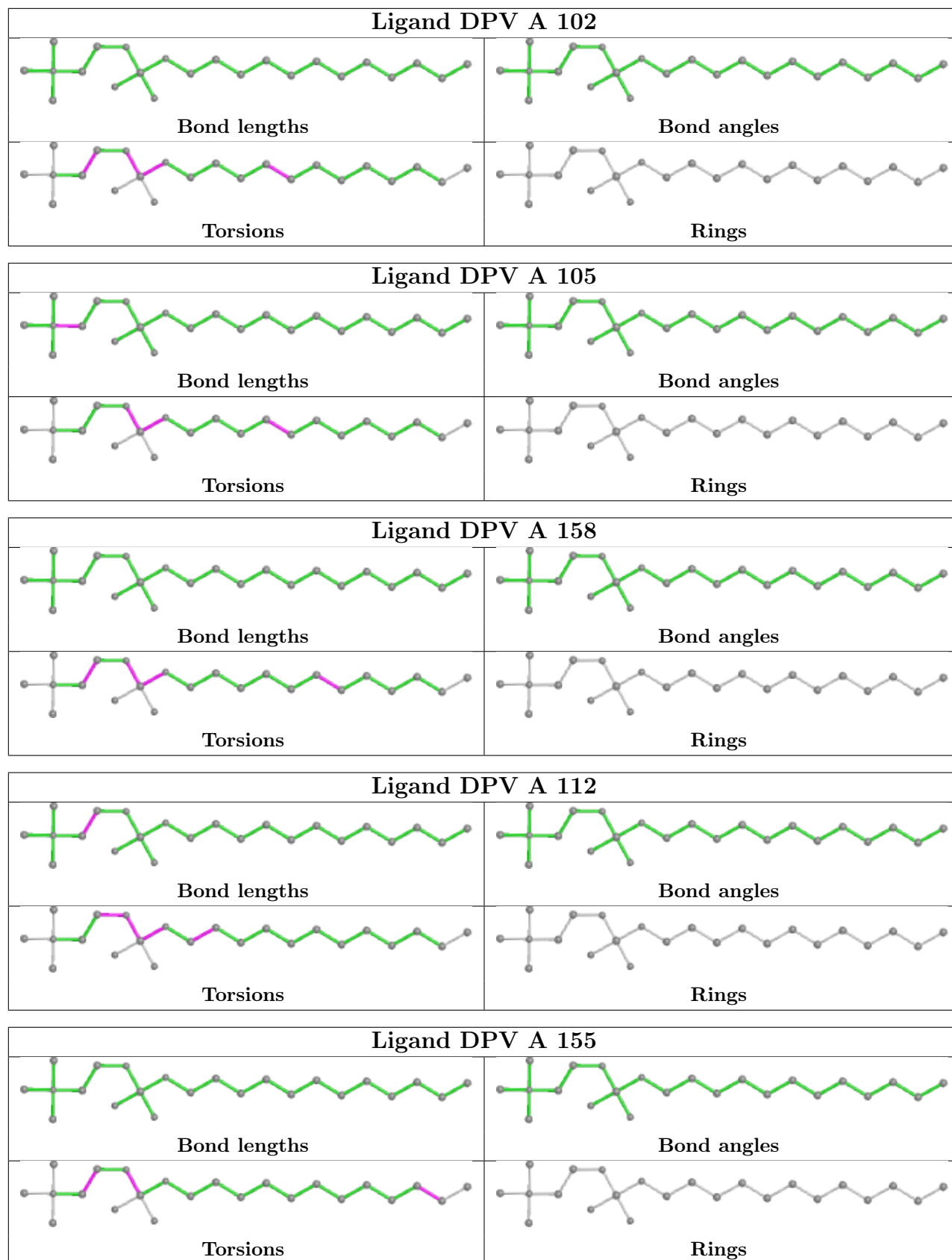
There are no torsion outliers.

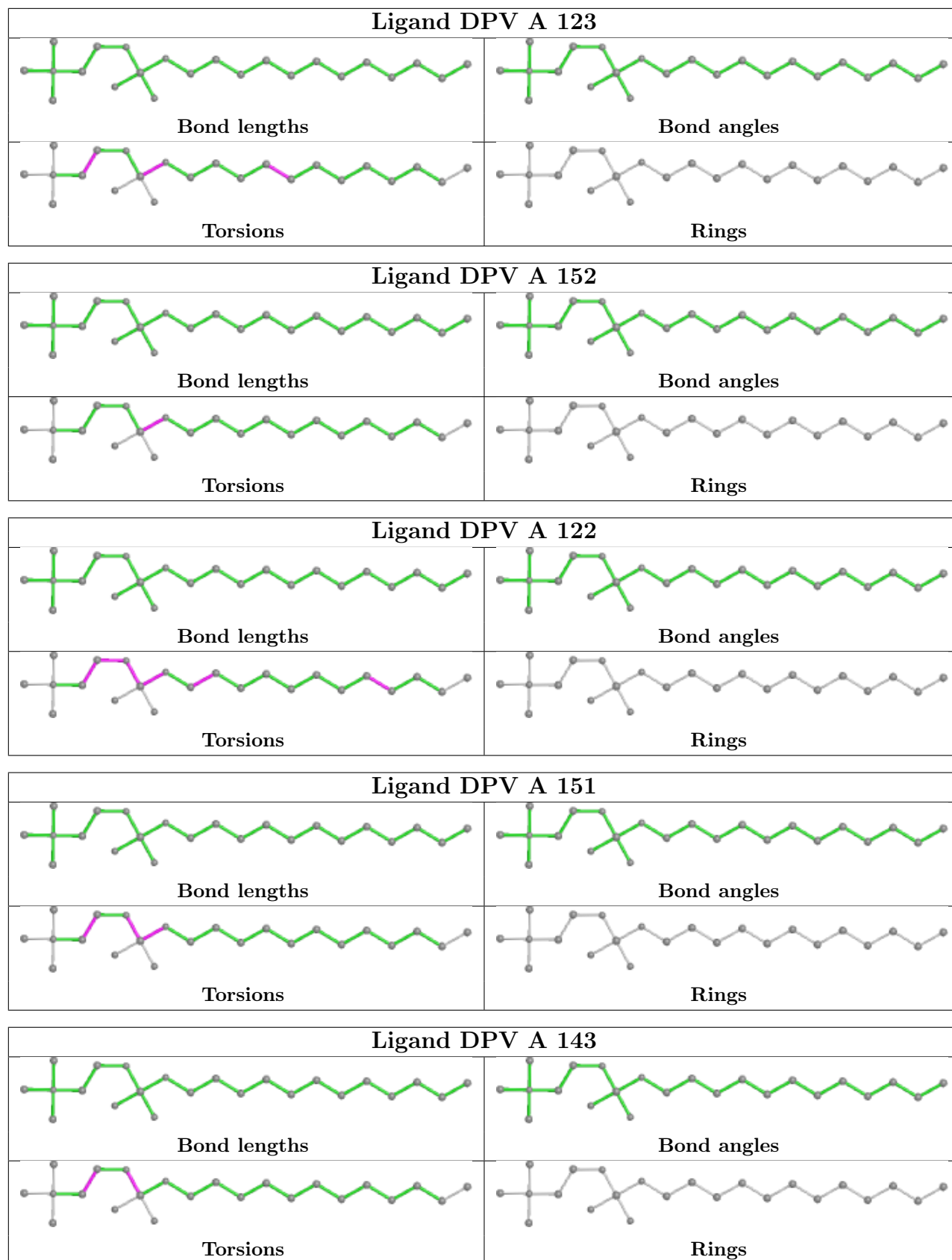
There are no ring outliers.

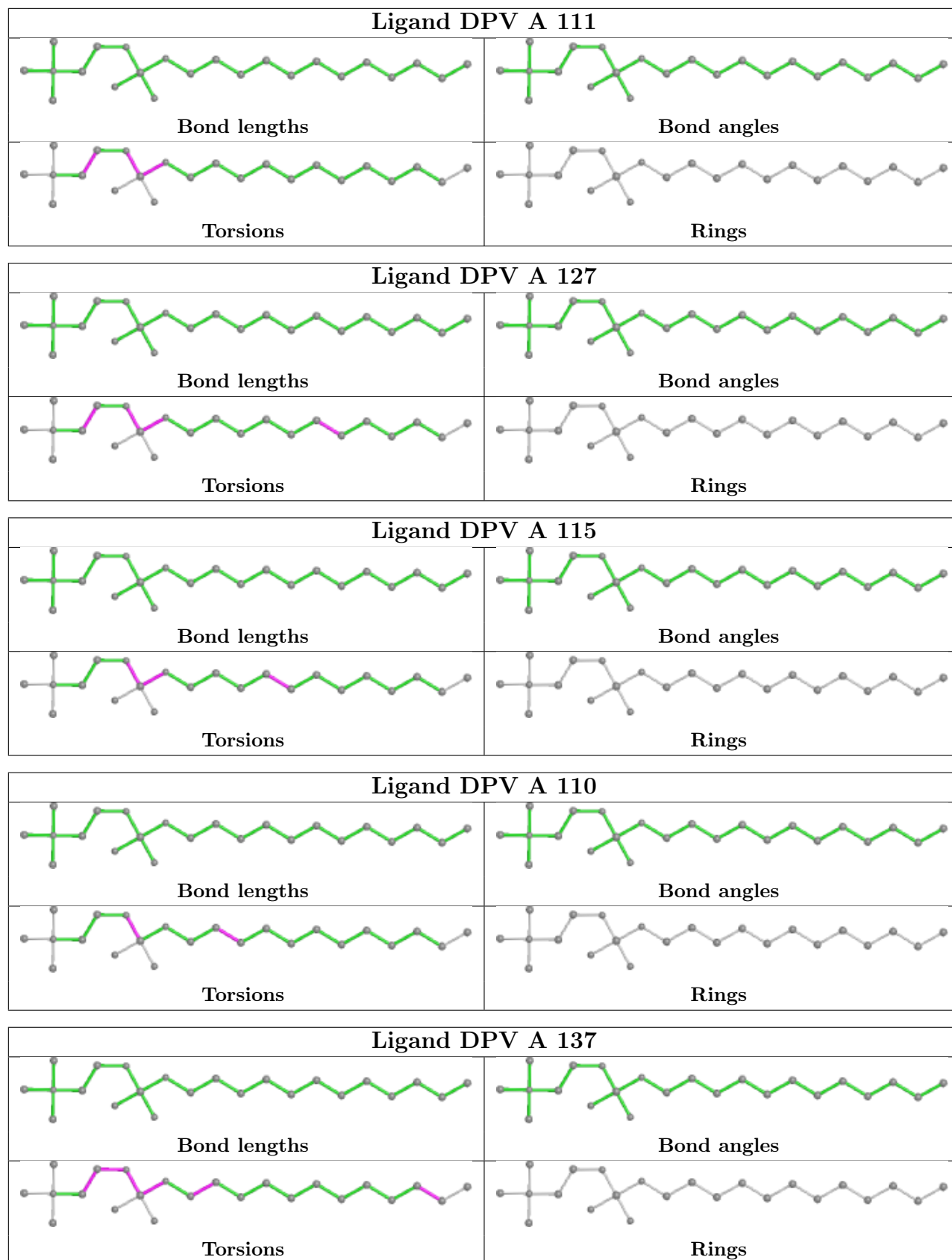
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

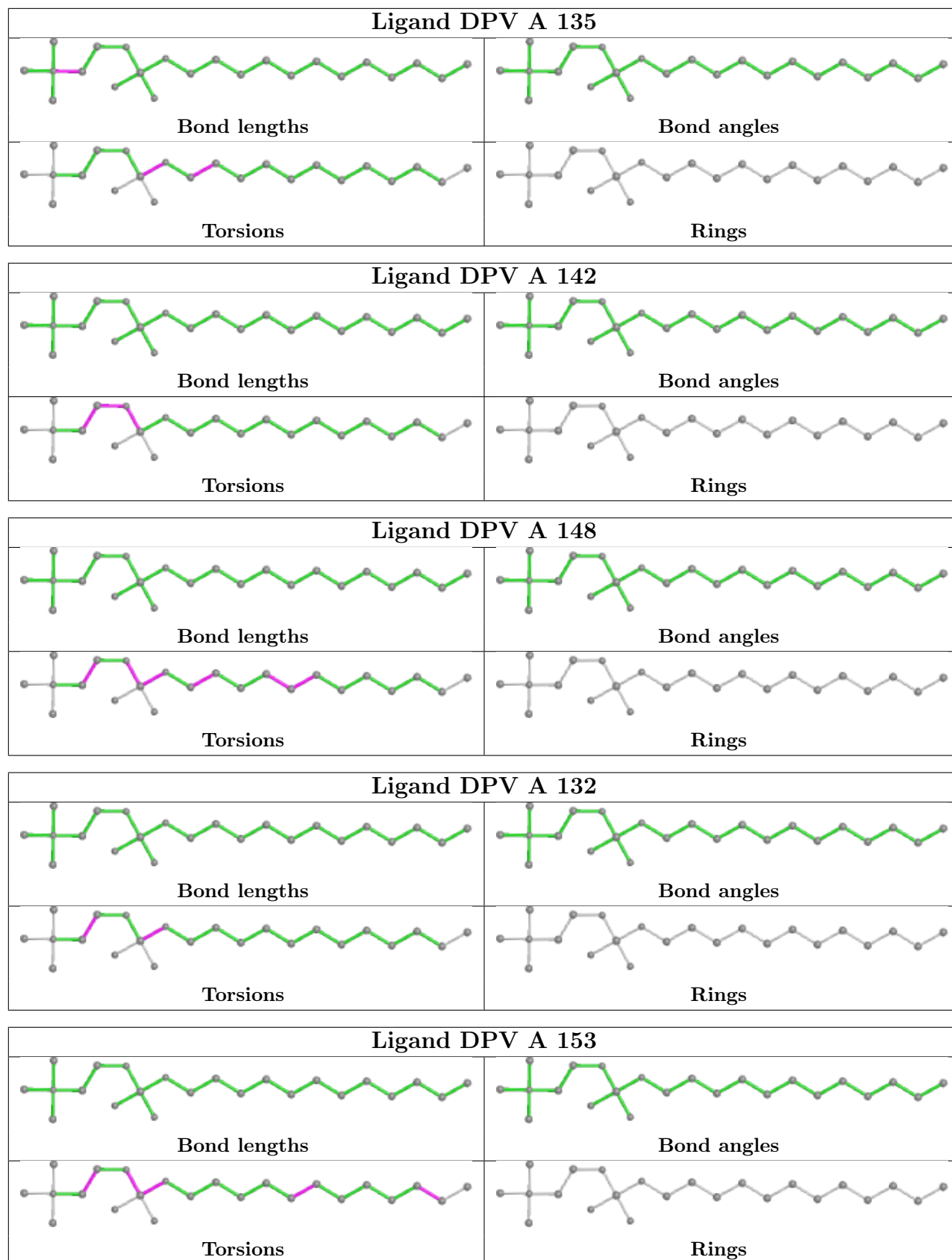


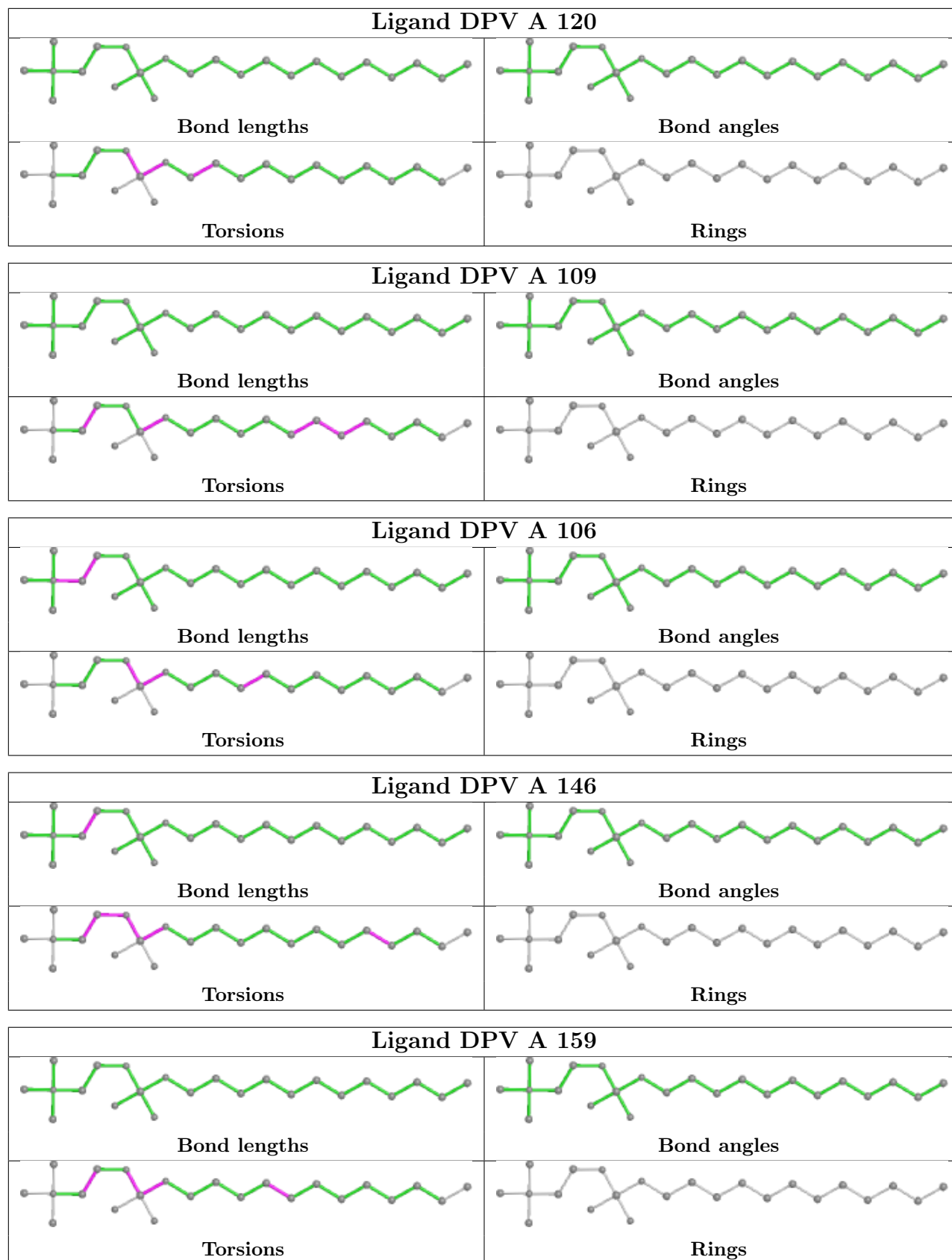


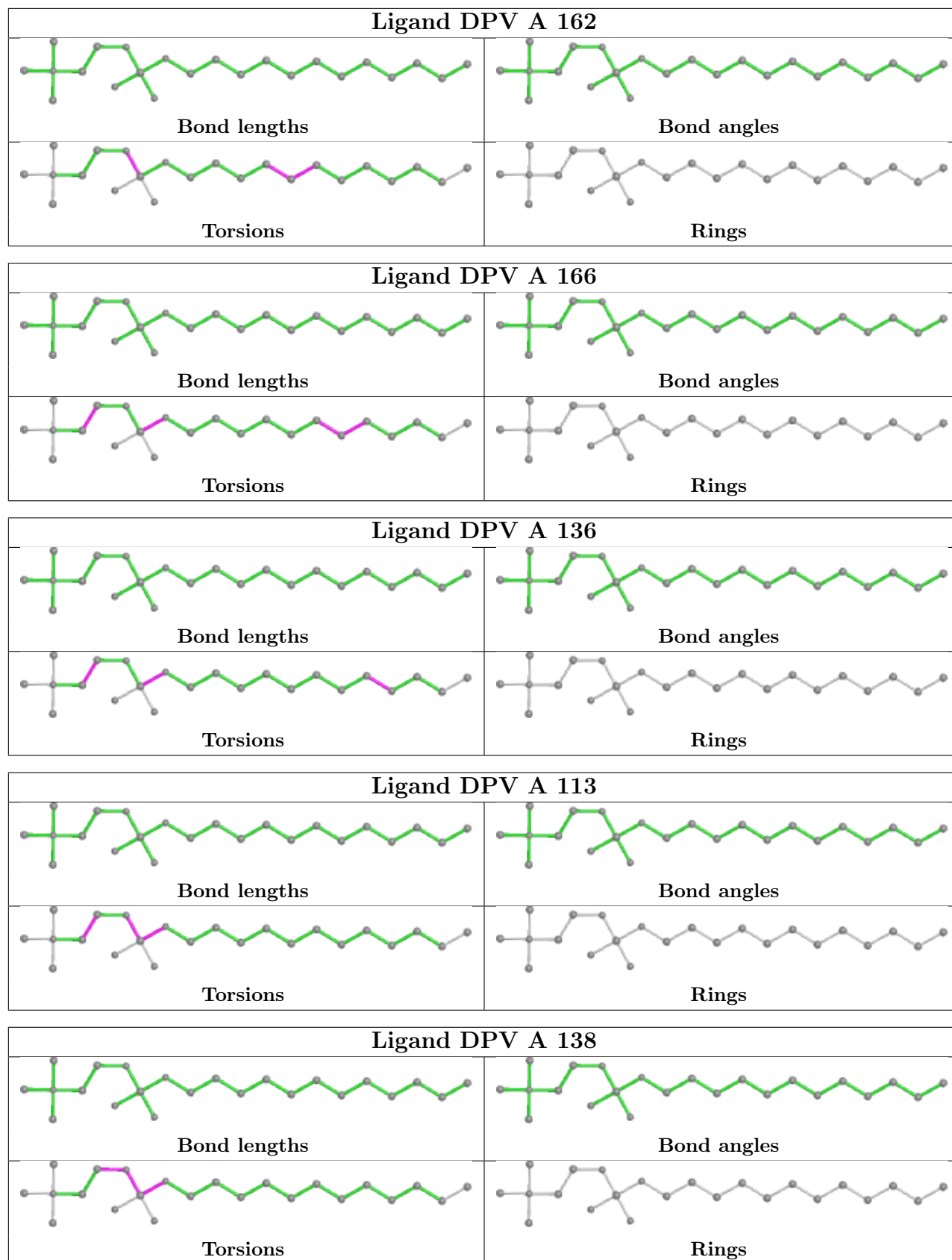


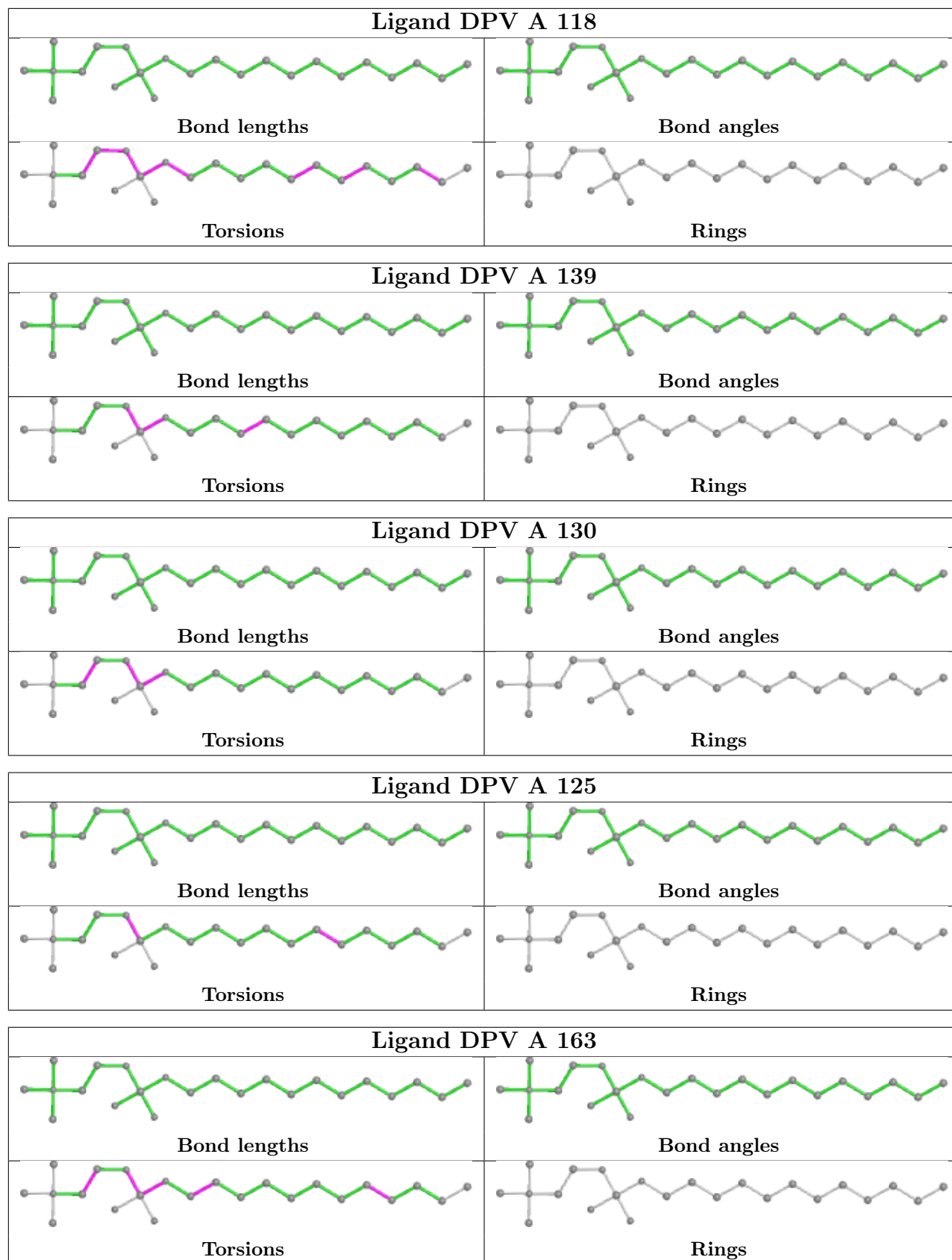


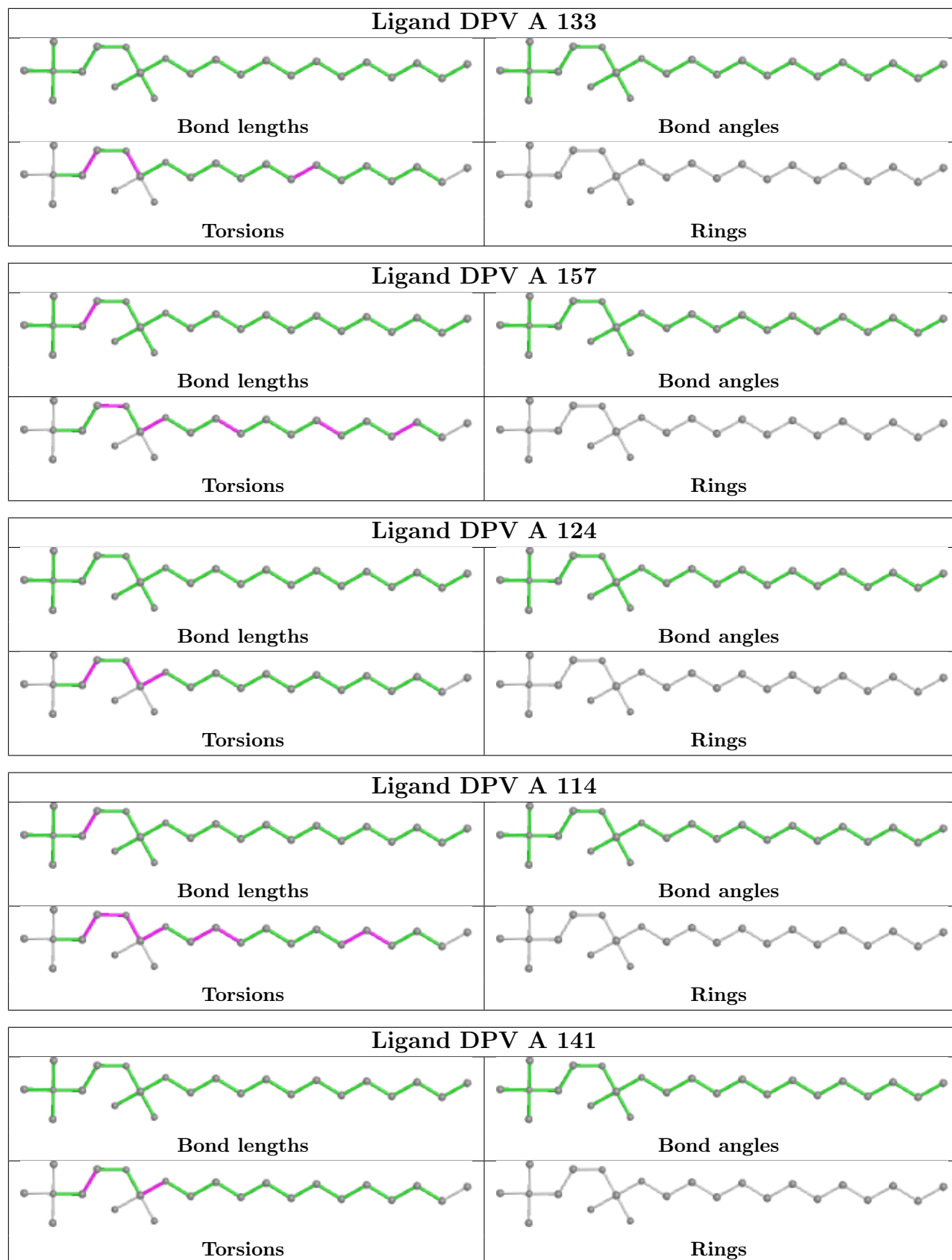


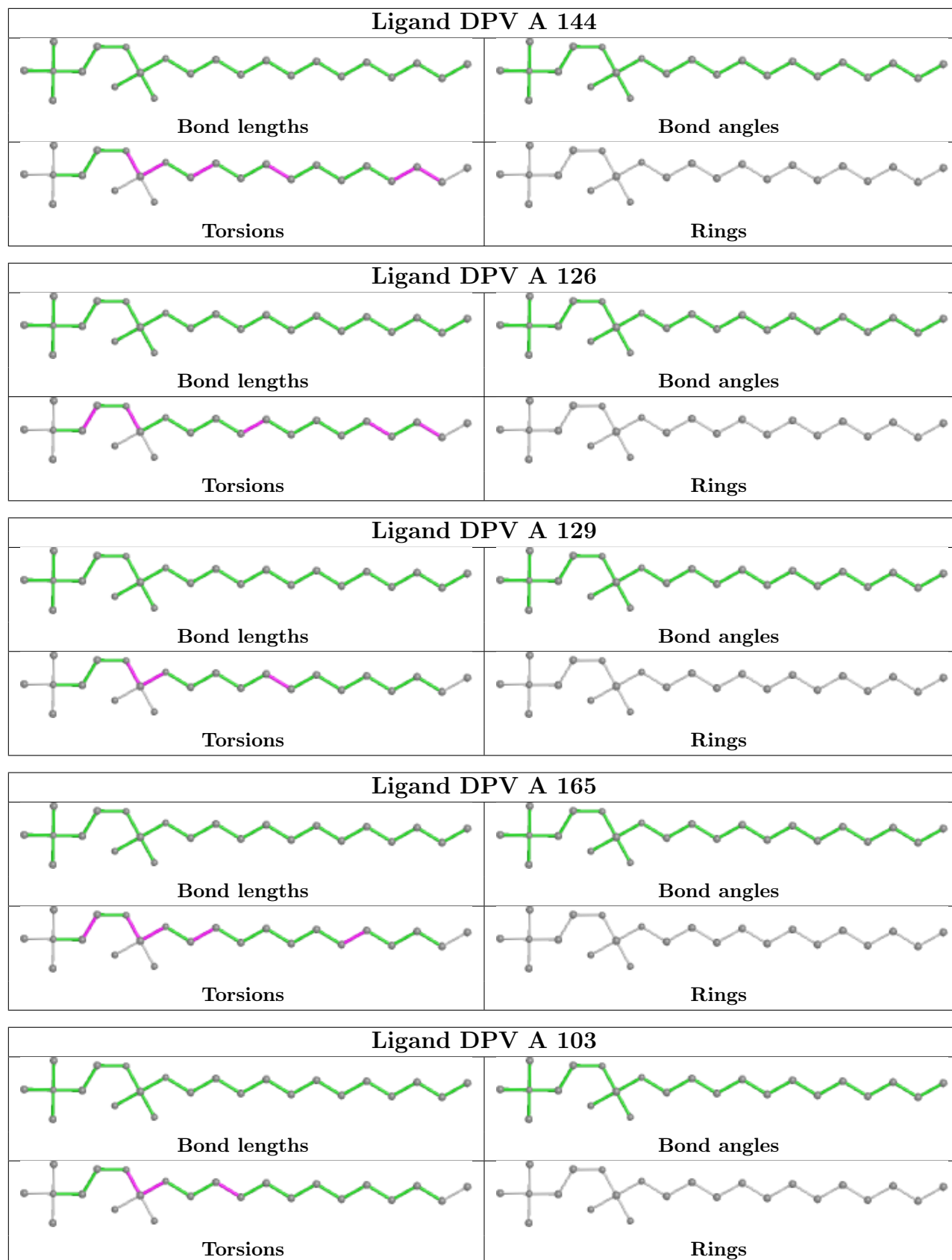


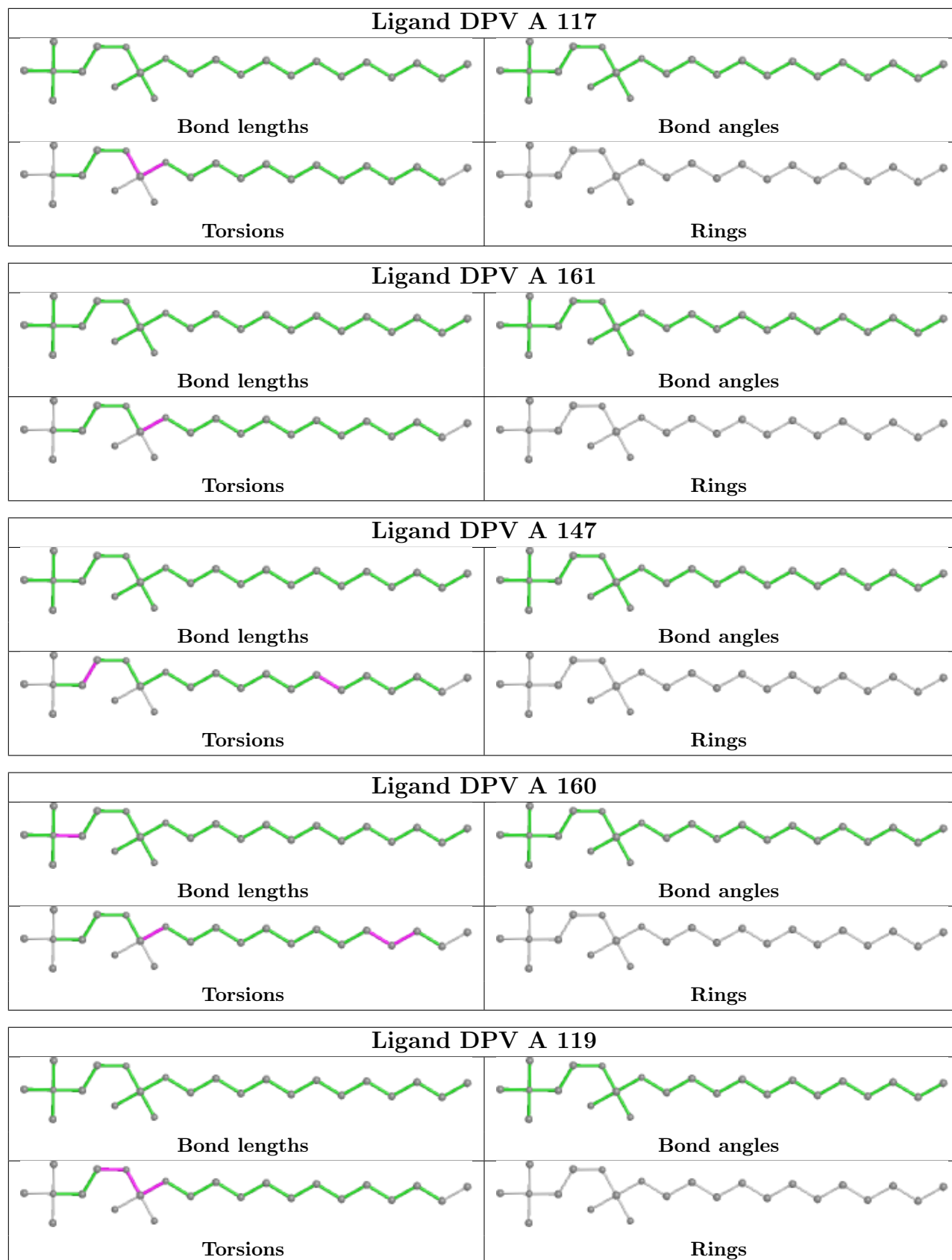


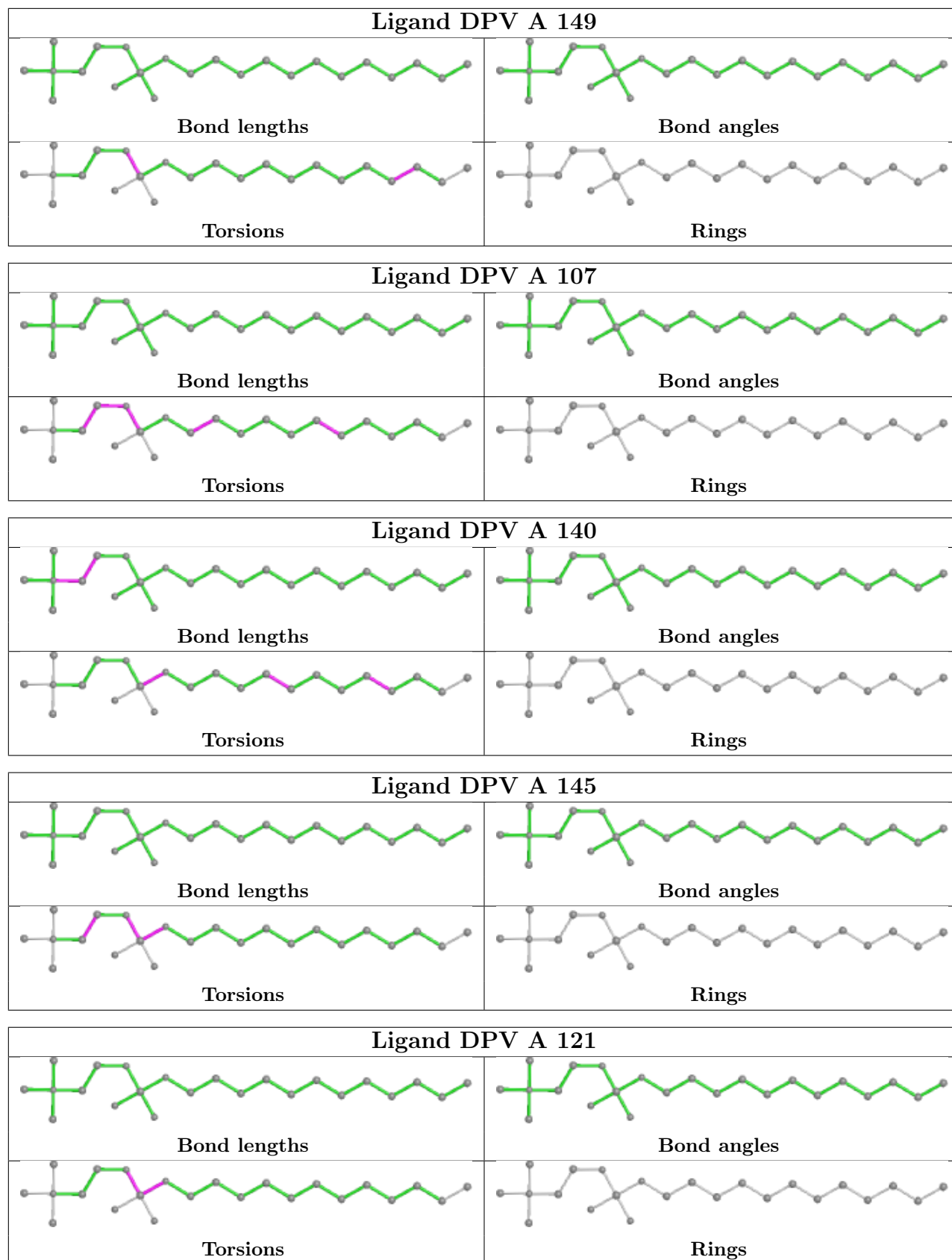


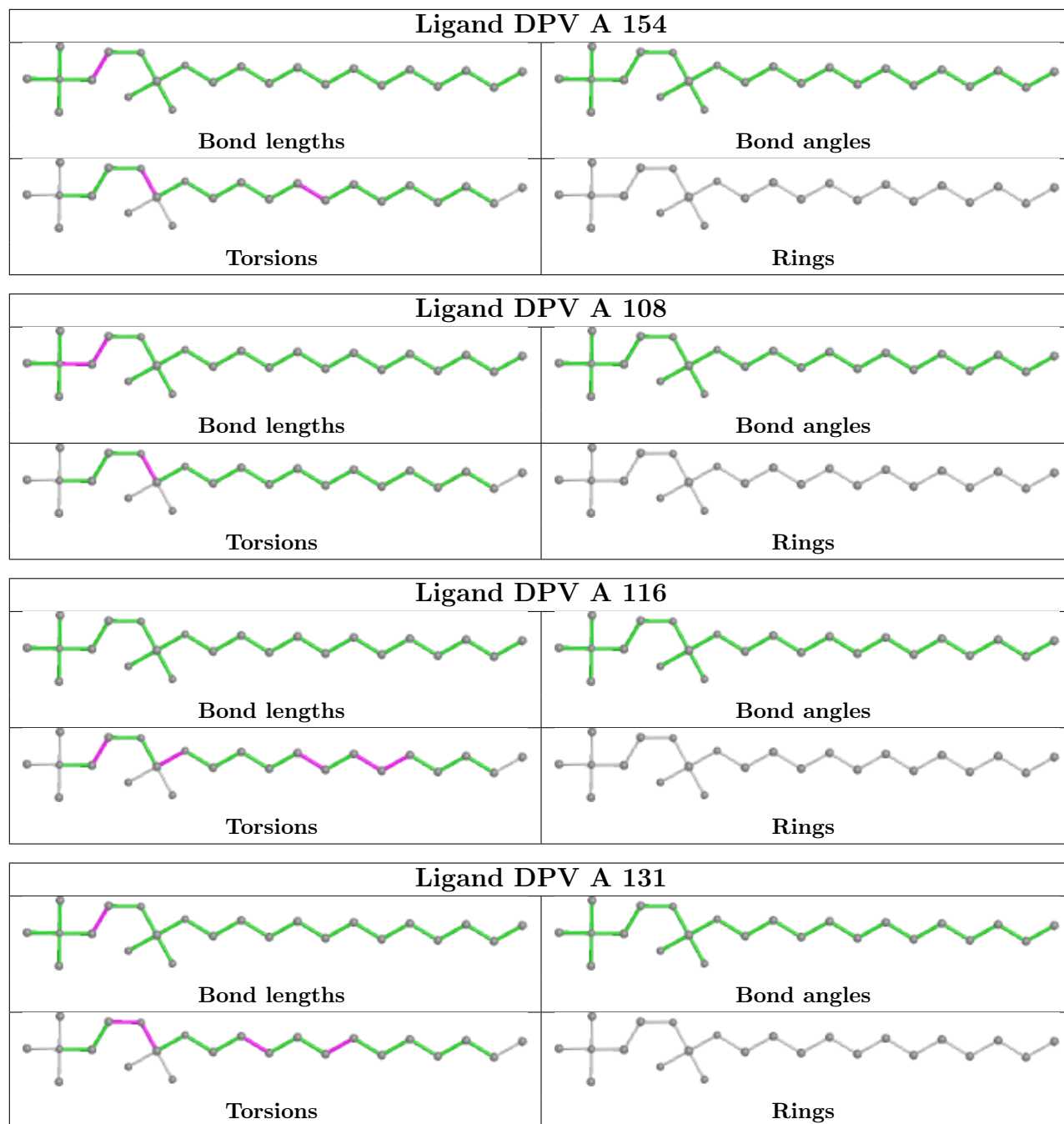












6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|-----|
| Total number of shifts | 134 |
| Number of shifts mapped to atoms | 134 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 132 atoms were assigned a chemical shift out of a possible 170. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone | 27/51 (53%) | 19/21 (90%) | 8/20 (40%) | 0/10 (0%) |
| Sidechain | 94/107 (88%) | 65/71 (92%) | 29/33 (88%) | 0/3 (0%) |
| Aromatic | 11/12 (92%) | 6/6 (100%) | 5/5 (100%) | 0/1 (0%) |
| Overall | 132/170 (78%) | 90/98 (92%) | 42/58 (72%) | 0/14 (0%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 132 atoms were assigned a chemical shift out of a possible 170. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone | 27/51 (53%) | 19/21 (90%) | 8/20 (40%) | 0/10 (0%) |
| Sidechain | 94/107 (88%) | 65/71 (92%) | 29/33 (88%) | 0/3 (0%) |
| Aromatic | 11/12 (92%) | 6/6 (100%) | 5/5 (100%) | 0/1 (0%) |
| Overall | 132/170 (78%) | 90/98 (92%) | 42/58 (72%) | 0/14 (0%) |

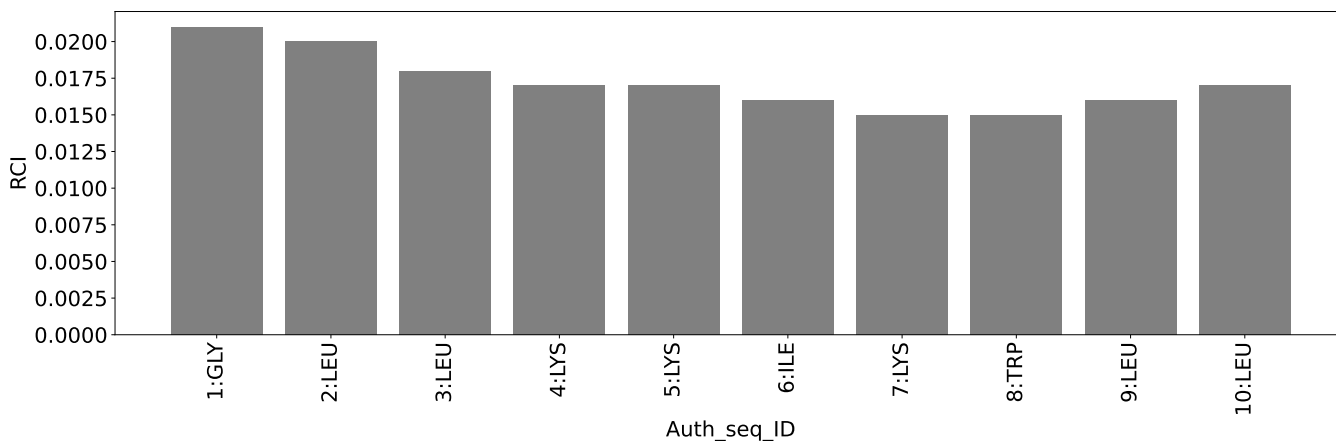
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

| Description | Value |
|--|-------|
| Total distance restraints | 107 |
| Intra-residue ($ i-j =0$) | 64 |
| Sequential ($ i-j =1$) | 28 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 15 |
| Long range ($ i-j \geq 5$) | 0 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 14 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 11.0 |
| Number of long range restraints per residue ¹ | 0.0 |

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation. There are no distance violations

8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis

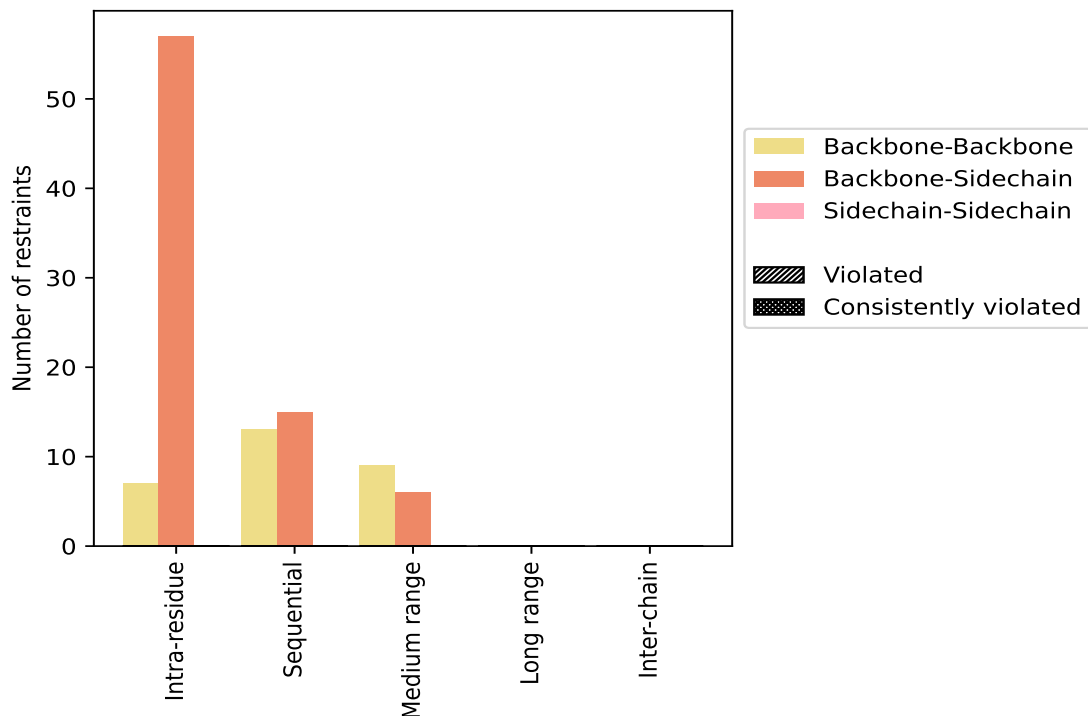
9.1 Summary of distance violations

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue (i-j =0) | 64 | 59.8 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 7 | 6.5 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 57 | 53.3 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sequential (i-j =1) | 28 | 26.2 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 13 | 12.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 15 | 14.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Medium range (i-j >1 & i-j <5) | 15 | 14.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 9 | 8.4 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 6 | 5.6 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Long range (i-j ≥5) | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Inter-chain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 107 | 100.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 29 | 27.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 78 | 72.9 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfid bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

No violations found

9.3 Distance violation statistics for the ensemble [i](#)

No violations found

9.4 Most violated distance restraints in the ensemble [i](#)

No violations found

9.5 All violated distance restraints [i](#)

No violations found

10 Dihedral-angle violation analysis [i](#)

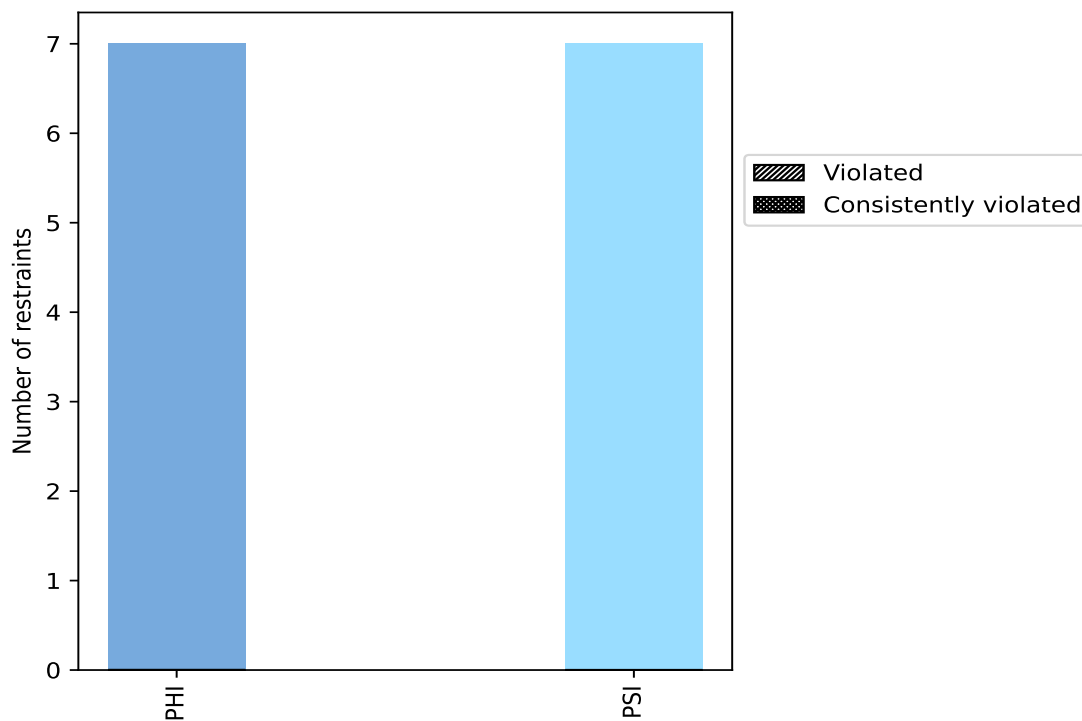
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

| Angle type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| PHI | 7 | 50.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| PSI | 7 | 50.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 14 | 100.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

No violations found

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

No violations found

10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

No violations found

10.5 All violated dihedral-angle restraints [i](#)

No violations found