



## wwPDB EM Validation Summary Report ⓘ

Sep 8, 2025 – 02:04 pm BST

PDB ID : 9HEO / pdb\_00009heo  
EMDB ID : EMD-52085  
Title : Open-state RyR1 in 0.05% POPC micelles, in complex with a nanobody and FKBP  
Authors : Li, C.; Efremov, R.G.  
Deposited on : 2024-11-14  
Resolution : 3.40 Å(reported)

This is a wwPDB EM Validation Summary 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.dev126  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

# 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 3.40 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 146783 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4327	Total	C	N	O	S	1	0
			34225	21798	5895	6303	229		
1	C	4327	Total	C	N	O	S	1	0
			34225	21798	5895	6303	229		
1	G	4327	Total	C	N	O	S	1	0
			34225	21798	5895	6303	229		
1	J	4327	Total	C	N	O	S	1	0
			34224	21797	5895	6303	229		

- Molecule 2 is a protein called Nanobody 9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	126	Total	C	N	O	S	0	0
			961	594	167	195	5		
2	D	126	Total	C	N	O	S	0	0
			961	594	167	195	5		
2	H	126	Total	C	N	O	S	0	0
			961	594	167	195	5		
2	K	126	Total	C	N	O	S	0	0
			961	594	167	195	5		

- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
3	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
3	I	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
3	L	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

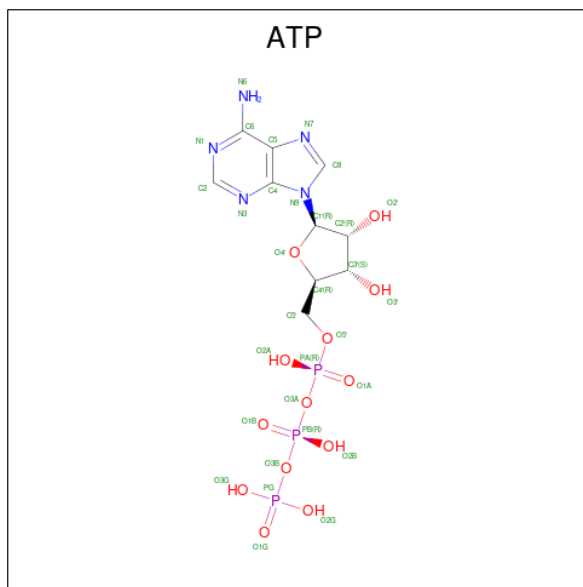
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	100	ASP	GLY	conflict	UNP Q8HYX6
F	100	ASP	GLY	conflict	UNP Q8HYX6
I	100	ASP	GLY	conflict	UNP Q8HYX6
L	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	G	1	Total	Zn	0
			1	1	
4	J	1	Total	Zn	0
			1	1	

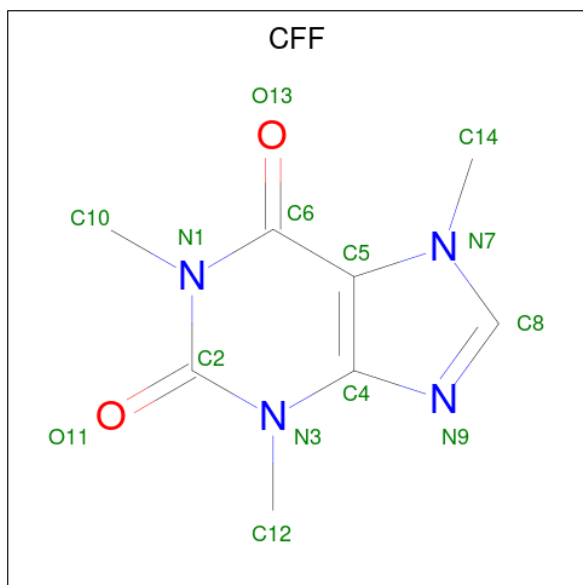
- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
5	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula:  $C_8H_{10}N_4O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	
6	J	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

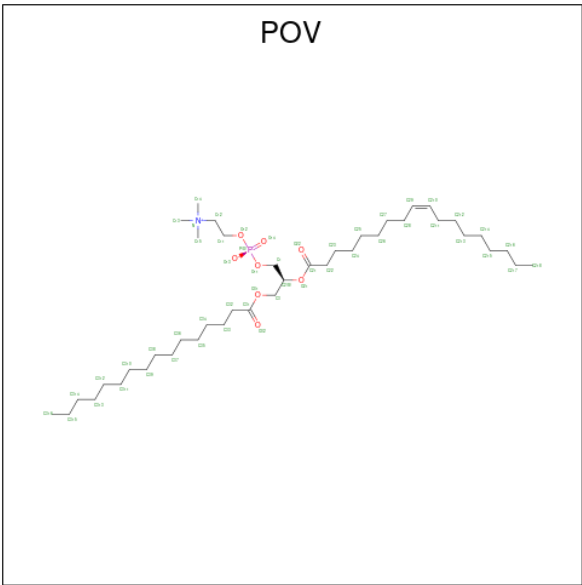
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Ca	0
			1	1	
7	C	1	Total	Ca	0
			1	1	
7	G	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
7	J	1	Total	Ca	0
			1	1	

- Molecule 8 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
8	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
8	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
8	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
8	A	1	Total	C	N	O	P	0
			20	11	1	7	1	
8	A	1	Total	C	N	O	P	0
			20	11	1	7	1	
8	A	1	Total	C	N	O	P	0
			20	12	1	6	1	
8	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
8	A	1	Total	C	N	O	P	0
			28	18	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			24	15	1	7	1	
8	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
8	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
8	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
8	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
8	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
8	A	1	Total	C	N	O	P	0
			48	38	1	8	1	
8	A	1	Total	C				0
			13	13				
8	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
8	C	1	Total	C	N	O	P	0
			48	38	1	8	1	
8	C	1	Total	C				0
			13	13				
8	C	1	Total	C	N	O	P	0
			49	39	1	8	1	
8	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
8	C	1	Total	C	N	O	P	0
			50	40	1	8	1	
8	C	1	Total	C	N	O	P	0
			46	36	1	8	1	
8	C	1	Total	C	N	O	P	0
			20	11	1	7	1	
8	C	1	Total	C	N	O	P	0
			20	11	1	7	1	
8	C	1	Total	C	N	O	P	0
			20	12	1	6	1	
8	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
8	C	1	Total	C	N	O	P	0
			28	18	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	N	O	P	0
			24	15	1	7	1	
8	C	1	Total	C	N	O	P	0
			34	24	1	8	1	
8	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
8	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
8	C	1	Total	C	N	O	P	0
			31	21	1	8	1	
8	G	1	Total	C	N	O	P	0
			40	30	1	8	1	
8	G	1	Total	C	N	O	P	0
			48	38	1	8	1	
8	G	1	Total	C				0
			13	13				
8	G	1	Total	C	N	O	P	0
			49	39	1	8	1	
8	G	1	Total	C	N	O	P	0
			47	37	1	8	1	
8	G	1	Total	C	N	O	P	0
			50	40	1	8	1	
8	G	1	Total	C	N	O	P	0
			46	36	1	8	1	
8	G	1	Total	C	N	O	P	0
			20	11	1	7	1	
8	G	1	Total	C	N	O	P	0
			20	11	1	7	1	
8	G	1	Total	C	N	O	P	0
			20	12	1	6	1	
8	G	1	Total	C	N	O	P	0
			35	25	1	8	1	
8	G	1	Total	C	N	O	P	0
			28	18	1	8	1	
8	G	1	Total	C	N	O	P	0
			24	15	1	7	1	
8	G	1	Total	C	N	O	P	0
			34	24	1	8	1	
8	G	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
8	G	1	Total	C	N	O	P	0
			47	37	1	8	1	
8	G	1	Total	C	N	O	P	0
			41	31	1	8	1	
8	G	1	Total	C	N	O	P	0
			31	21	1	8	1	
8	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
8	J	1	Total	C	N	O	P	0
			47	37	1	8	1	
8	J	1	Total	C	N	O	P	0
			41	31	1	8	1	
8	J	1	Total	C	N	O	P	0
			31	21	1	8	1	
8	J	1	Total	C	N	O	P	0
			40	30	1	8	1	
8	J	1	Total	C	N	O	P	0
			48	38	1	8	1	
8	J	1	Total	C				0
			13	13				
8	J	1	Total	C	N	O	P	0
			49	39	1	8	1	
8	J	1	Total	C	N	O	P	0
			47	37	1	8	1	
8	J	1	Total	C	N	O	P	0
			50	40	1	8	1	
8	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
8	J	1	Total	C	N	O	P	0
			20	11	1	7	1	
8	J	1	Total	C	N	O	P	0
			20	11	1	7	1	
8	J	1	Total	C	N	O	P	0
			20	12	1	6	1	
8	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
8	J	1	Total	C	N	O	P	0
			28	18	1	8	1	
8	J	1	Total	C	N	O	P	0
			24	15	1	7	1	
8	J	1	Total	C	N	O	P	0
			34	24	1	8	1	

MolProbity failed to run properly - this section is therefore empty.

### 3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	279776	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.280	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.043	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	479.136, 479.136, 479.136	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.426, 1.426, 1.426	Depositor

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

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

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

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 8 are monoatomic - leaving 80 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	POV	A	5105	-	48,48,51	0.51	0	54,56,59	0.47	0
8	POV	G	5120	-	46,46,51	0.31	0	52,54,59	0.34	0
8	POV	J	5105	-	39,39,51	0.53	0	45,47,59	0.64	1 (2%)
8	POV	C	5114	-	19,19,51	0.65	0	24,25,59	0.57	0
8	POV	G	5113	-	19,19,51	0.39	0	24,26,59	0.52	0
8	POV	J	5106	-	47,47,51	0.51	0	53,55,59	0.47	0
8	POV	A	5108	-	45,45,51	0.52	0	51,53,59	0.47	0
8	POV	G	5118	-	33,33,51	0.60	0	39,41,59	0.53	0
8	POV	C	5112	-	19,19,51	0.72	0	24,26,59	0.70	0
8	POV	G	5112	-	19,19,51	0.72	0	24,26,59	0.70	0
8	POV	J	5118	-	19,19,51	0.66	0	24,25,59	0.57	0
8	POV	A	5119	-	30,30,51	0.81	1 (3%)	34,37,59	0.59	0
8	POV	C	5121	-	40,40,51	0.54	0	46,48,59	0.62	1 (2%)
8	POV	J	5101	-	51,51,51	0.49	0	57,59,59	0.47	0
8	POV	A	5106	-	46,46,51	0.52	0	52,54,59	0.49	0
6	CFF	J	5110	-	8,15,15	0.89	0	8,23,23	2.89	2 (25%)
8	POV	A	5111	-	19,19,51	0.65	0	24,25,59	0.57	0
5	ATP	A	5102	-	26,33,33	0.66	0	31,52,52	0.80	1 (3%)
8	POV	J	5116	-	19,19,51	0.72	0	24,26,59	0.71	0
8	POV	J	5114	-	49,49,51	0.50	0	55,57,59	0.48	0
8	POV	J	5117	-	19,19,51	0.39	0	24,26,59	0.51	0
8	POV	A	5107	-	49,49,51	0.50	0	55,57,59	0.48	0
8	POV	C	5120	-	46,46,51	0.31	0	52,54,59	0.31	0
8	POV	C	5122	-	30,30,51	0.81	1 (3%)	34,37,59	0.59	0
8	POV	C	5113	-	19,19,51	0.40	0	24,26,59	0.52	0
6	CFF	G	5106	-	8,15,15	0.87	0	8,23,23	2.88	2 (25%)
8	POV	C	5116	-	27,27,51	0.65	0	33,35,59	0.59	0
8	POV	A	5115	-	33,33,51	0.34	0	39,41,59	0.38	0
8	POV	J	5102	-	46,46,51	0.31	0	52,54,59	0.29	0
8	POV	G	5101	-	39,39,51	0.54	0	45,47,59	0.64	1 (2%)
8	POV	A	5114	-	23,23,51	0.66	0	28,30,59	0.67	0
8	POV	G	5114	-	19,19,51	0.65	0	24,25,59	0.57	0
8	POV	G	5119	-	51,51,51	0.49	0	57,59,59	0.47	0
8	POV	J	5115	-	45,45,51	0.52	0	51,53,59	0.47	0
8	POV	C	5103	-	12,12,51	0.22	0	11,11,59	0.22	0
8	POV	A	5113	-	27,27,51	0.65	0	33,35,59	0.59	0
6	CFF	C	5106	-	8,15,15	0.87	0	8,23,23	2.90	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	POV	A	5117	-	46,46,51	0.32	0	52,54,59	0.30	0
8	POV	G	5110	-	49,49,51	0.50	0	55,57,59	0.48	0
8	POV	J	5104	-	30,30,51	0.81	1 (3%)	34,37,59	0.59	0
8	POV	G	5111	-	45,45,51	0.52	0	51,53,59	0.47	0
8	POV	A	5120	-	39,39,51	0.55	0	45,47,59	0.64	1 (2%)
8	POV	G	5117	-	23,23,51	0.65	0	28,30,59	0.67	0
8	POV	C	5108	-	48,48,51	0.51	0	54,56,59	0.47	0
8	POV	G	5103	-	12,12,51	0.23	0	11,11,59	0.23	0
8	POV	G	5102	-	47,47,51	0.50	0	53,55,59	0.47	0
8	POV	C	5109	-	46,46,51	0.52	0	52,54,59	0.49	0
8	POV	J	5113	-	46,46,51	0.52	0	52,54,59	0.49	0
8	POV	A	5118	-	40,40,51	0.54	0	46,48,59	0.62	1 (2%)
8	POV	G	5122	-	30,30,51	0.80	1 (3%)	34,37,59	0.59	0
8	POV	C	5115	-	34,34,51	0.59	0	40,42,59	0.56	0
5	ATP	J	5109	-	26,33,33	0.67	0	31,52,52	0.80	1 (3%)
8	POV	C	5110	-	49,49,51	0.50	0	55,57,59	0.48	0
5	ATP	G	5105	-	26,33,33	0.66	0	31,52,52	0.81	1 (3%)
8	POV	J	5103	-	40,40,51	0.54	0	46,48,59	0.62	1 (2%)
8	POV	G	5109	-	46,46,51	0.52	0	52,54,59	0.48	0
8	POV	J	5112	-	48,48,51	0.51	0	54,56,59	0.47	0
8	POV	G	5115	-	34,34,51	0.59	0	40,42,59	0.56	0
8	POV	A	5112	-	34,34,51	0.59	0	40,42,59	0.56	0
8	POV	A	5110	-	19,19,51	0.38	0	24,26,59	0.52	0
8	POV	C	5101	-	39,39,51	0.54	0	45,47,59	0.64	1 (2%)
8	POV	A	5116	-	51,51,51	0.50	0	57,59,59	0.47	0
8	POV	C	5118	-	33,33,51	0.60	0	39,41,59	0.53	0
8	POV	C	5102	-	47,47,51	0.51	0	53,55,59	0.48	0
8	POV	J	5121	-	23,23,51	0.66	0	28,30,59	0.67	0
8	POV	A	5109	-	19,19,51	0.72	0	24,26,59	0.71	0
8	POV	C	5119	-	51,51,51	0.49	0	57,59,59	0.47	0
8	POV	A	5121	-	47,47,51	0.50	0	53,55,59	0.48	0
8	POV	J	5122	-	33,33,51	0.60	0	39,41,59	0.53	0
8	POV	G	5121	-	40,40,51	0.54	0	46,48,59	0.62	1 (2%)
6	CFF	A	5103	-	8,15,15	0.87	0	8,23,23	2.88	2 (25%)
8	POV	G	5108	-	48,48,51	0.51	0	54,56,59	0.47	0
5	ATP	C	5105	-	26,33,33	0.66	0	31,52,52	0.80	1 (3%)
8	POV	J	5119	-	34,34,51	0.59	0	40,42,59	0.56	0
8	POV	J	5120	-	27,27,51	0.65	0	33,35,59	0.59	0
8	POV	G	5116	-	27,27,51	0.66	0	33,35,59	0.59	0
8	POV	A	5122	-	12,12,51	0.23	0	11,11,59	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	POV	C	5111	-	45,45,51	0.52	0	51,53,59	0.47	0
8	POV	J	5107	-	12,12,51	0.23	0	11,11,59	0.23	0
8	POV	C	5117	-	23,23,51	0.66	0	28,30,59	0.67	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
8	POV	A	5105	-	-	23/52/52/55	-
8	POV	G	5120	-	-	8/50/50/55	-
8	POV	J	5105	-	-	10/43/43/55	-
8	POV	C	5114	-	-	8/20/20/55	-
8	POV	G	5113	-	-	9/22/22/55	-
8	POV	J	5106	-	-	13/51/51/55	-
8	POV	A	5108	-	-	12/49/49/55	-
8	POV	G	5118	-	-	11/37/37/55	-
8	POV	C	5112	-	-	8/22/22/55	-
8	POV	G	5112	-	-	8/22/22/55	-
8	POV	J	5118	-	-	8/20/20/55	-
8	POV	A	5119	-	-	14/33/33/55	-
8	POV	C	5121	-	-	16/44/44/55	-
8	POV	J	5101	-	-	16/55/55/55	-
8	POV	A	5106	-	-	13/50/50/55	-
6	CFF	J	5110	-	-	-	0/2/2/2
8	POV	A	5111	-	-	8/20/20/55	-
5	ATP	A	5102	-	-	1/18/38/38	0/3/3/3
8	POV	J	5116	-	-	8/22/22/55	-
8	POV	J	5114	-	-	24/53/53/55	-
8	POV	J	5117	-	-	9/22/22/55	-
8	POV	A	5107	-	-	24/53/53/55	-
8	POV	C	5120	-	-	6/50/50/55	-
8	POV	C	5122	-	-	14/33/33/55	-
8	POV	C	5113	-	-	6/22/22/55	-
6	CFF	G	5106	-	-	-	0/2/2/2
8	POV	C	5116	-	-	8/31/31/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	POV	A	5115	-	-	11/37/37/55	-
8	POV	J	5102	-	-	6/50/50/55	-
8	POV	G	5101	-	-	10/43/43/55	-
8	POV	A	5114	-	-	8/26/26/55	-
8	POV	G	5114	-	-	8/20/20/55	-
8	POV	G	5119	-	-	16/55/55/55	-
8	POV	J	5115	-	-	12/49/49/55	-
8	POV	C	5103	-	-	1/10/10/55	-
8	POV	A	5113	-	-	8/31/31/55	-
8	POV	A	5117	-	-	7/50/50/55	-
8	POV	G	5110	-	-	24/53/53/55	-
6	CFF	C	5106	-	-	-	0/2/2/2
8	POV	J	5104	-	-	14/33/33/55	-
8	POV	G	5111	-	-	12/49/49/55	-
8	POV	A	5120	-	-	10/43/43/55	-
8	POV	G	5117	-	-	8/26/26/55	-
8	POV	C	5108	-	-	23/52/52/55	-
8	POV	G	5103	-	-	1/10/10/55	-
8	POV	G	5102	-	-	13/51/51/55	-
8	POV	C	5109	-	-	13/50/50/55	-
8	POV	J	5113	-	-	13/50/50/55	-
8	POV	A	5118	-	-	16/44/44/55	-
8	POV	G	5122	-	-	14/33/33/55	-
8	POV	C	5115	-	-	12/38/38/55	-
5	ATP	J	5109	-	-	1/18/38/38	0/3/3/3
8	POV	C	5110	-	-	24/53/53/55	-
5	ATP	G	5105	-	-	1/18/38/38	0/3/3/3
8	POV	J	5103	-	-	16/44/44/55	-
8	POV	G	5109	-	-	13/50/50/55	-
8	POV	J	5112	-	-	23/52/52/55	-
8	POV	G	5115	-	-	12/38/38/55	-
8	POV	A	5112	-	-	12/38/38/55	-
8	POV	A	5110	-	-	8/22/22/55	-
8	POV	C	5101	-	-	10/43/43/55	-
8	POV	A	5116	-	-	16/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	POV	C	5118	-	-	11/37/37/55	-
8	POV	C	5102	-	-	13/51/51/55	-
8	POV	J	5121	-	-	8/26/26/55	-
8	POV	A	5109	-	-	8/22/22/55	-
8	POV	C	5119	-	-	16/55/55/55	-
8	POV	A	5121	-	-	13/51/51/55	-
8	POV	J	5122	-	-	11/37/37/55	-
8	POV	G	5121	-	-	16/44/44/55	-
6	CFF	A	5103	-	-	-	0/2/2/2
8	POV	G	5108	-	-	23/52/52/55	-
5	ATP	C	5105	-	-	1/18/38/38	0/3/3/3
8	POV	J	5119	-	-	12/38/38/55	-
8	POV	J	5120	-	-	8/31/31/55	-
8	POV	G	5116	-	-	8/31/31/55	-
8	POV	A	5122	-	-	1/10/10/55	-
8	POV	C	5111	-	-	12/49/49/55	-
8	POV	J	5107	-	-	1/10/10/55	-
8	POV	C	5117	-	-	8/26/26/55	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	5119	POV	O21-C2	-3.18	1.43	1.46
8	C	5122	POV	O21-C2	-3.18	1.43	1.46
8	J	5104	POV	O21-C2	-3.18	1.43	1.46
8	G	5122	POV	O21-C2	-3.08	1.43	1.46

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	5110	CFF	C5-C6-N1	-6.04	111.76	118.20
6	C	5106	CFF	C5-C6-N1	-6.02	111.78	118.20
6	G	5106	CFF	C5-C6-N1	-6.02	111.78	118.20
6	A	5103	CFF	C5-C6-N1	-6.01	111.79	118.20
6	C	5106	CFF	C4-C5-C6	4.94	123.13	119.96

There are no chirality outliers.

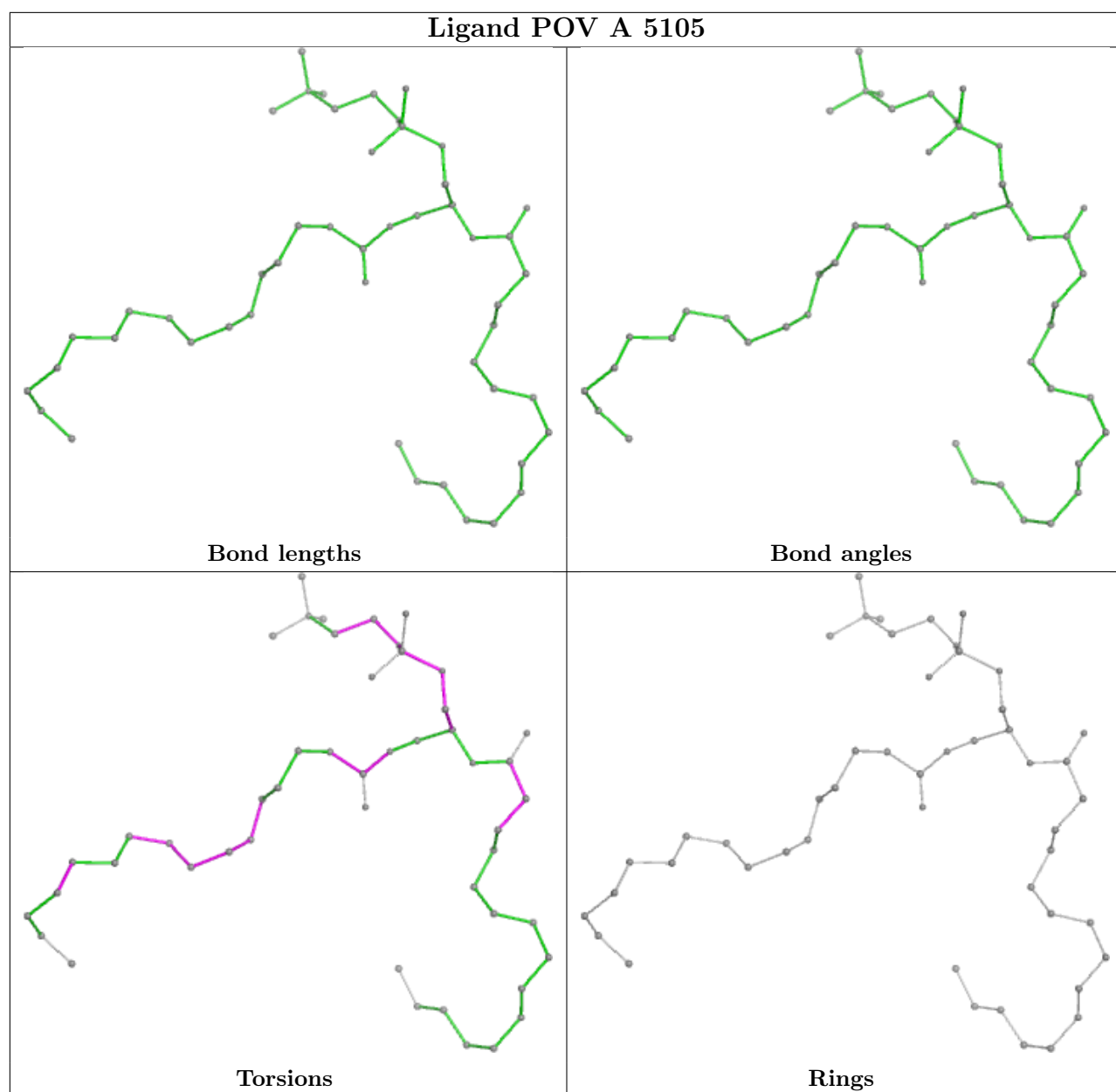
5 of 851 torsion outliers are listed below:

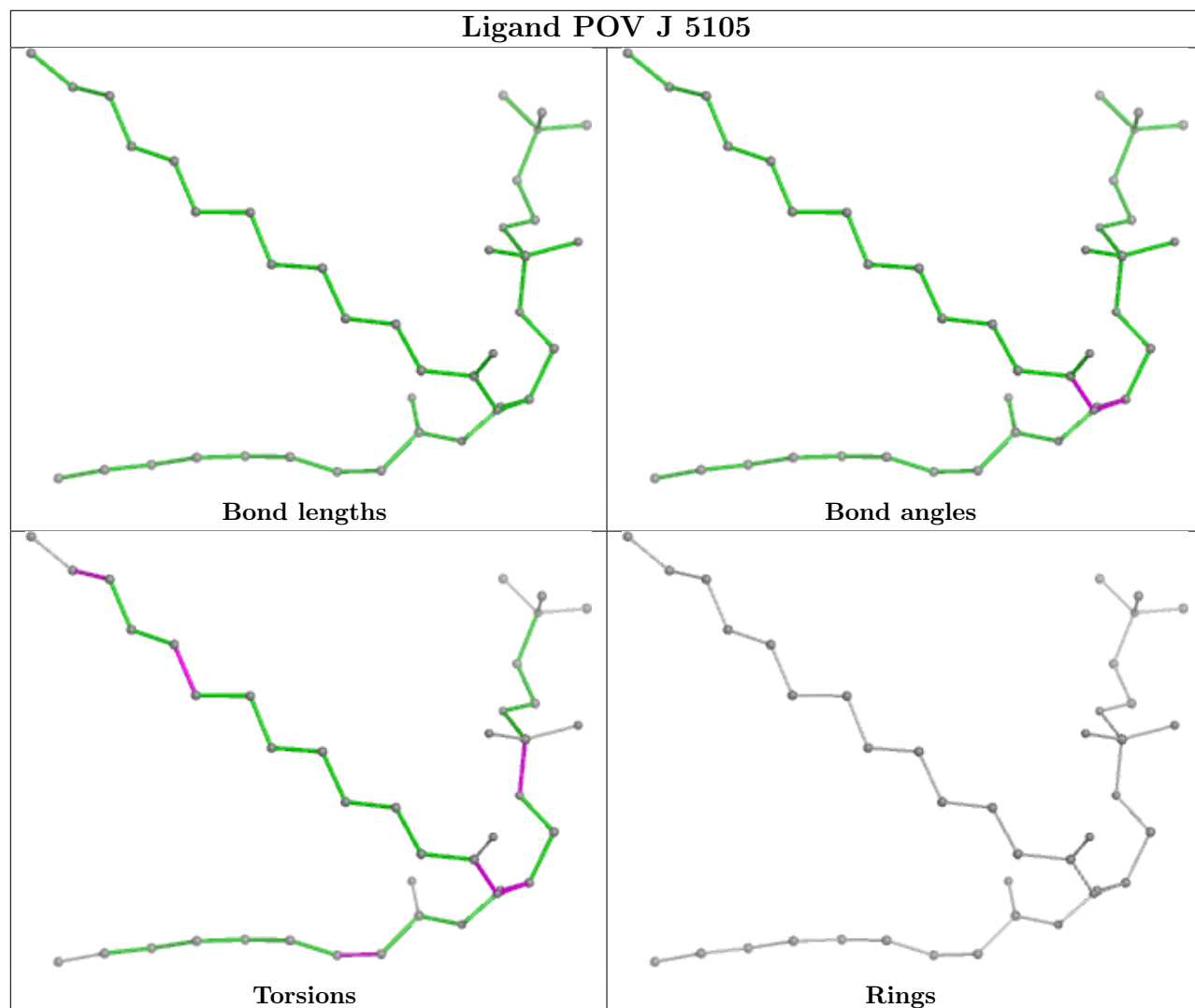
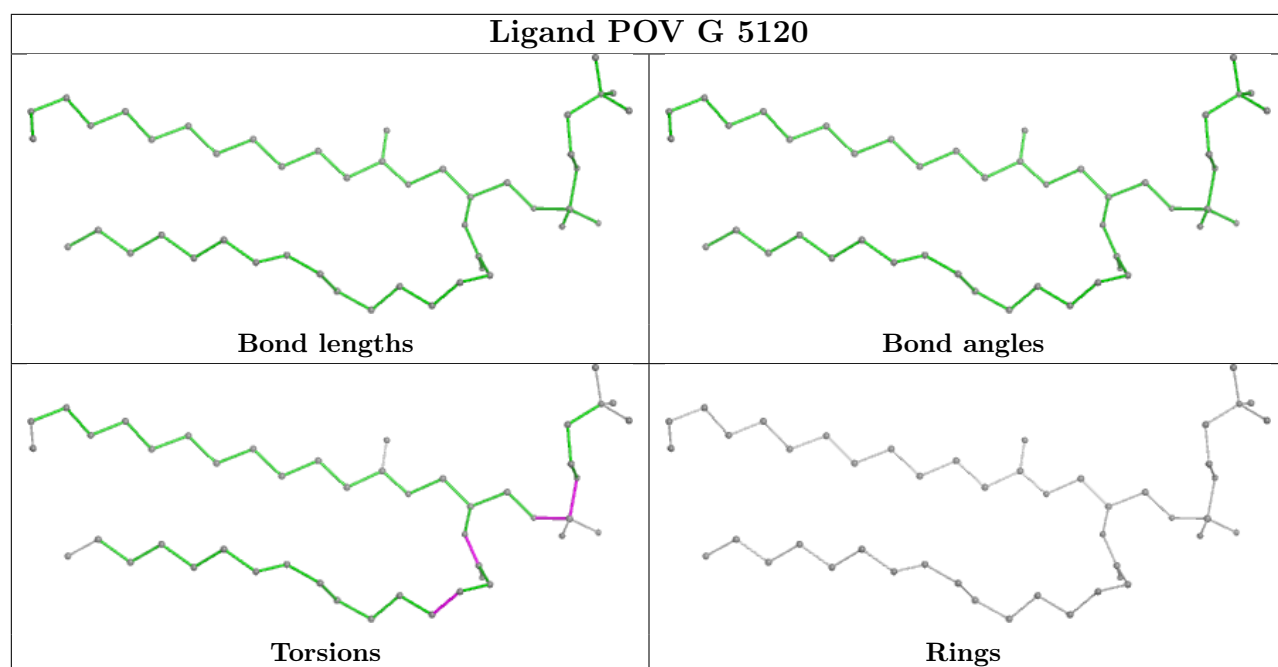
Mol	Chain	Res	Type	Atoms
8	A	5105	POV	C1-O11-P-O14
8	A	5105	POV	C11-O12-P-O11
8	A	5105	POV	C11-O12-P-O14
8	A	5105	POV	O12-C11-C12-N
8	A	5106	POV	C1-O11-P-O13

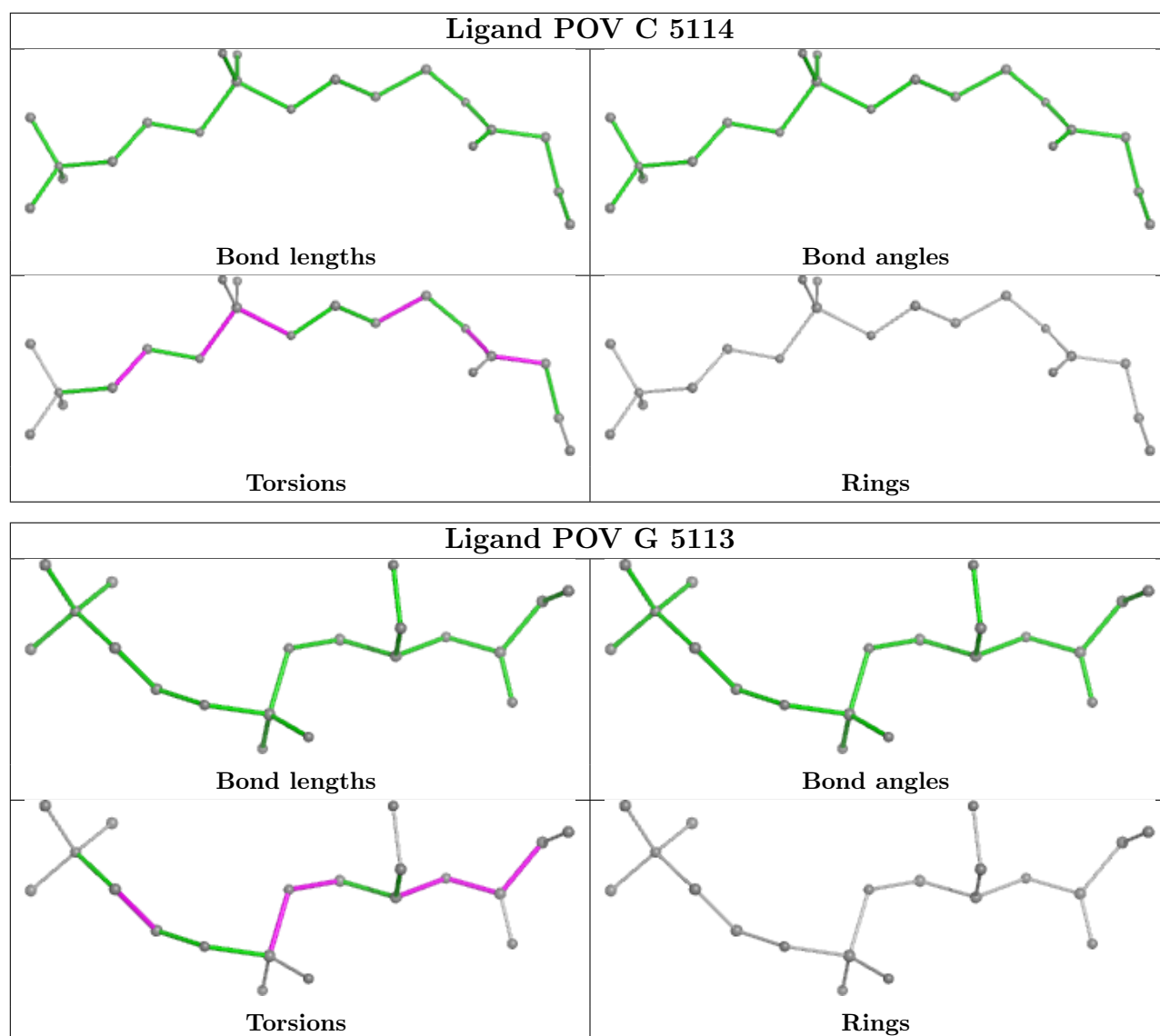
There are no ring outliers.

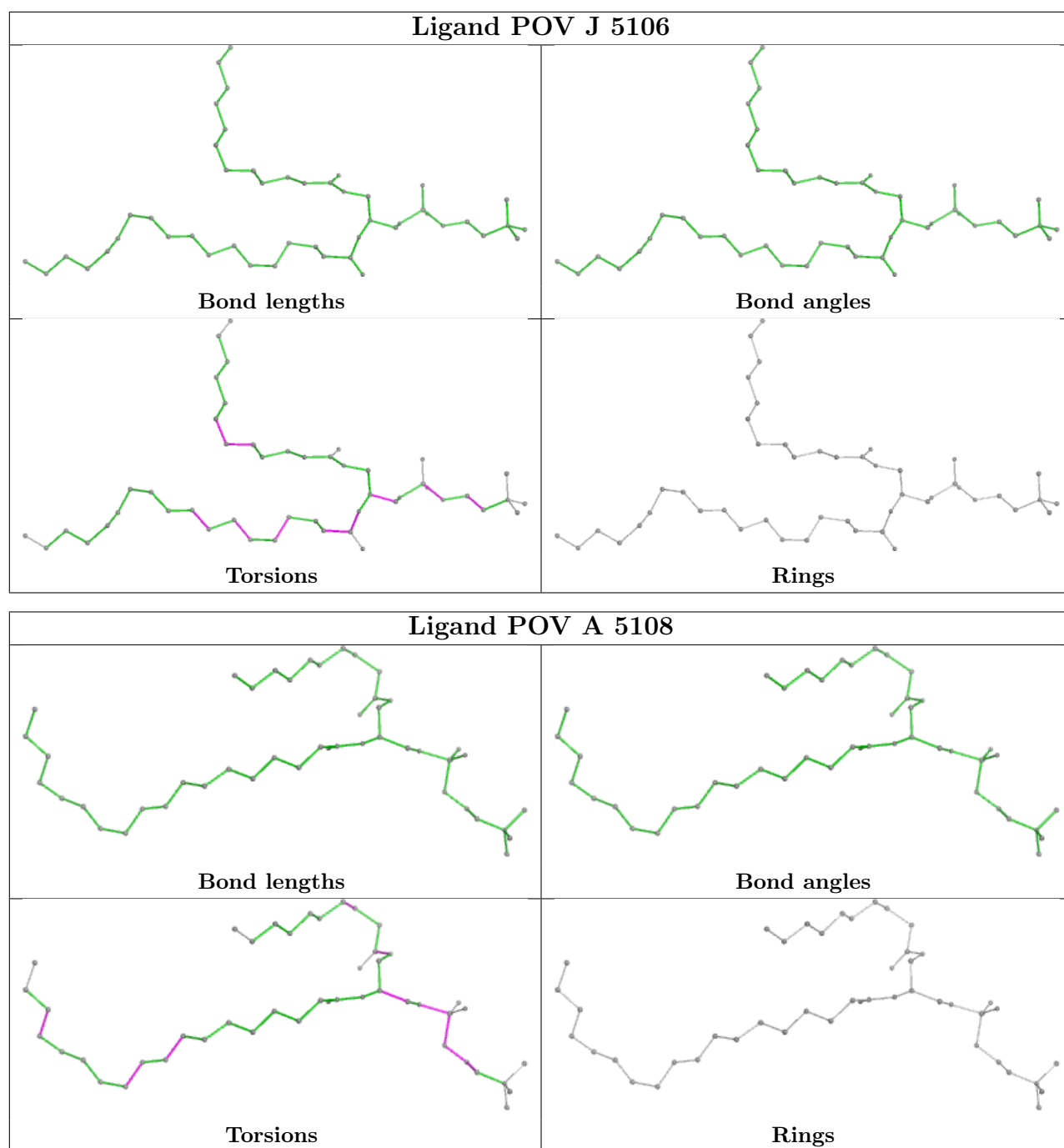
No monomer is involved in short contacts.

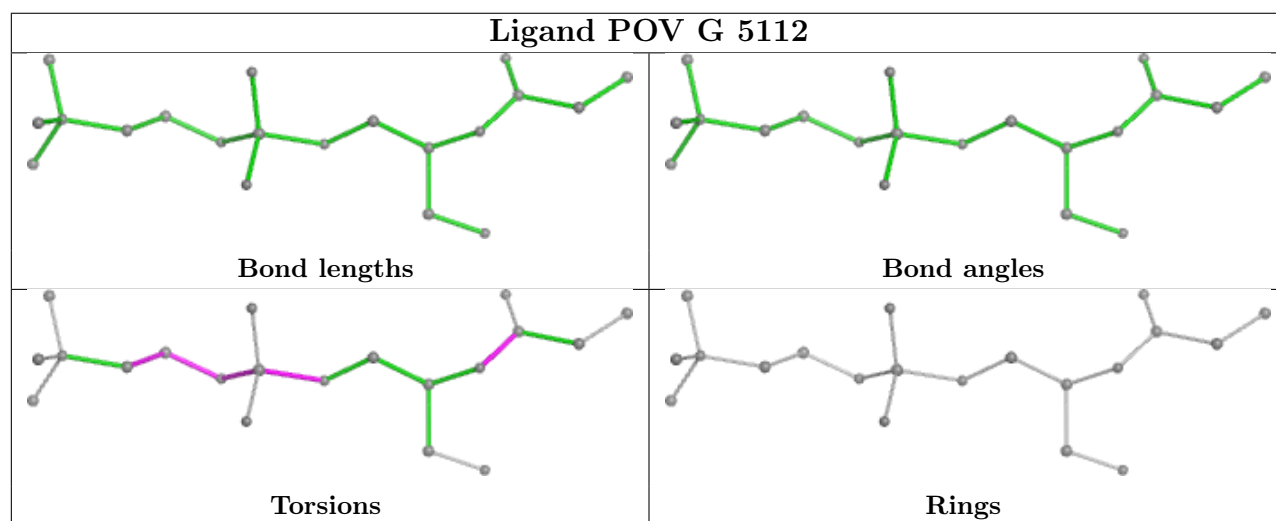
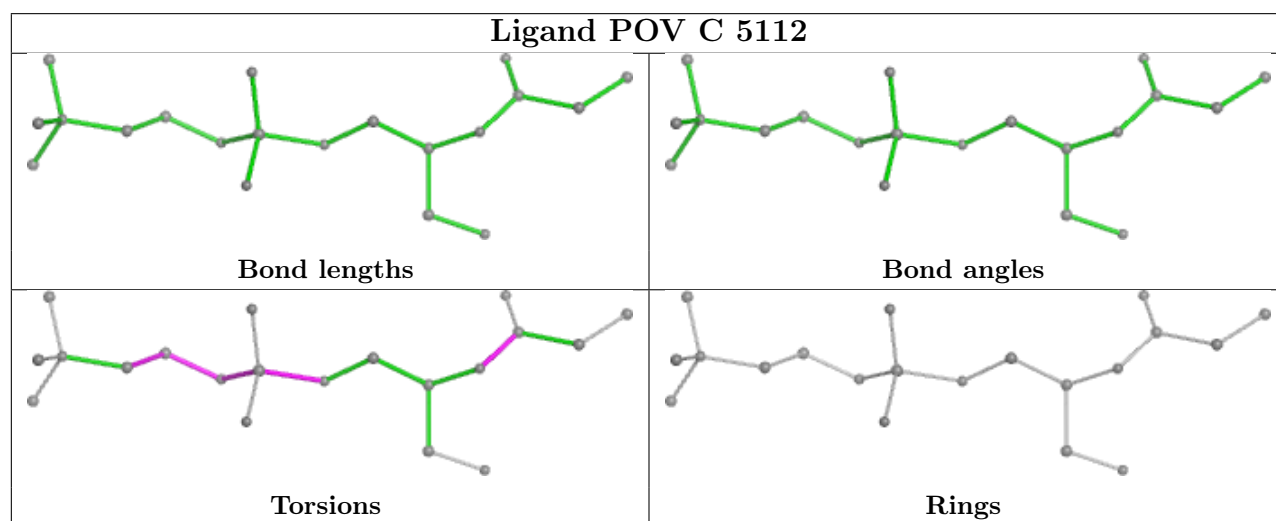
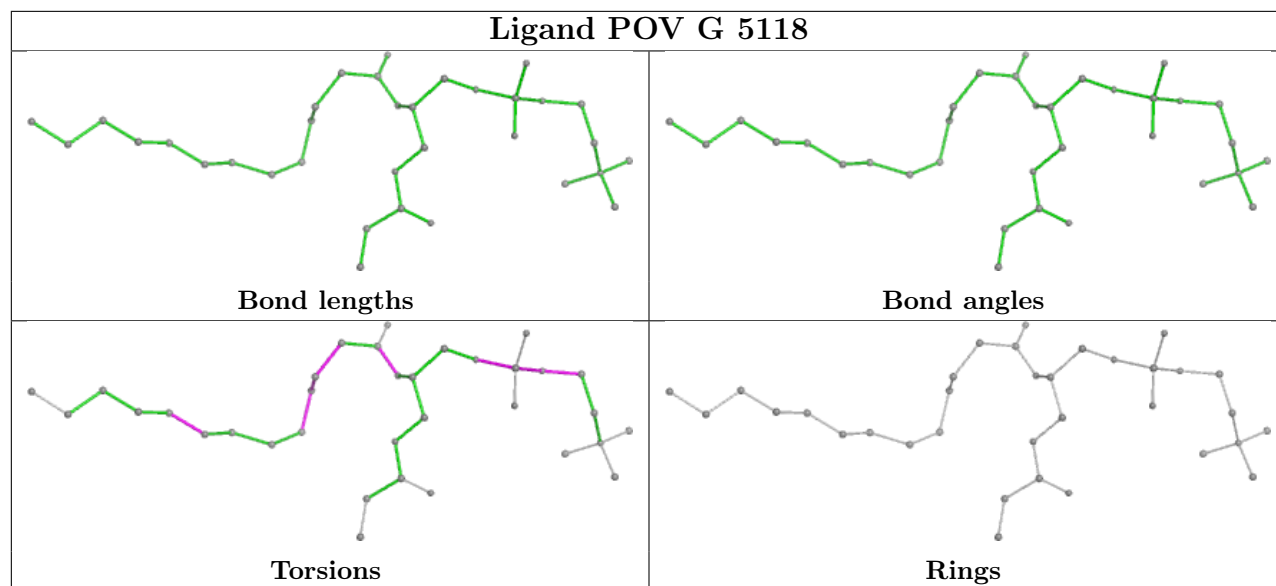
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

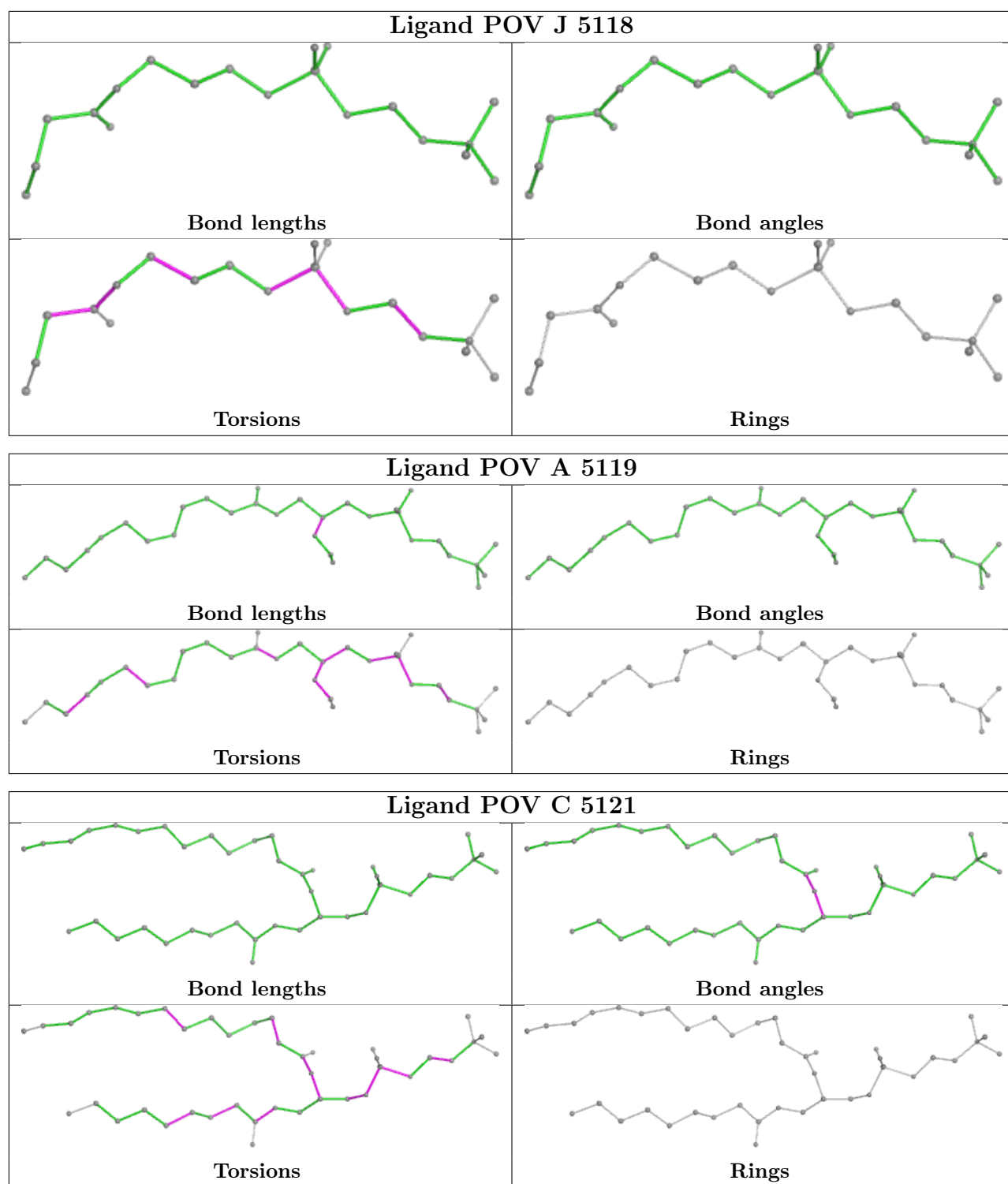




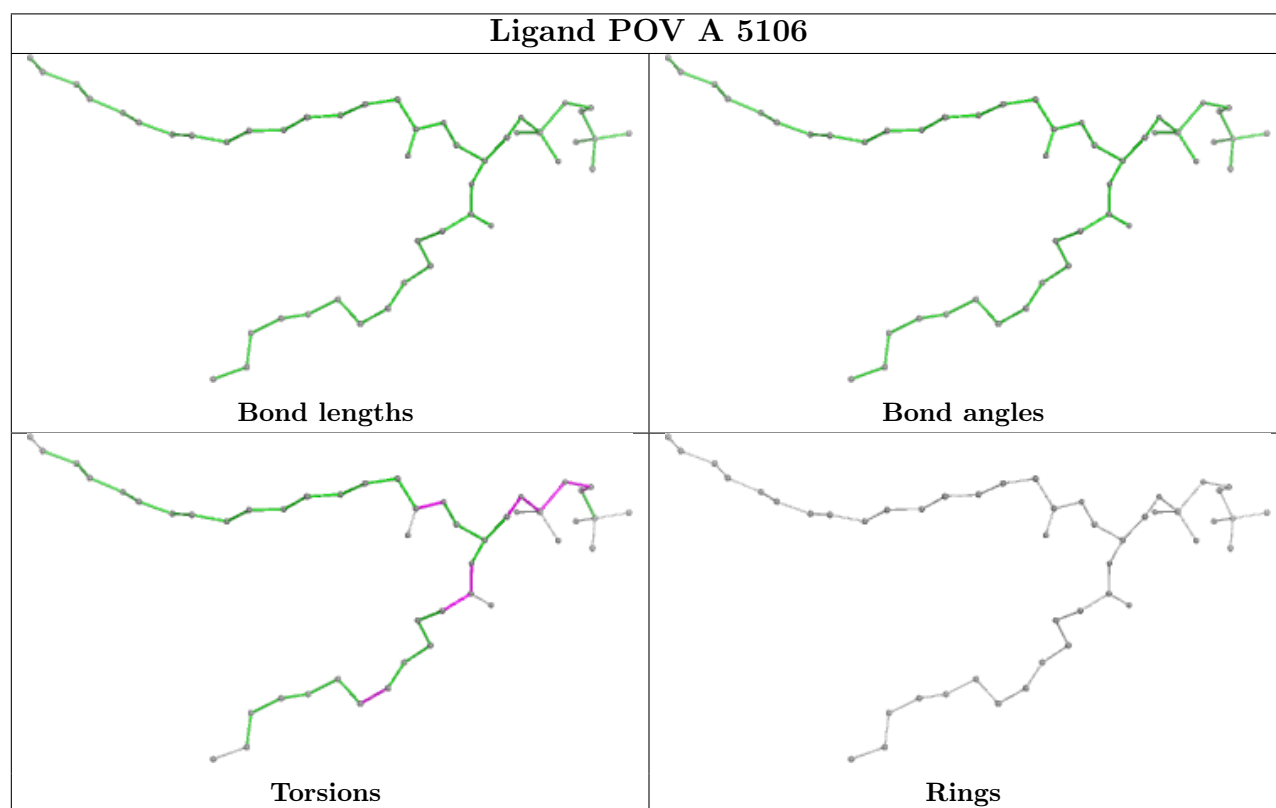
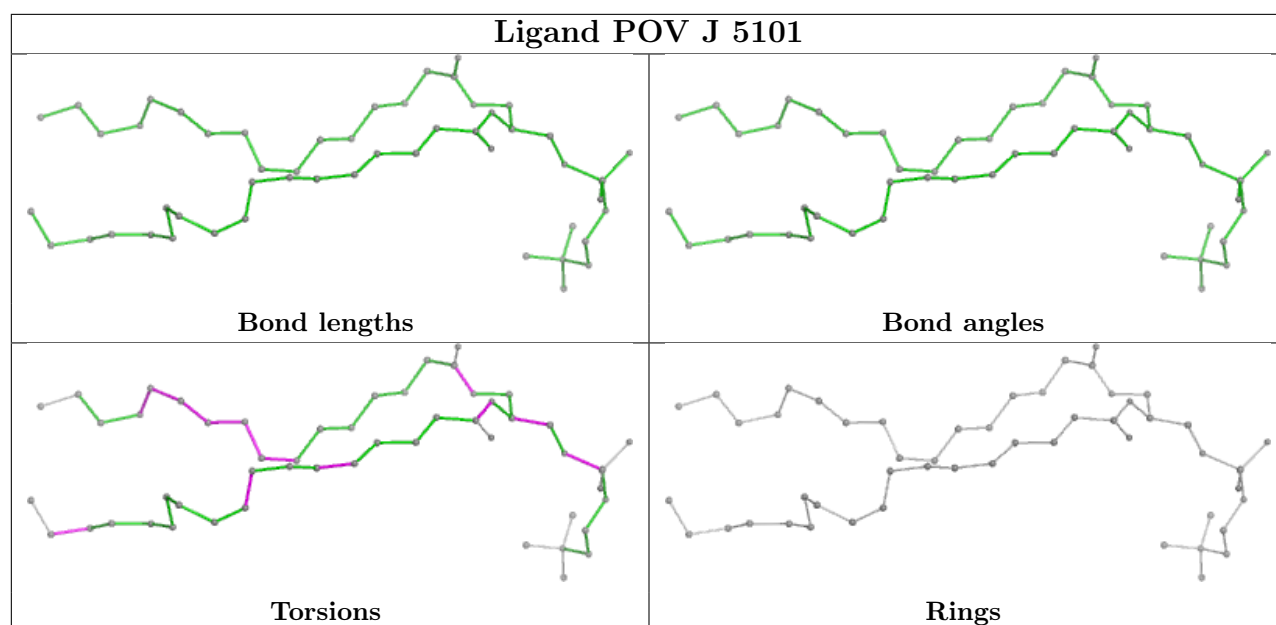


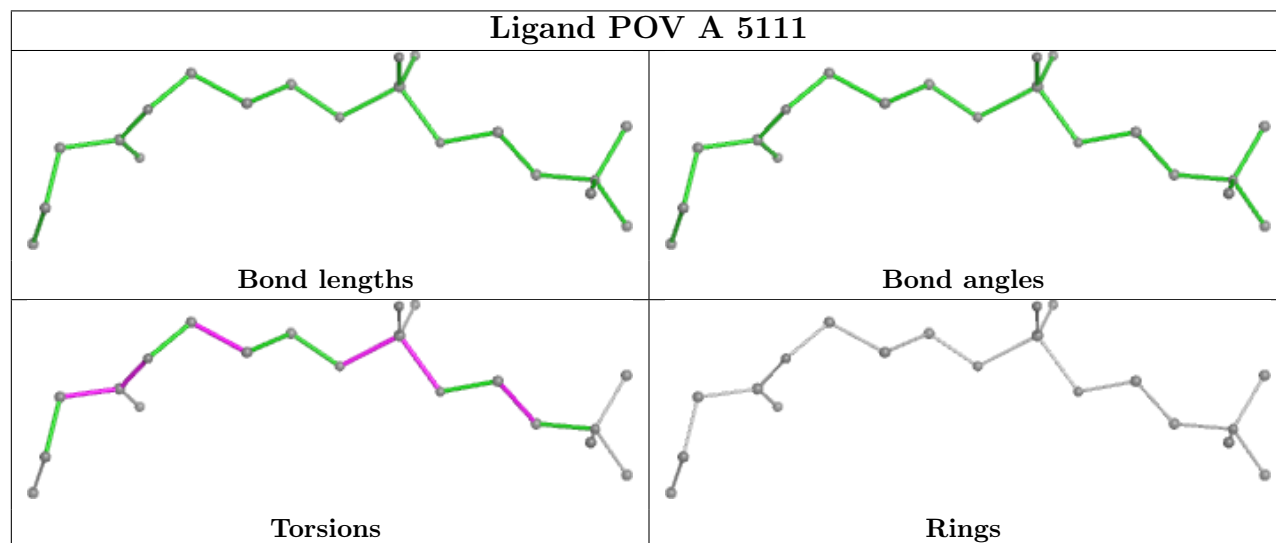
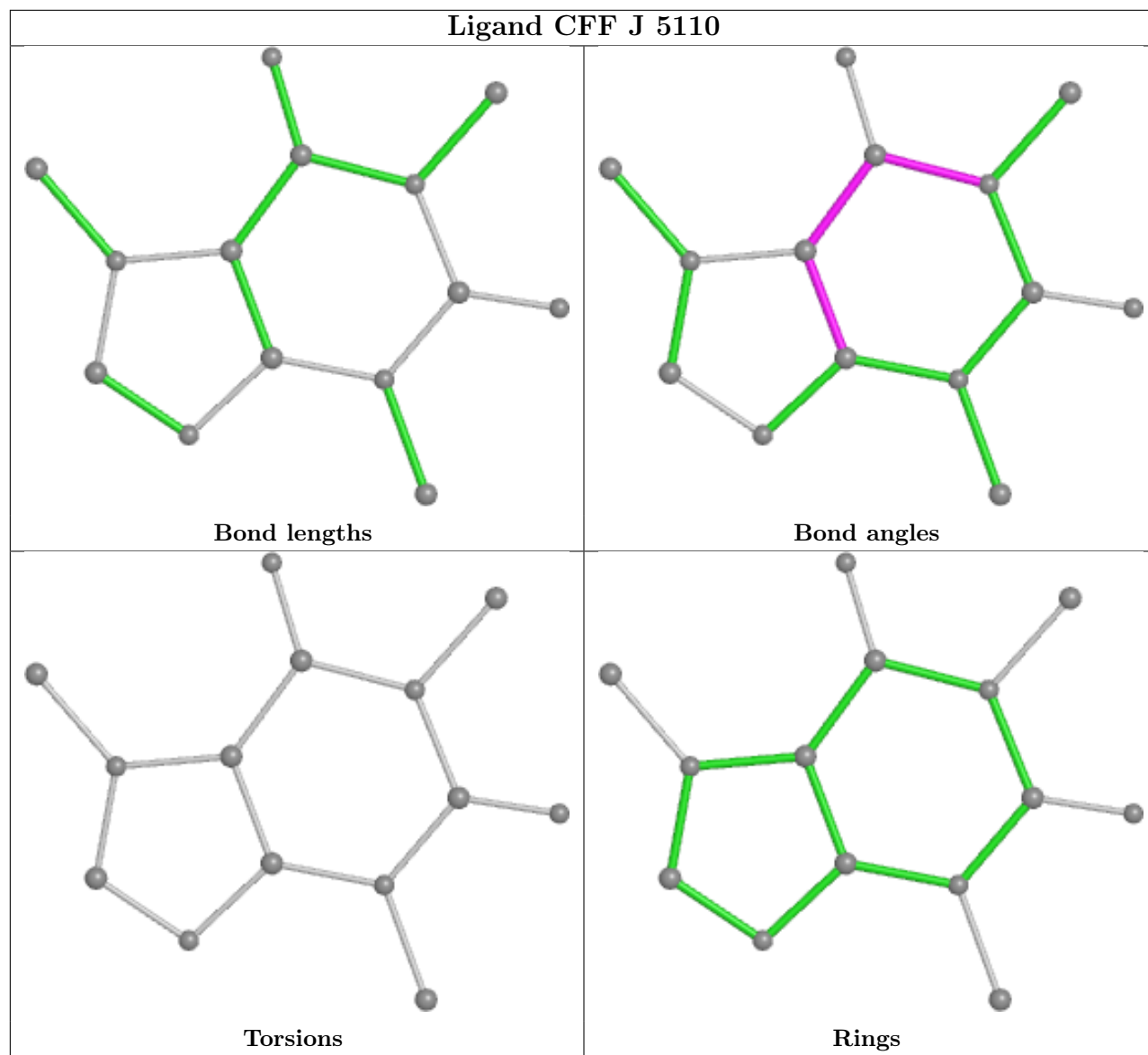


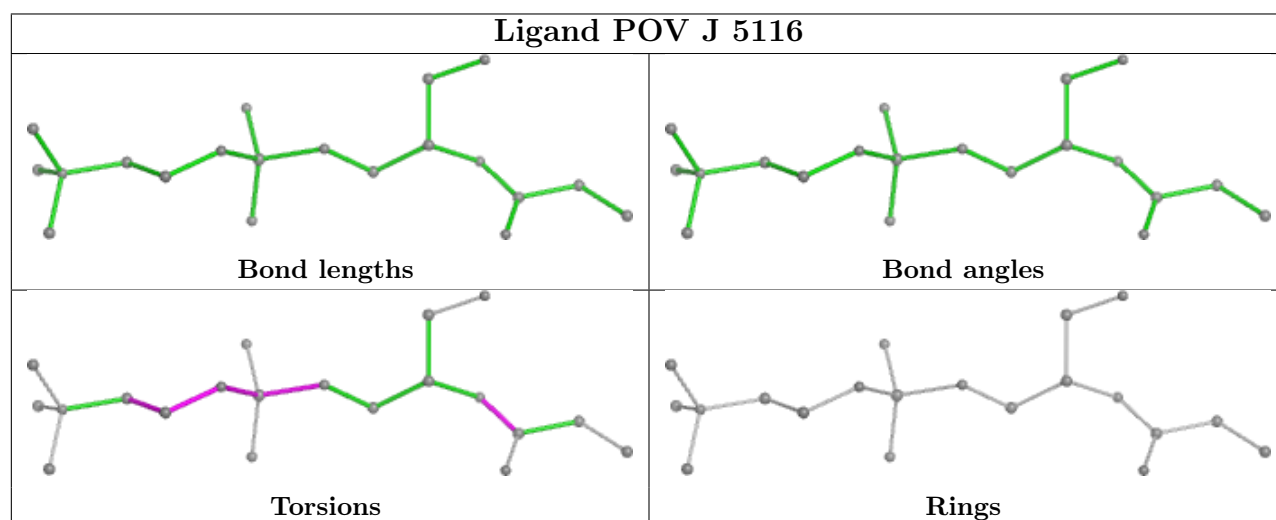
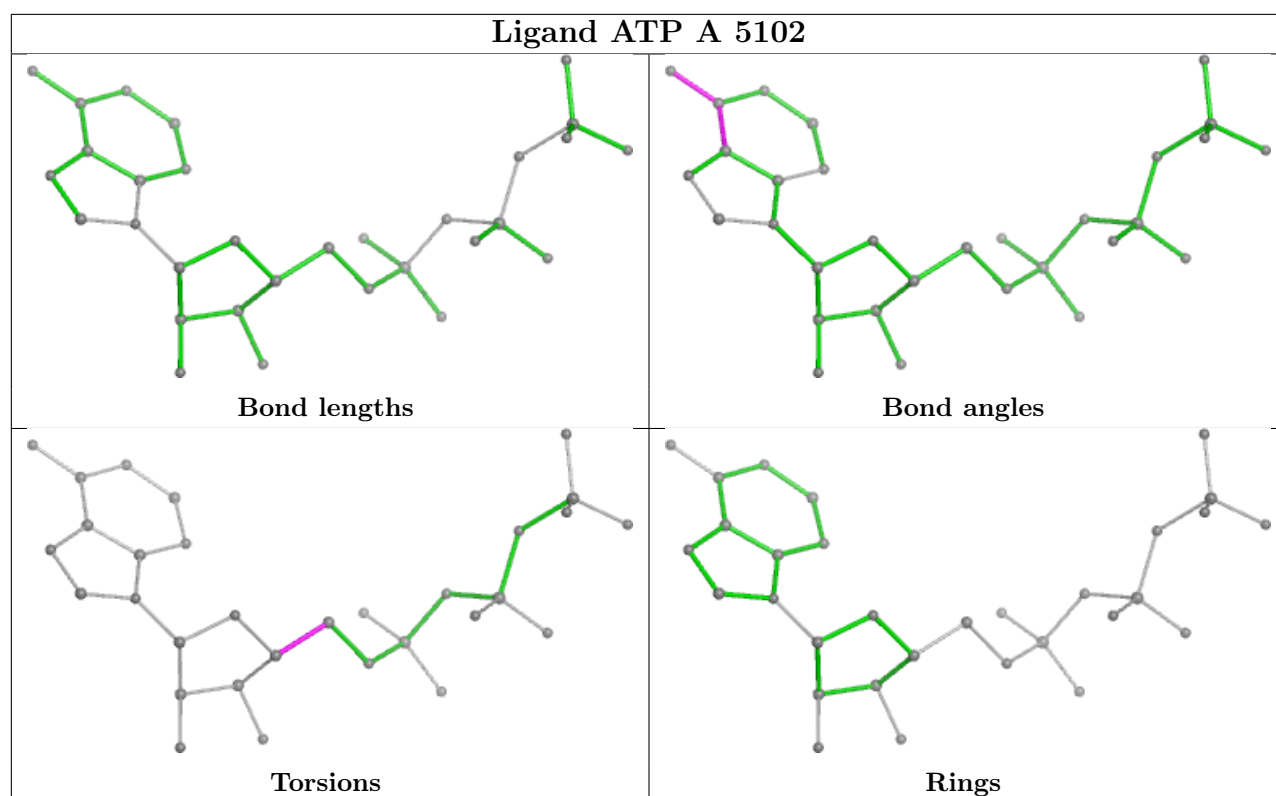


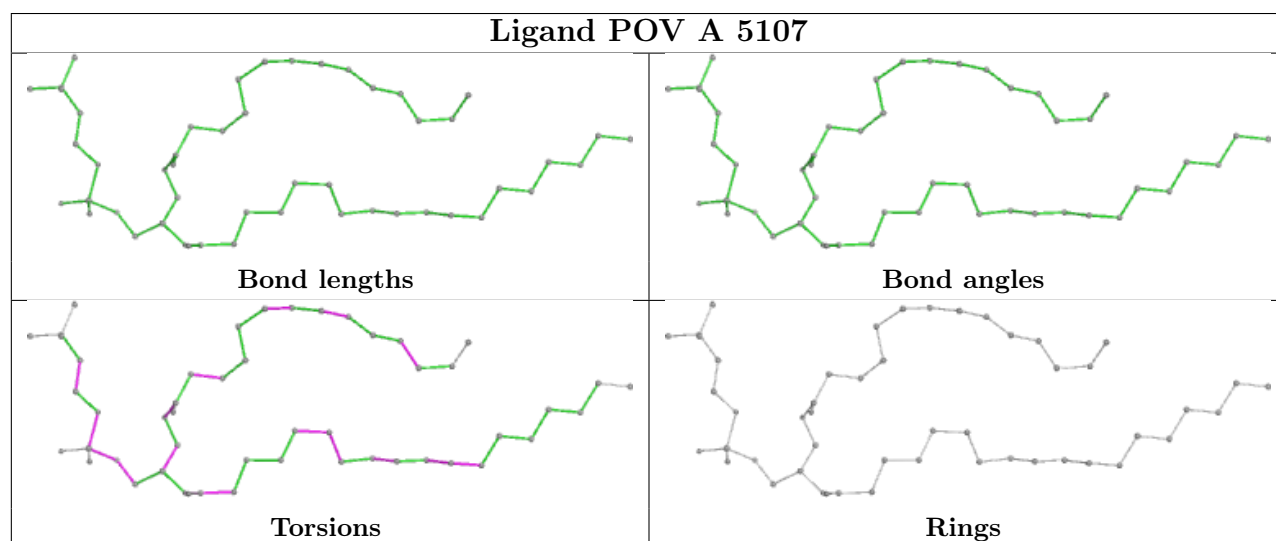
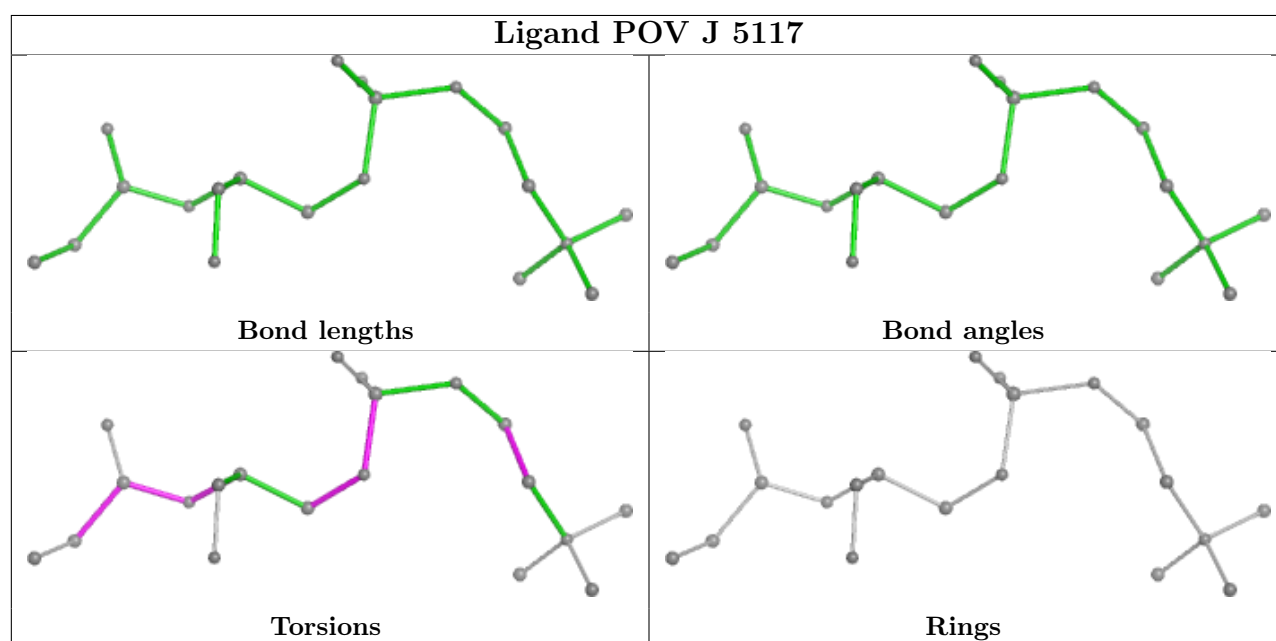
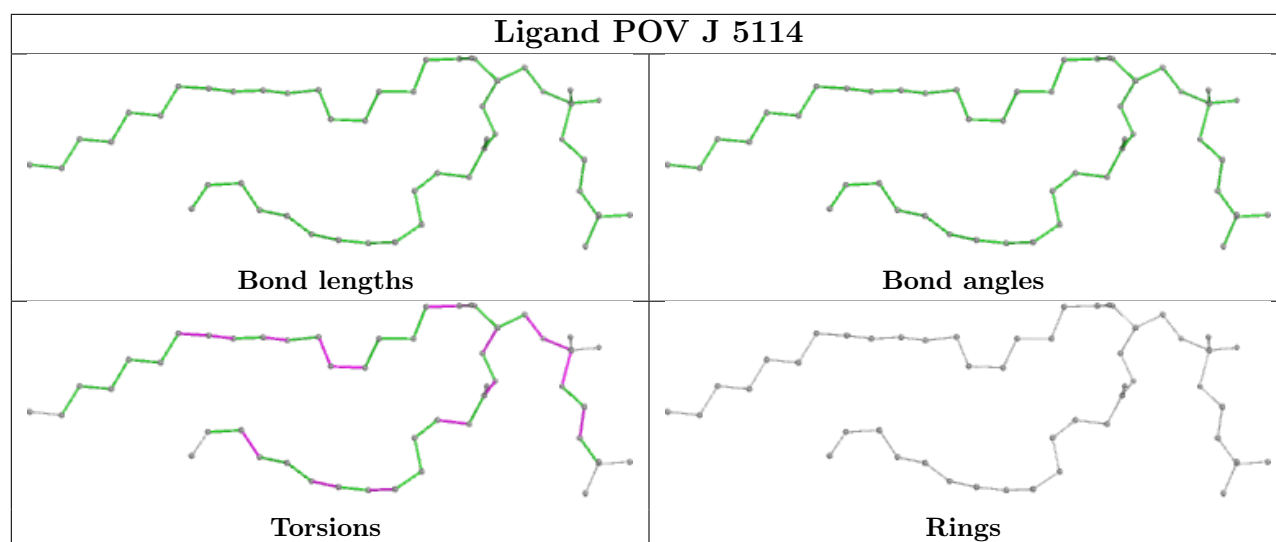


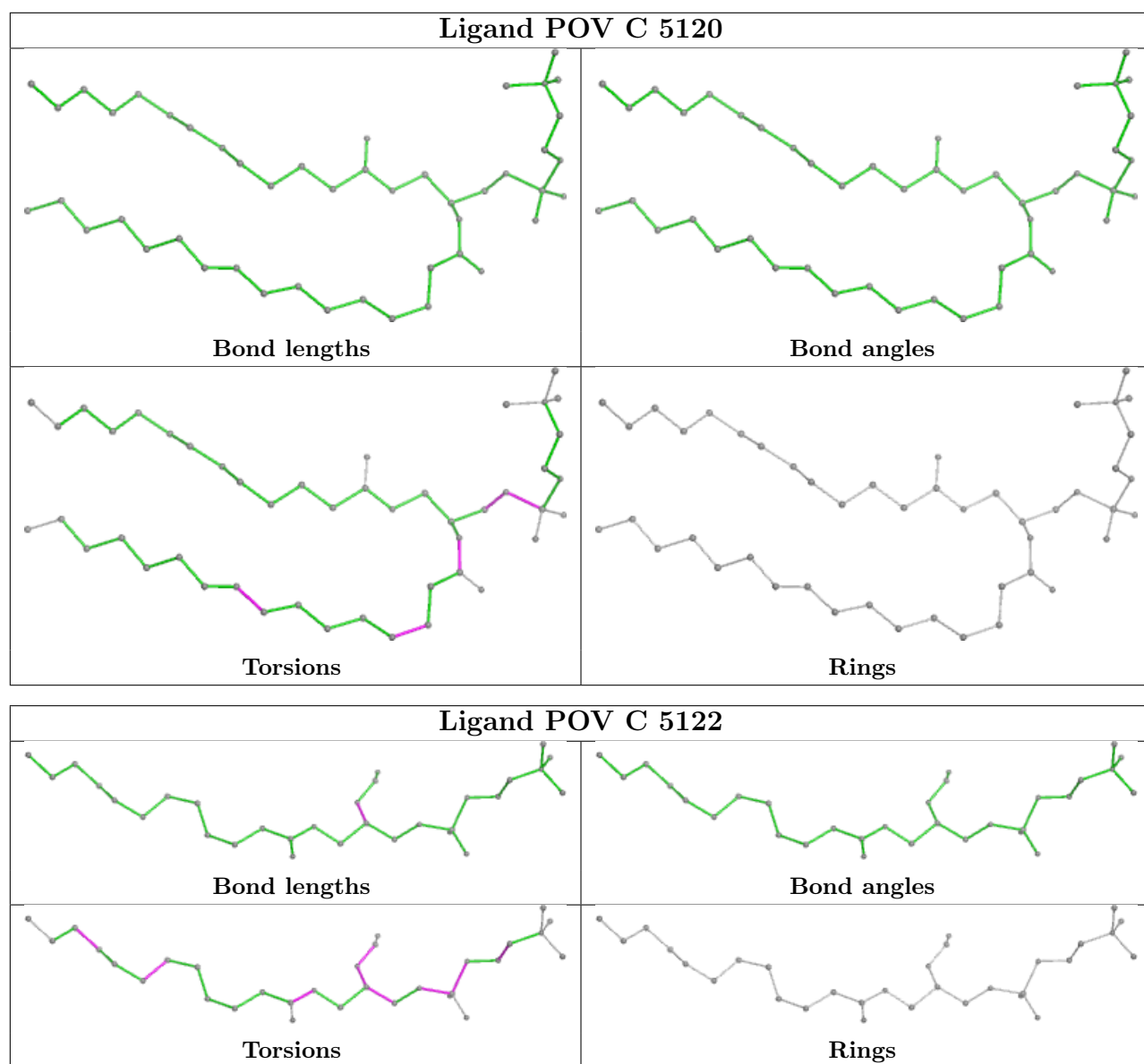


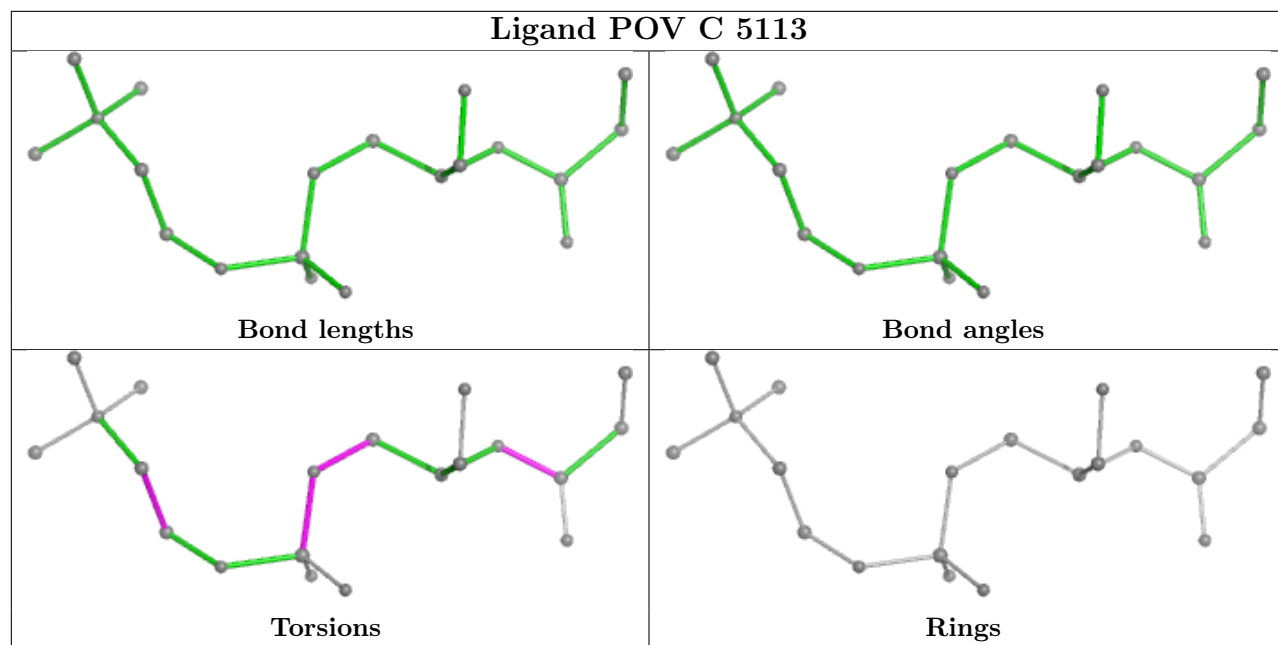


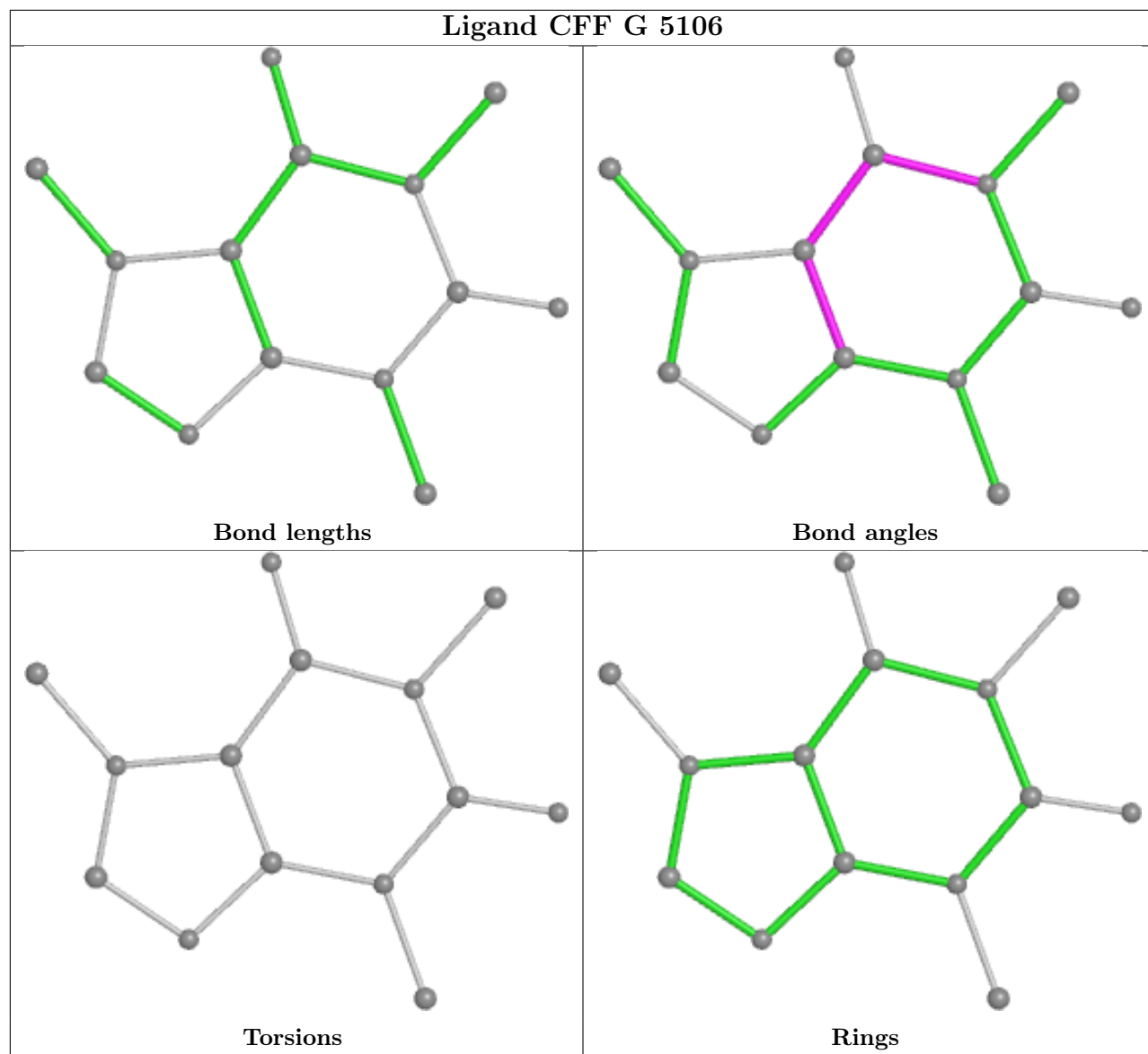


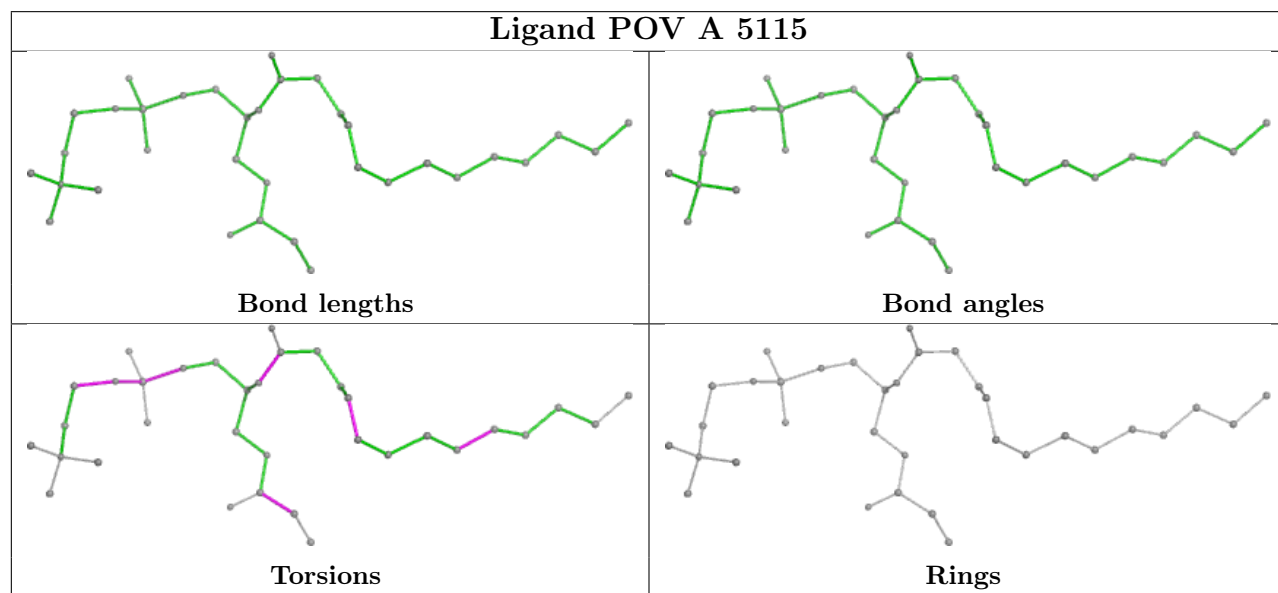
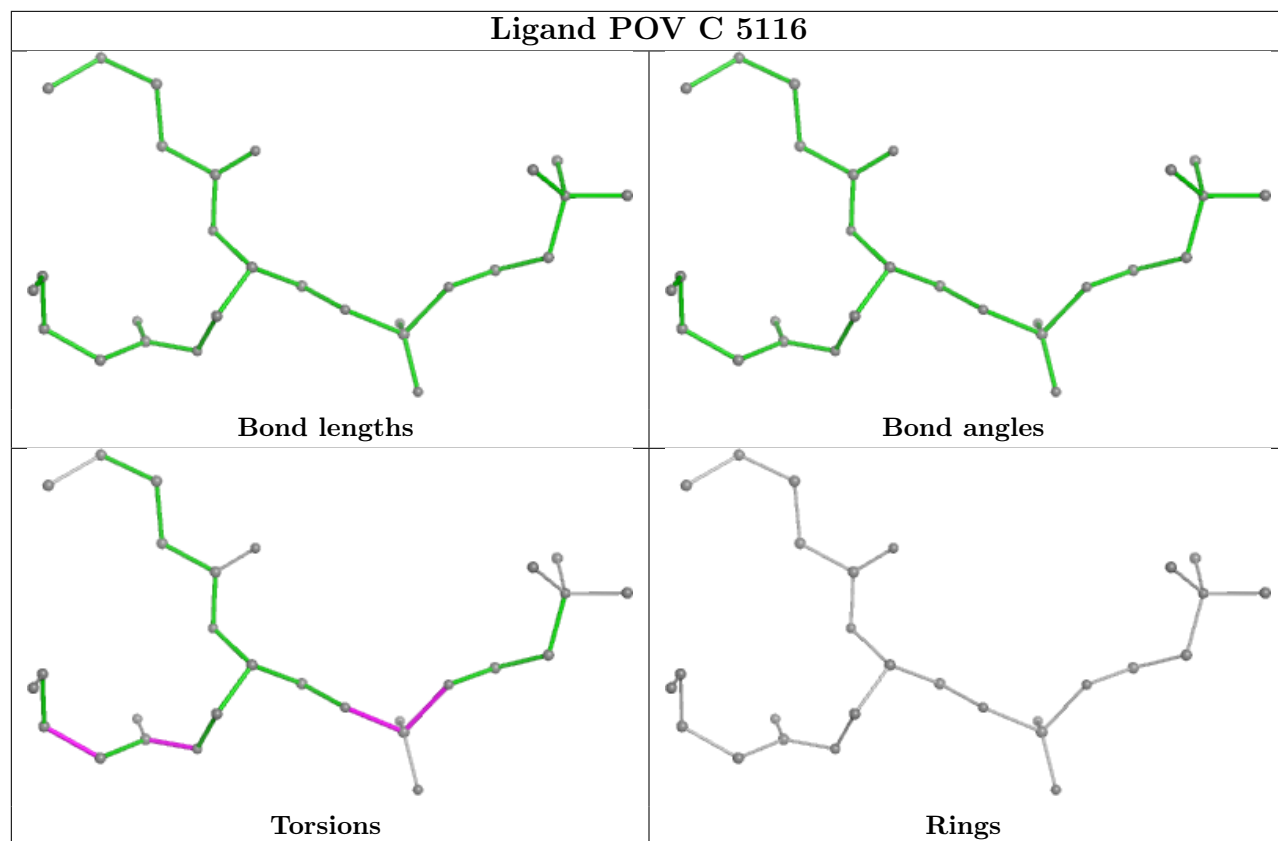




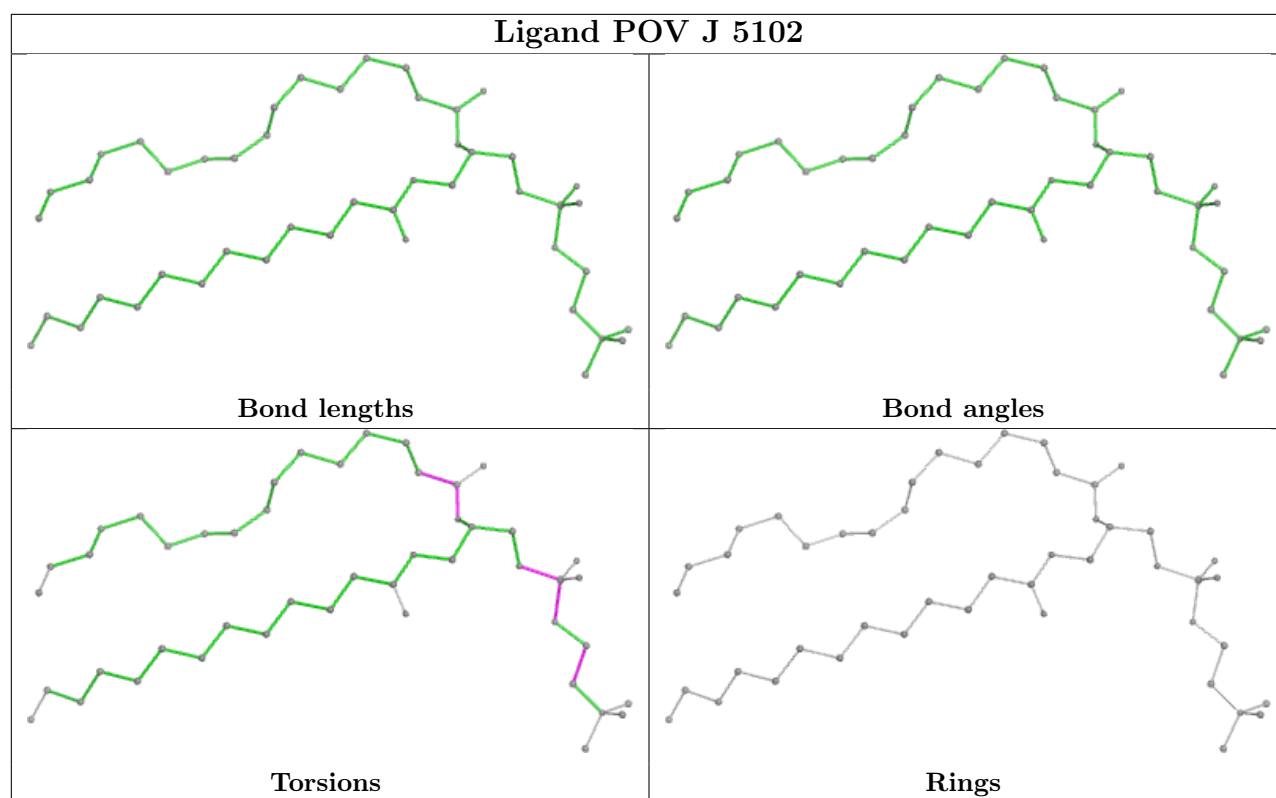


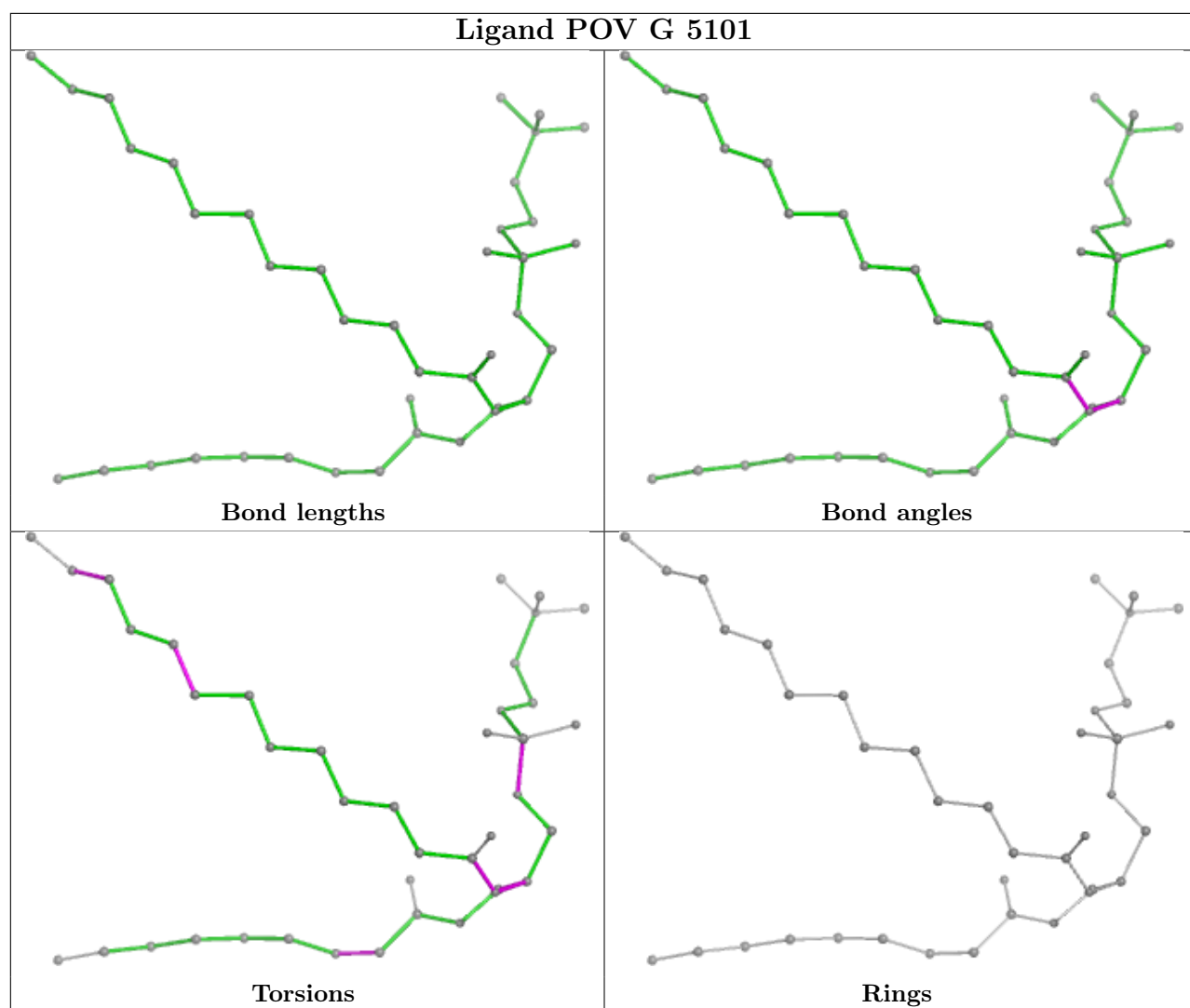


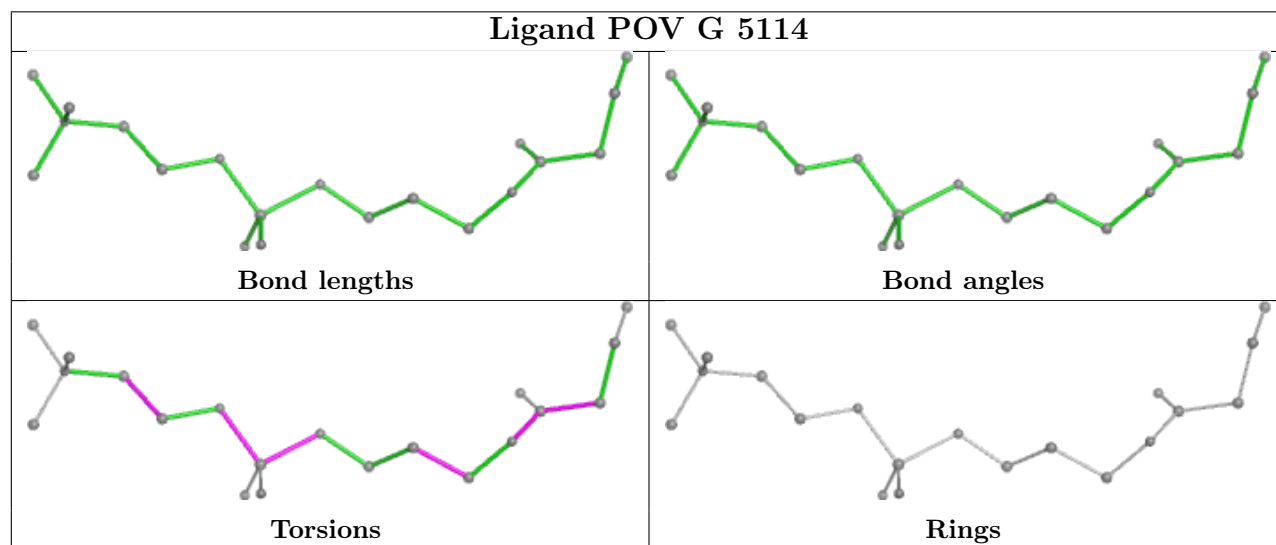
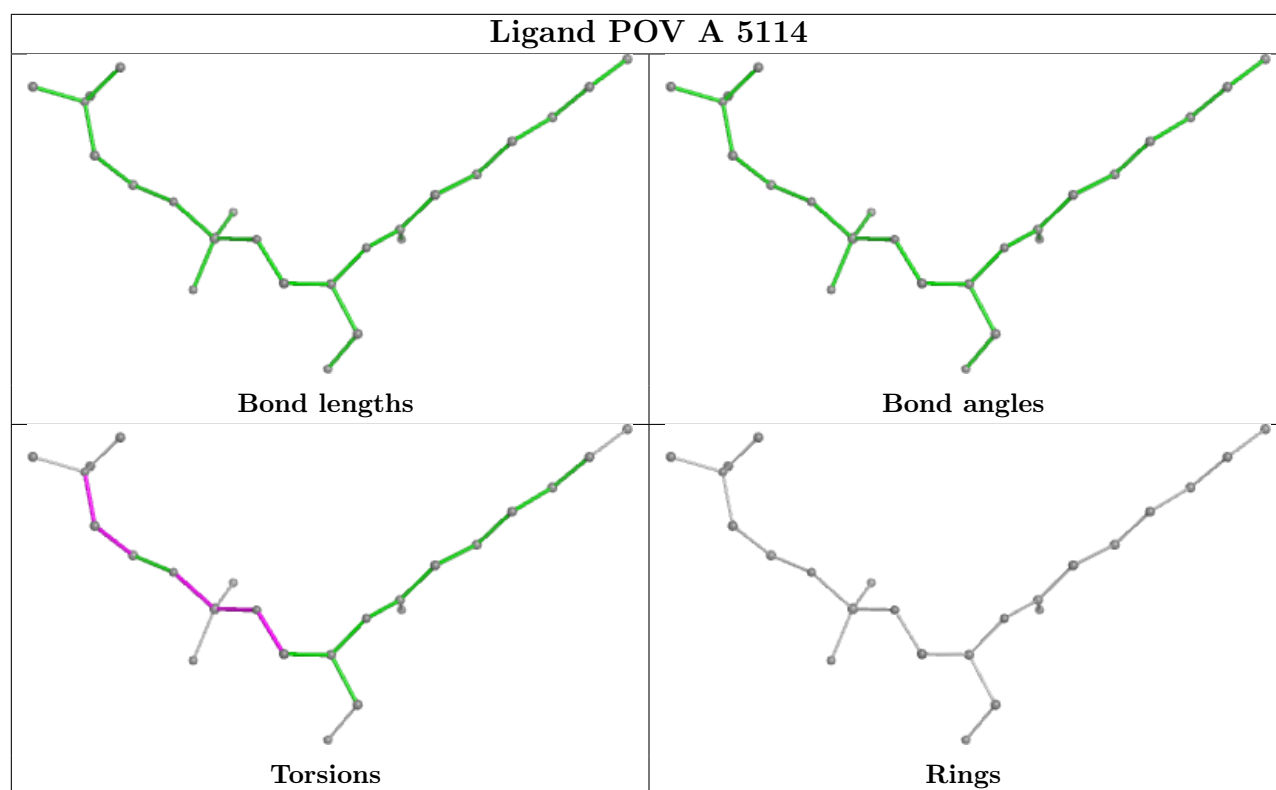


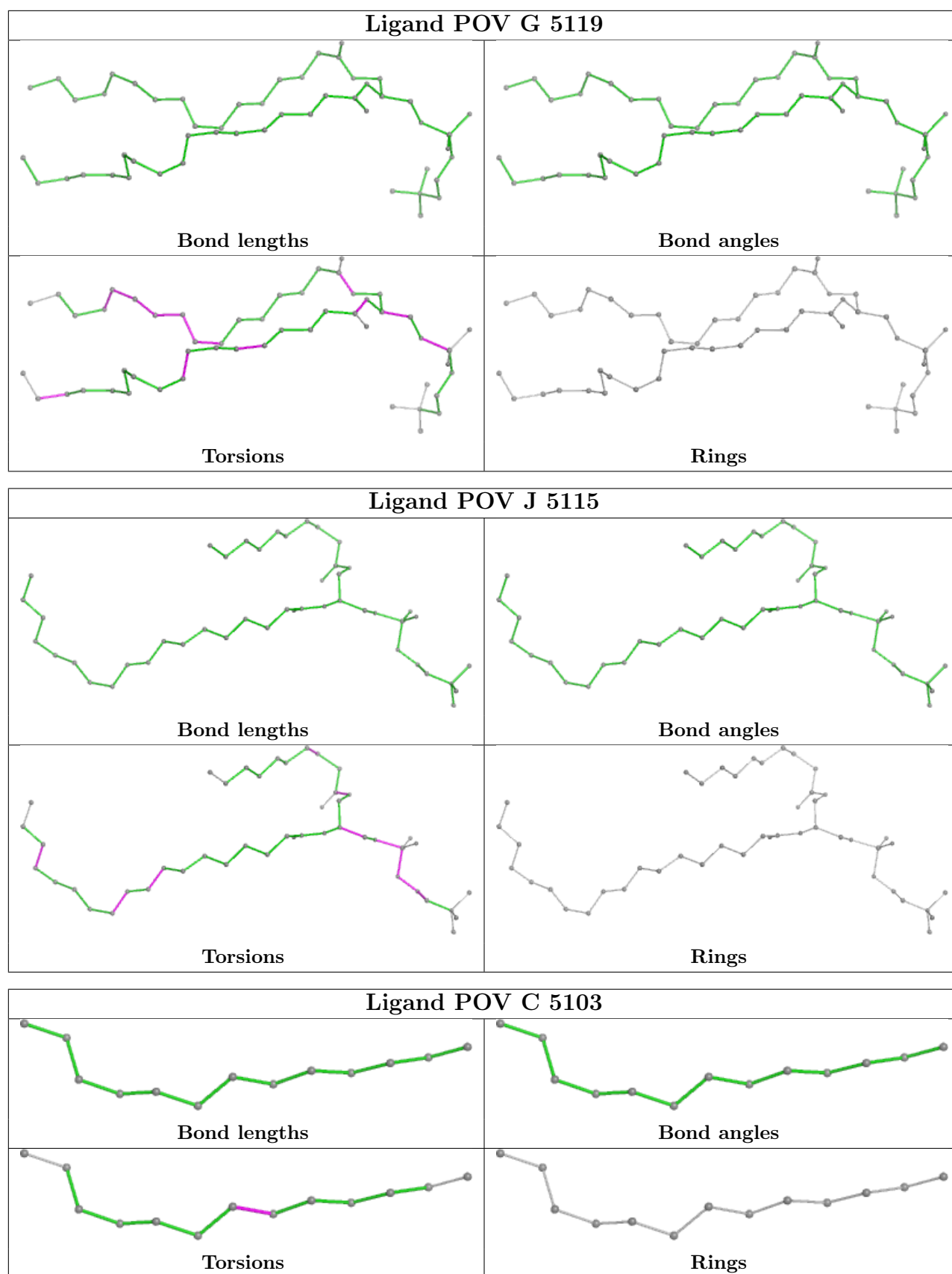


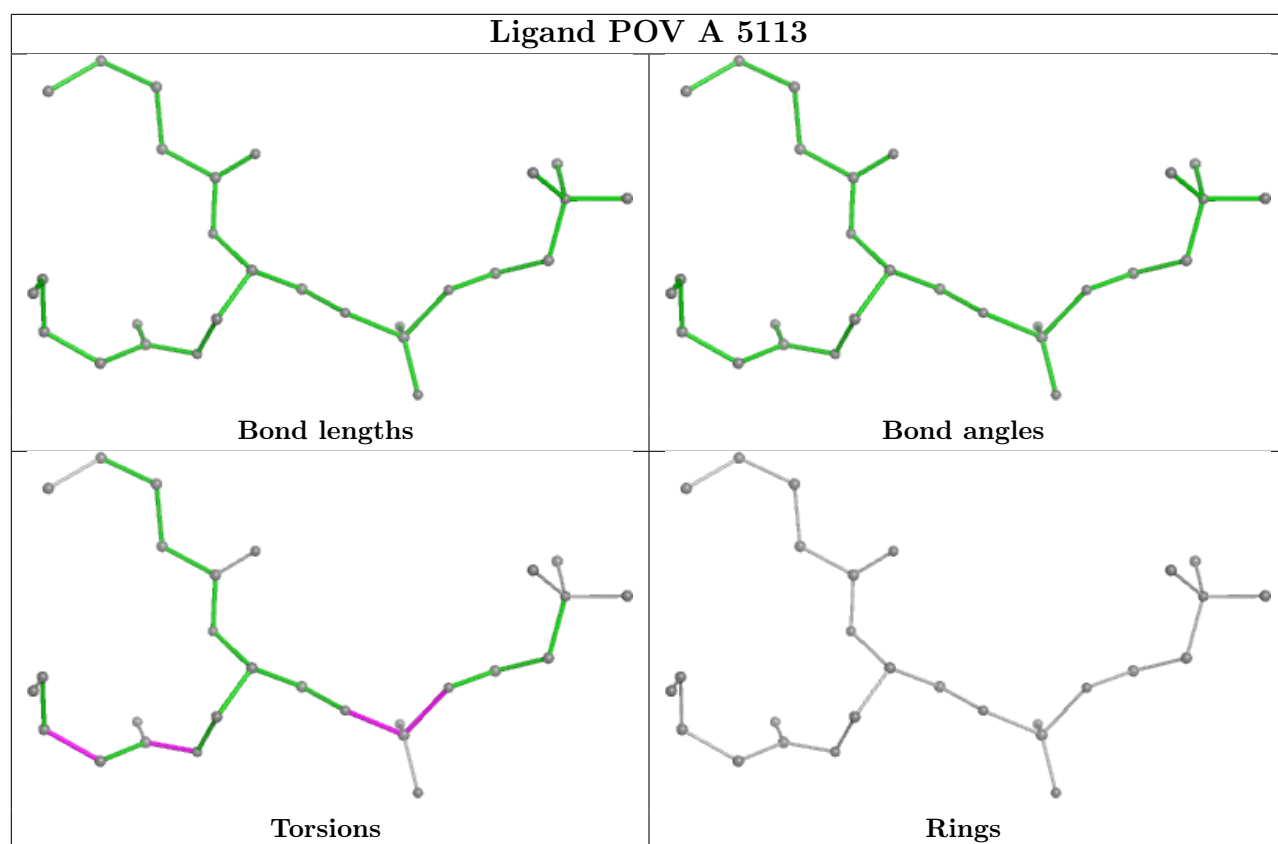


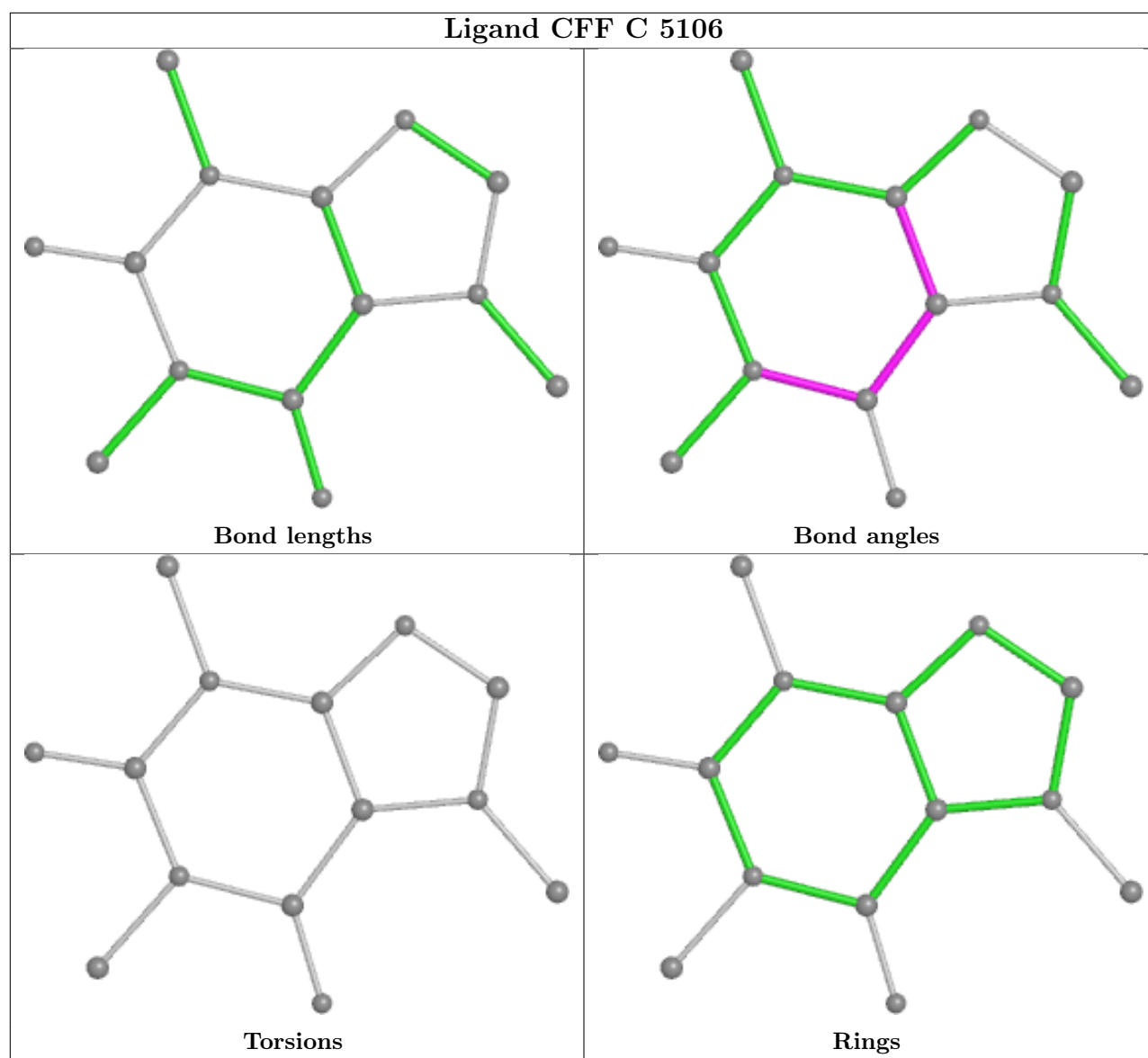


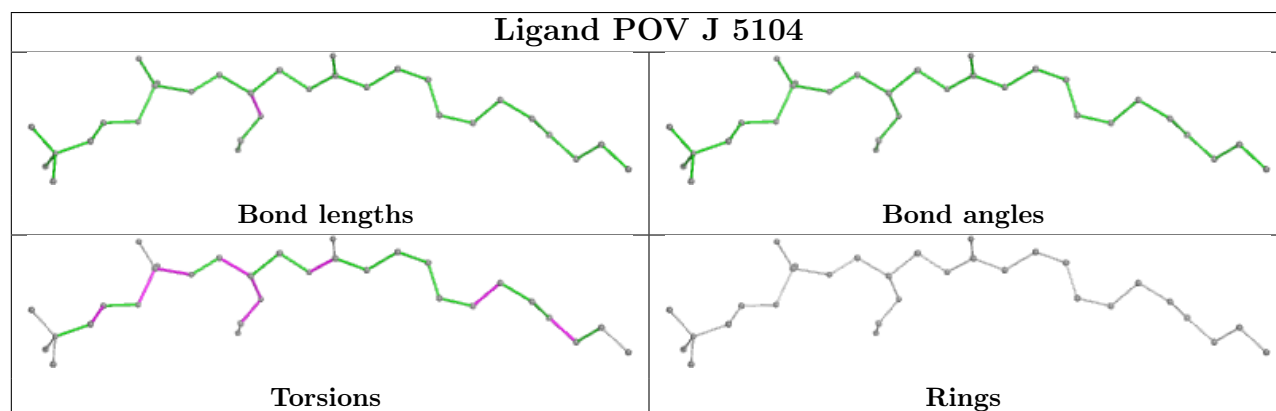
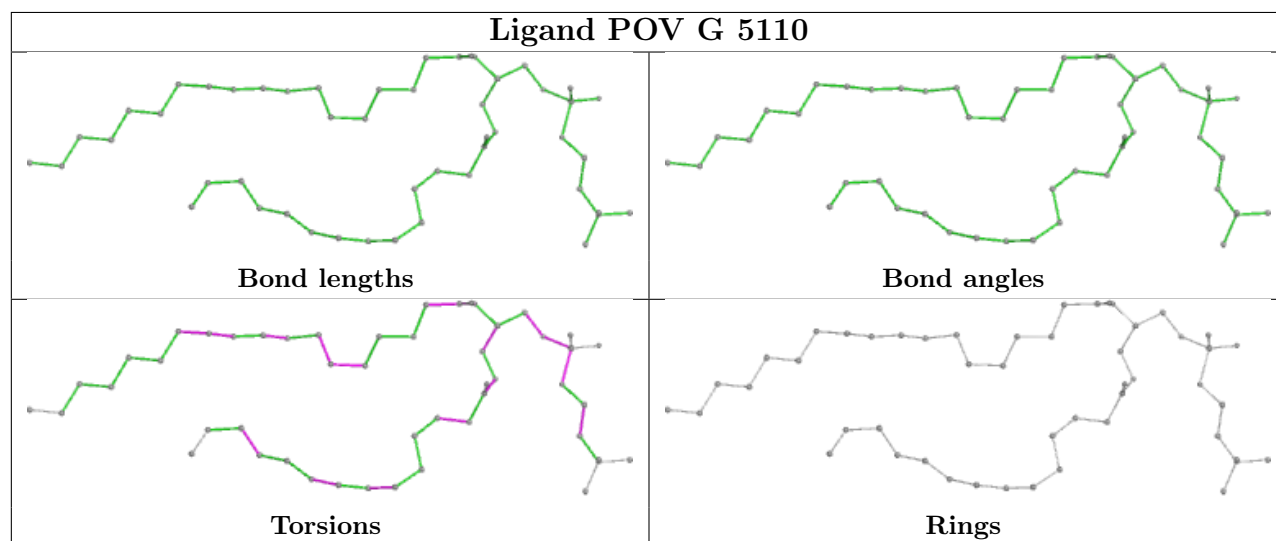
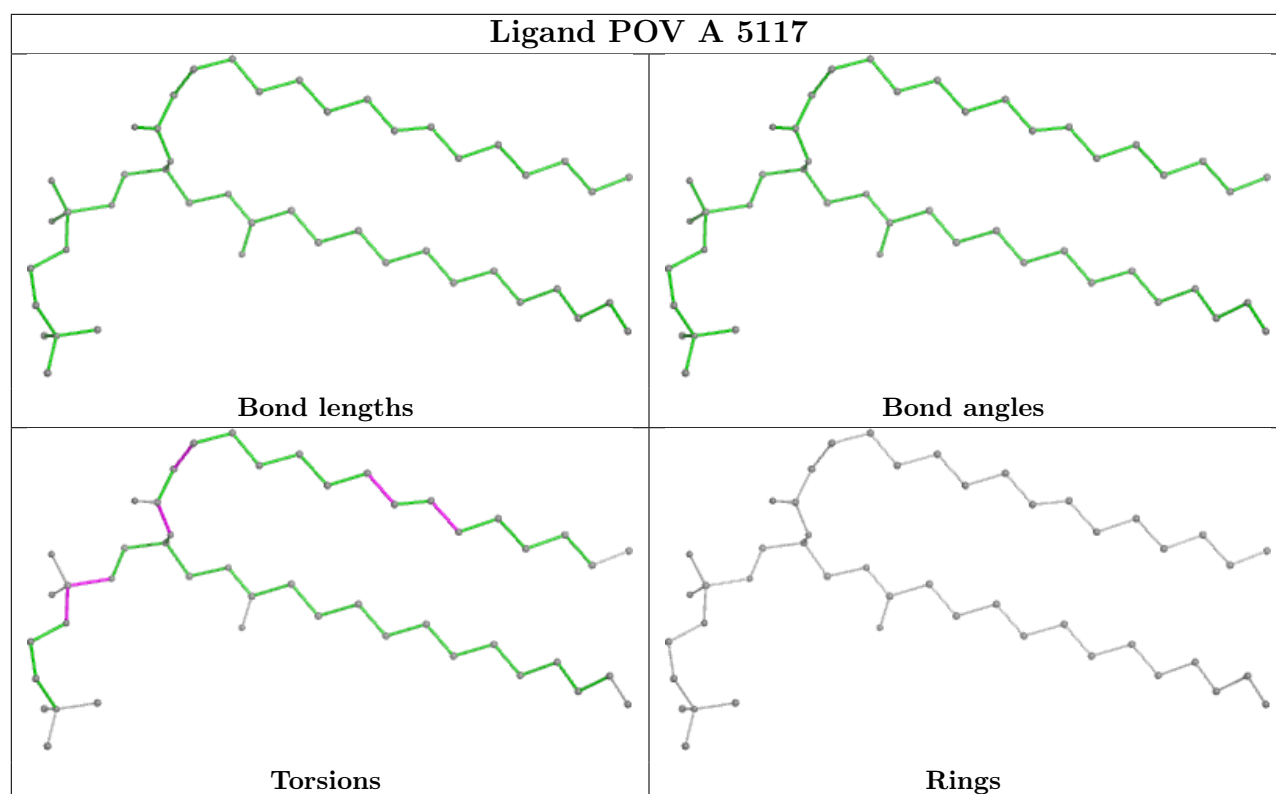


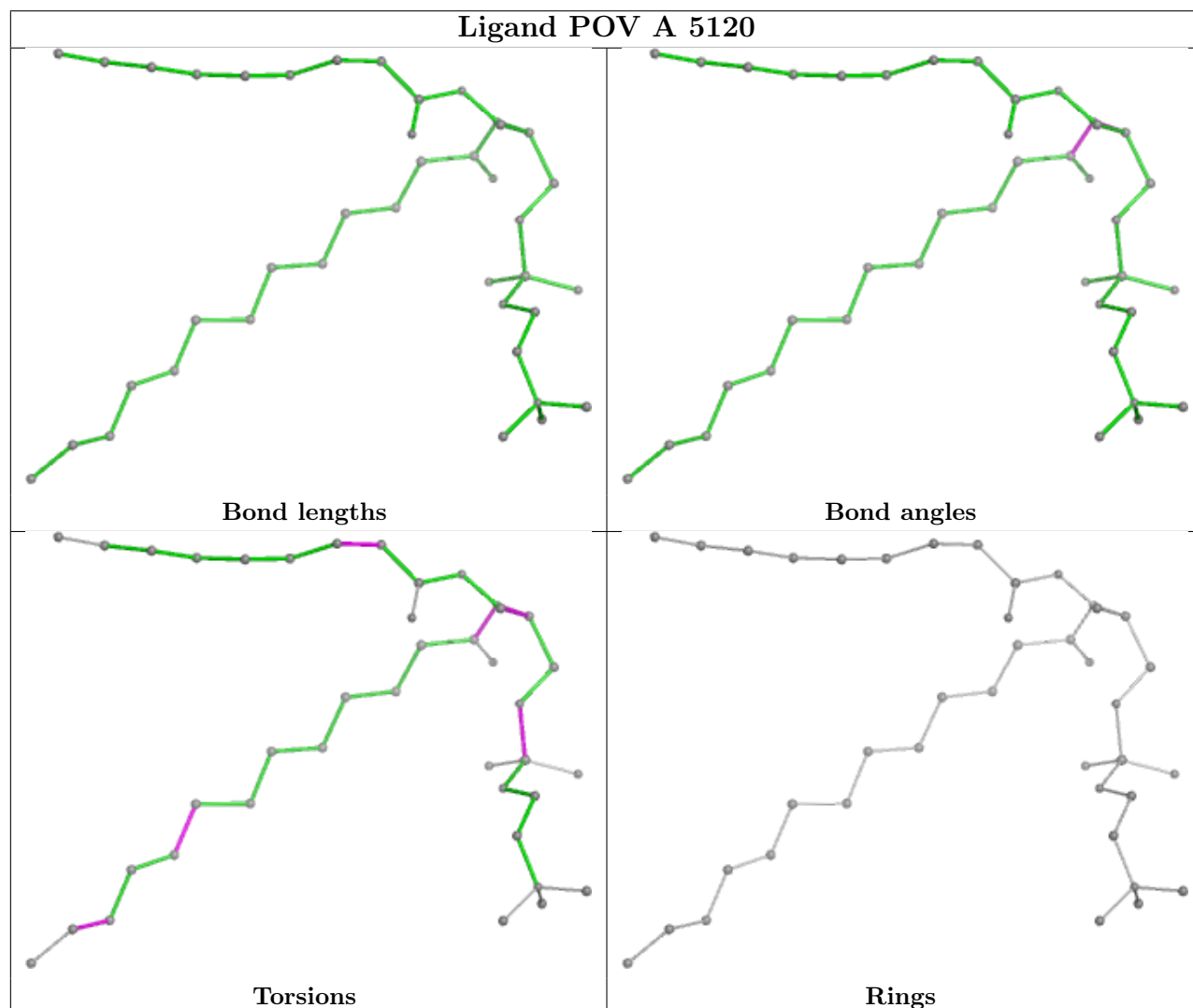
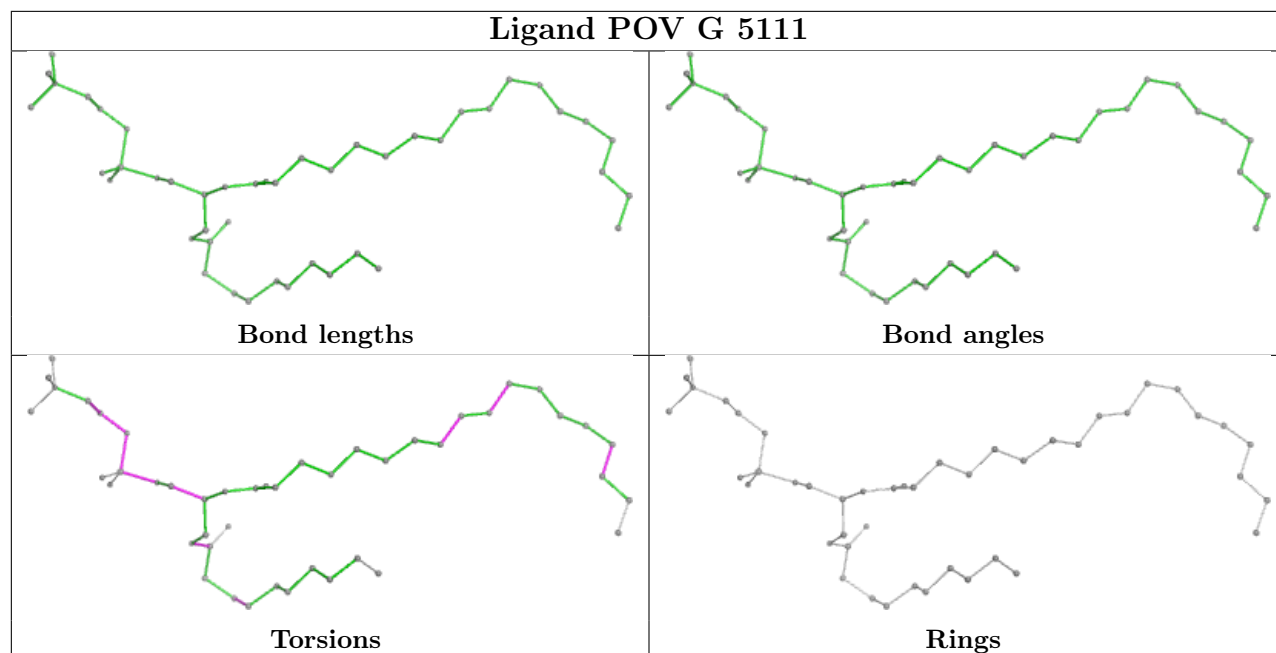




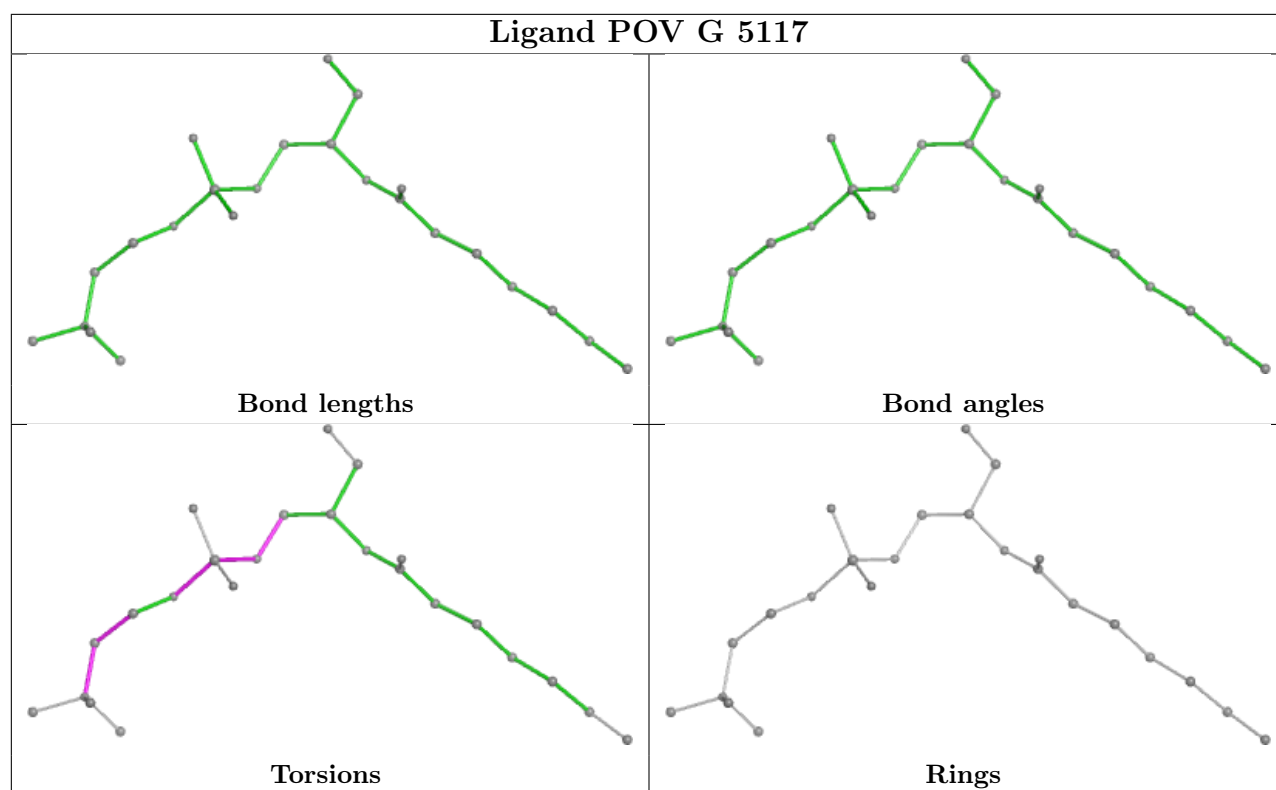


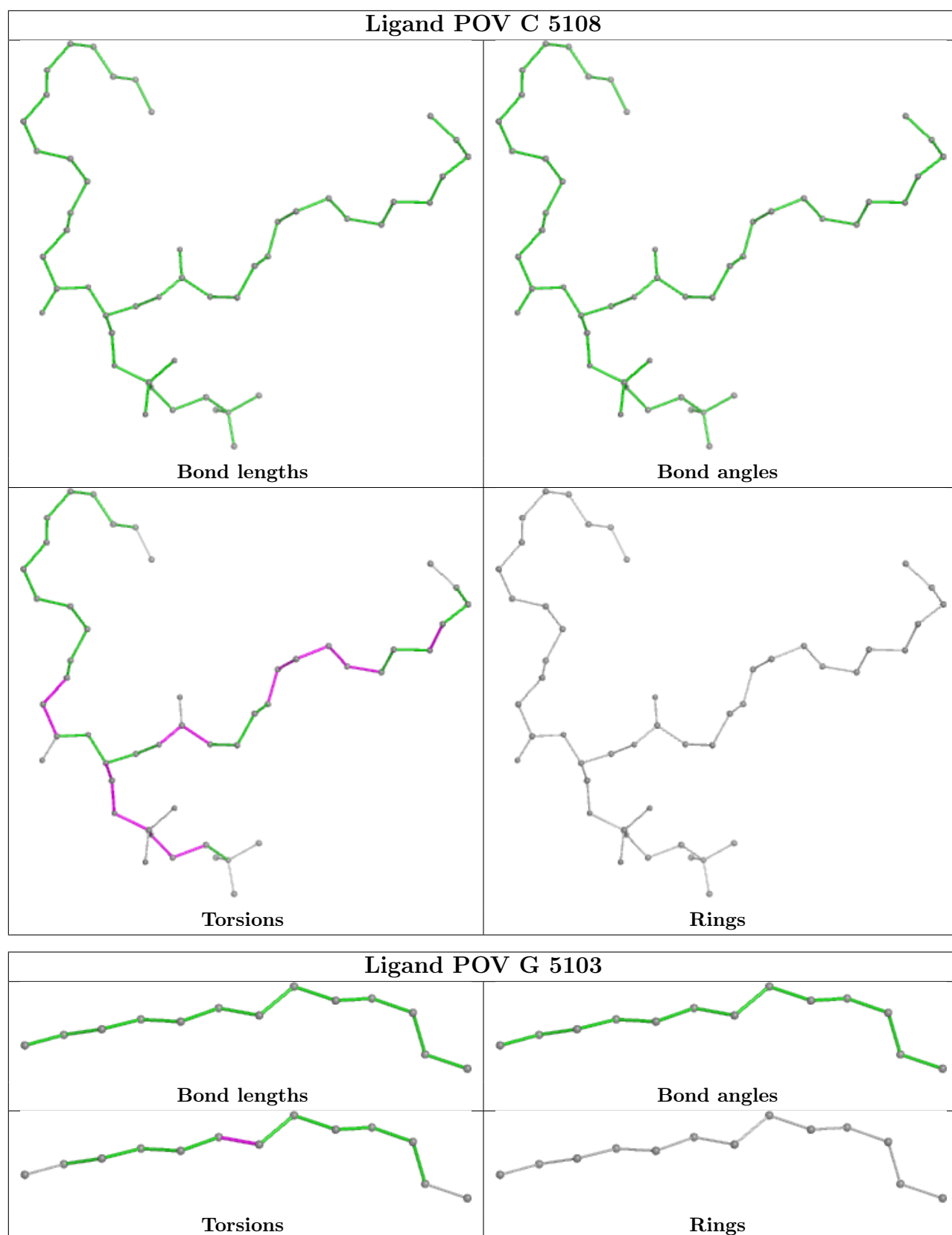


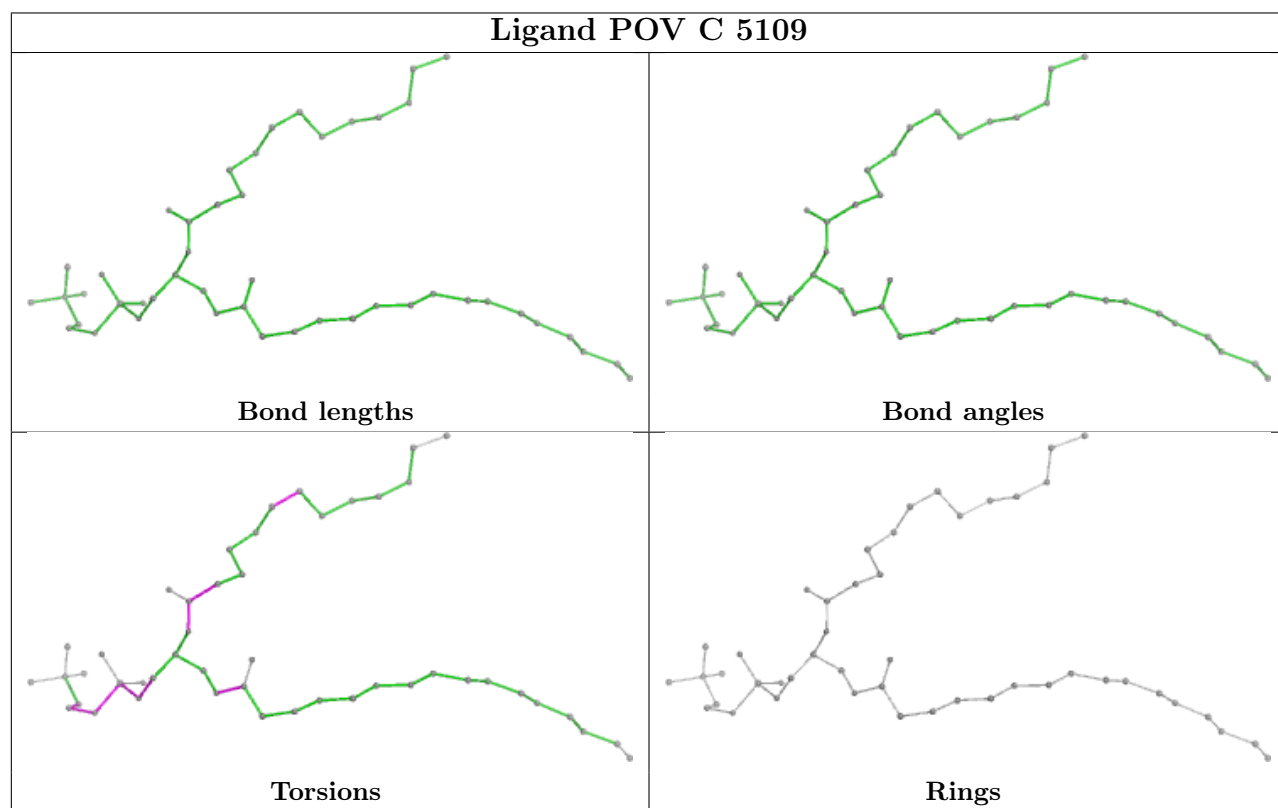
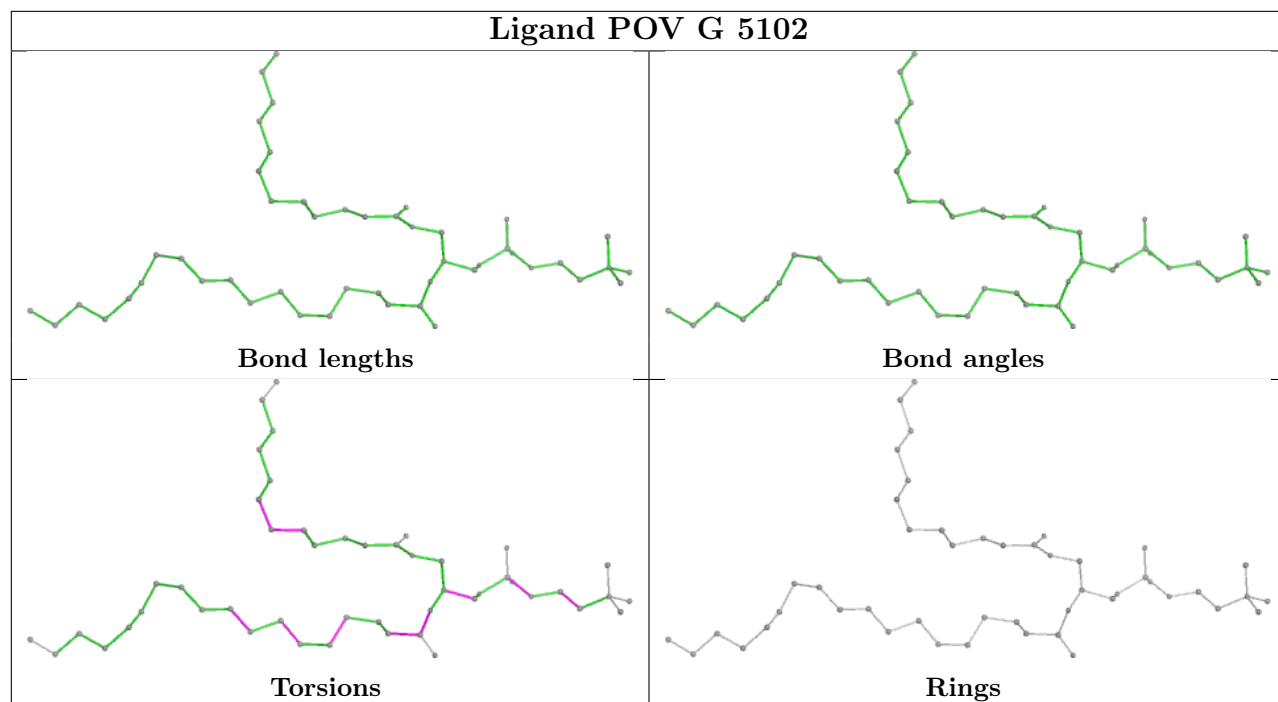


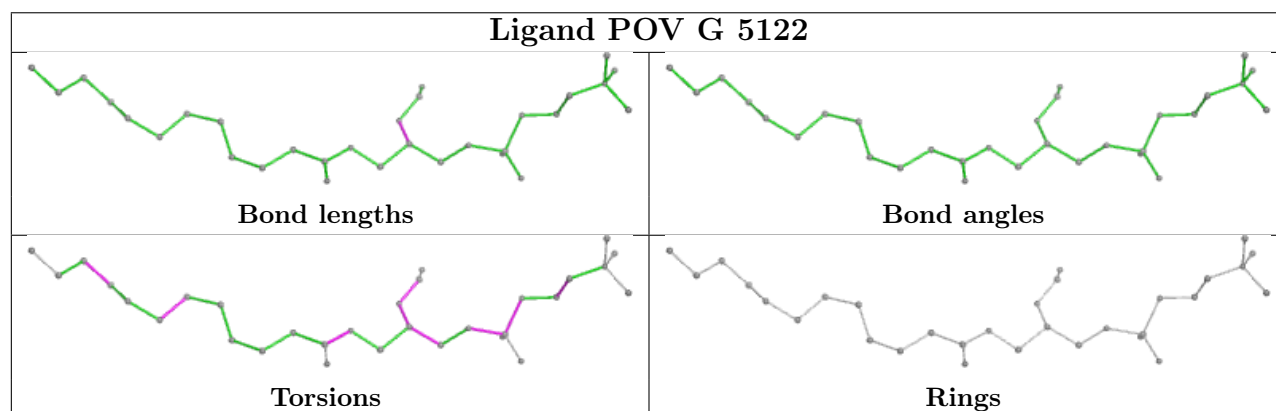
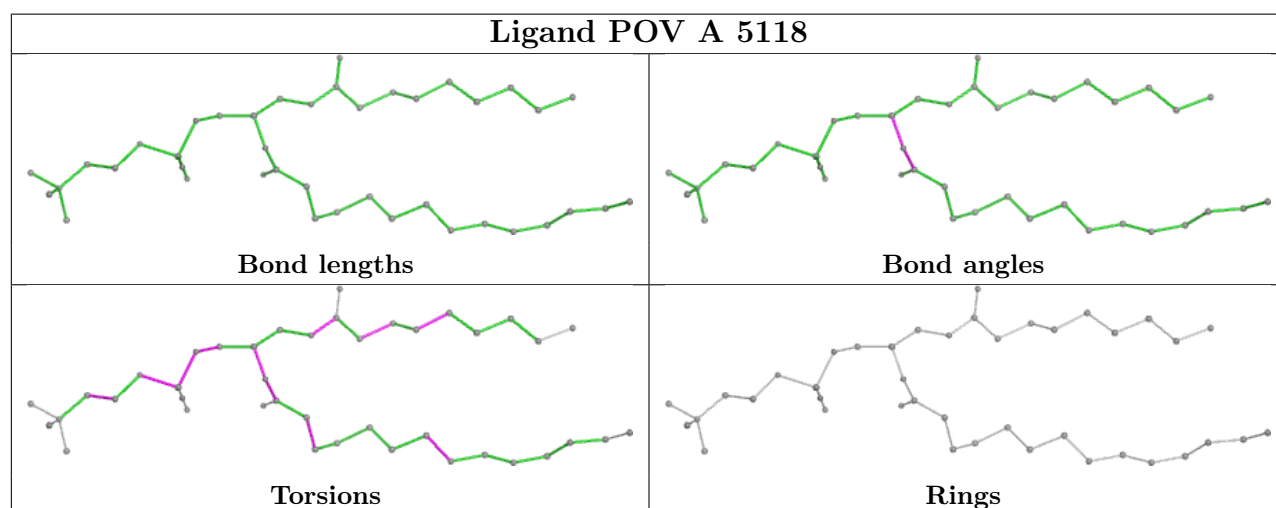
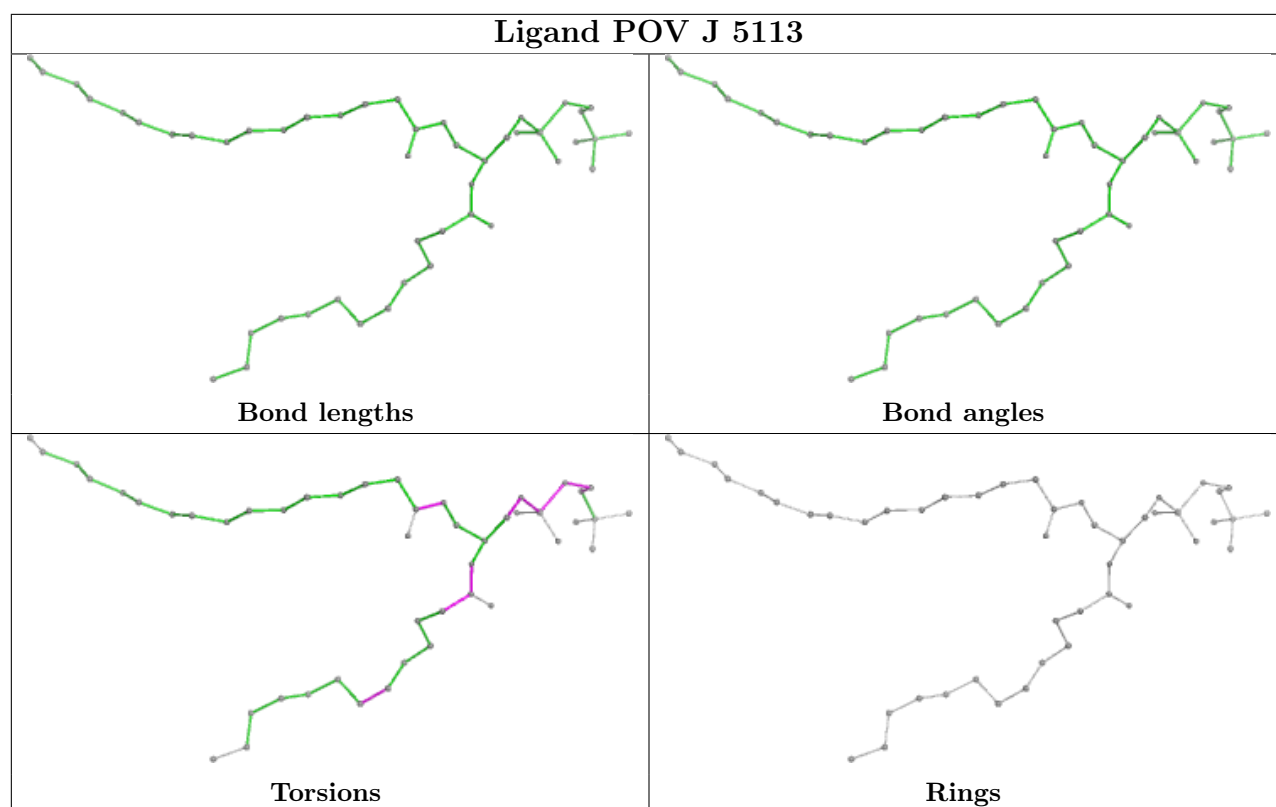


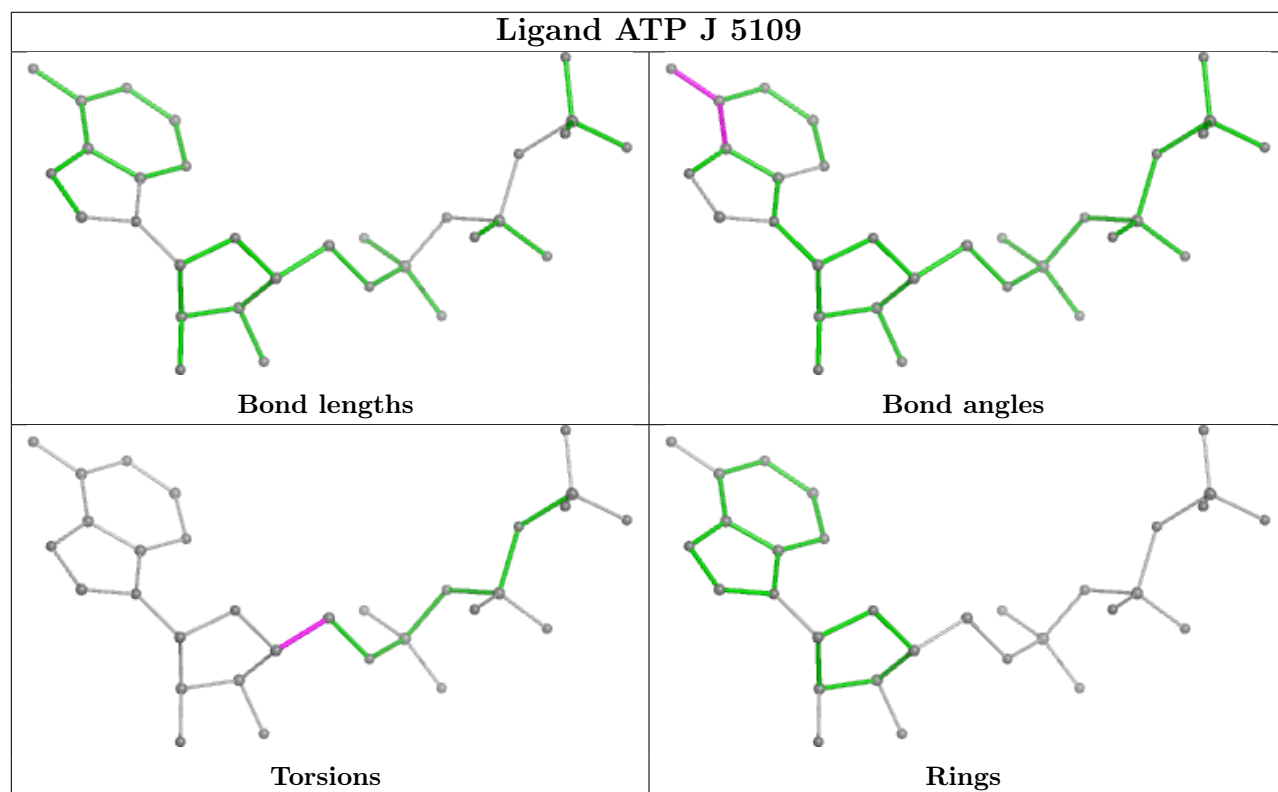
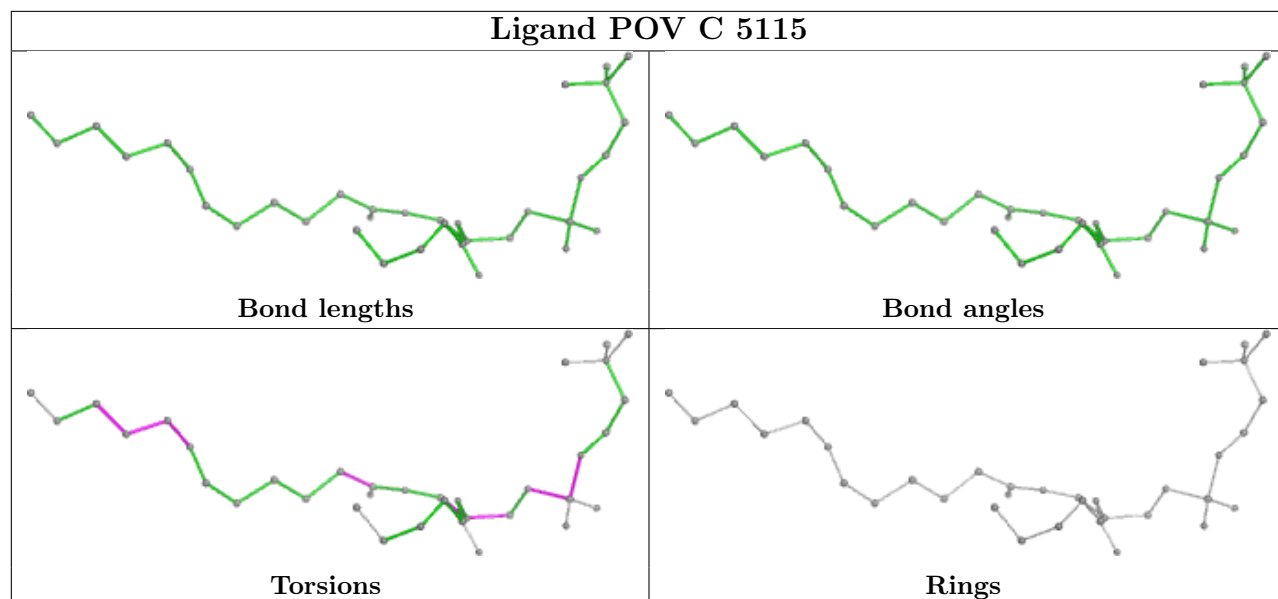


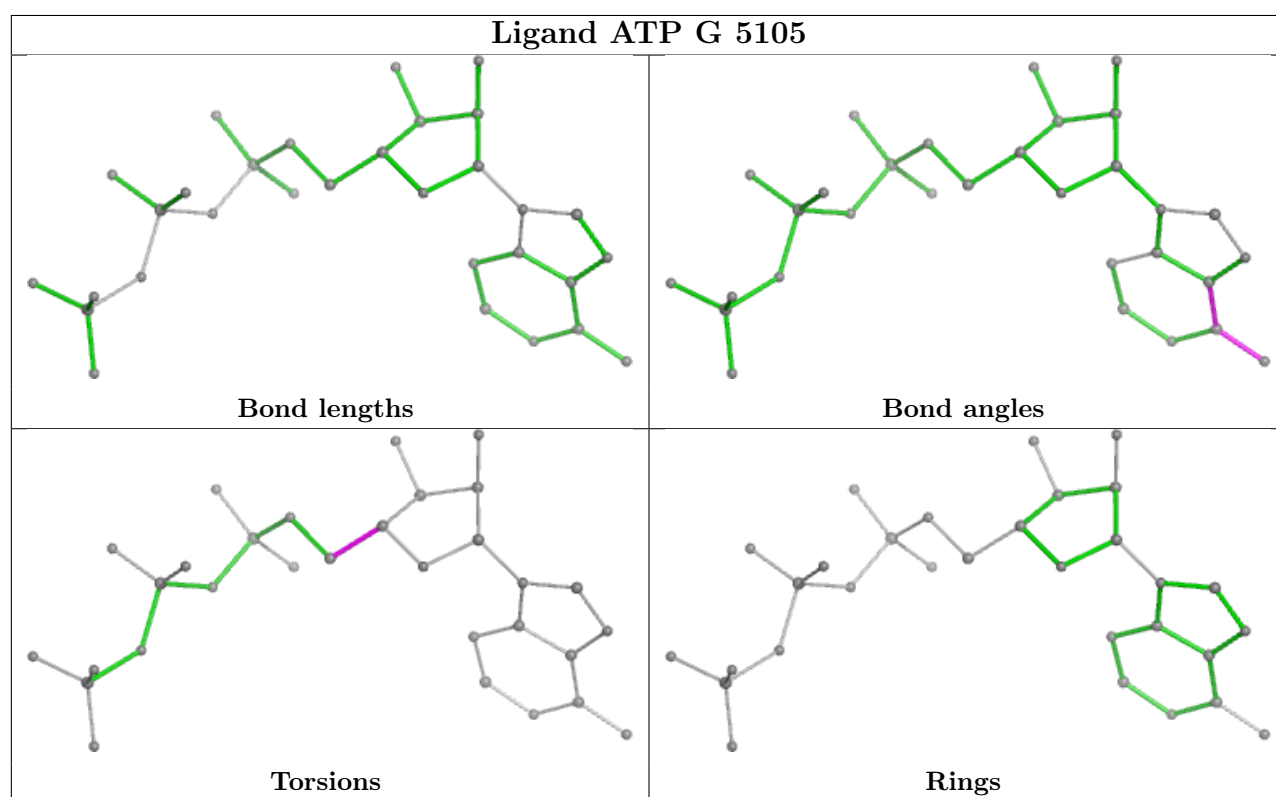
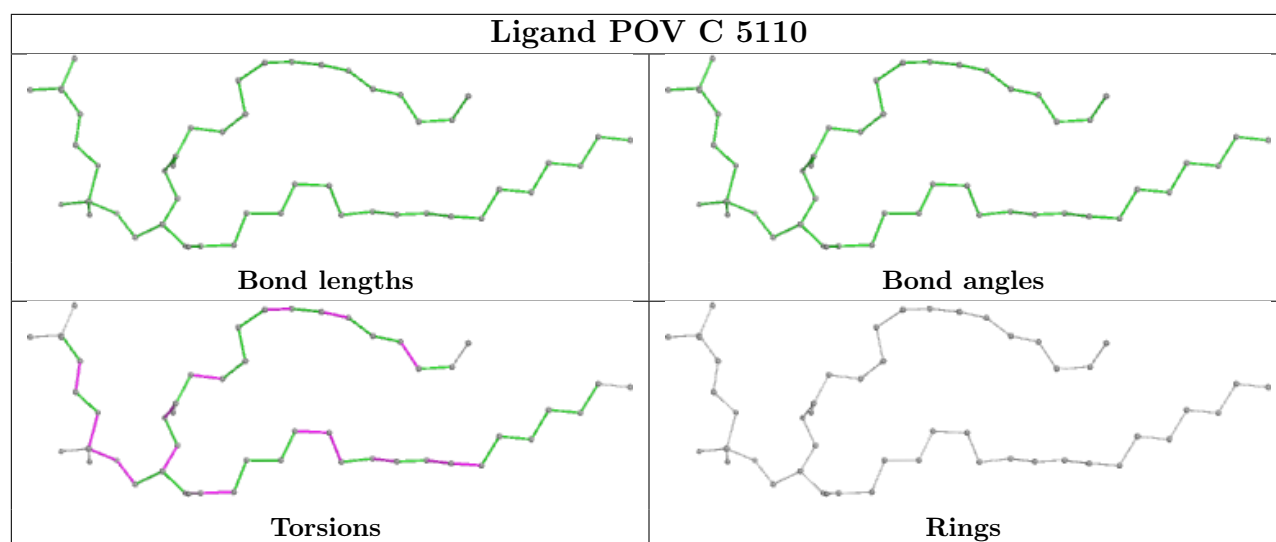


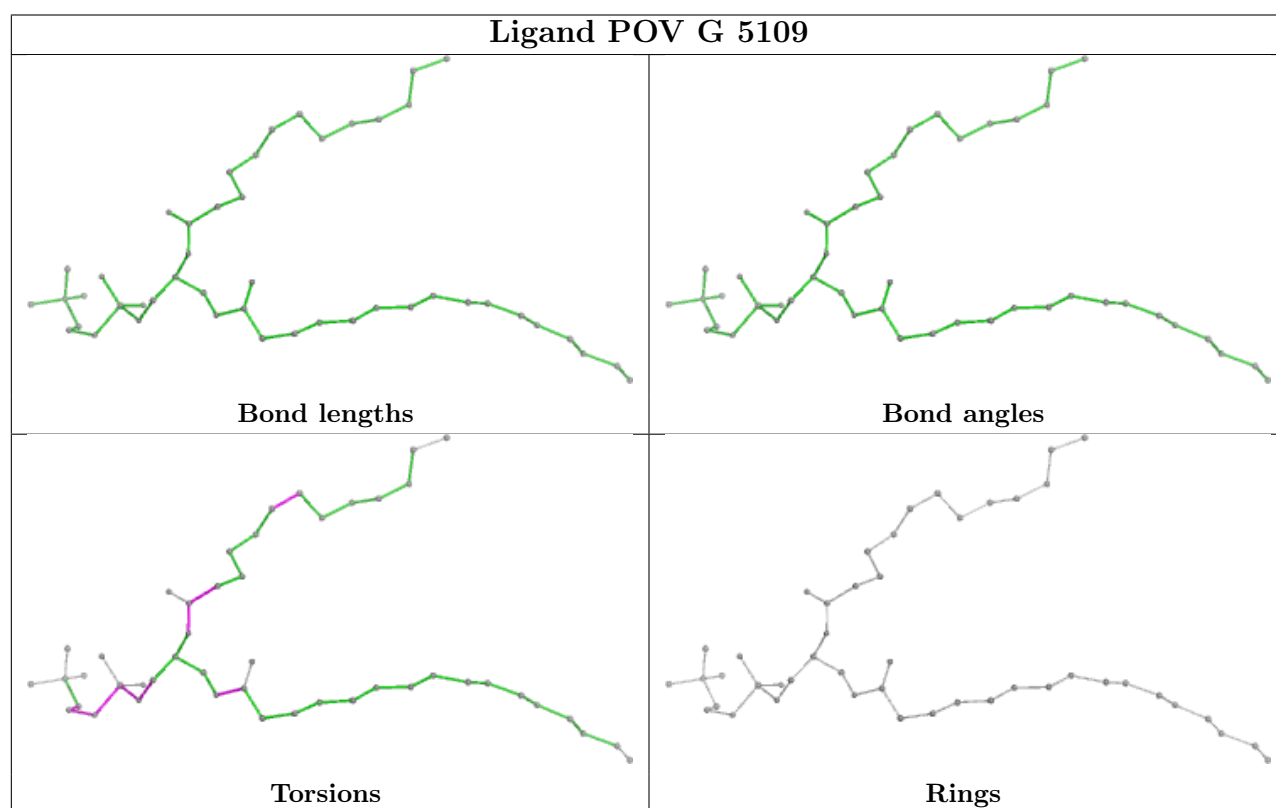
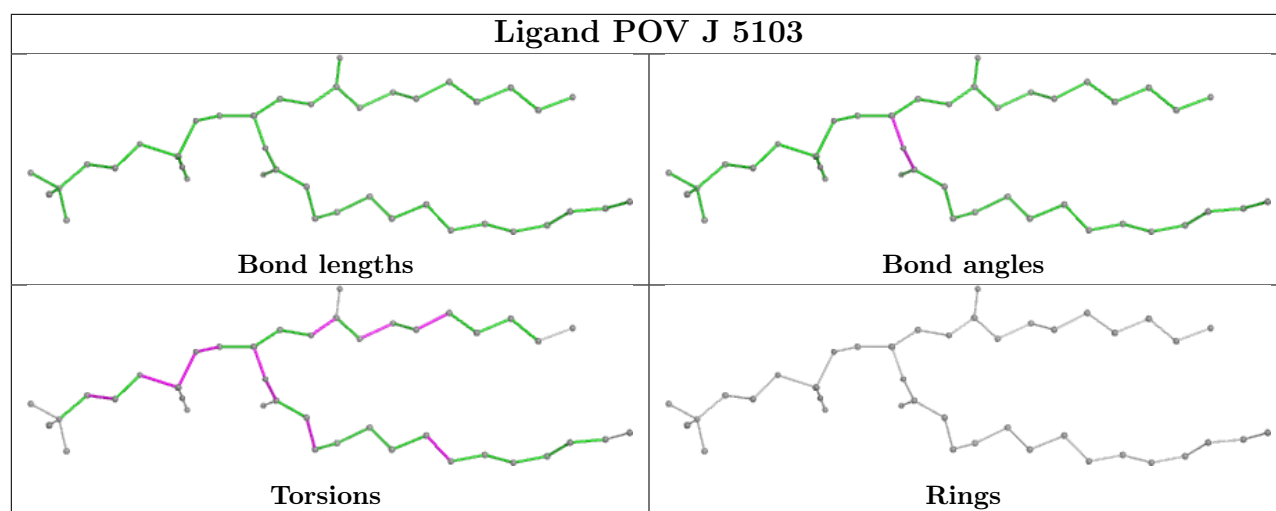


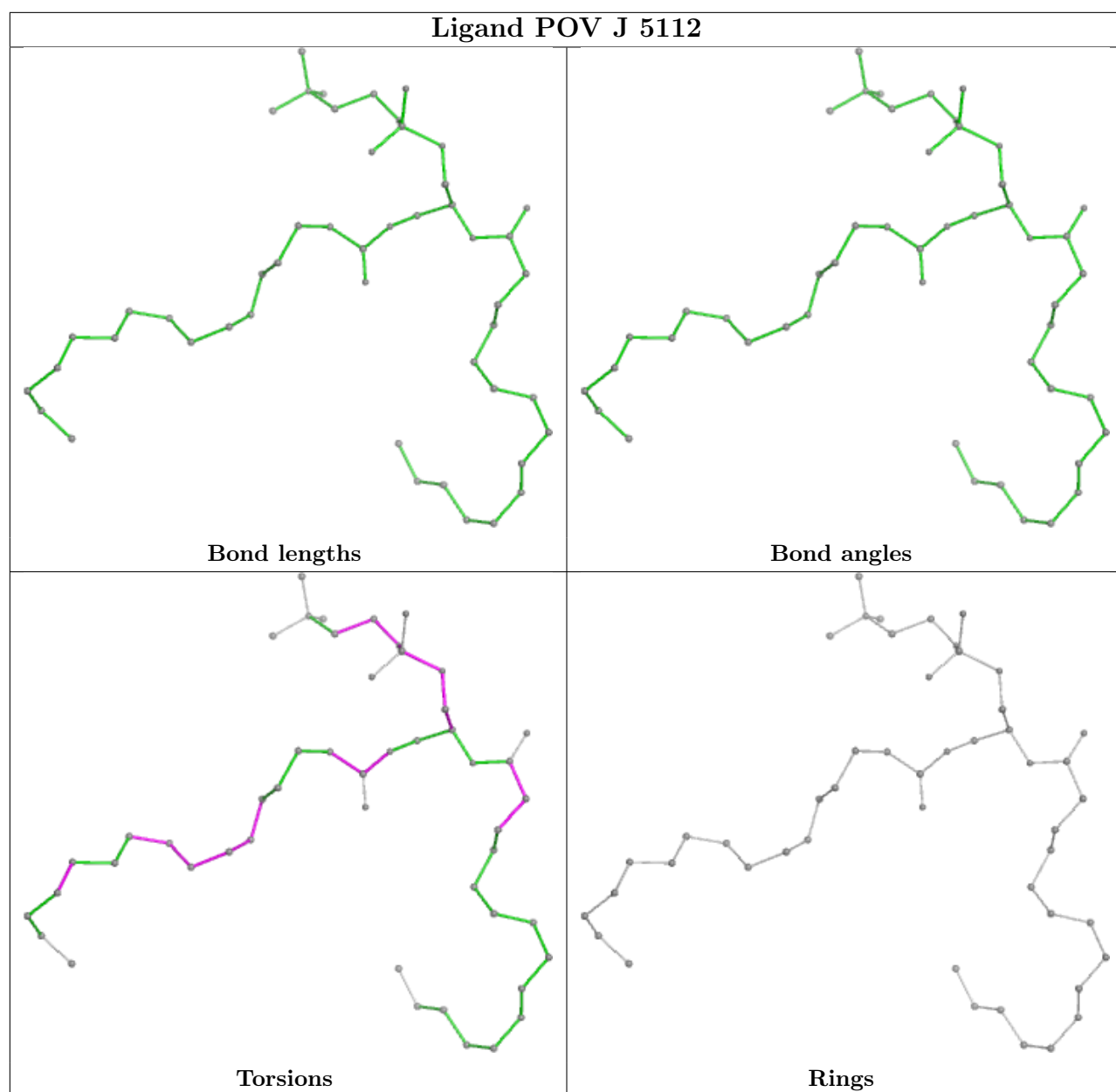




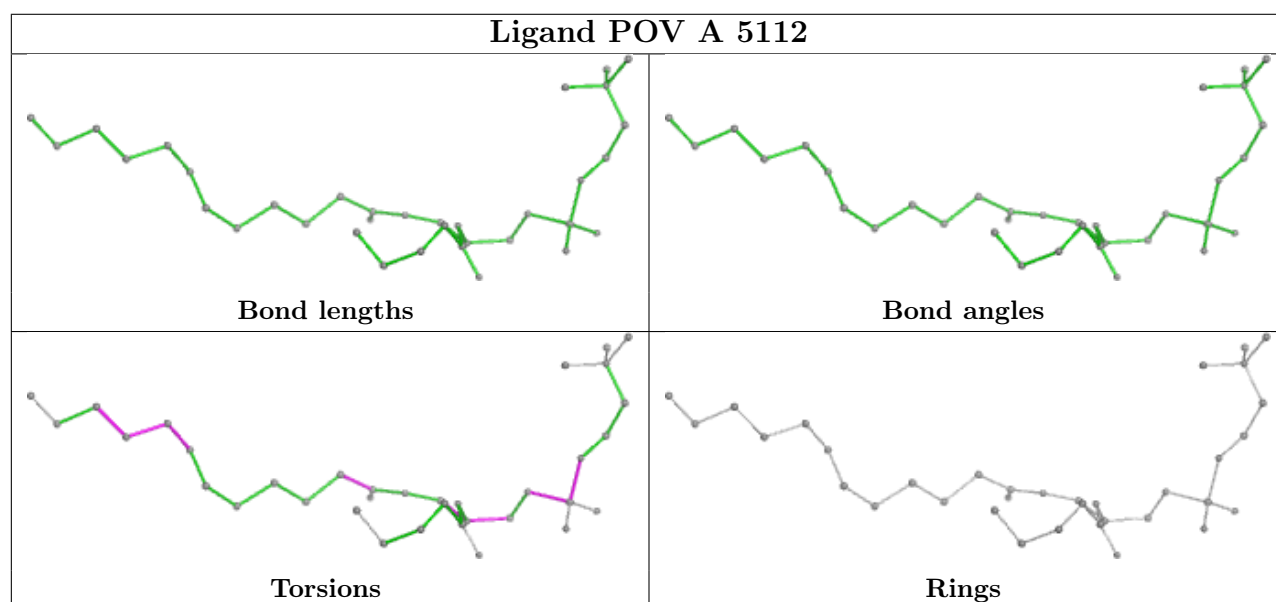
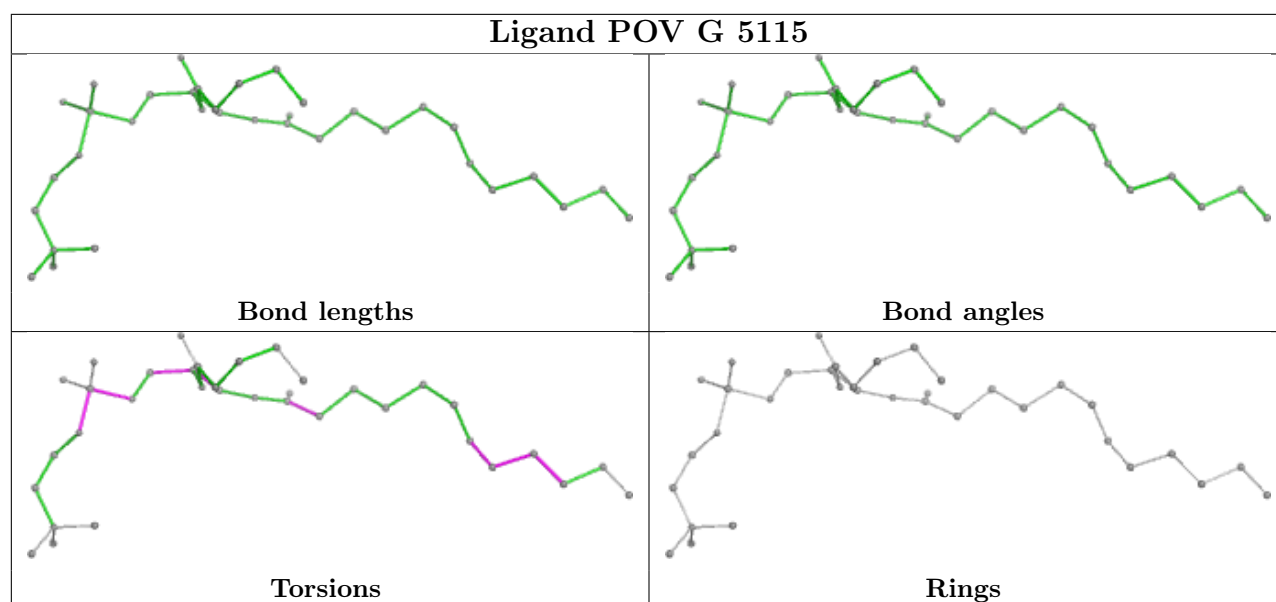


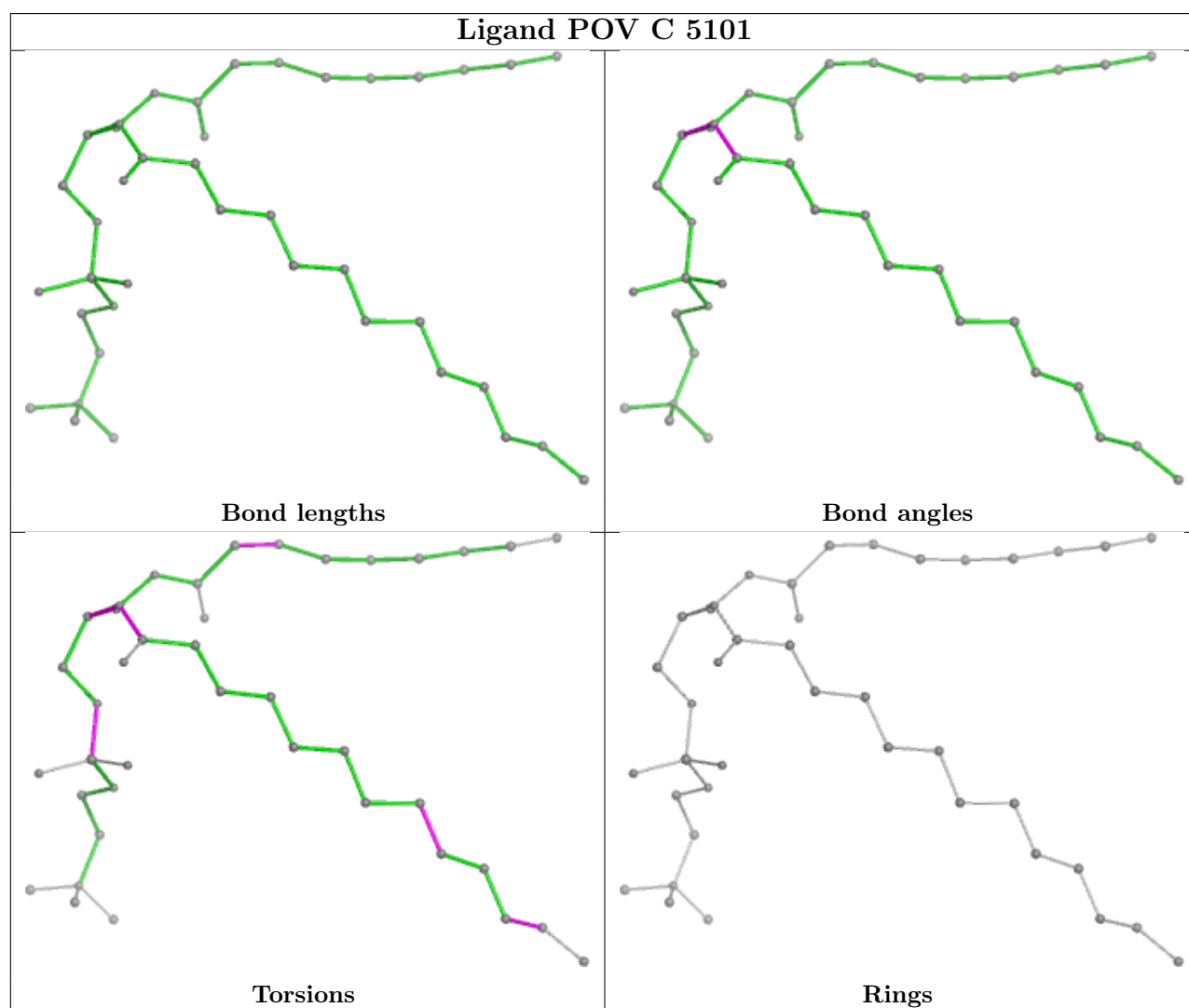
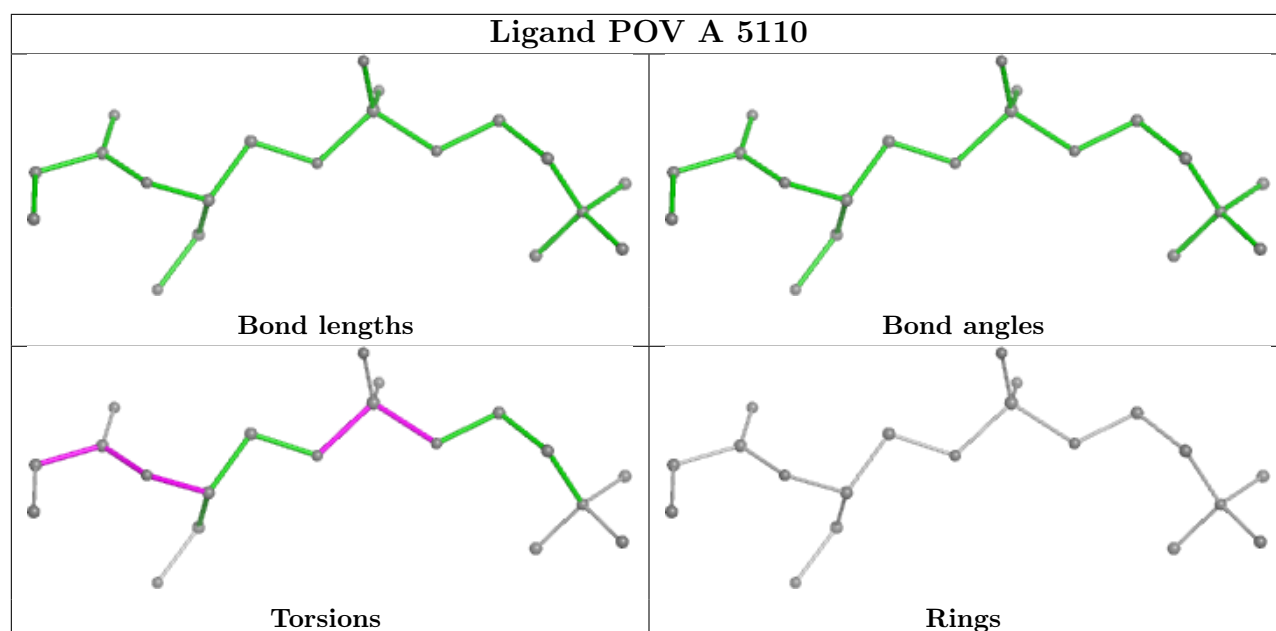


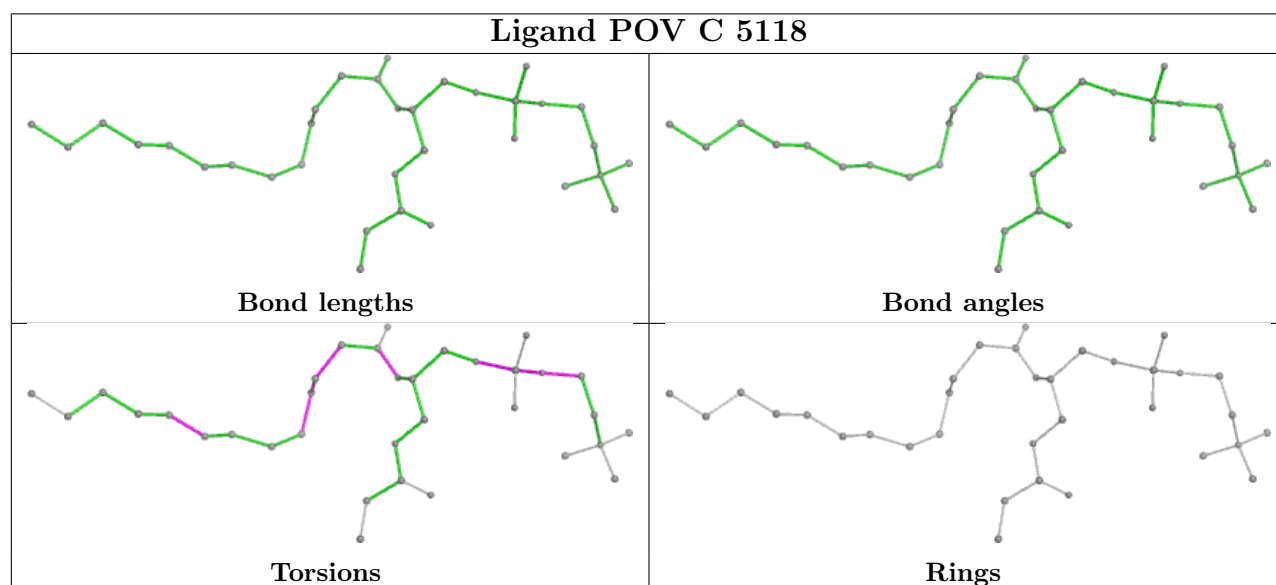
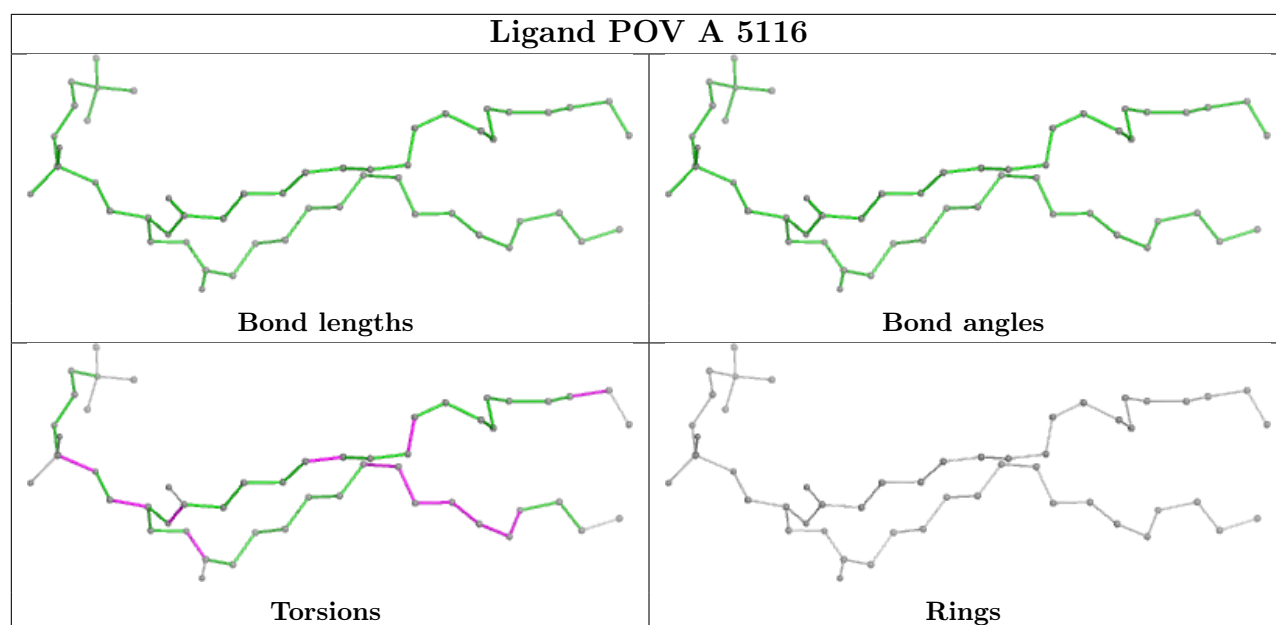


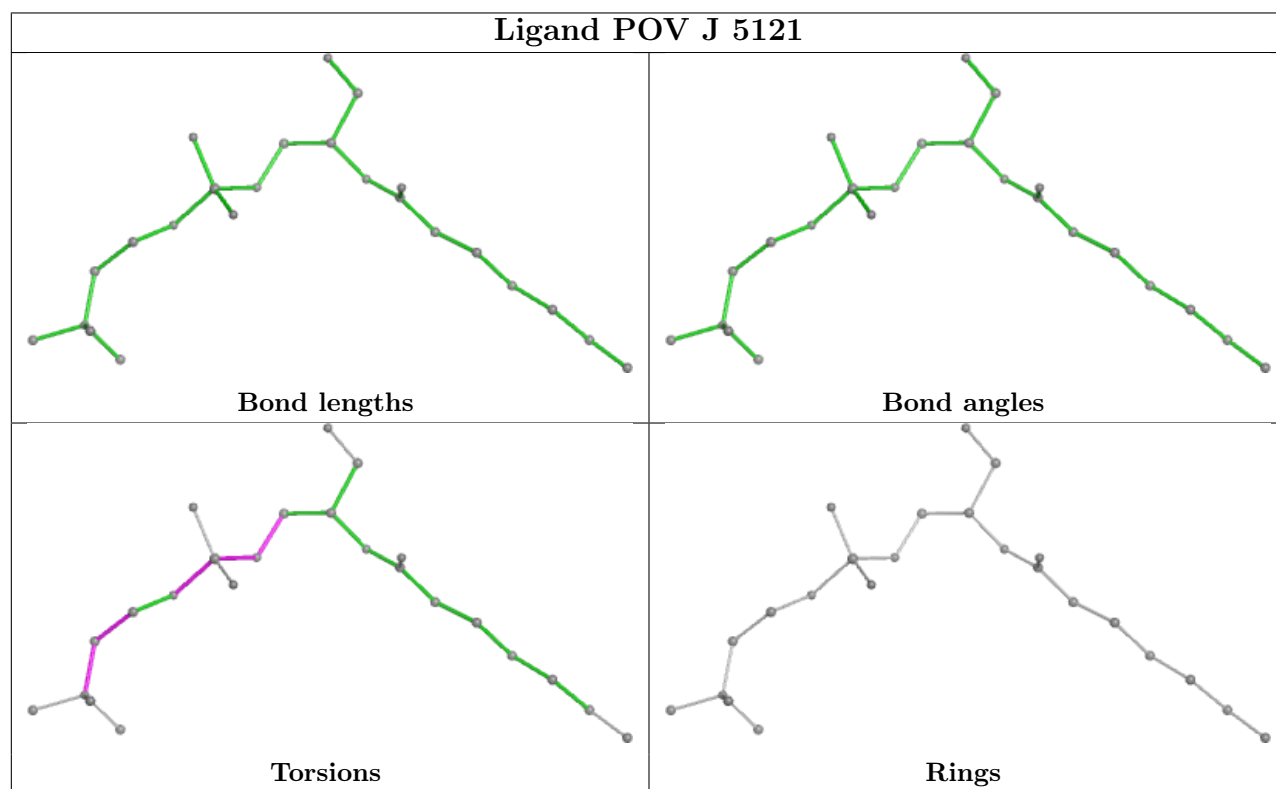
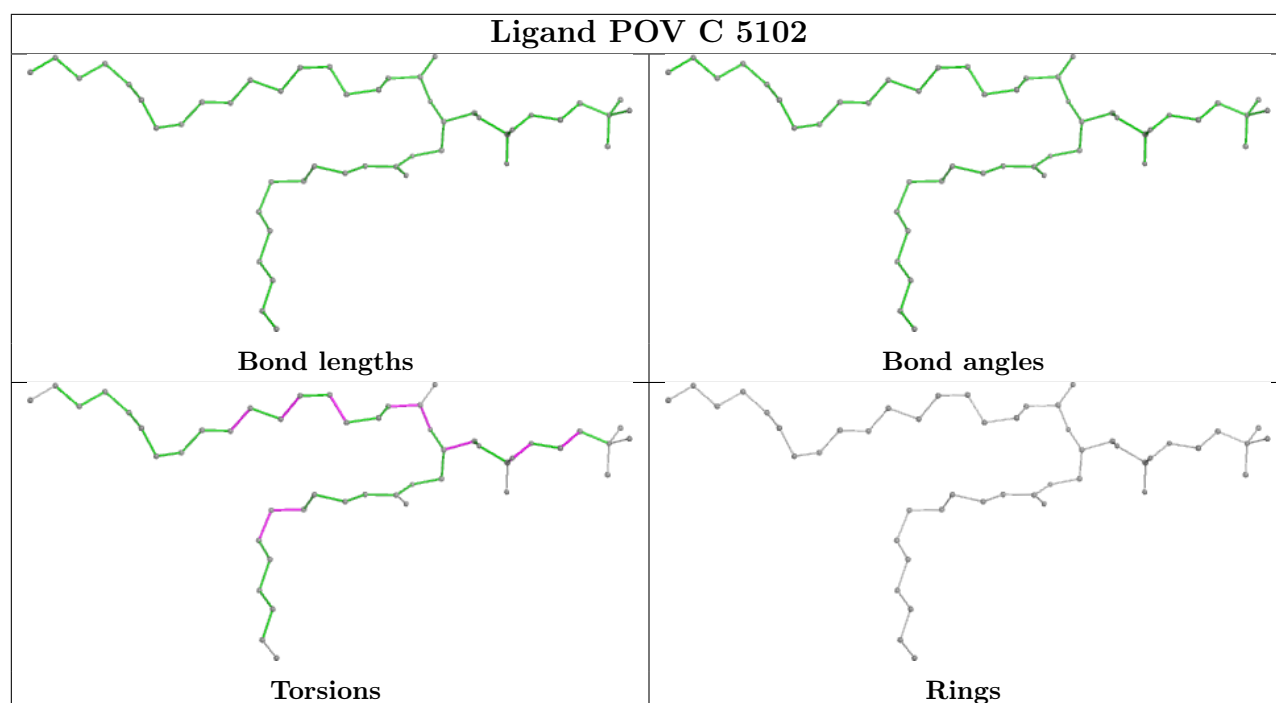


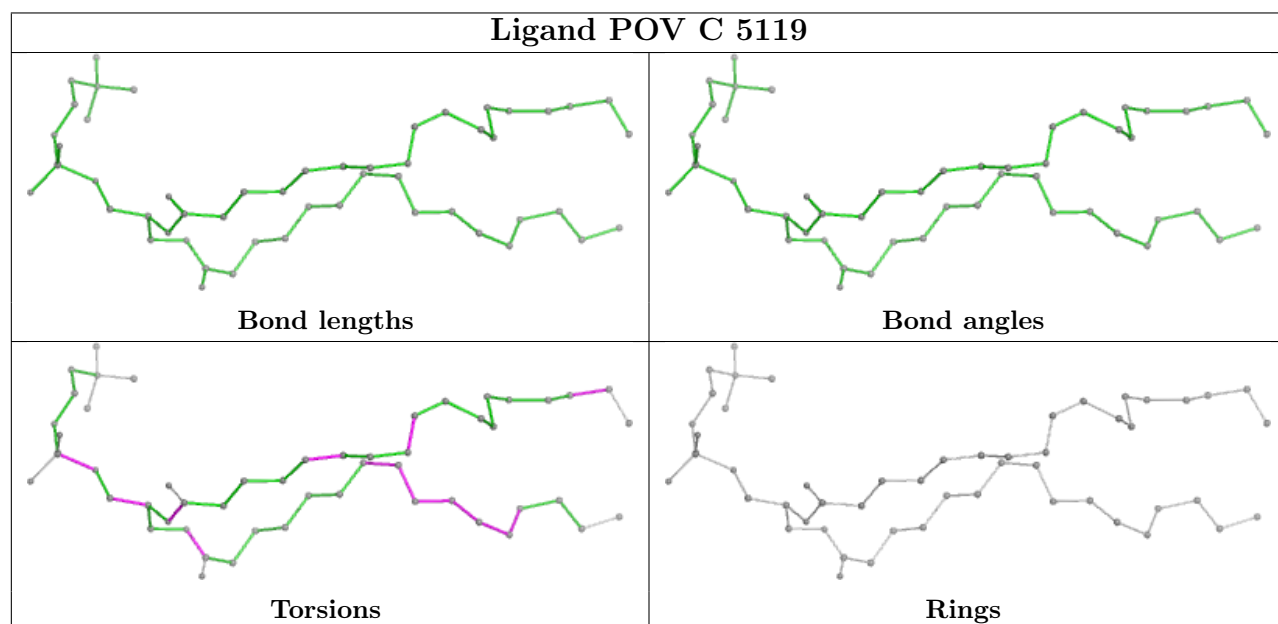
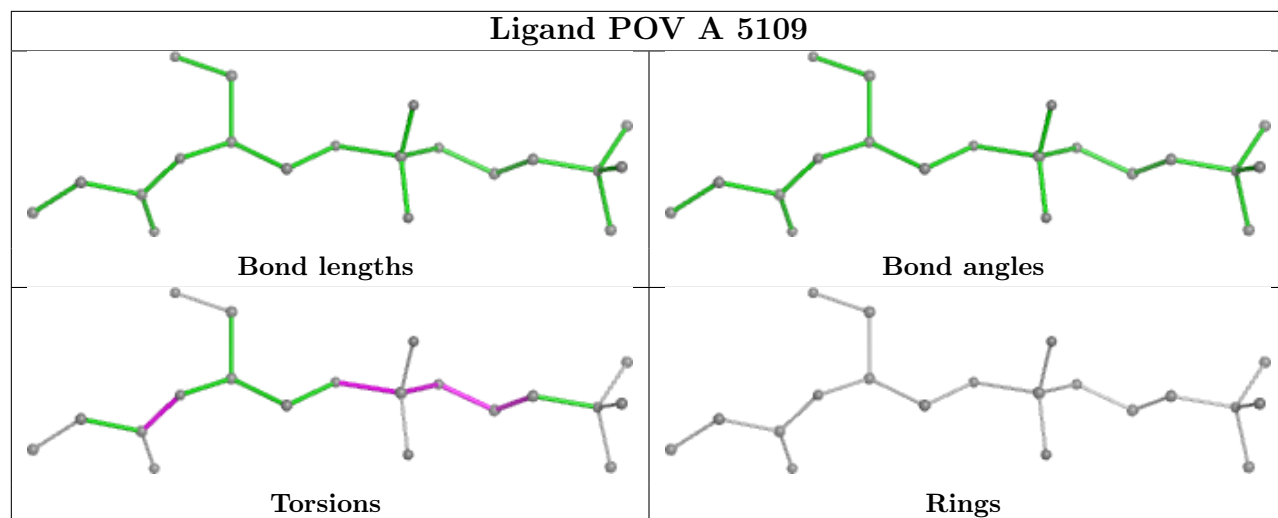


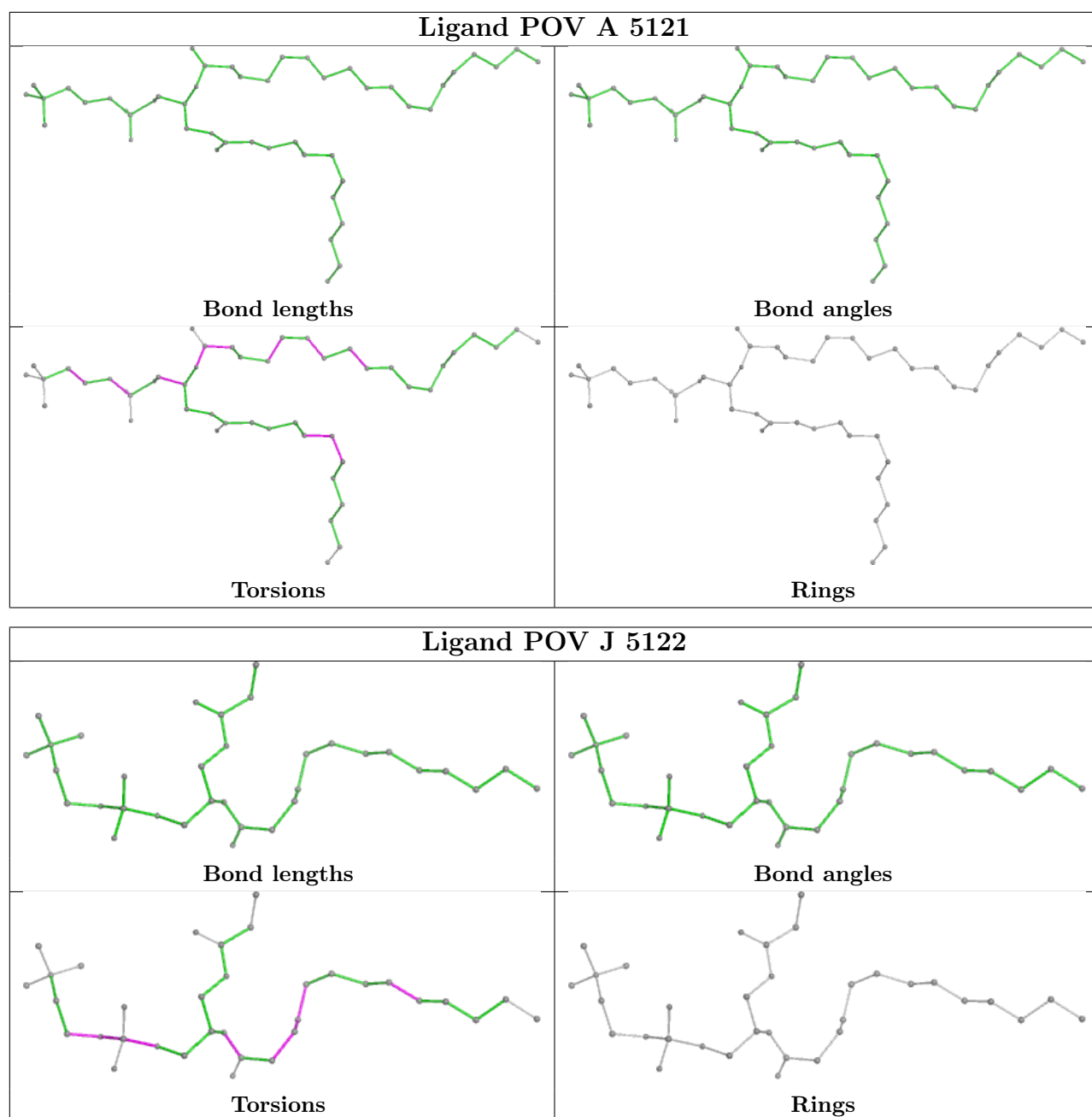


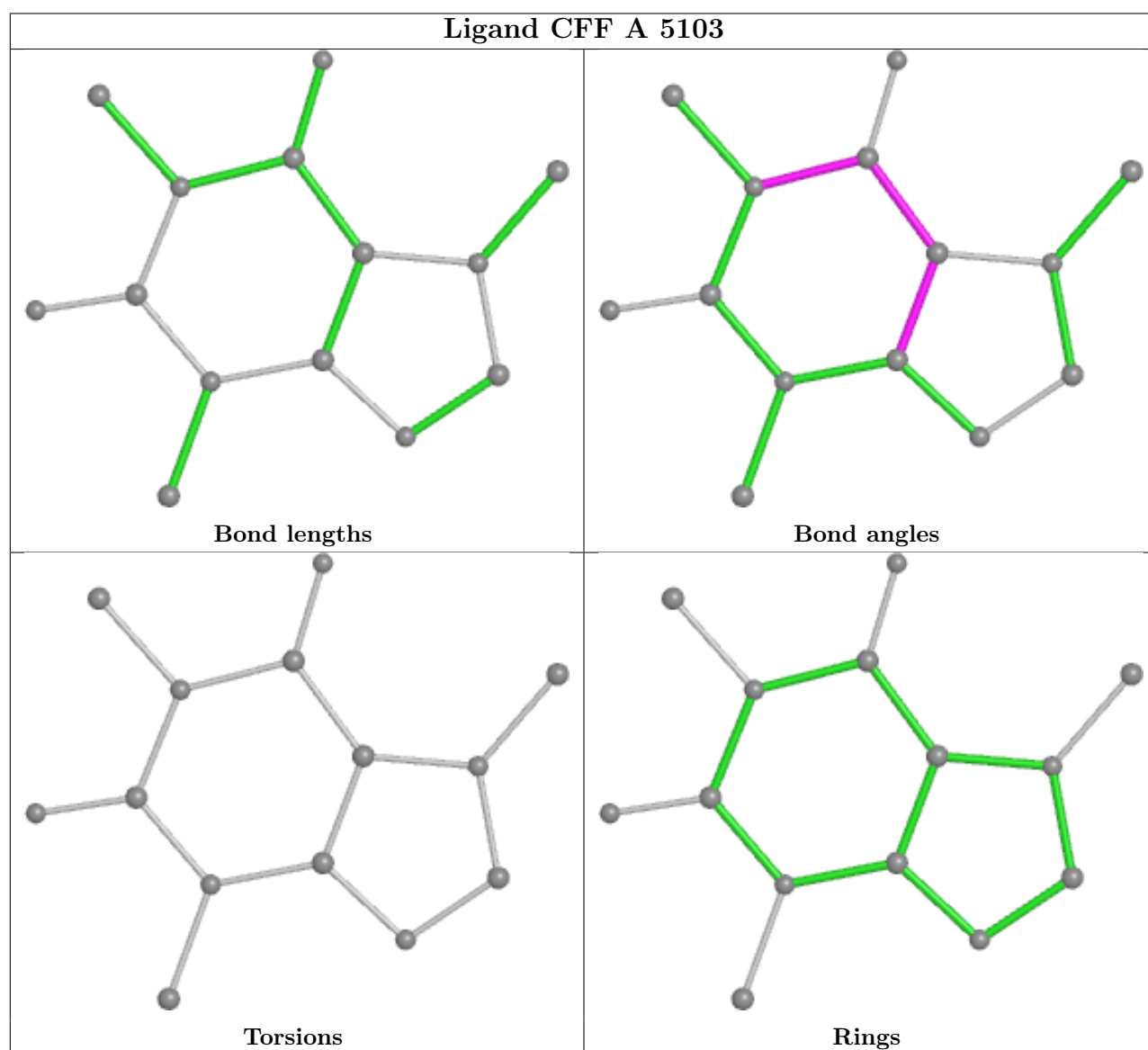
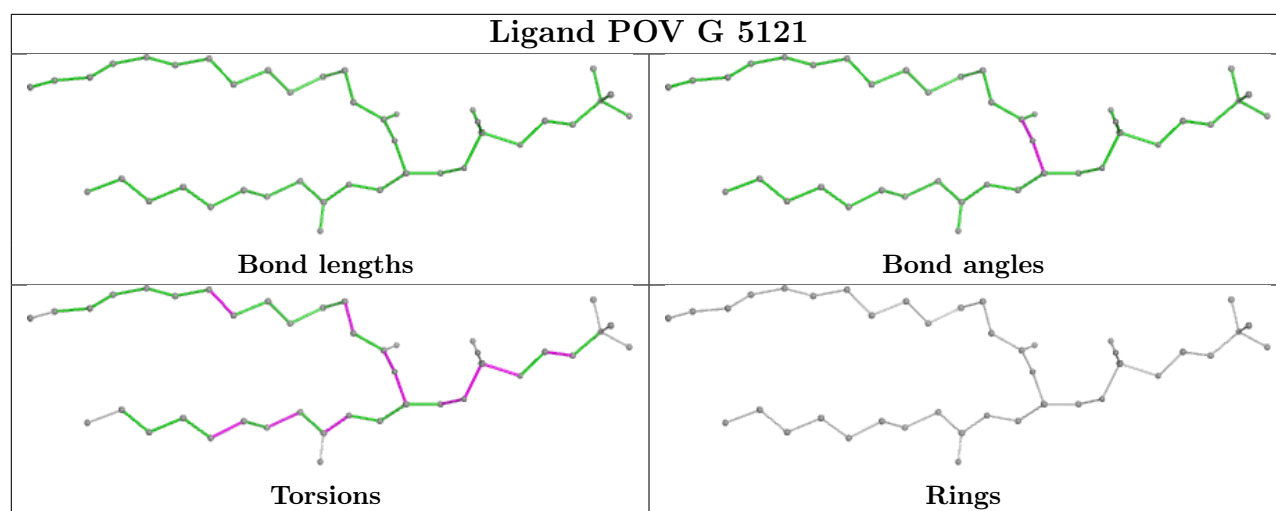


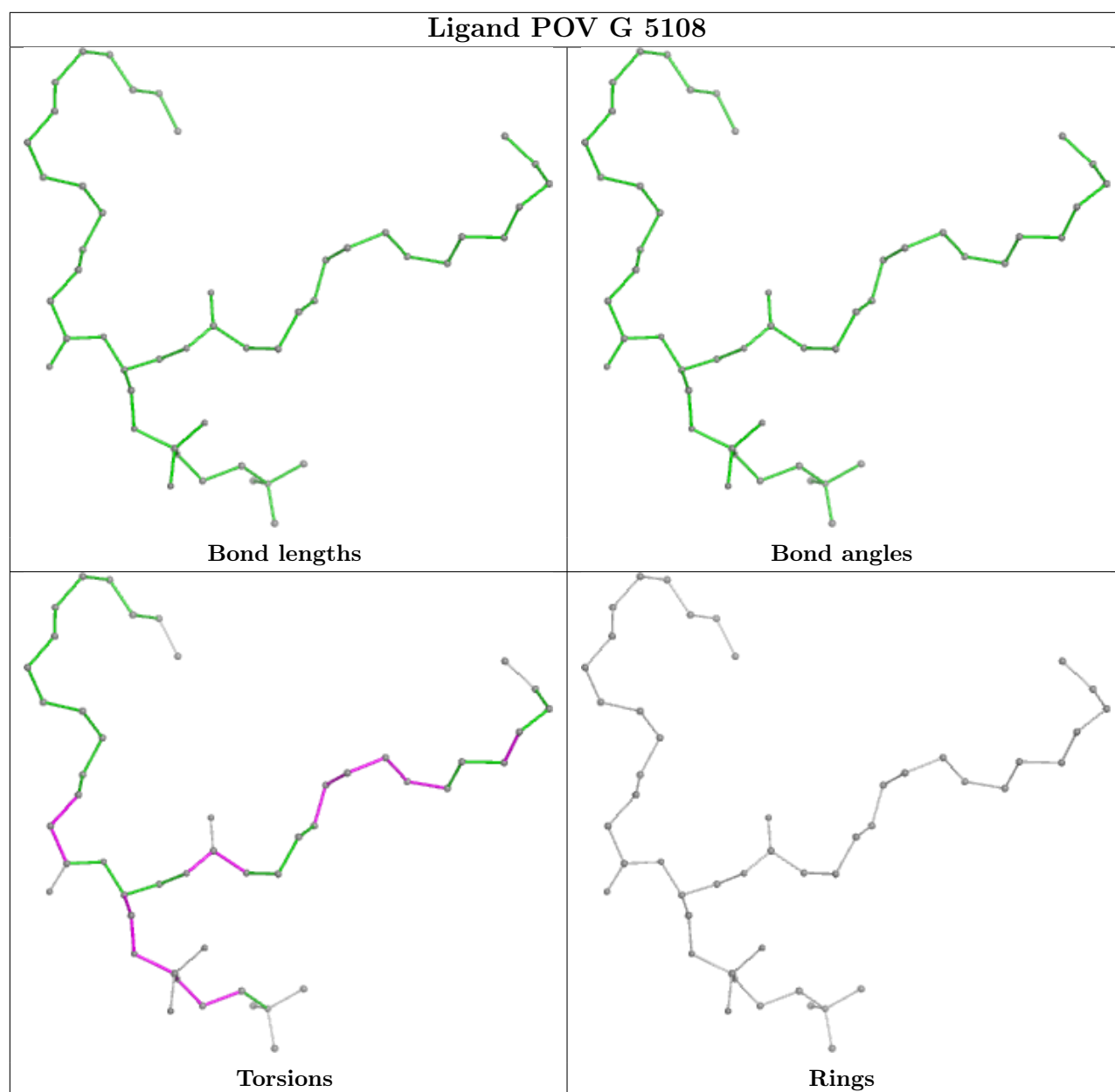




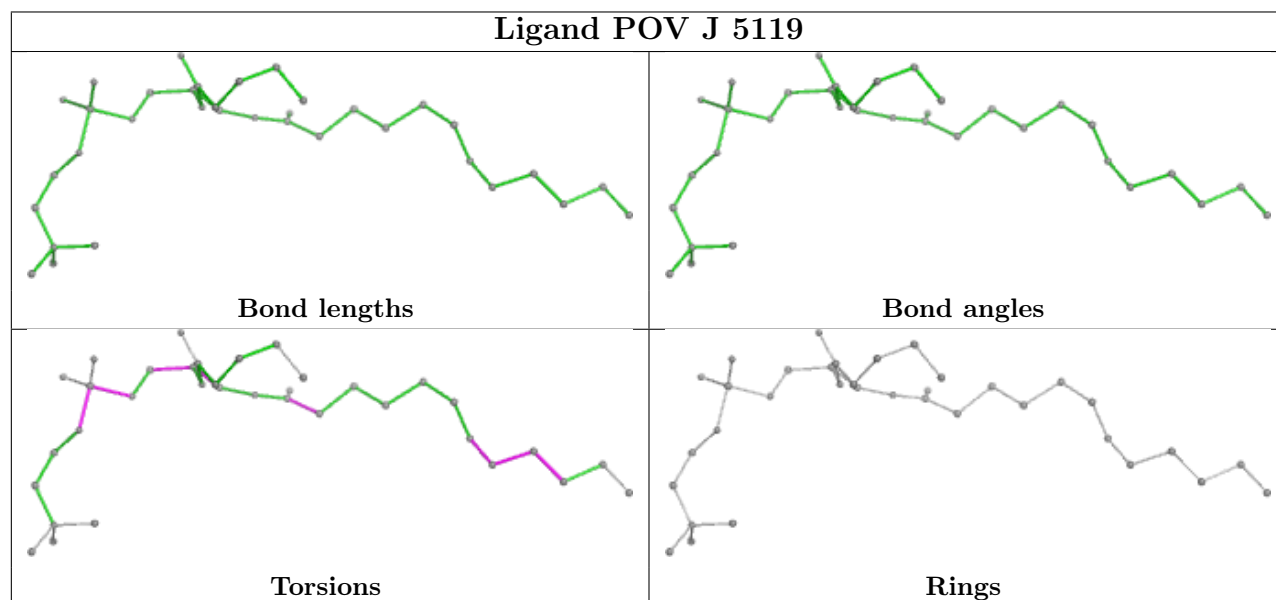
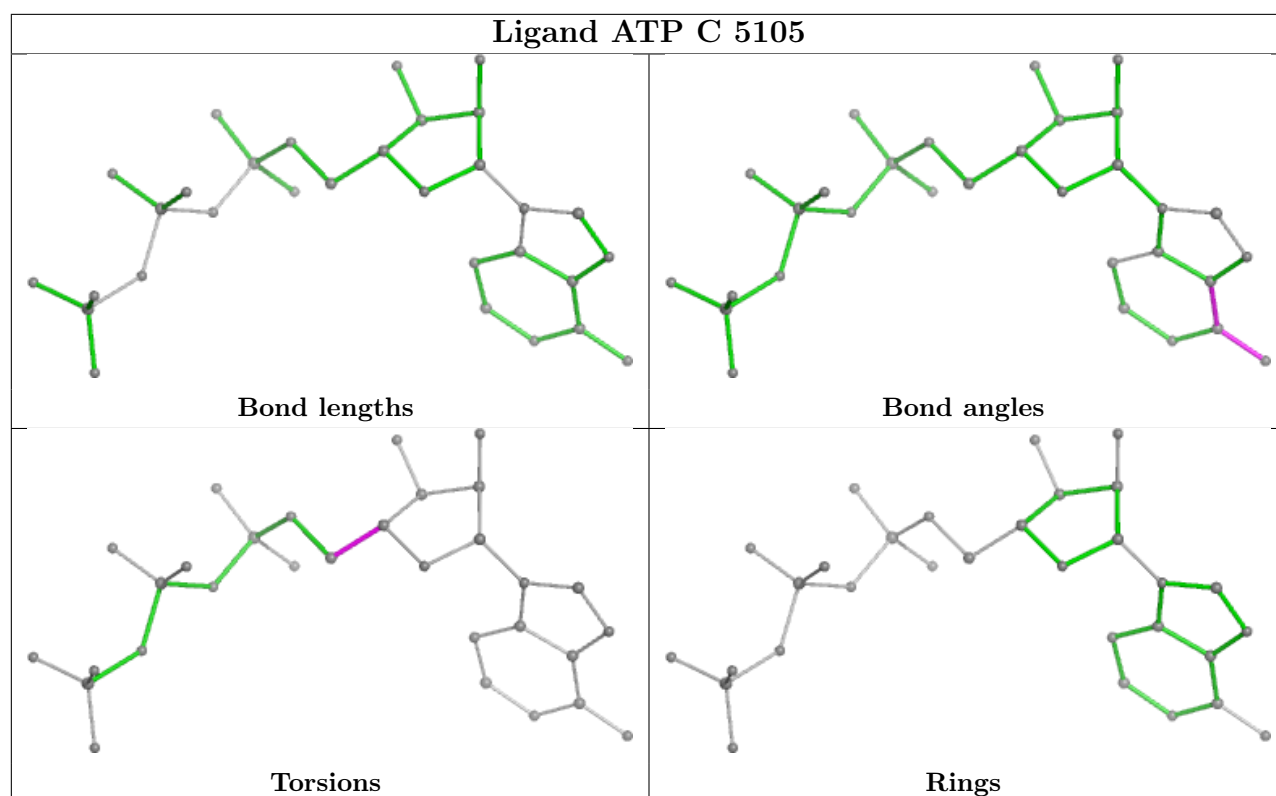


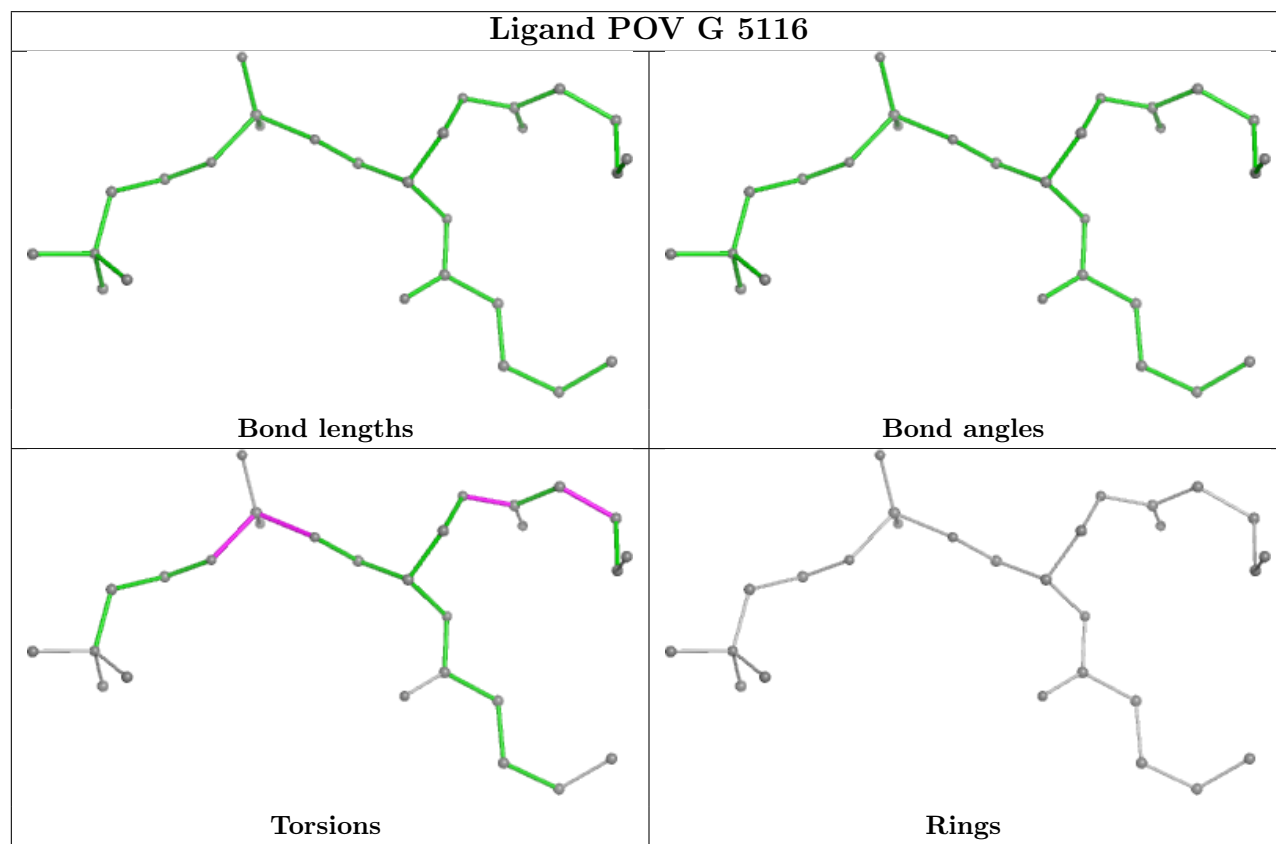
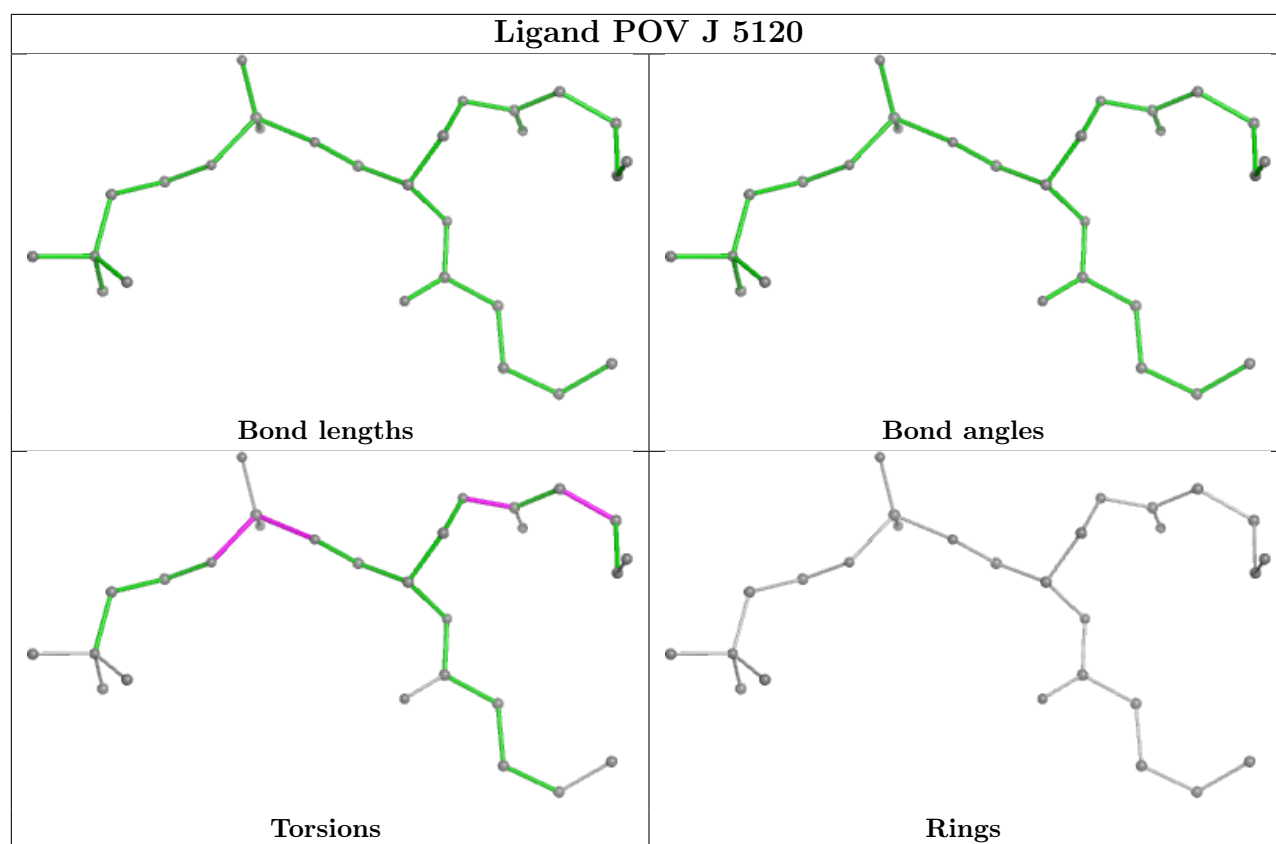


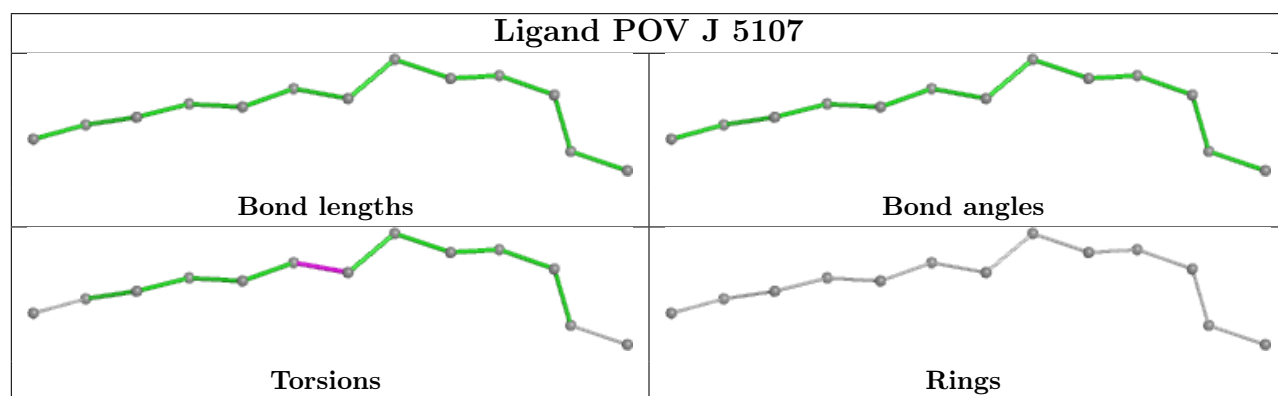
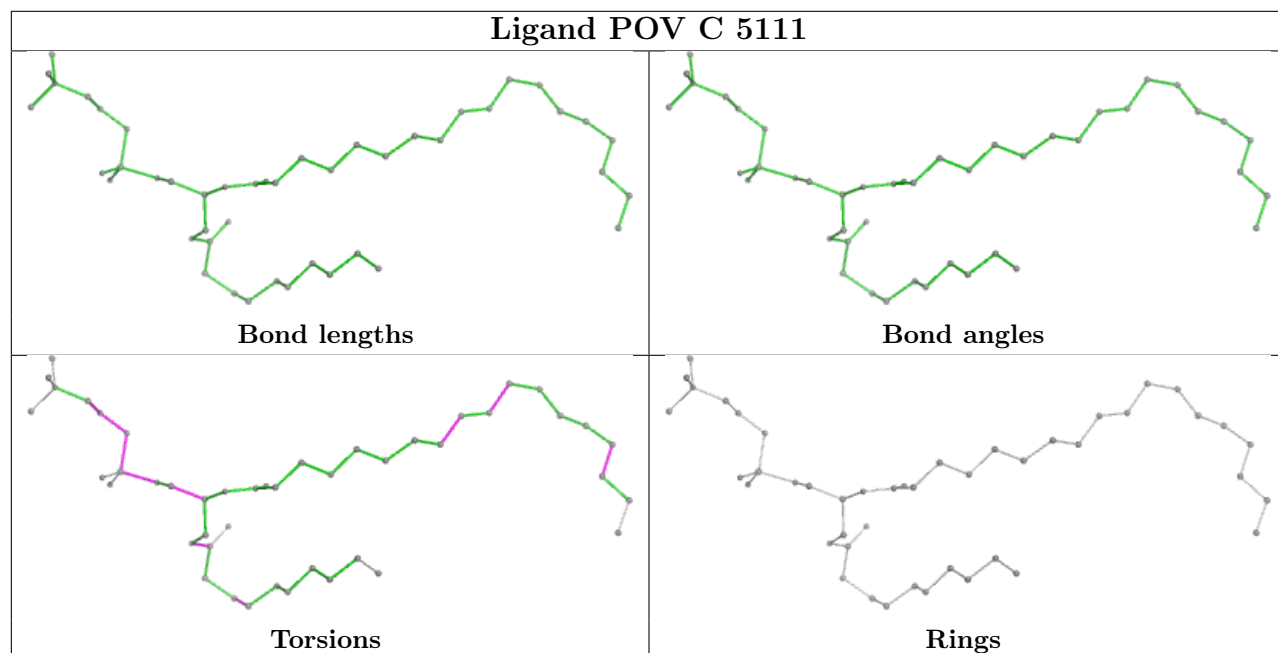
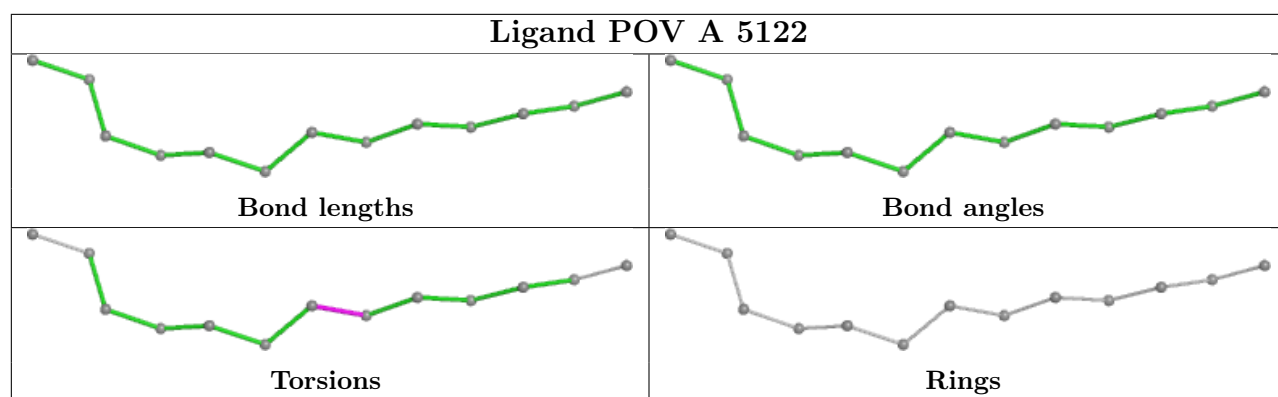


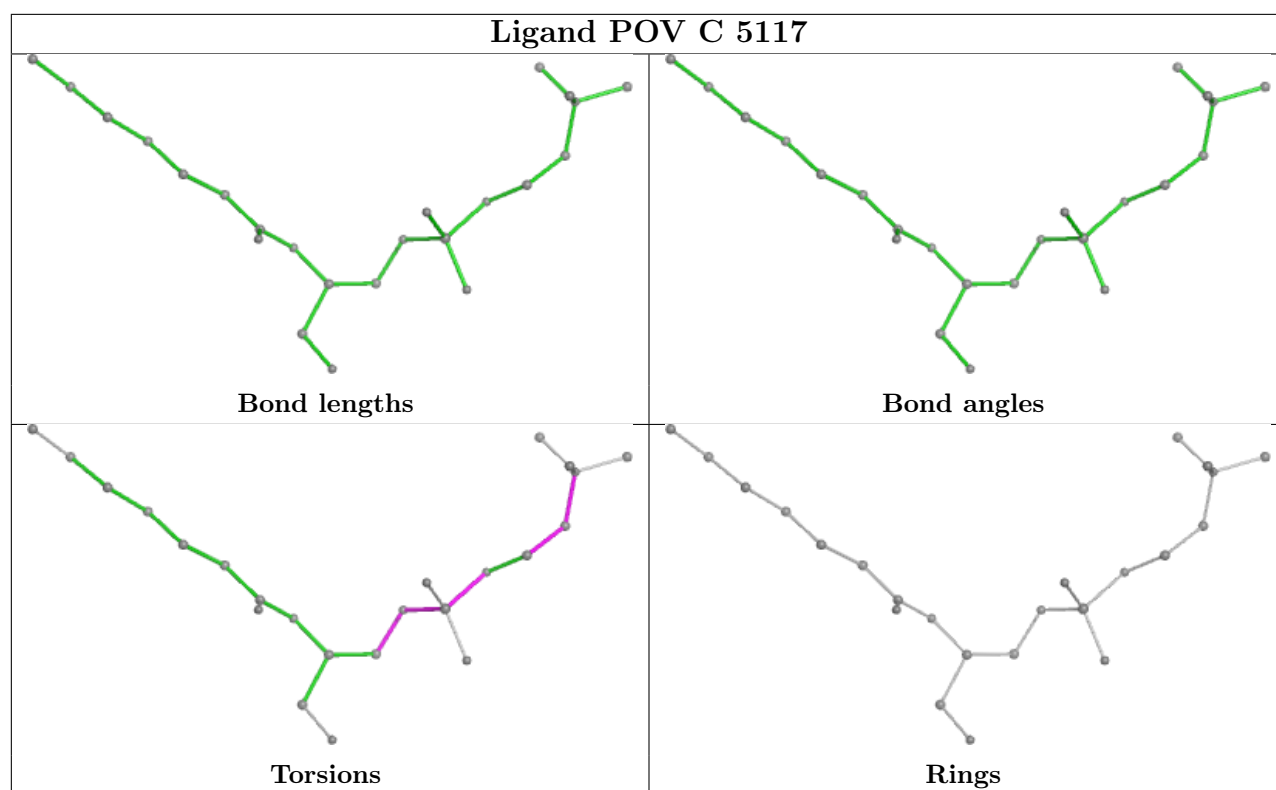












#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

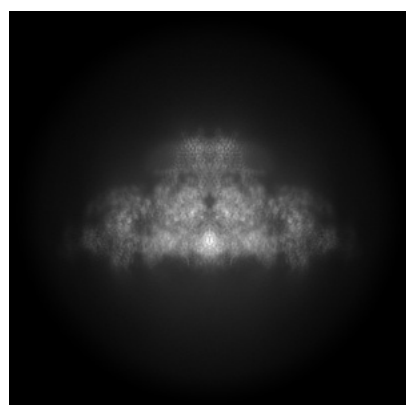
## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52085. These allow visual inspection of the internal detail of the map and identification of artifacts.

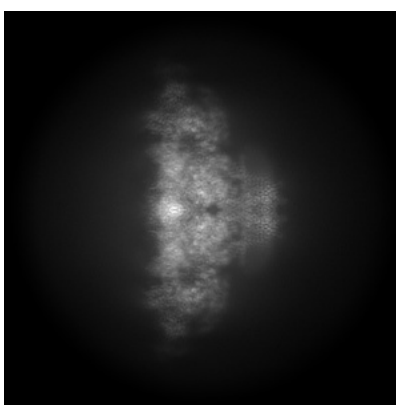
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

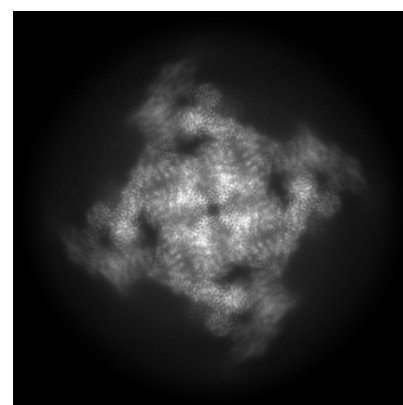
#### 5.1.1 Primary map



X



Y



Z

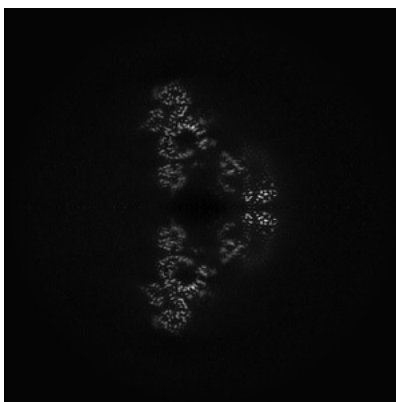
The images above show the map projected in three orthogonal directions.

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

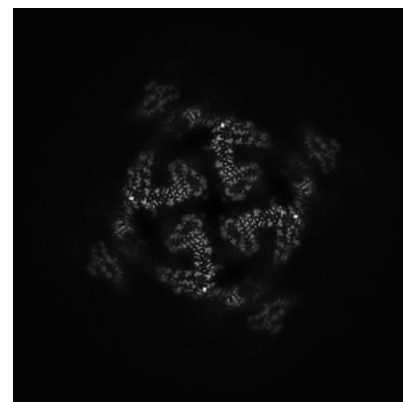
#### 5.2.1 Primary map



X Index: 168



Y Index: 168



Z Index: 168

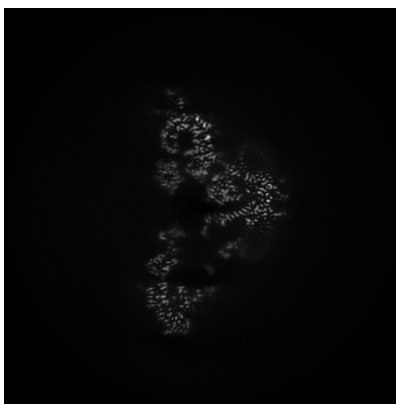
The images above show central slices of the map in three orthogonal directions.

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

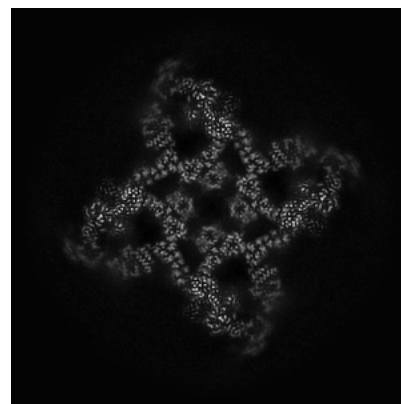
### 5.3.1 Primary map



X Index: 161



Y Index: 161

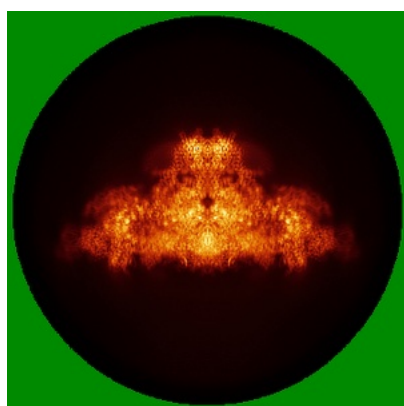


Z Index: 144

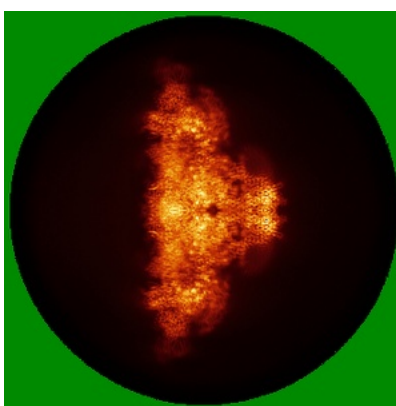
The images above show the largest variance slices of the map in three orthogonal directions.

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

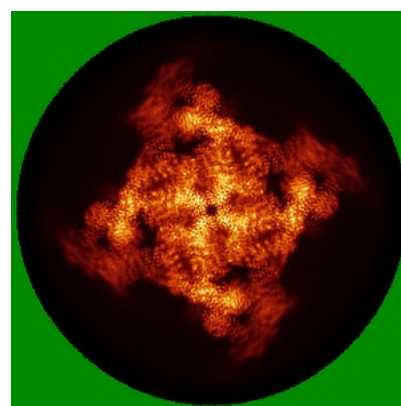
### 5.4.1 Primary map



X



Y

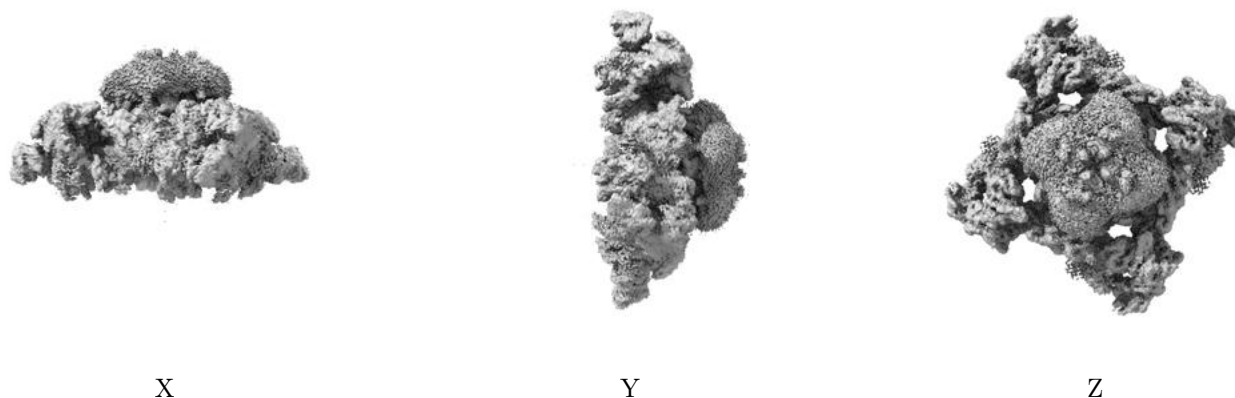


Z

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

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

### 5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

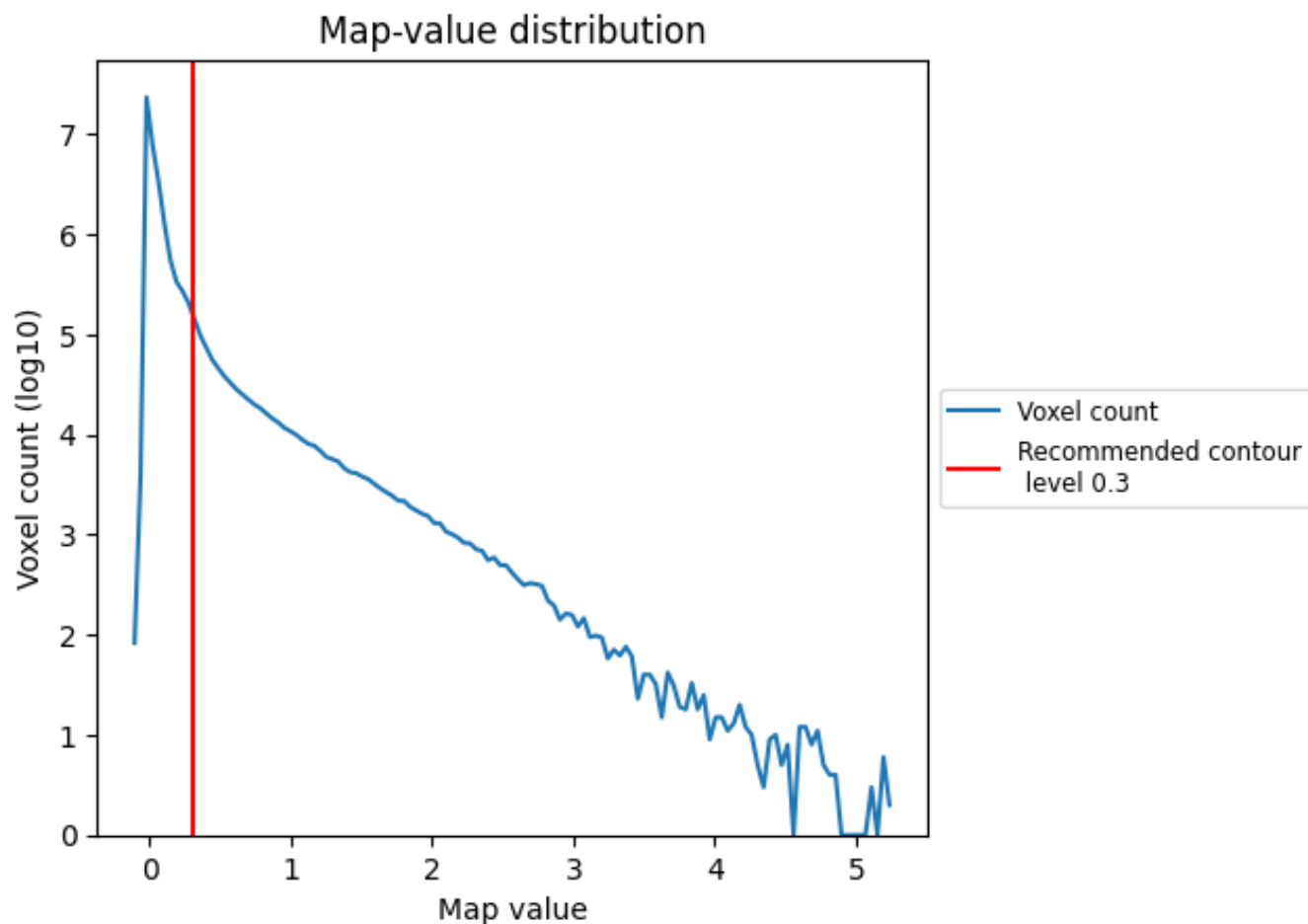
## 5.6 Mask visualisation [i](#)

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

## 6 Map analysis [i](#)

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

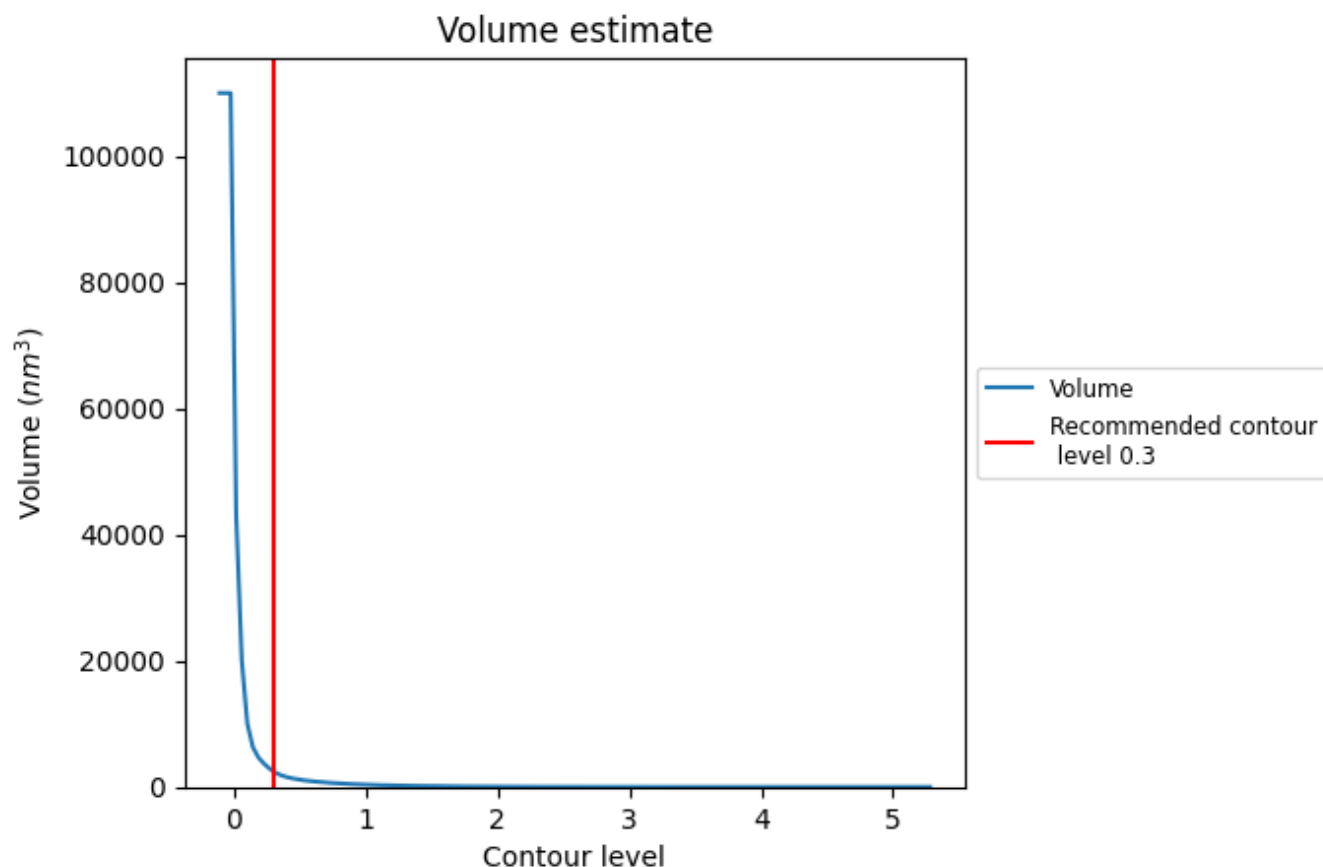
### 6.1 Map-value distribution [i](#)



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.



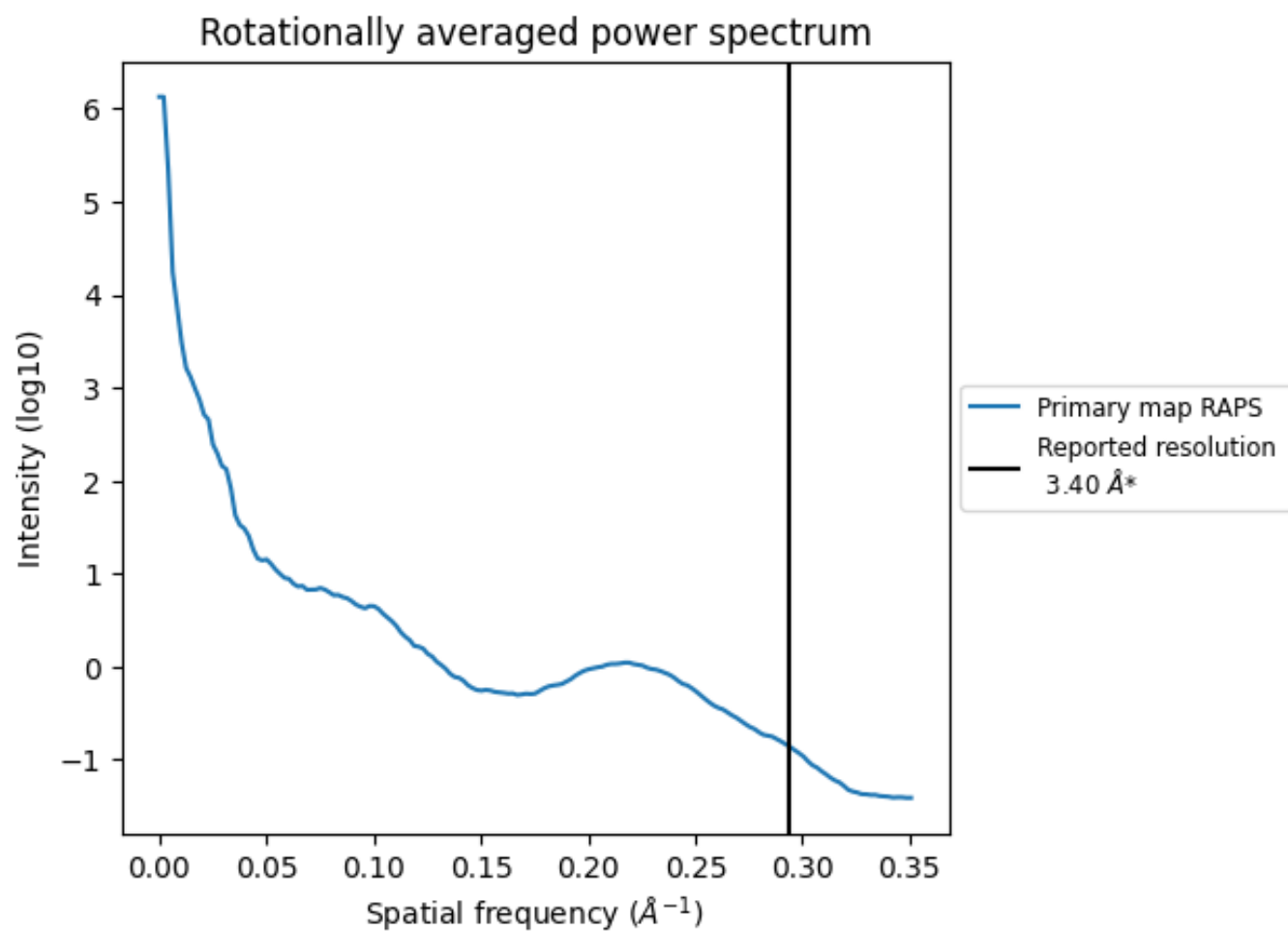
## 6.2 Volume estimate [i](#)



The volume at the recommended contour level is  $2518 \text{ nm}^3$ ; this corresponds to an approximate mass of 2275 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.

### 6.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

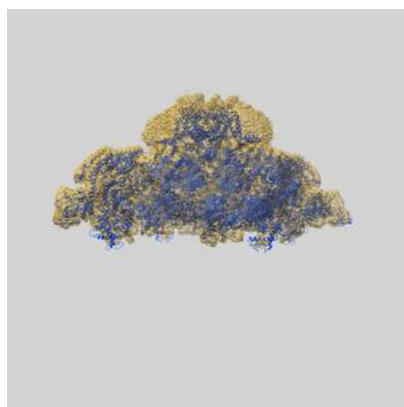
## 7 Fourier-Shell correlation ⓘ

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

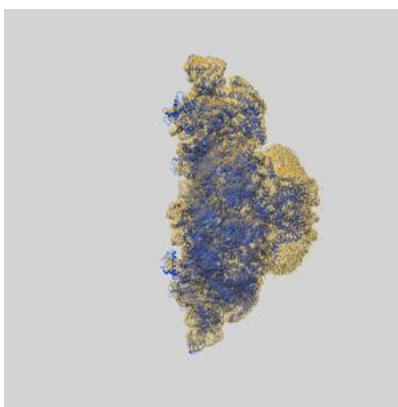
## 8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52085 and PDB model 9HEO. Per-residue inclusion information can be found in section ?? on page ??.

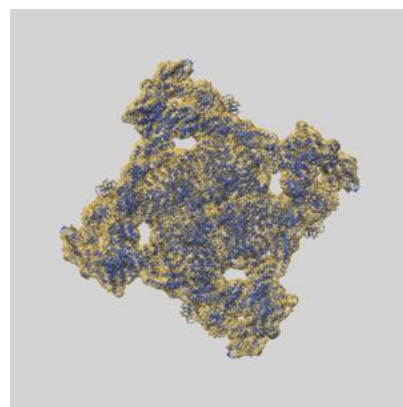
### 8.1 Map-model overlay [i](#)



X



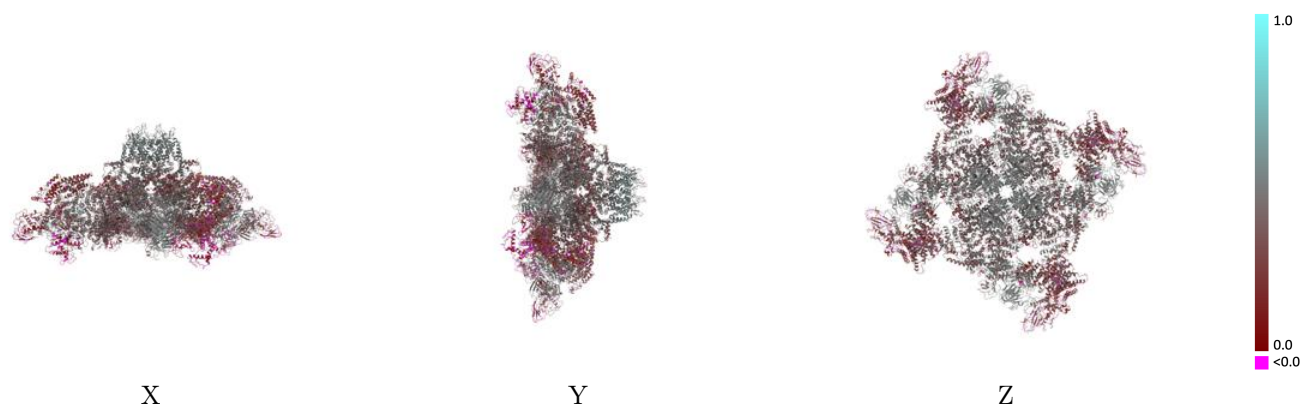
Y



Z

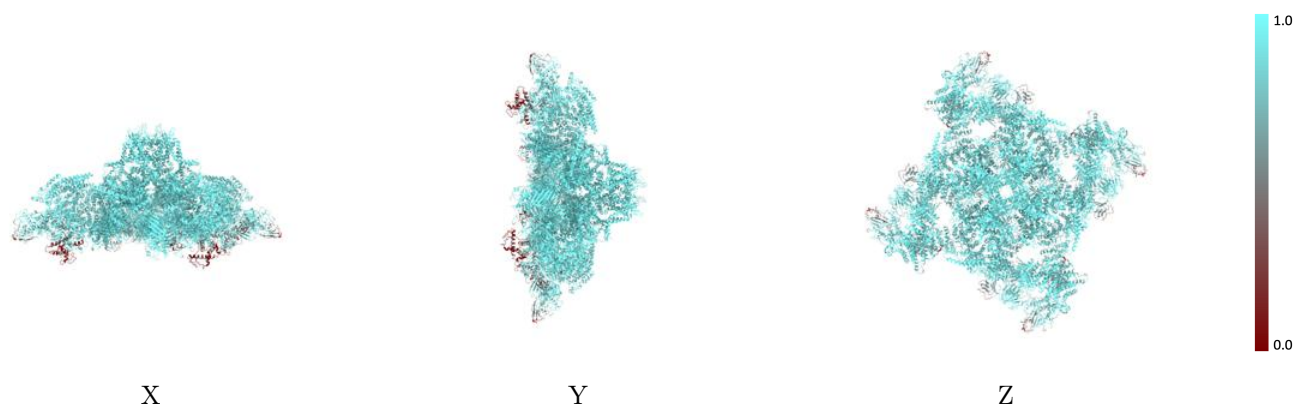
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



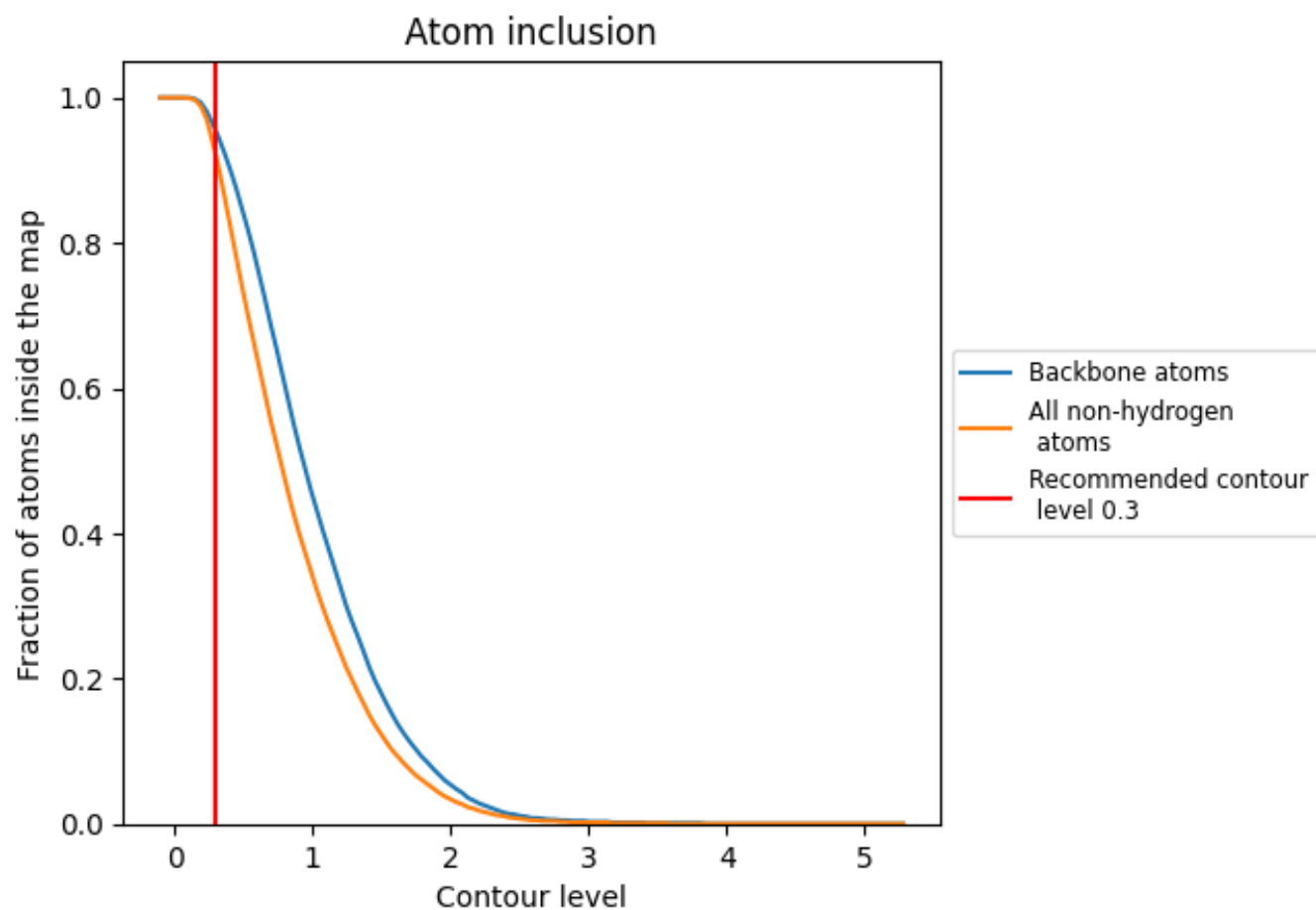
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

## 8.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9180	<div></div> 0.3600
A	<div></div> 0.9340	<div></div> 0.3650
B	<div></div> 0.6020	<div></div> 0.1630
C	<div></div> 0.9340	<div></div> 0.3660
D	<div></div> 0.6020	<div></div> 0.1660
E	<div></div> 0.6010	<div></div> 0.3560
F	<div></div> 0.5980	<div></div> 0.3610
G	<div></div> 0.9340	<div></div> 0.3650
H	<div></div> 0.6160	<div></div> 0.1670
I	<div></div> 0.6080	<div></div> 0.3710
J	<div></div> 0.9340	<div></div> 0.3650
K	<div></div> 0.6030	<div></div> 0.1660
L	<div></div> 0.6080	<div></div> 0.3670

