



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Oct 29, 2019 – 05:20 PM EDT

PDB ID : 6JB1
EMDB ID: : EMD-9787
Title : Structure of pancreatic ATP-sensitive potassium channel bound with repaglinide and ATPgammaS at 3.3A resolution
Authors : Chen, L.; Ding, D.; Wang, M.; Wu, J.-X.; Kang, Y.
Deposited on : 2019-01-25
Resolution : 3.30 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

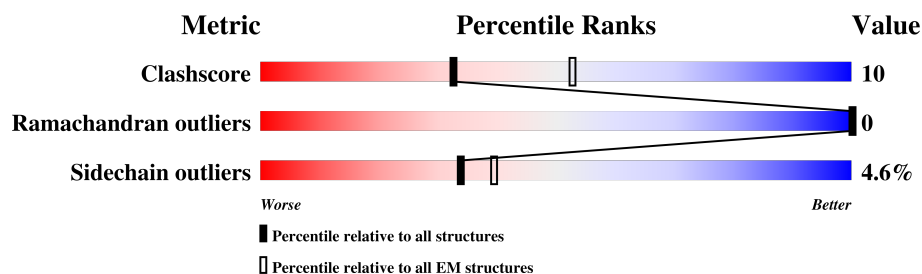
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	390	55% 27% • 16%
1	C	390	55% 28% • 16%
1	E	390	54% 28% • 16%
1	G	390	54% 28% • 16%
2	B	1582	69% 16% • 14%
2	D	1582	69% 16% • 14%
2	F	1582	70% 16% • 14%
2	H	1582	70% 15% • 14%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 52028 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.

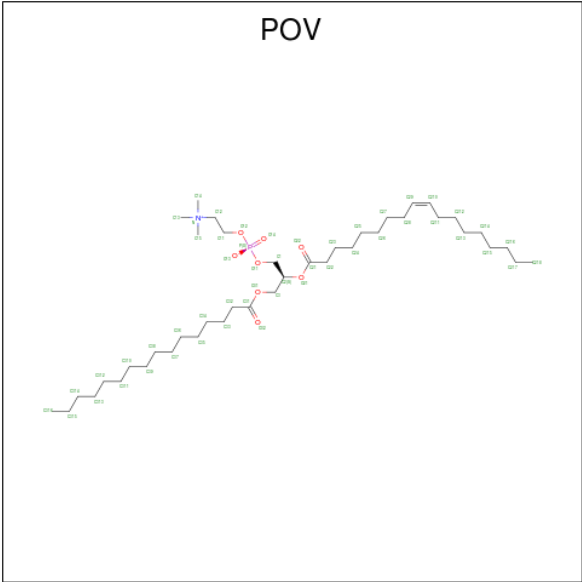
- Molecule 1 is a protein called ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	327	Total	C	N	O	S	0	0
			2543	1641	440	446	16		
1	C	327	Total	C	N	O	S	0	0
			2543	1641	440	446	16		
1	E	327	Total	C	N	O	S	0	0
			2543	1641	440	446	16		
1	G	327	Total	C	N	O	S	0	0
			2543	1641	440	446	16		

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8 isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1366	Total	C	N	O	S	0	0
			9890	6419	1693	1735	43		
2	D	1366	Total	C	N	O	S	0	0
			9890	6419	1693	1735	43		
2	F	1366	Total	C	N	O	S	0	0
			9890	6419	1693	1735	43		
2	H	1366	Total	C	N	O	S	0	0
			9890	6419	1693	1735	43		

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	22	1	7	1	
3	B	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	B	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	B	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	B	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	B	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	B	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	B	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	C	1	Total	C	N	O	P	0
			31	22	1	7	1	
3	D	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	D	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	D	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	D	1	Total	C	N	O	P	0
			272	199	7	59	7	

Continued on next page...

Continued from previous page...

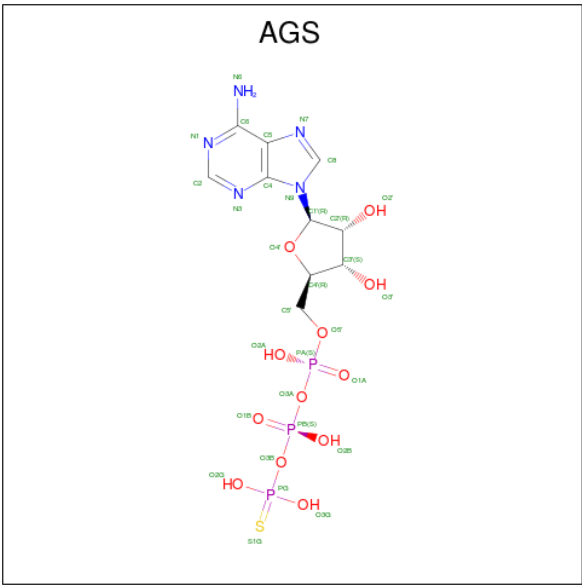
Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	D	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	D	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	D	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	E	1	Total	C	N	O	P	0
			31	22	1	7	1	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	F	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	G	1	Total	C	N	O	P	0
			31	22	1	7	1	
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	

Continued on next page...

Continued from previous page...

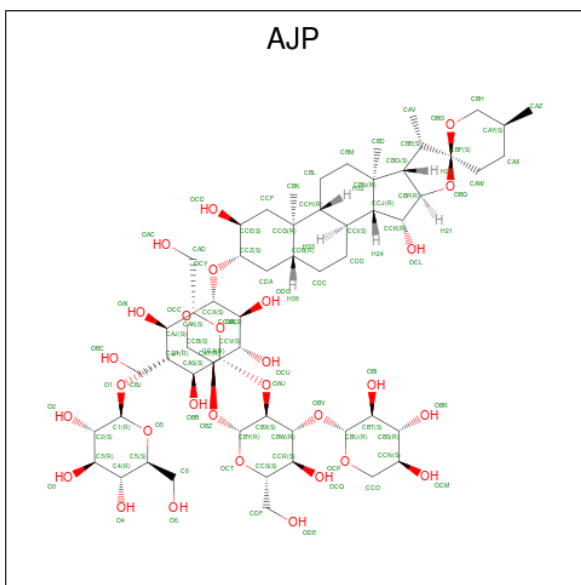
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	H	1	272	199	7	59	7	0

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



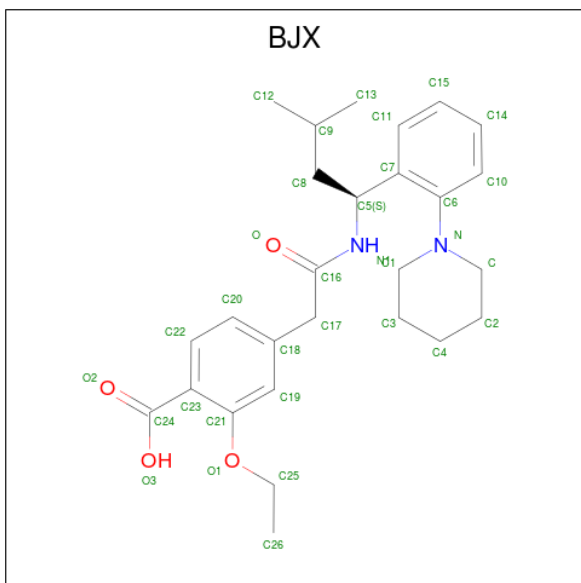
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
4	A	1	31	10	5	12	3	1	0
4	B	1	31	10	5	12	3	1	0
4	C	1	31	10	5	12	3	1	0
4	D	1	31	10	5	12	3	1	0
4	E	1	31	10	5	12	3	1	0
4	F	1	31	10	5	12	3	1	0
4	G	1	31	10	5	12	3	1	0
4	H	1	31	10	5	12	3	1	0

- Molecule 5 is Digitonin (three-letter code: AJP) (formula: C₅₆H₉₂O₂₉).



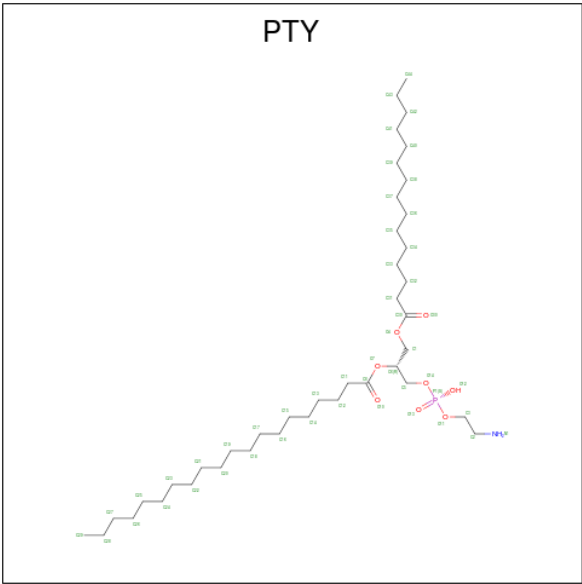
Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total 74	C 50	O 24	0
5	D	1	Total 74	C 50	O 24	0
5	F	1	Total 74	C 50	O 24	0
5	H	1	Total 74	C 50	O 24	0

- Molecule 6 is Repaglinide (three-letter code: BJX) (formula: $\text{C}_{27}\text{H}_{36}\text{N}_2\text{O}_4$).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			33	27	2	4	
6	D	1	Total	C	N	O	0
			33	27	2	4	
6	F	1	Total	C	N	O	0
			33	27	2	4	
6	H	1	Total	C	N	O	0
			33	27	2	4	

- Molecule 7 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	B	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	B	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	B	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	D	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	D	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	D	1	Total	C	N	O	P	0
			102	65	4	29	4	

Continued on next page...

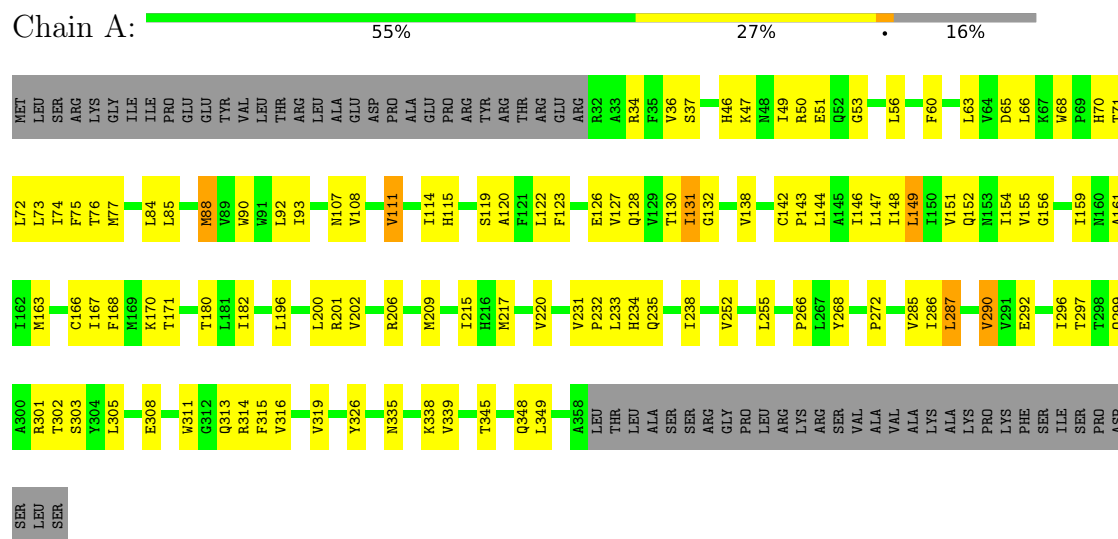
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	F	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	F	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	F	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	F	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	H	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	H	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	H	1	Total	C	N	O	P	0
			102	65	4	29	4	

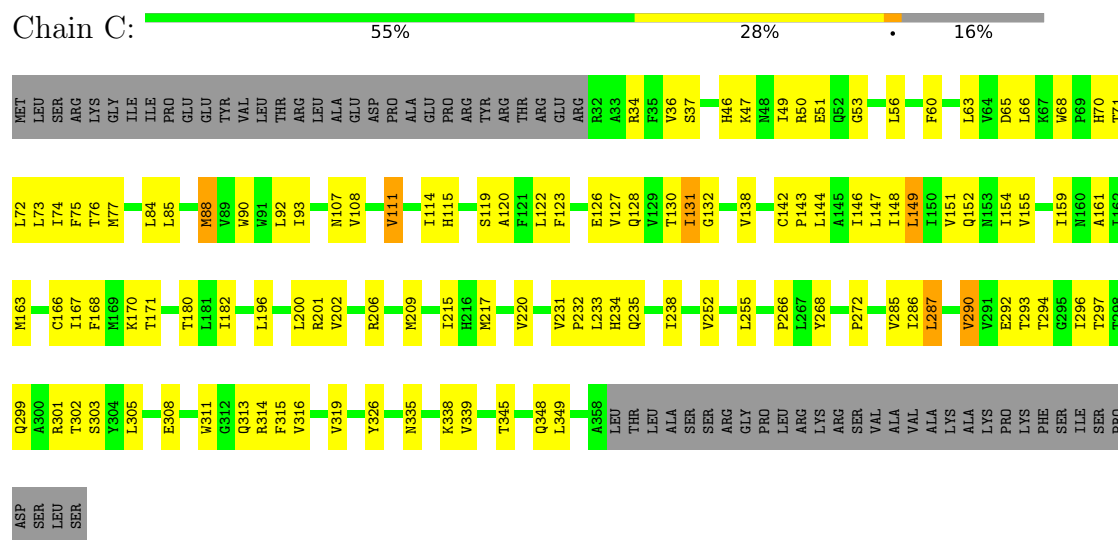
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

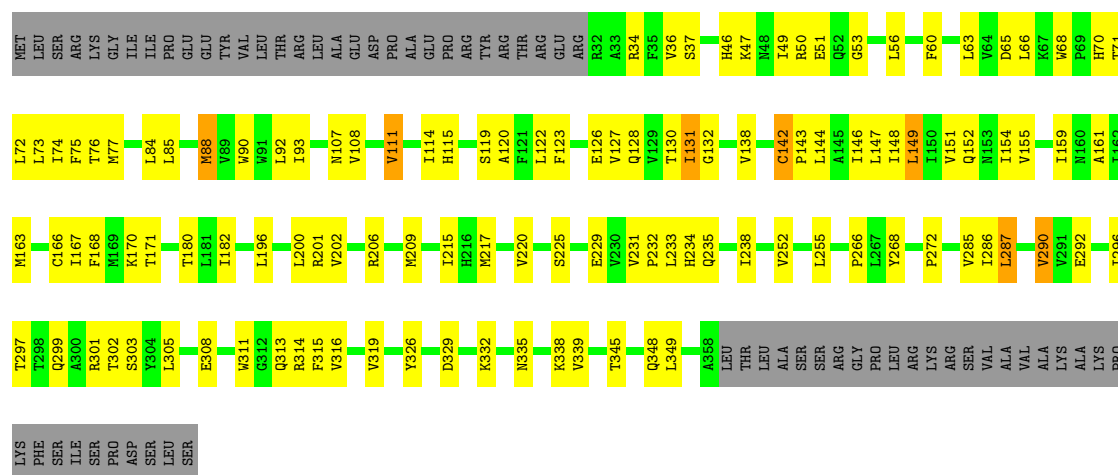


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



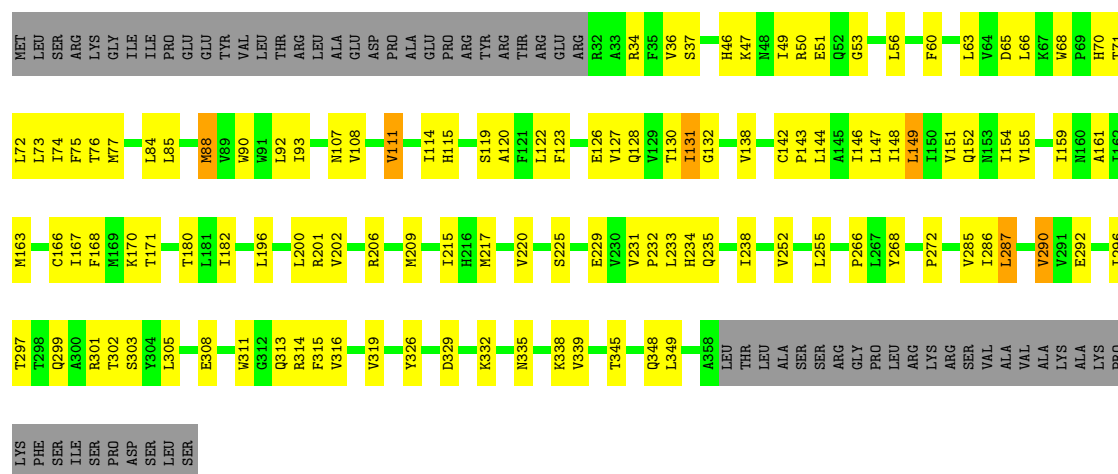
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11





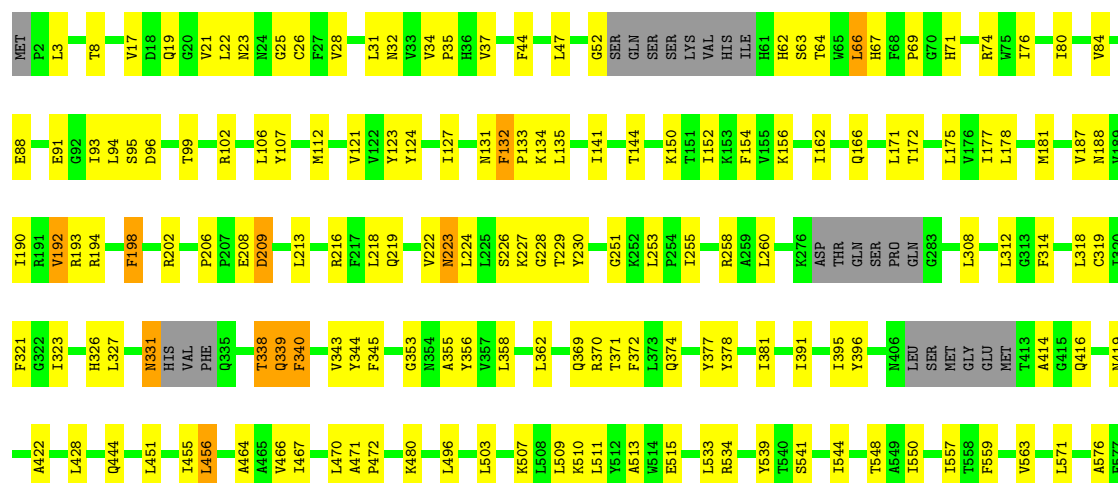
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

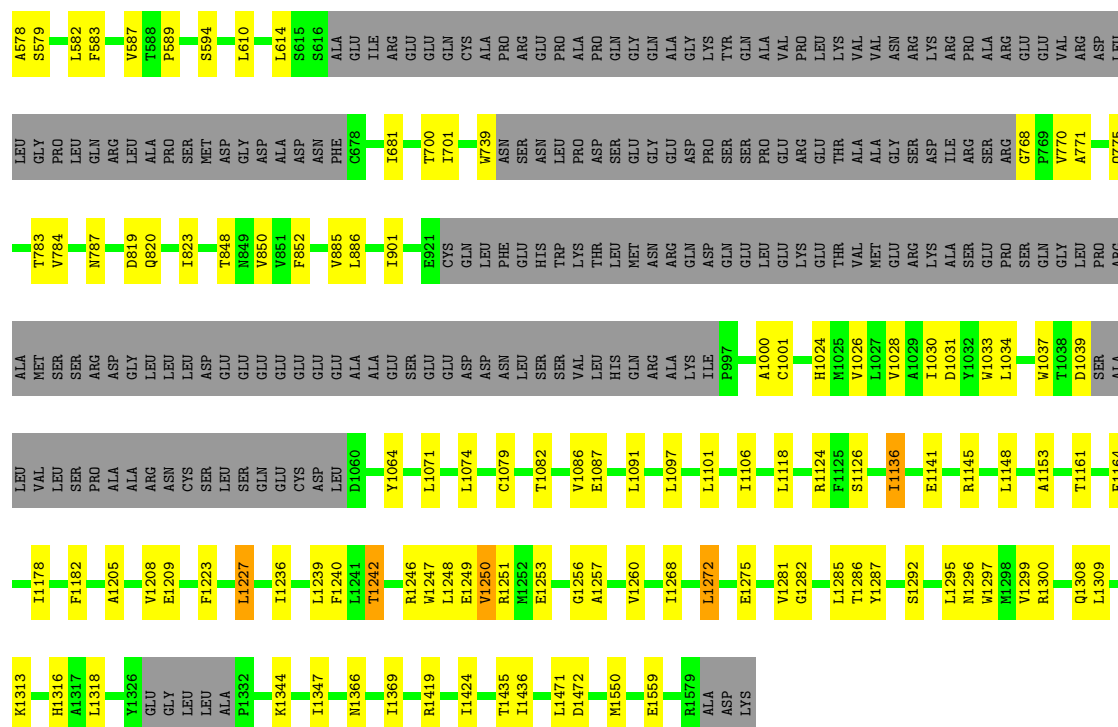
Chain G: 54% 28% 16%



- Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

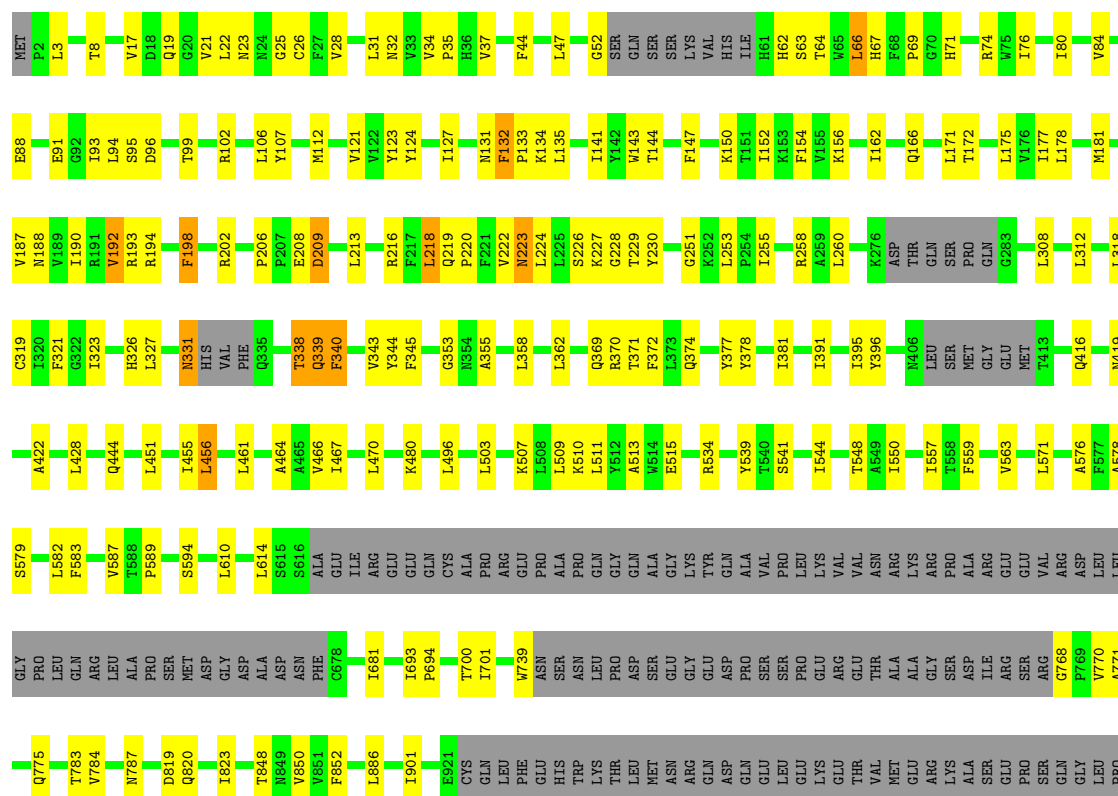
Chain B: 69% 16% 14%

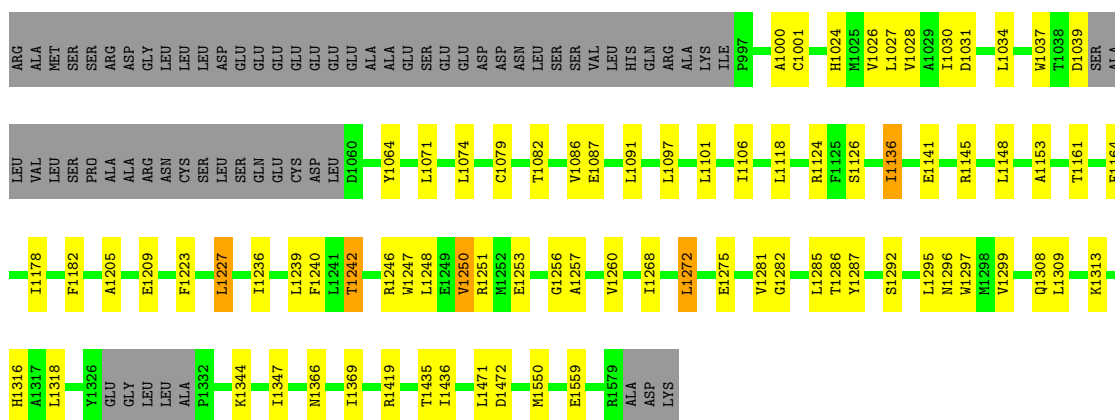




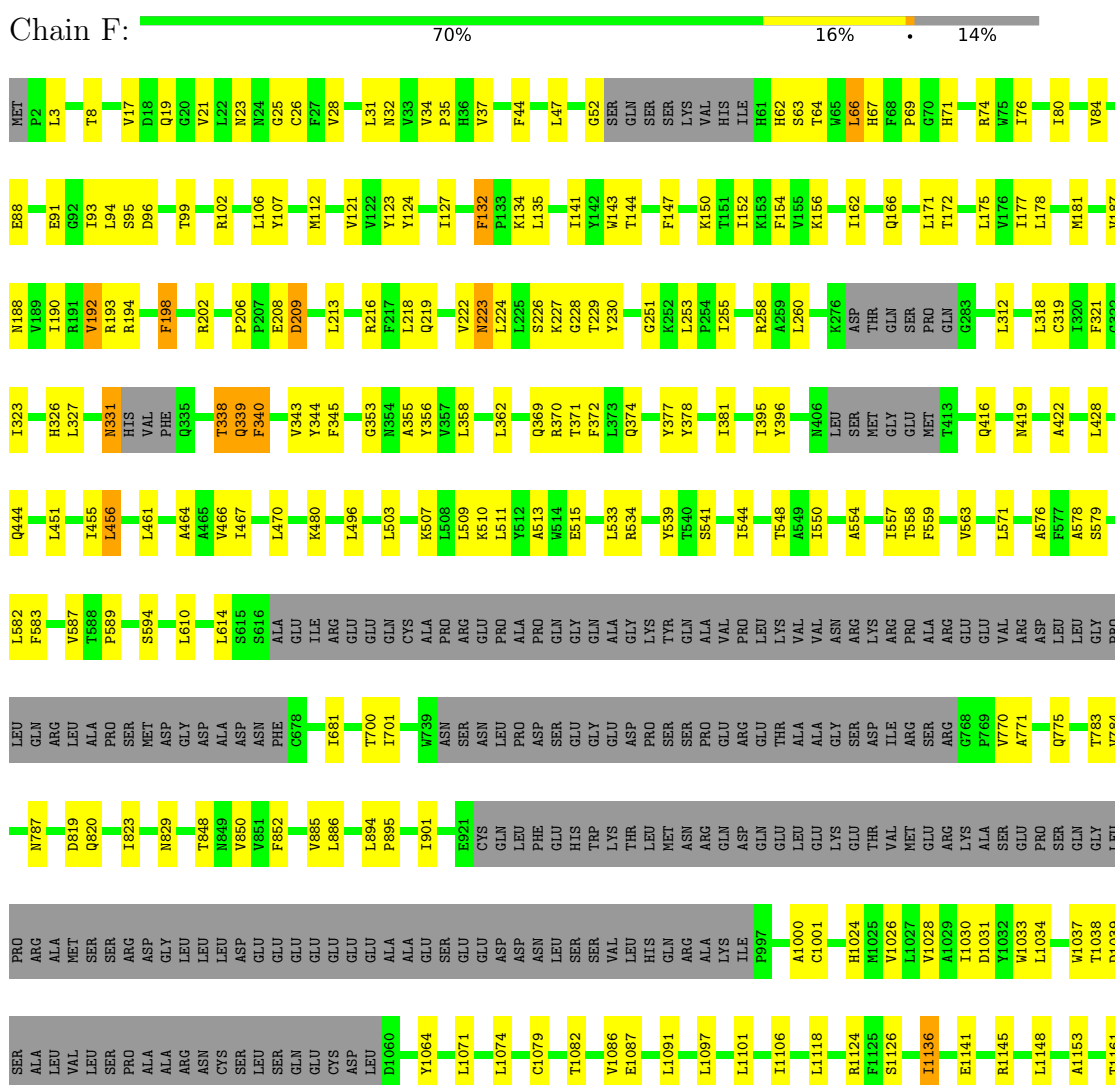
● Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

Chain D: 69% 16% 14%





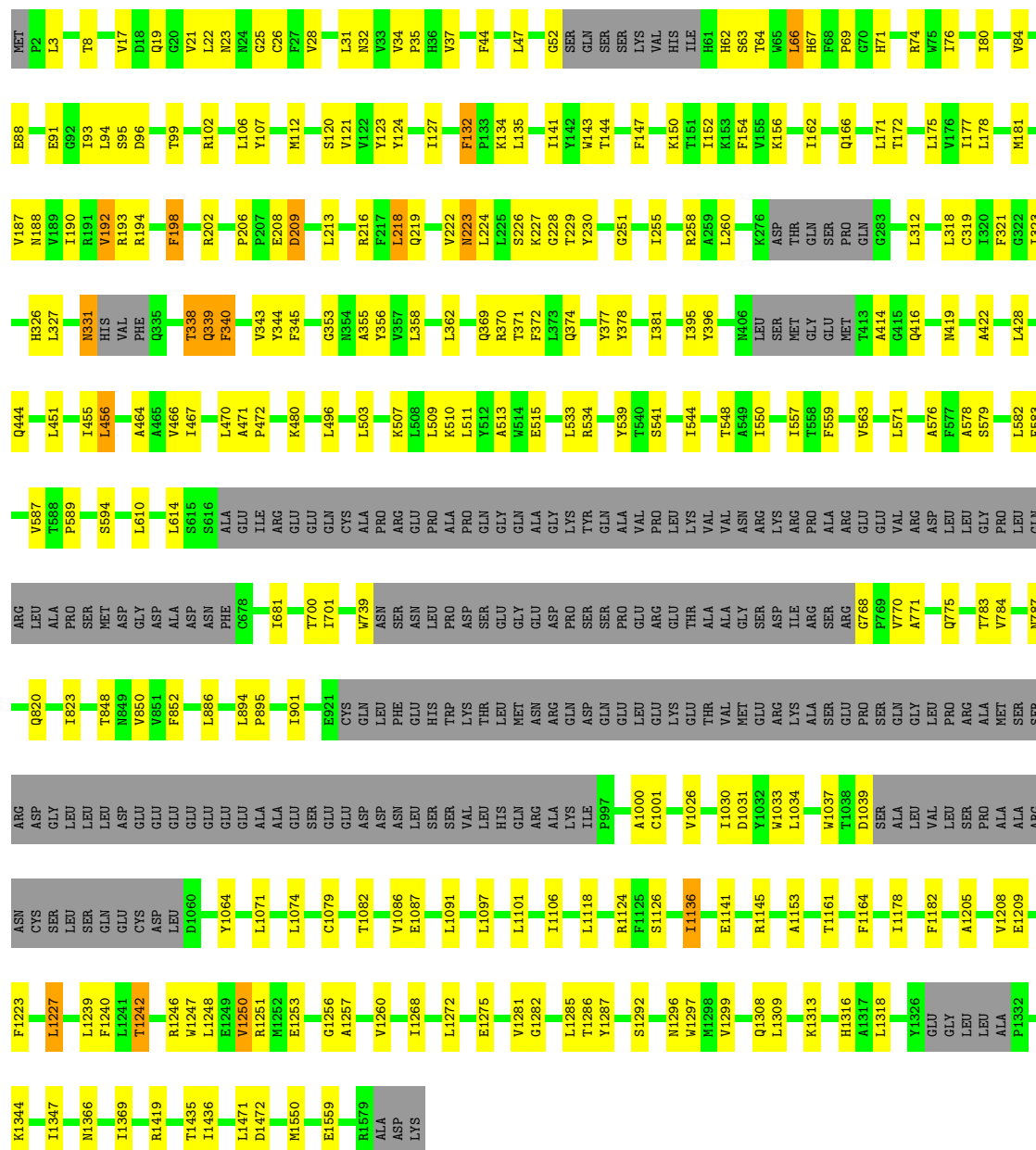
- Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2





• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

Chain H: 70% 15% 14%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	277548	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AJP, POV, AGS, PTY, BJX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.36	0/2600	0.54	0/3535
1	C	0.36	0/2600	0.54	0/3535
1	E	0.36	0/2600	0.54	0/3535
1	G	0.36	0/2600	0.54	0/3535
2	B	0.28	0/10097	0.43	0/13798
2	D	0.28	0/10097	0.43	0/13798
2	F	0.28	0/10097	0.43	0/13798
2	H	0.28	0/10097	0.43	0/13798
All	All	0.30	0/50788	0.45	0/69332

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2543	0	2571	79	0
1	C	2543	0	2571	80	0
1	E	2543	0	2571	78	0
1	G	2543	0	2571	79	0
2	B	9890	0	9397	178	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	9890	0	9397	180	0
2	F	9890	0	9397	172	0
2	H	9890	0	9397	170	0
3	A	31	0	40	4	0
3	B	272	0	346	21	0
3	C	31	0	40	3	0
3	D	272	0	346	19	0
3	E	31	0	40	4	0
3	F	272	0	346	18	0
3	G	31	0	40	4	0
3	H	272	0	346	19	0
4	A	31	0	12	2	0
4	B	31	0	12	1	0
4	C	31	0	12	2	0
4	D	31	0	12	1	0
4	E	31	0	12	2	0
4	F	31	0	12	1	0
4	G	31	0	12	2	0
4	H	31	0	12	1	0
5	B	74	0	0	1	0
5	D	74	0	0	1	0
5	F	74	0	0	1	0
5	H	74	0	0	1	0
6	B	33	0	0	2	0
6	D	33	0	0	2	0
6	F	33	0	0	2	0
6	H	33	0	0	2	0
7	B	102	0	108	7	0
7	D	102	0	108	7	0
7	F	102	0	108	7	0
7	H	102	0	108	7	0
All	All	52028	0	49944	1026	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 1026 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:THR:HA	1:G:131:ILE:HG22	1.59	0.85
1:E:131:ILE:HG22	1:G:130:THR:HA	1.59	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:HG22	1:C:130:THR:HA	1.59	0.84
1:C:131:ILE:HG22	1:E:130:THR:HA	1.59	0.84
2:F:371:THR:HG21	7:F:1615:PTY:H141	1.63	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/390 (83%)	305 (94%)	20 (6%)	0	100	100
1	C	325/390 (83%)	305 (94%)	20 (6%)	0	100	100
1	E	325/390 (83%)	305 (94%)	20 (6%)	0	100	100
1	G	325/390 (83%)	305 (94%)	20 (6%)	0	100	100
2	B	1346/1582 (85%)	1284 (95%)	62 (5%)	0	100	100
2	D	1346/1582 (85%)	1284 (95%)	62 (5%)	0	100	100
2	F	1346/1582 (85%)	1284 (95%)	62 (5%)	0	100	100
2	H	1346/1582 (85%)	1284 (95%)	62 (5%)	0	100	100
All	All	6684/7888 (85%)	6356 (95%)	328 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/339 (81%)	256 (93%)	20 (7%)	16	46
1	C	276/339 (81%)	256 (93%)	20 (7%)	16	46
1	E	276/339 (81%)	256 (93%)	20 (7%)	16	46
1	G	276/339 (81%)	256 (93%)	20 (7%)	16	46
2	B	931/1371 (68%)	896 (96%)	35 (4%)	36	67
2	D	931/1371 (68%)	896 (96%)	35 (4%)	36	67
2	F	931/1371 (68%)	896 (96%)	35 (4%)	36	67
2	H	931/1371 (68%)	896 (96%)	35 (4%)	36	67
All	All	4828/6840 (71%)	4608 (95%)	220 (5%)	34	63

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	456	LEU
1	E	202	VAL
2	H	331	ASN
2	D	886	LEU
1	E	65	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	437	ASN
1	E	46	HIS
1	G	46	HIS
2	D	219	GLN
1	G	299	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

68 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	A	401	-	30,30,51	0.97	1 (3%)	35,37,59	1.03	2 (5%)
4	AGS	A	402	-	25,33,33	2.13	3 (12%)	24,52,52	1.38	4 (16%)
5	AJP	B	1601	-	83,83,95	0.63	0	122,131,149	1.21	9 (7%)
4	AGS	B	1602	-	25,33,33	2.14	3 (12%)	24,52,52	1.35	3 (12%)
6	BJX	B	1603	-	33,35,35	1.77	4 (12%)	40,47,47	1.39	5 (12%)
3	POV	B	1604	-	35,35,51	1.16	2 (5%)	41,43,59	1.08	2 (4%)
3	POV	B	1605	-	40,40,51	1.10	2 (5%)	46,48,59	1.01	2 (4%)
3	POV	B	1606	-	39,39,51	1.12	2 (5%)	45,47,59	1.05	2 (4%)
3	POV	B	1607	-	40,40,51	1.09	2 (5%)	46,48,59	1.10	4 (8%)
3	POV	B	1608	-	35,35,51	1.18	2 (5%)	41,43,59	1.25	4 (9%)
3	POV	B	1609	-	24,24,51	1.07	1 (4%)	29,31,59	1.03	1 (3%)
3	POV	B	1610	-	24,24,51	1.02	1 (4%)	29,31,59	1.14	2 (6%)
3	POV	B	1611	-	27,27,51	1.26	2 (7%)	29,29,59	1.22	2 (6%)
7	PTY	B	1612	-	31,31,49	1.23	2 (6%)	34,36,54	1.25	2 (5%)
7	PTY	B	1613	-	26,26,49	1.35	2 (7%)	29,31,54	1.14	2 (6%)
7	PTY	B	1614	-	21,21,49	1.11	1 (4%)	23,25,54	0.91	1 (4%)
7	PTY	B	1615	-	20,20,49	1.20	2 (10%)	22,24,54	1.30	3 (13%)
4	AGS	C	401	-	25,33,33	2.13	3 (12%)	24,52,52	1.38	4 (16%)
3	POV	C	402	-	30,30,51	0.97	1 (3%)	35,37,59	1.03	2 (5%)
5	AJP	D	1601	-	83,83,95	0.63	0	122,131,149	1.21	9 (7%)
4	AGS	D	1602	-	25,33,33	2.14	3 (12%)	24,52,52	1.35	3 (12%)
6	BJX	D	1603	-	33,35,35	1.77	4 (12%)	40,47,47	1.39	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	D	1604	-	35,35,51	1.16	2 (5%)	41,43,59	1.08	2 (4%)
3	POV	D	1605	-	40,40,51	1.10	2 (5%)	46,48,59	1.01	2 (4%)
3	POV	D	1606	-	39,39,51	1.12	2 (5%)	45,47,59	1.05	2 (4%)
3	POV	D	1607	-	40,40,51	1.09	2 (5%)	46,48,59	1.10	4 (8%)
3	POV	D	1608	-	35,35,51	1.18	2 (5%)	41,43,59	1.25	4 (9%)
3	POV	D	1609	-	24,24,51	1.07	1 (4%)	29,31,59	1.03	1 (3%)
3	POV	D	1610	-	24,24,51	1.02	1 (4%)	29,31,59	1.14	2 (6%)
3	POV	D	1611	-	27,27,51	1.26	2 (7%)	29,29,59	1.22	2 (6%)
7	PTY	D	1612	-	31,31,49	1.23	2 (6%)	34,36,54	1.25	2 (5%)
7	PTY	D	1613	-	26,26,49	1.35	2 (7%)	29,31,54	1.14	2 (6%)
7	PTY	D	1614	-	21,21,49	1.11	1 (4%)	23,25,54	0.91	1 (4%)
7	PTY	D	1615	-	20,20,49	1.20	2 (10%)	22,24,54	1.30	3 (13%)
4	AGS	E	401	-	25,33,33	2.13	3 (12%)	24,52,52	1.38	4 (16%)
3	POV	E	402	-	30,30,51	0.97	1 (3%)	35,37,59	1.03	2 (5%)
5	AJP	F	1601	-	83,83,95	0.63	0	122,131,149	1.21	9 (7%)
4	AGS	F	1602	-	25,33,33	2.14	3 (12%)	24,52,52	1.35	3 (12%)
6	BJX	F	1603	-	33,35,35	1.77	4 (12%)	40,47,47	1.39	5 (12%)
3	POV	F	1604	-	35,35,51	1.16	2 (5%)	41,43,59	1.08	2 (4%)
3	POV	F	1605	-	40,40,51	1.10	2 (5%)	46,48,59	1.01	2 (4%)
3	POV	F	1606	-	39,39,51	1.12	2 (5%)	45,47,59	1.05	2 (4%)
3	POV	F	1607	-	40,40,51	1.09	2 (5%)	46,48,59	1.10	4 (8%)
3	POV	F	1608	-	35,35,51	1.18	2 (5%)	41,43,59	1.25	4 (9%)
3	POV	F	1609	-	24,24,51	1.07	1 (4%)	29,31,59	1.03	1 (3%)
3	POV	F	1610	-	24,24,51	1.02	1 (4%)	29,31,59	1.14	2 (6%)
3	POV	F	1611	-	27,27,51	1.26	2 (7%)	29,29,59	1.22	2 (6%)
7	PTY	F	1612	-	31,31,49	1.23	2 (6%)	34,36,54	1.25	2 (5%)
7	PTY	F	1613	-	26,26,49	1.35	2 (7%)	29,31,54	1.14	2 (6%)
7	PTY	F	1614	-	21,21,49	1.11	1 (4%)	23,25,54	0.91	1 (4%)
7	PTY	F	1615	-	20,20,49	1.20	2 (10%)	22,24,54	1.30	3 (13%)
4	AGS	G	401	-	25,33,33	2.13	3 (12%)	24,52,52	1.38	4 (16%)
3	POV	G	402	-	30,30,51	0.97	1 (3%)	35,37,59	1.03	2 (5%)
5	AJP	H	1601	-	83,83,95	0.63	0	122,131,149	1.21	9 (7%)
4	AGS	H	1602	-	25,33,33	2.14	3 (12%)	24,52,52	1.35	3 (12%)
6	BJX	H	1603	-	33,35,35	1.77	4 (12%)	40,47,47	1.39	5 (12%)
3	POV	H	1604	-	35,35,51	1.16	2 (5%)	41,43,59	1.08	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	H	1605	-	40,40,51	1.10	2 (5%)	46,48,59	1.01	2 (4%)
3	POV	H	1606	-	39,39,51	1.12	2 (5%)	45,47,59	1.05	2 (4%)
3	POV	H	1607	-	40,40,51	1.09	2 (5%)	46,48,59	1.10	4 (8%)
3	POV	H	1608	-	35,35,51	1.18	2 (5%)	41,43,59	1.25	4 (9%)
3	POV	H	1609	-	24,24,51	1.07	1 (4%)	29,31,59	1.03	1 (3%)
3	POV	H	1610	-	24,24,51	1.02	1 (4%)	29,31,59	1.14	2 (6%)
3	POV	H	1611	-	27,27,51	1.26	2 (7%)	29,29,59	1.22	2 (6%)
7	PTY	H	1612	-	31,31,49	1.23	2 (6%)	34,36,54	1.25	2 (5%)
7	PTY	H	1613	-	26,26,49	1.35	2 (7%)	29,31,54	1.14	2 (6%)
7	PTY	H	1614	-	21,21,49	1.11	1 (4%)	23,25,54	0.91	1 (4%)
7	PTY	H	1615	-	20,20,49	1.20	2 (10%)	22,24,54	1.30	3 (13%)

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	POV	A	401	-	-	3/33/33/55	-
4	AGS	A	402	-	-	2/17/38/38	0/3/3/3
5	AJP	B	1601	-	-	11/22/194/220	0/10/10/11
4	AGS	B	1602	-	-	2/17/38/38	0/3/3/3
6	BJX	B	1603	-	-	11/23/35/35	0/3/3/3
3	POV	B	1604	-	-	12/39/39/55	-
3	POV	B	1605	-	-	14/44/44/55	-
3	POV	B	1606	-	-	17/43/43/55	-
3	POV	B	1607	-	-	14/44/44/55	-
3	POV	B	1608	-	-	12/39/39/55	-
3	POV	B	1609	-	-	10/27/27/55	-
3	POV	B	1610	-	-	6/27/27/55	-
3	POV	B	1611	-	-	10/29/29/55	-
7	PTY	B	1612	-	-	14/35/35/53	-
7	PTY	B	1613	-	-	13/30/30/53	-
7	PTY	B	1614	-	-	13/23/23/53	-
7	PTY	B	1615	-	-	14/22/22/53	-
4	AGS	C	401	-	-	2/17/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	C	402	-	-	3/33/33/55	-
5	AJP	D	1601	-	-	11/22/194/220	0/10/10/11
4	AGS	D	1602	-	-	2/17/38/38	0/3/3/3
6	BJX	D	1603	-	-	11/23/35/35	0/3/3/3
3	POV	D	1604	-	-	12/39/39/55	-
3	POV	D	1605	-	-	14/44/44/55	-
3	POV	D	1606	-	-	17/43/43/55	-
3	POV	D	1607	-	-	14/44/44/55	-
3	POV	D	1608	-	-	12/39/39/55	-
3	POV	D	1609	-	-	10/27/27/55	-
3	POV	D	1610	-	-	6/27/27/55	-
3	POV	D	1611	-	-	10/29/29/55	-
7	PTY	D	1612	-	-	14/35/35/53	-
7	PTY	D	1613	-	-	13/30/30/53	-
7	PTY	D	1614	-	-	13/23/23/53	-
7	PTY	D	1615	-	-	14/22/22/53	-
4	AGS	E	401	-	-	2/17/38/38	0/3/3/3
3	POV	E	402	-	-	3/33/33/55	-
5	AJP	F	1601	-	-	11/22/194/220	0/10/10/11
4	AGS	F	1602	-	-	2/17/38/38	0/3/3/3
6	BJX	F	1603	-	-	11/23/35/35	0/3/3/3
3	POV	F	1604	-	-	12/39/39/55	-
3	POV	F	1605	-	-	14/44/44/55	-
3	POV	F	1606	-	-	17/43/43/55	-
3	POV	F	1607	-	-	14/44/44/55	-
3	POV	F	1608	-	-	12/39/39/55	-
3	POV	F	1609	-	-	10/27/27/55	-
3	POV	F	1610	-	-	6/27/27/55	-
3	POV	F	1611	-	-	10/29/29/55	-
7	PTY	F	1612	-	-	14/35/35/53	-
7	PTY	F	1613	-	-	13/30/30/53	-
7	PTY	F	1614	-	-	13/23/23/53	-
7	PTY	F	1615	-	-	14/22/22/53	-
4	AGS	G	401	-	-	2/17/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	G	402	-	-	3/33/33/55	-
5	AJP	H	1601	-	-	11/22/194/220	0/10/10/11
4	AGS	H	1602	-	-	2/17/38/38	0/3/3/3
6	BJX	H	1603	-	-	11/23/35/35	0/3/3/3
3	POV	H	1604	-	-	12/39/39/55	-
3	POV	H	1605	-	-	14/44/44/55	-
3	POV	H	1606	-	-	17/43/43/55	-
3	POV	H	1607	-	-	14/44/44/55	-
3	POV	H	1608	-	-	12/39/39/55	-
3	POV	H	1609	-	-	10/27/27/55	-
3	POV	H	1610	-	-	6/27/27/55	-
3	POV	H	1611	-	-	10/29/29/55	-
7	PTY	H	1612	-	-	14/35/35/53	-
7	PTY	H	1613	-	-	13/30/30/53	-
7	PTY	H	1614	-	-	13/23/23/53	-
7	PTY	H	1615	-	-	14/22/22/53	-

The worst 5 of 128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	401	AGS	PG-S1G	9.19	2.08	1.90
4	C	401	AGS	PG-S1G	9.19	2.08	1.90
4	G	401	AGS	PG-S1G	9.19	2.08	1.90
4	A	402	AGS	PG-S1G	9.19	2.08	1.90
4	B	1602	AGS	PG-S1G	9.18	2.08	1.90

The worst 5 of 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1608	POV	O21-C21-C22	4.99	122.41	111.51
3	H	1608	POV	O21-C21-C22	4.99	122.41	111.51
3	D	1608	POV	O21-C21-C22	4.99	122.41	111.51
3	B	1608	POV	O21-C21-C22	4.99	122.41	111.51
7	F	1612	PTY	O7-C8-C11	4.96	122.34	111.51

There are no chirality outliers.

5 of 712 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1602	AGS	PB-O3B-PG-O2G
4	B	1602	AGS	PB-O3B-PG-O3G
4	D	1602	AGS	PB-O3B-PG-O2G
4	D	1602	AGS	PB-O3B-PG-O3G
3	H	1611	POV	C22-C21-O21-C2

There are no ring outliers.

60 monomers are involved in 137 short contacts:

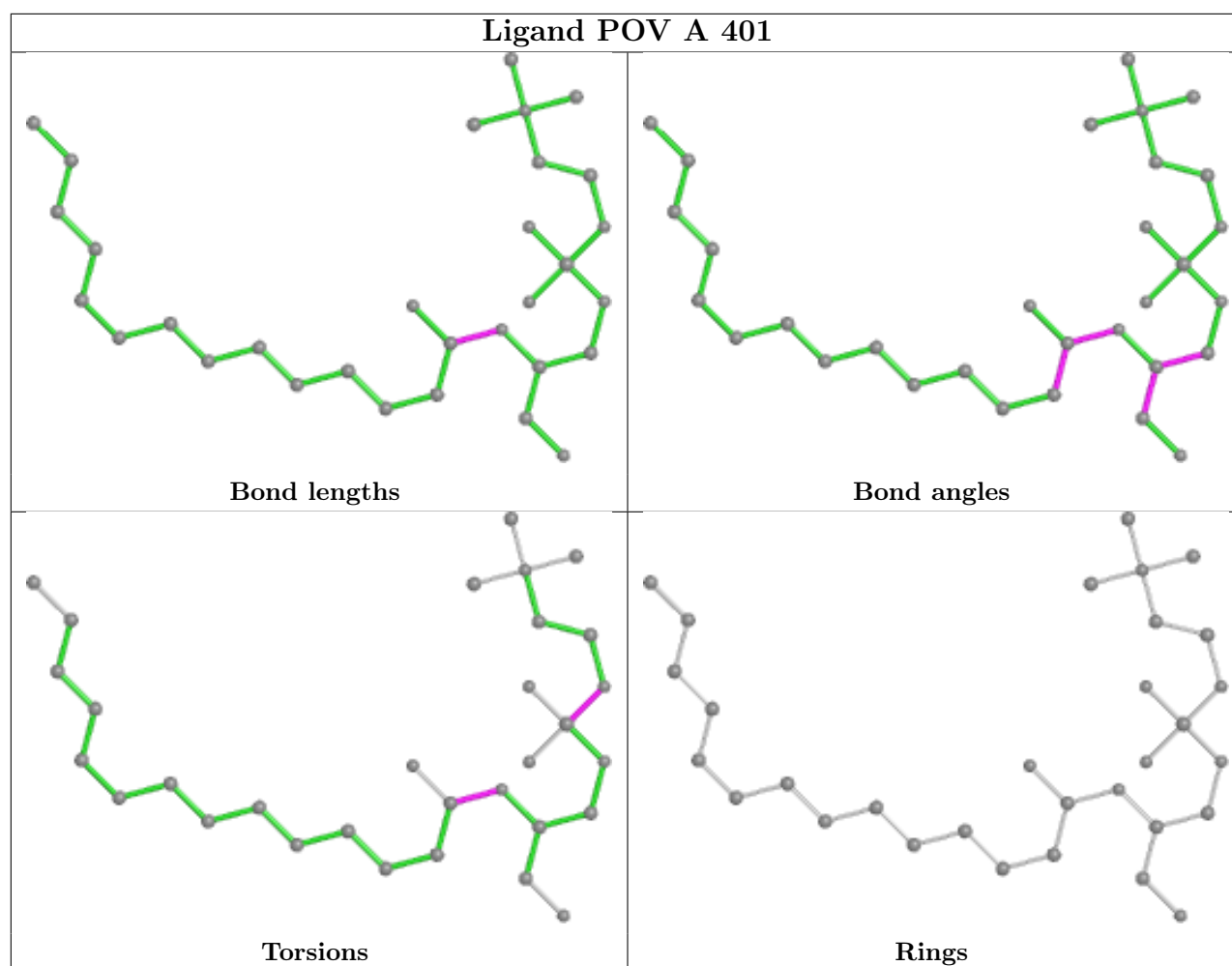
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	POV	4	0
4	A	402	AGS	2	0
5	B	1601	AJP	1	0
4	B	1602	AGS	1	0
6	B	1603	BJX	2	0
3	B	1604	POV	5	0
3	B	1605	POV	3	0
3	B	1606	POV	1	0
3	B	1607	POV	2	0
3	B	1608	POV	8	0
3	B	1609	POV	3	0
3	B	1611	POV	2	0
7	B	1613	PTY	4	0
7	B	1614	PTY	1	0
7	B	1615	PTY	2	0
4	C	401	AGS	2	0
3	C	402	POV	3	0
5	D	1601	AJP	1	0
4	D	1602	AGS	1	0
6	D	1603	BJX	2	0
3	D	1604	POV	5	0
3	D	1605	POV	3	0
3	D	1606	POV	1	0
3	D	1607	POV	2	0
3	D	1608	POV	8	0
3	D	1609	POV	2	0
3	D	1611	POV	1	0
7	D	1613	PTY	4	0
7	D	1614	PTY	1	0
7	D	1615	PTY	2	0
4	E	401	AGS	2	0
3	E	402	POV	4	0
5	F	1601	AJP	1	0

Continued on next page...

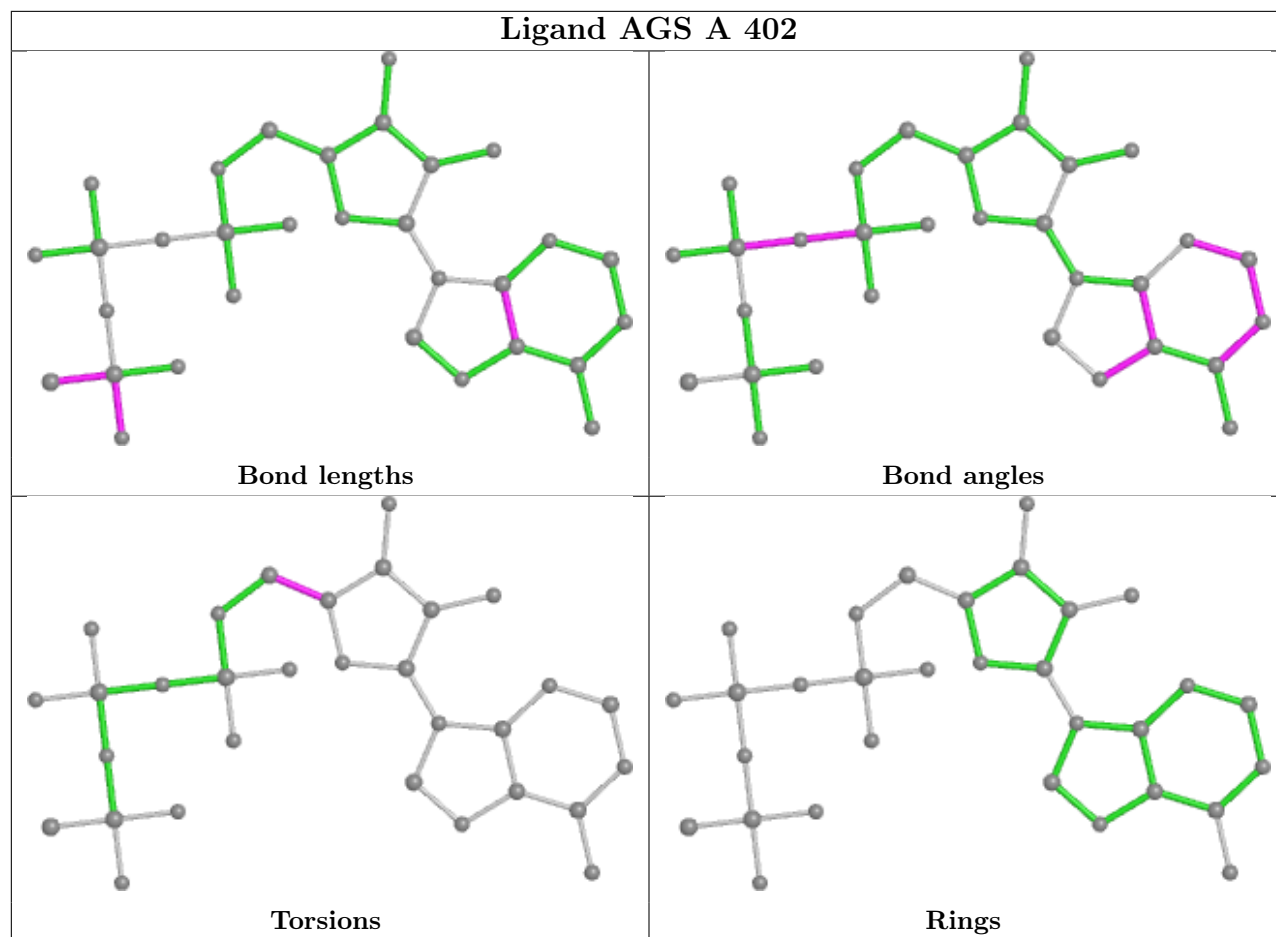
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1602	AGS	1	0
6	F	1603	BJX	2	0
3	F	1604	POV	4	0
3	F	1605	POV	2	0
3	F	1606	POV	1	0
3	F	1607	POV	2	0
3	F	1608	POV	7	0
3	F	1609	POV	3	0
3	F	1611	POV	2	0
7	F	1613	PTY	4	0
7	F	1614	PTY	1	0
7	F	1615	PTY	2	0
4	G	401	AGS	2	0
3	G	402	POV	4	0
5	H	1601	AJP	1	0
4	H	1602	AGS	1	0
6	H	1603	BJX	2	0
3	H	1604	POV	4	0
3	H	1605	POV	2	0
3	H	1606	POV	1	0
3	H	1607	POV	2	0
3	H	1608	POV	8	0
3	H	1609	POV	3	0
3	H	1611	POV	2	0
7	H	1613	PTY	4	0
7	H	1614	PTY	1	0
7	H	1615	PTY	2	0

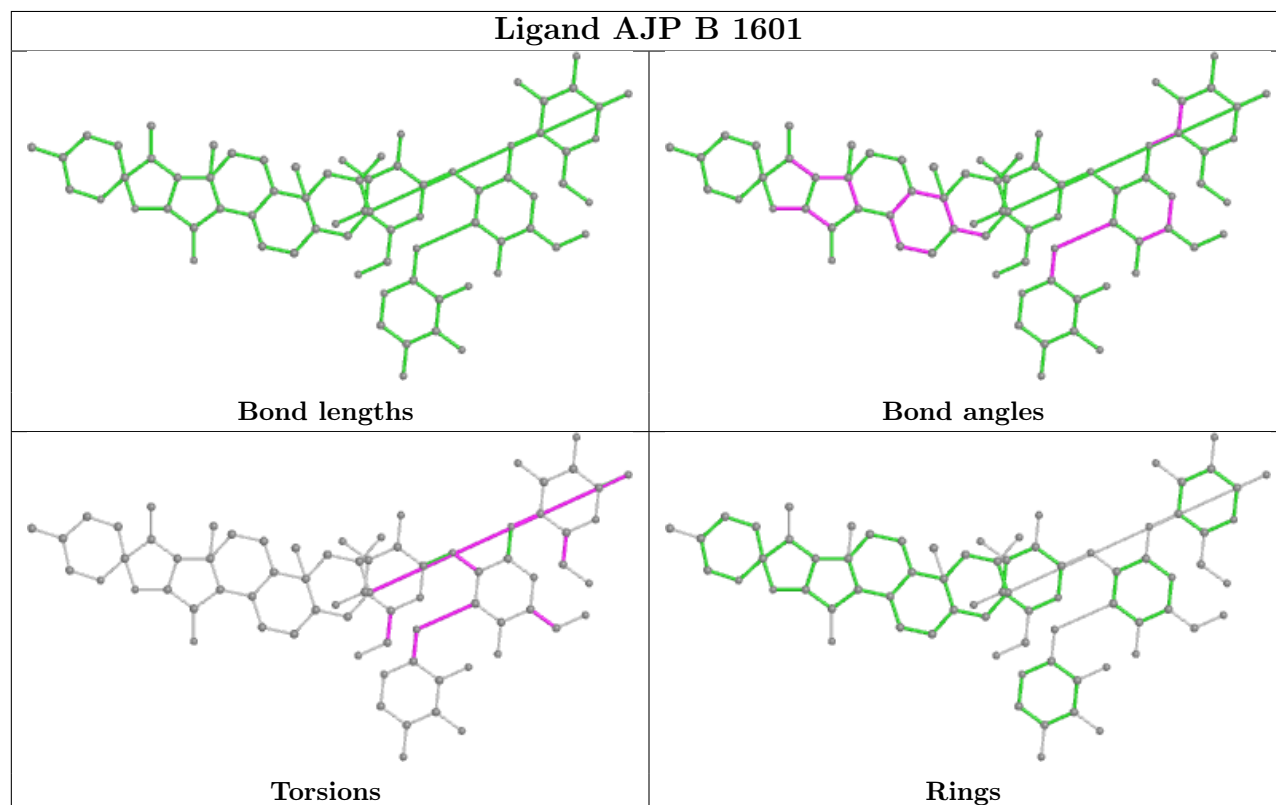
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

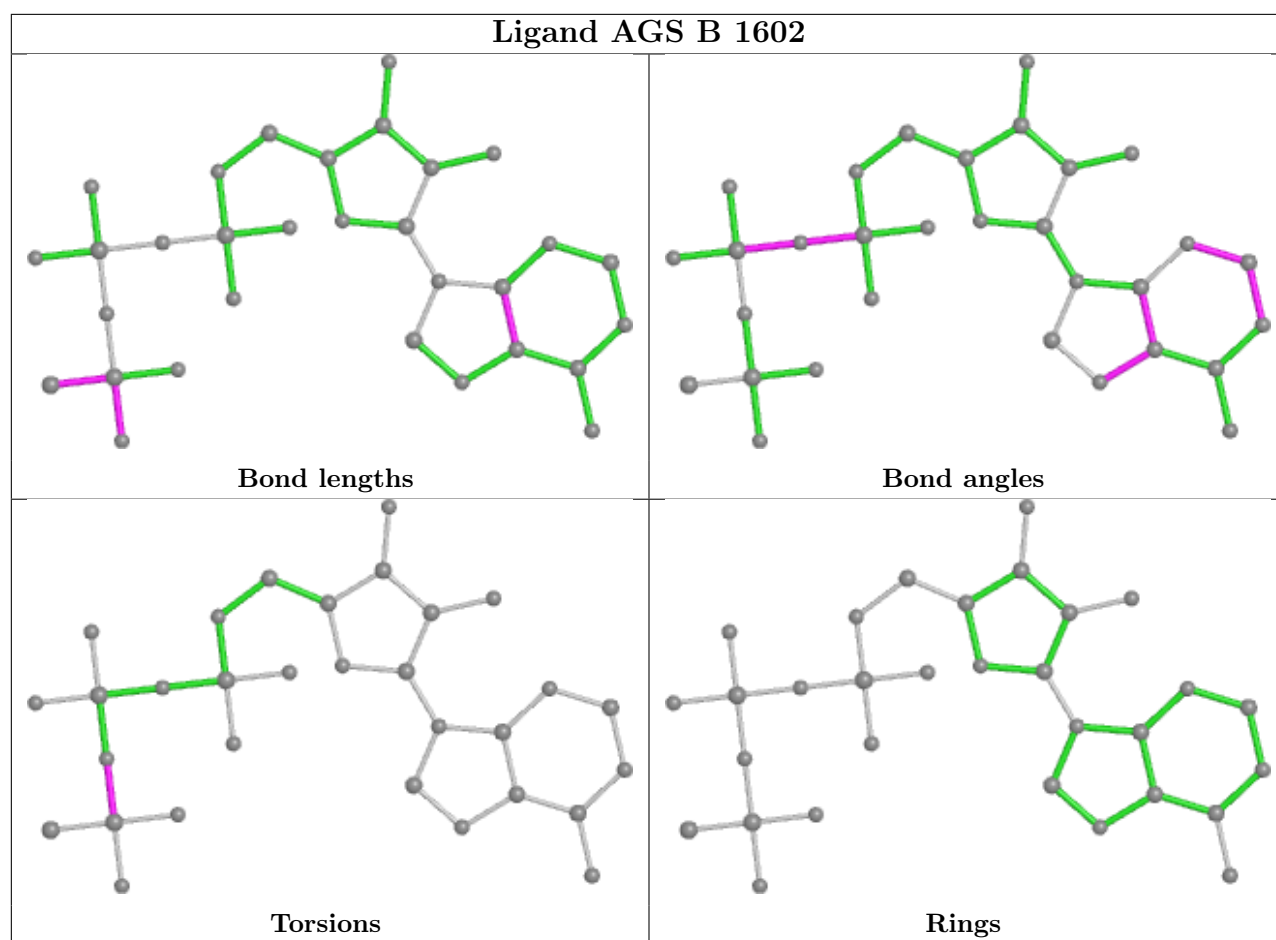


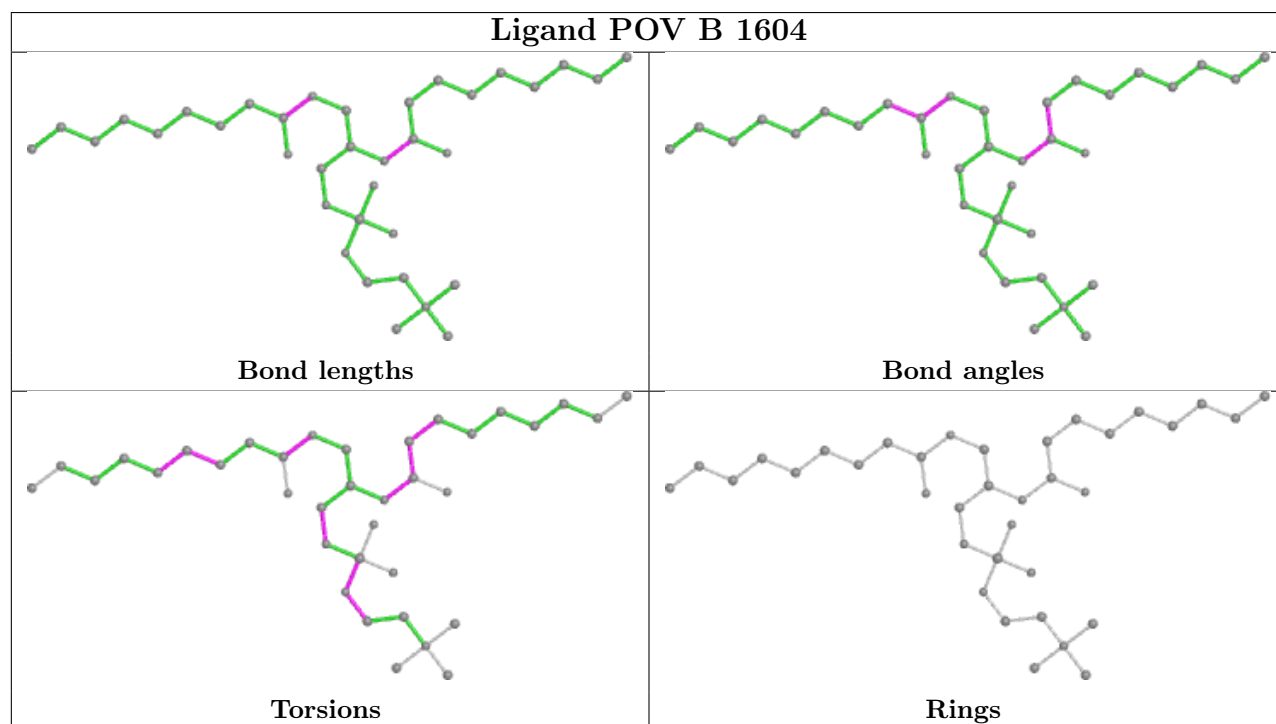
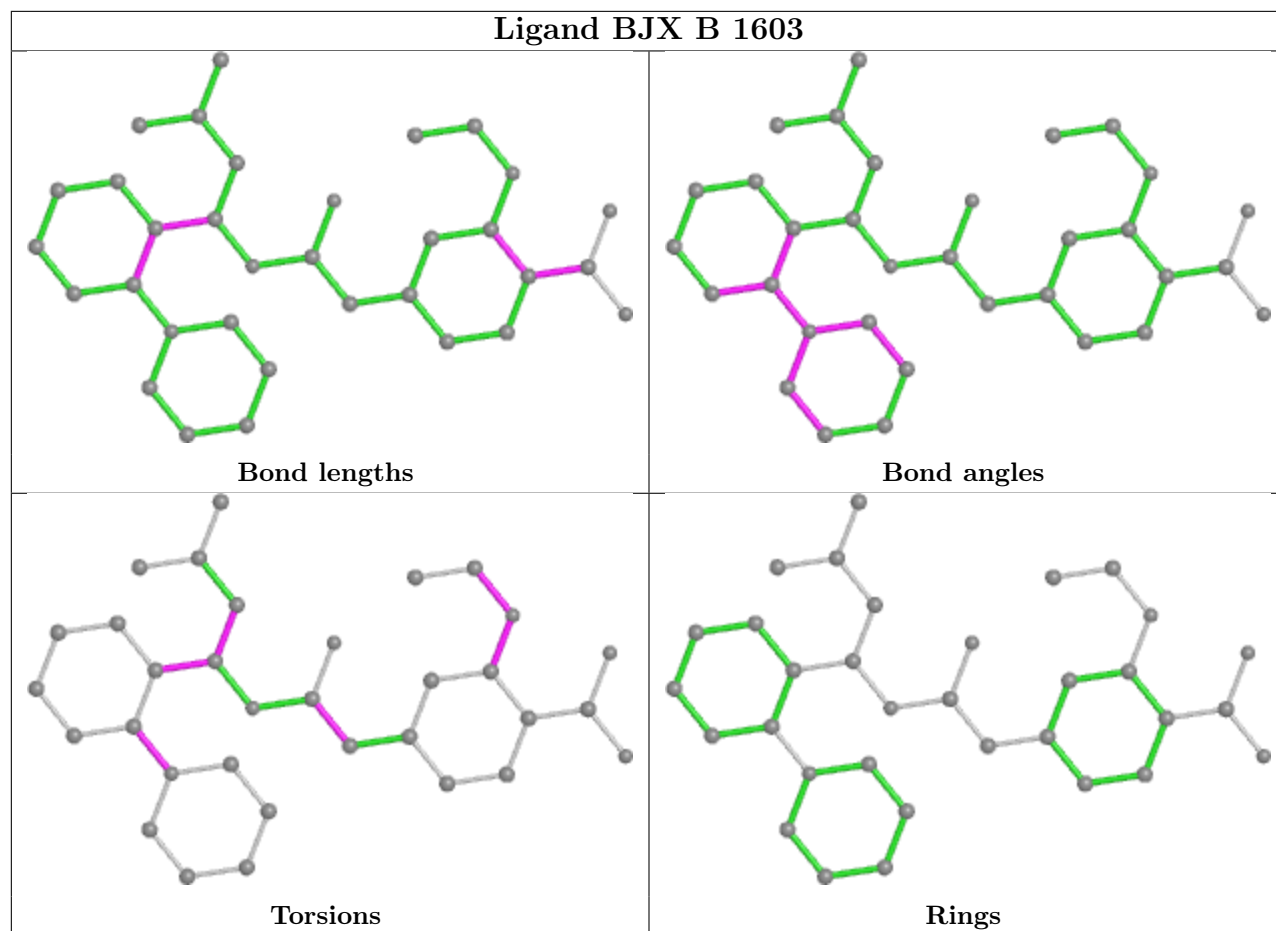
Ligand AGS A 402

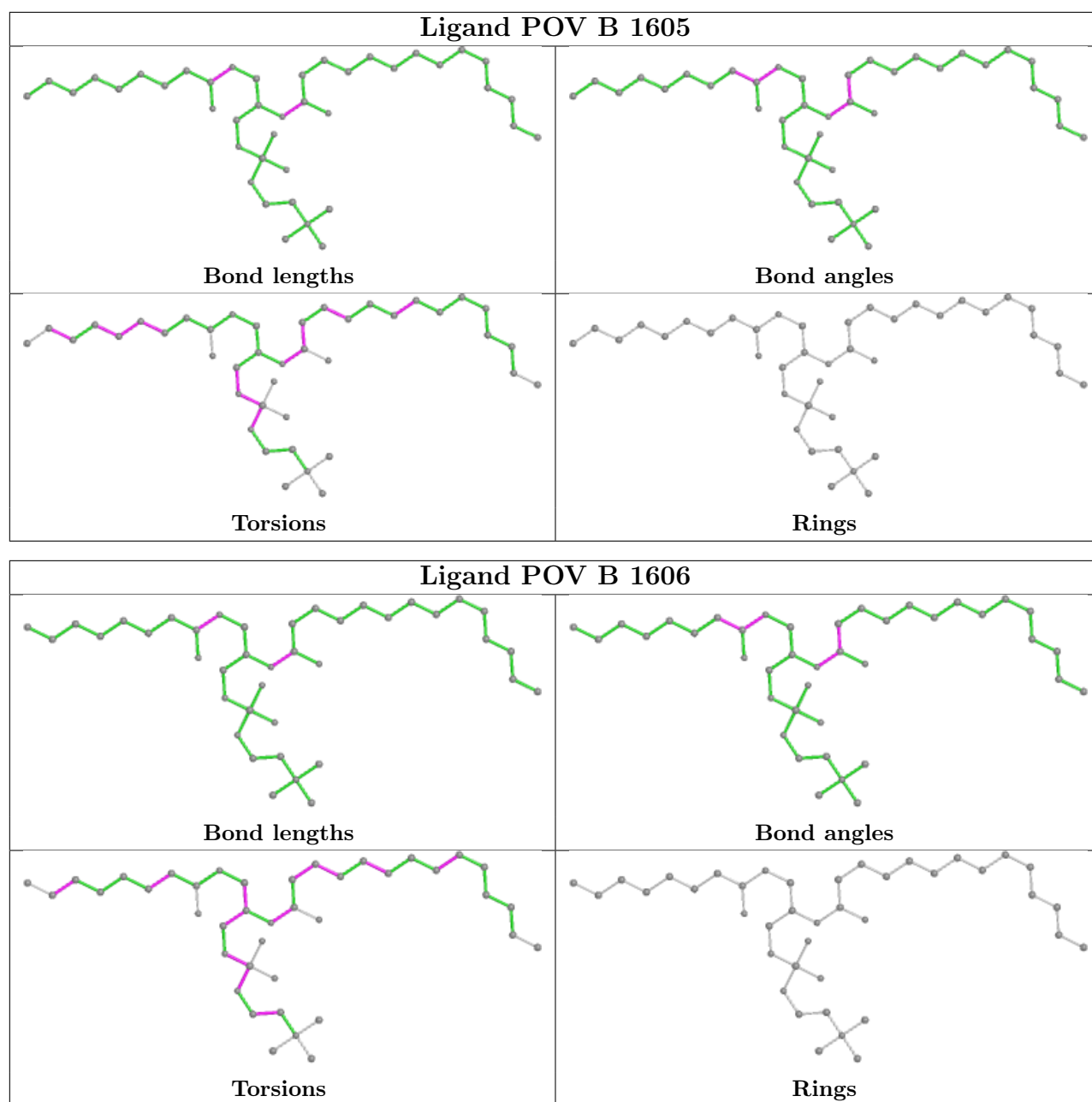


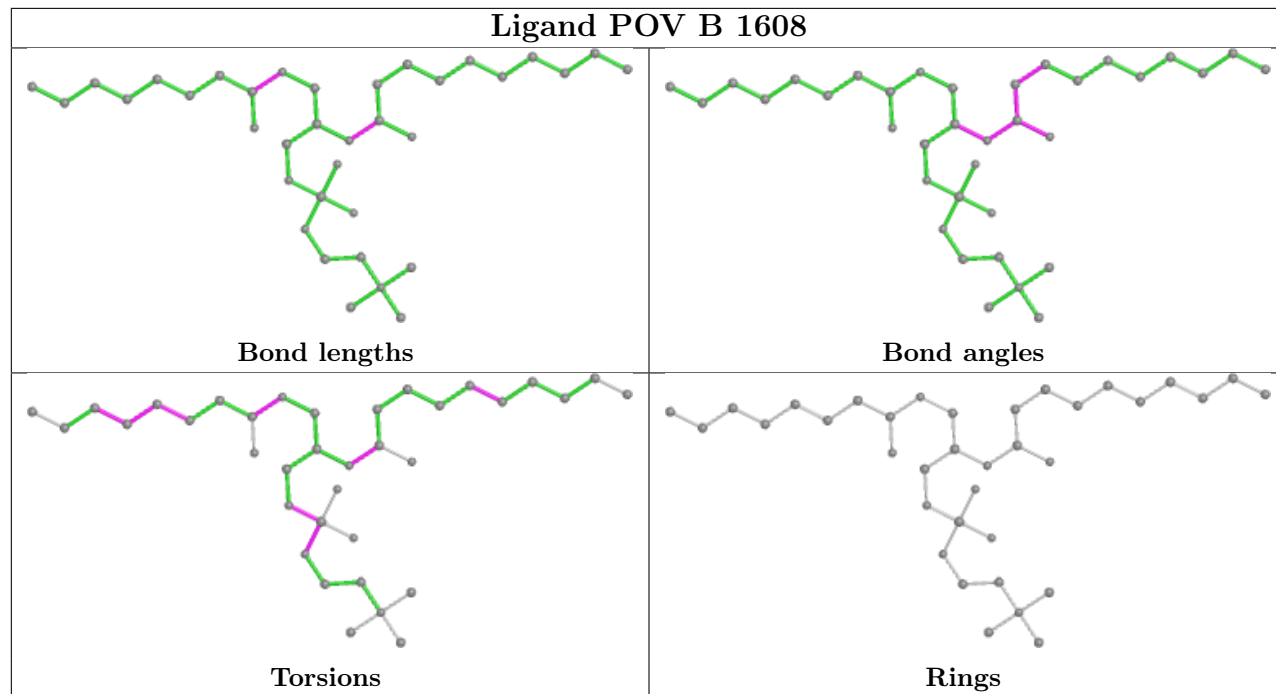
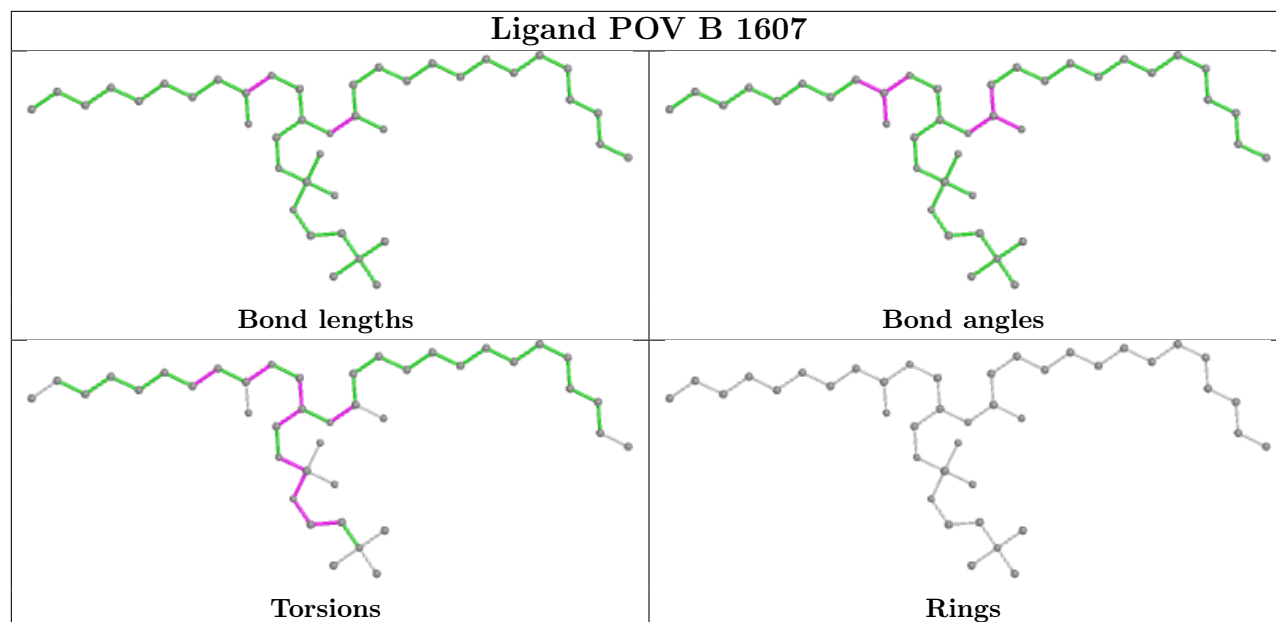
Ligand AJP B 1601

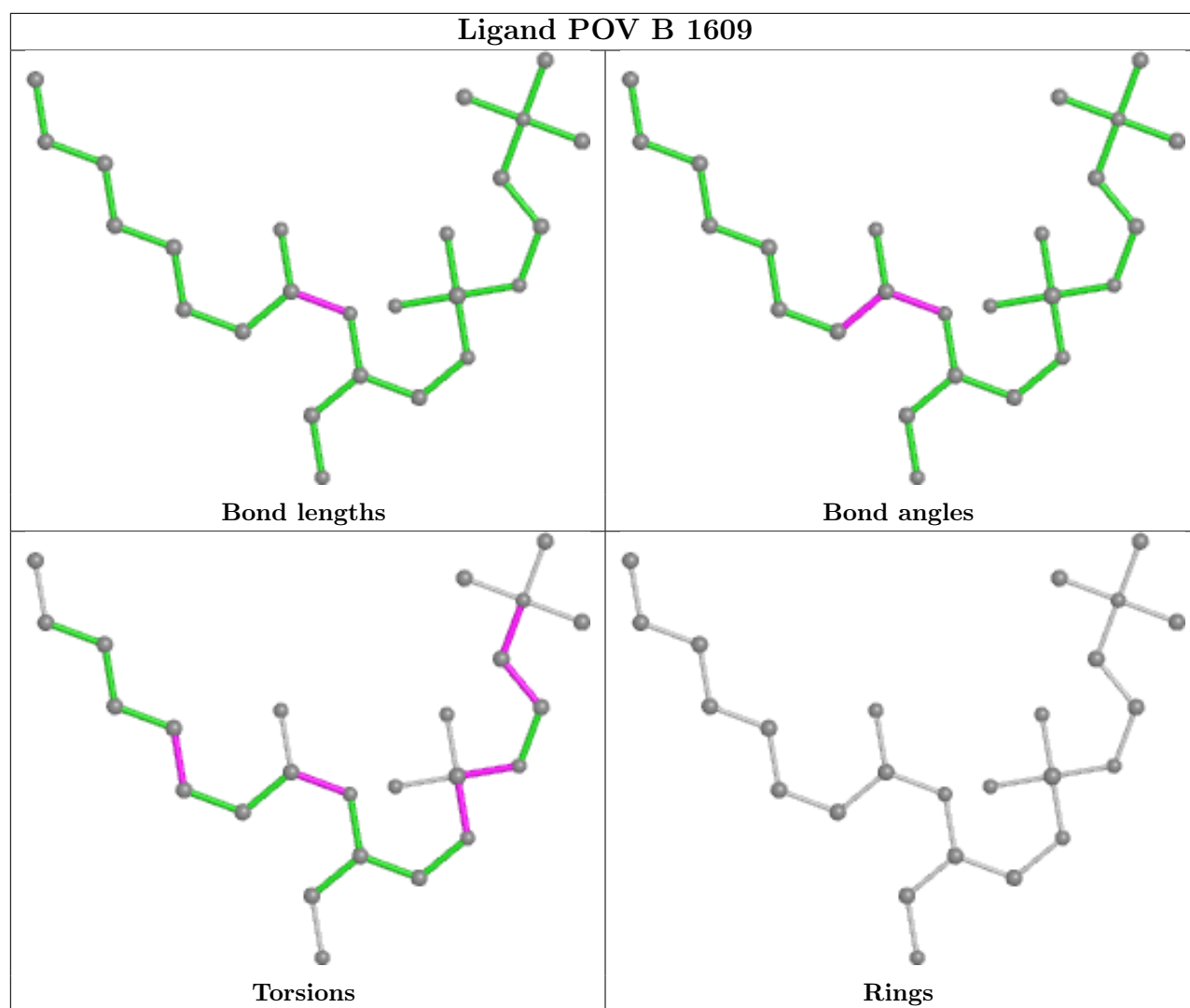


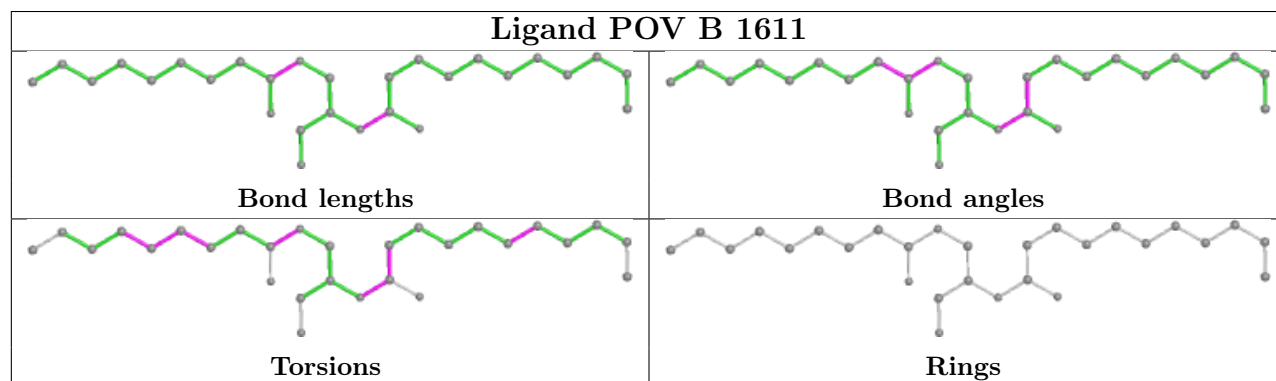
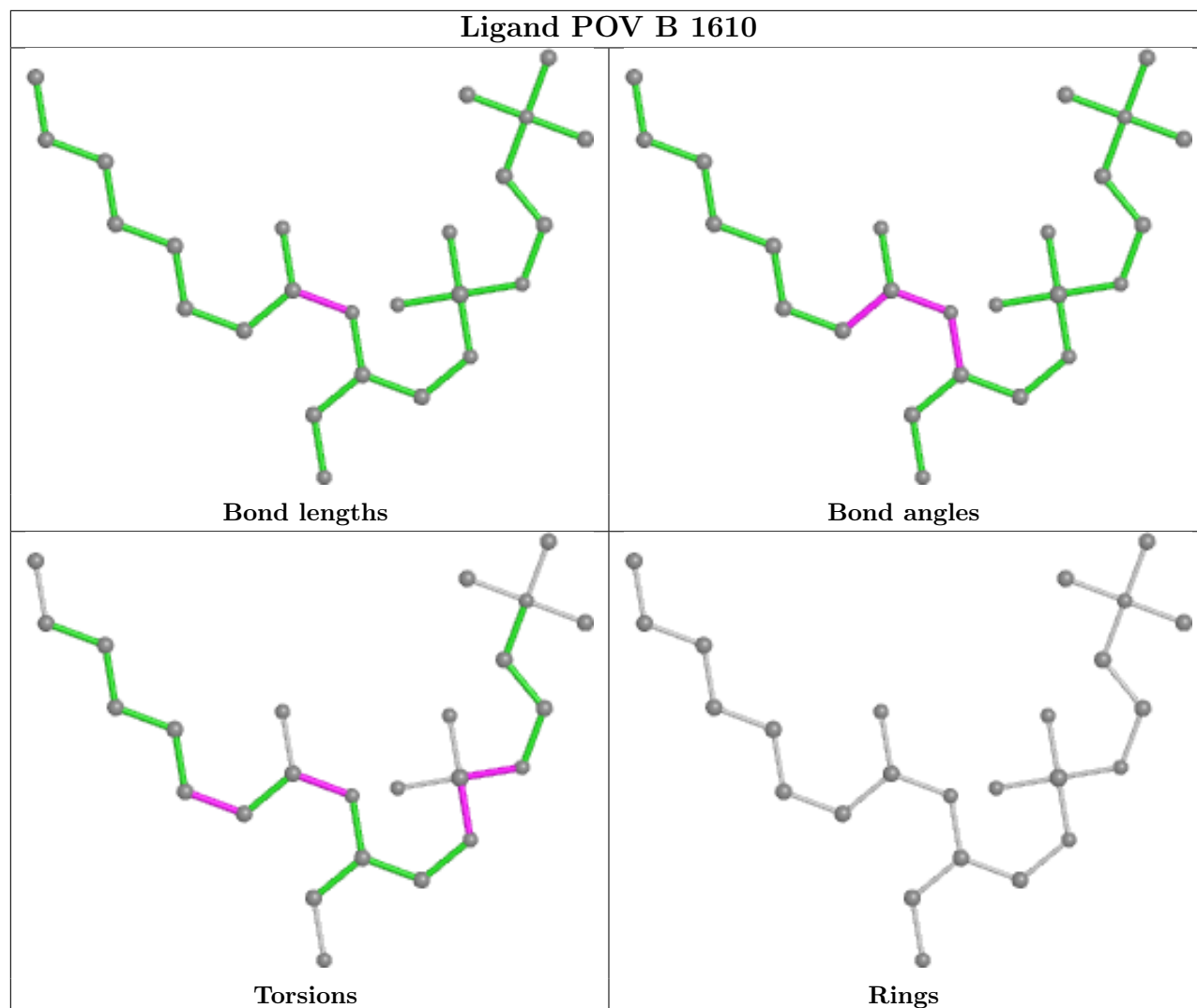


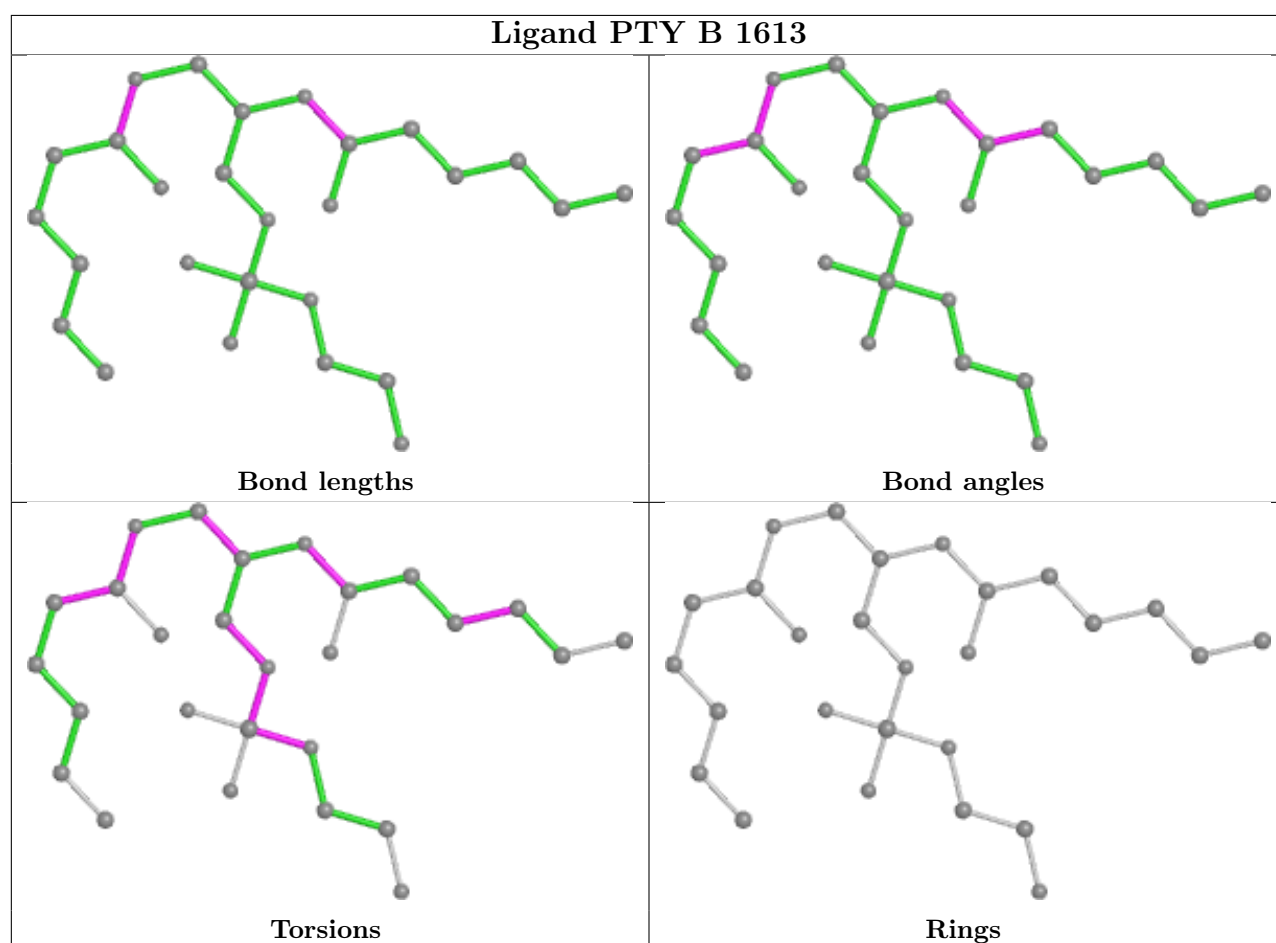
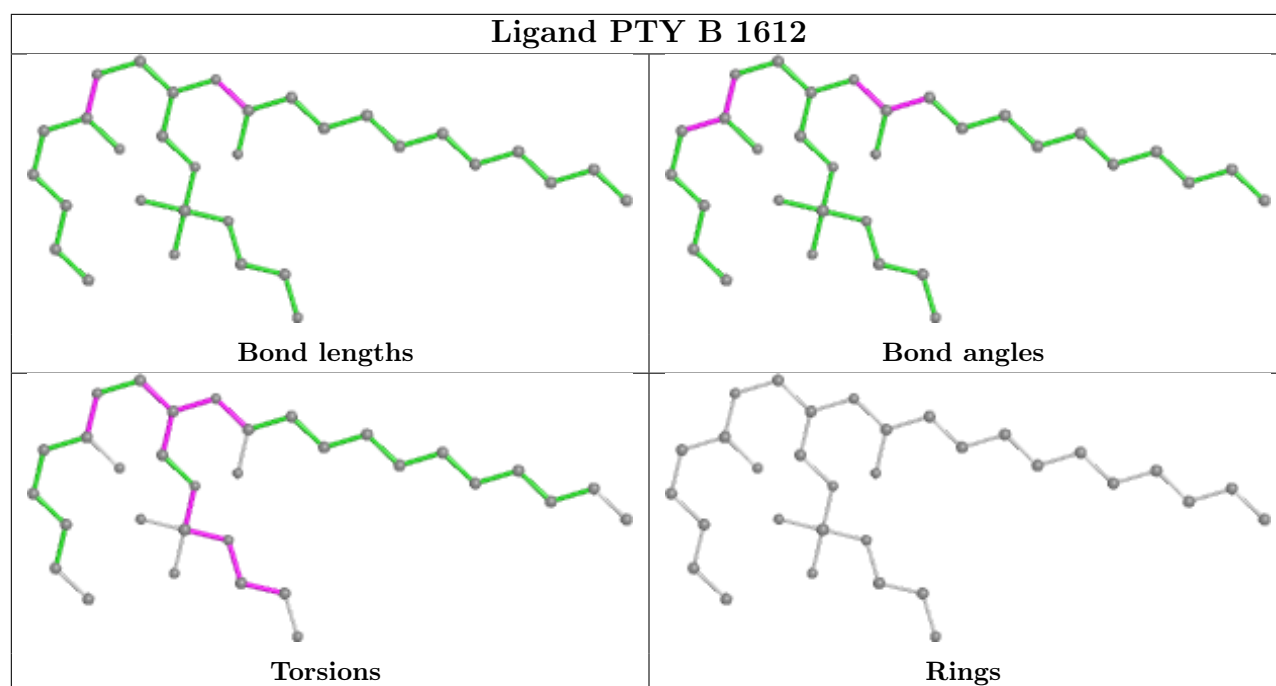




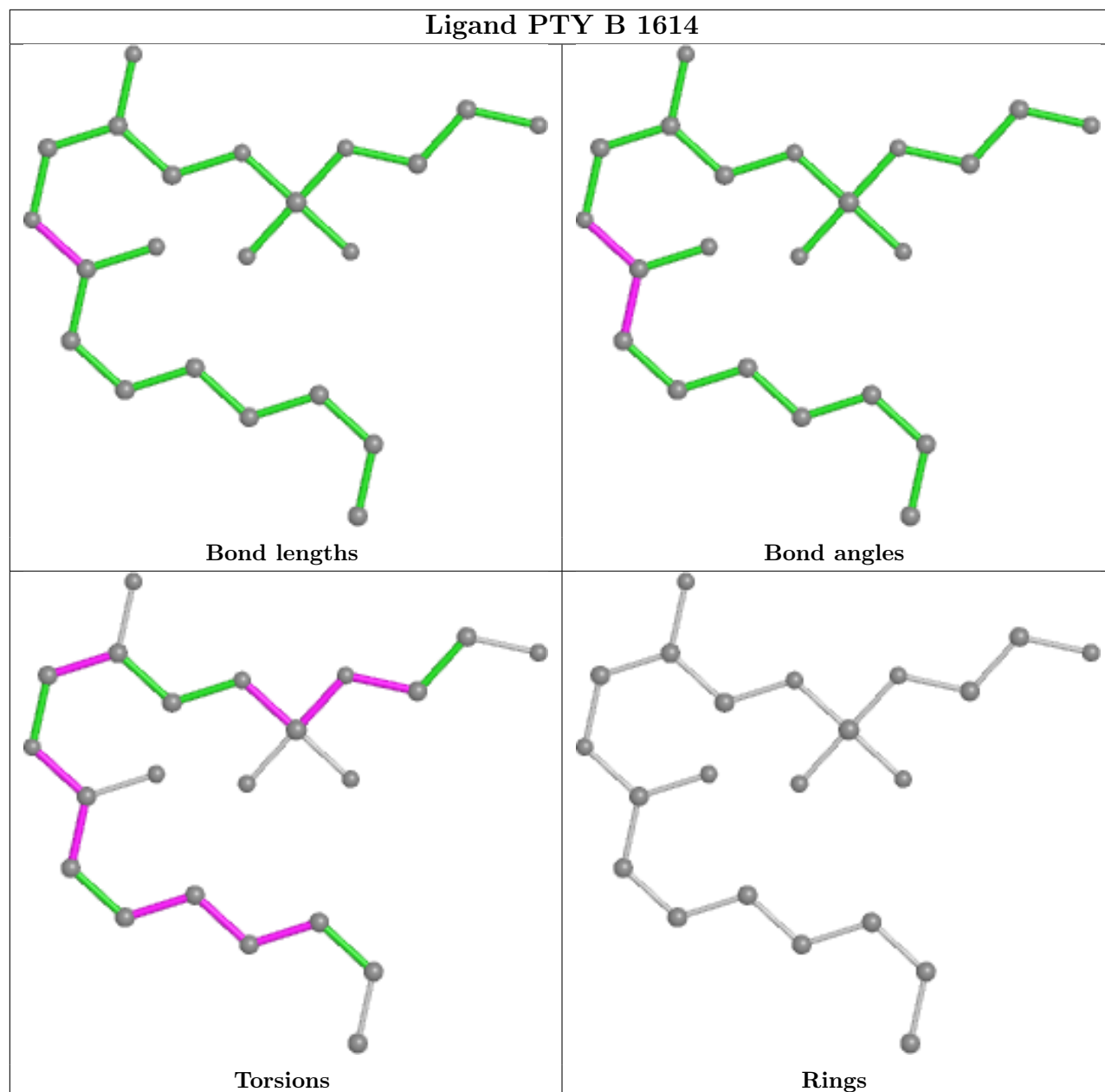


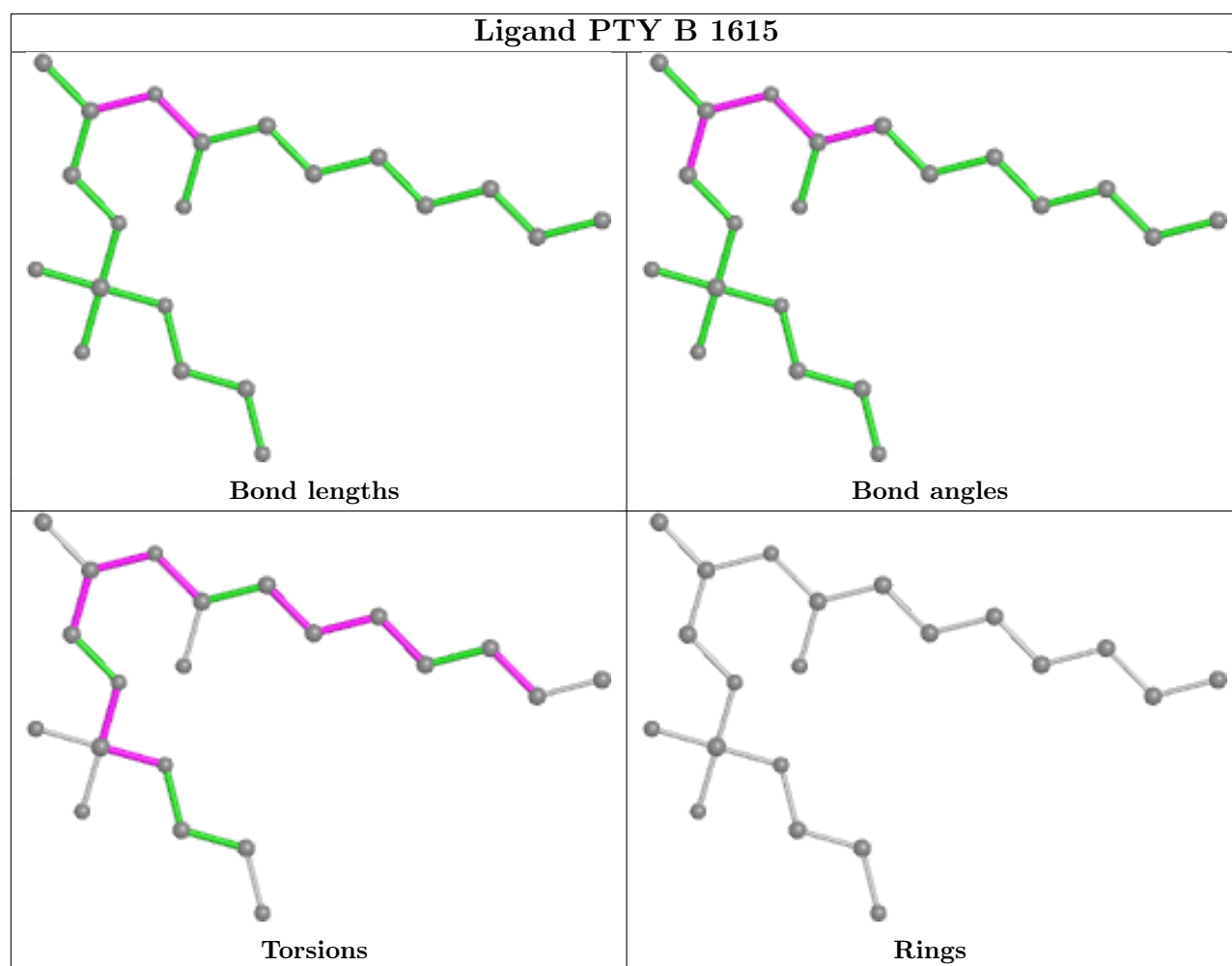


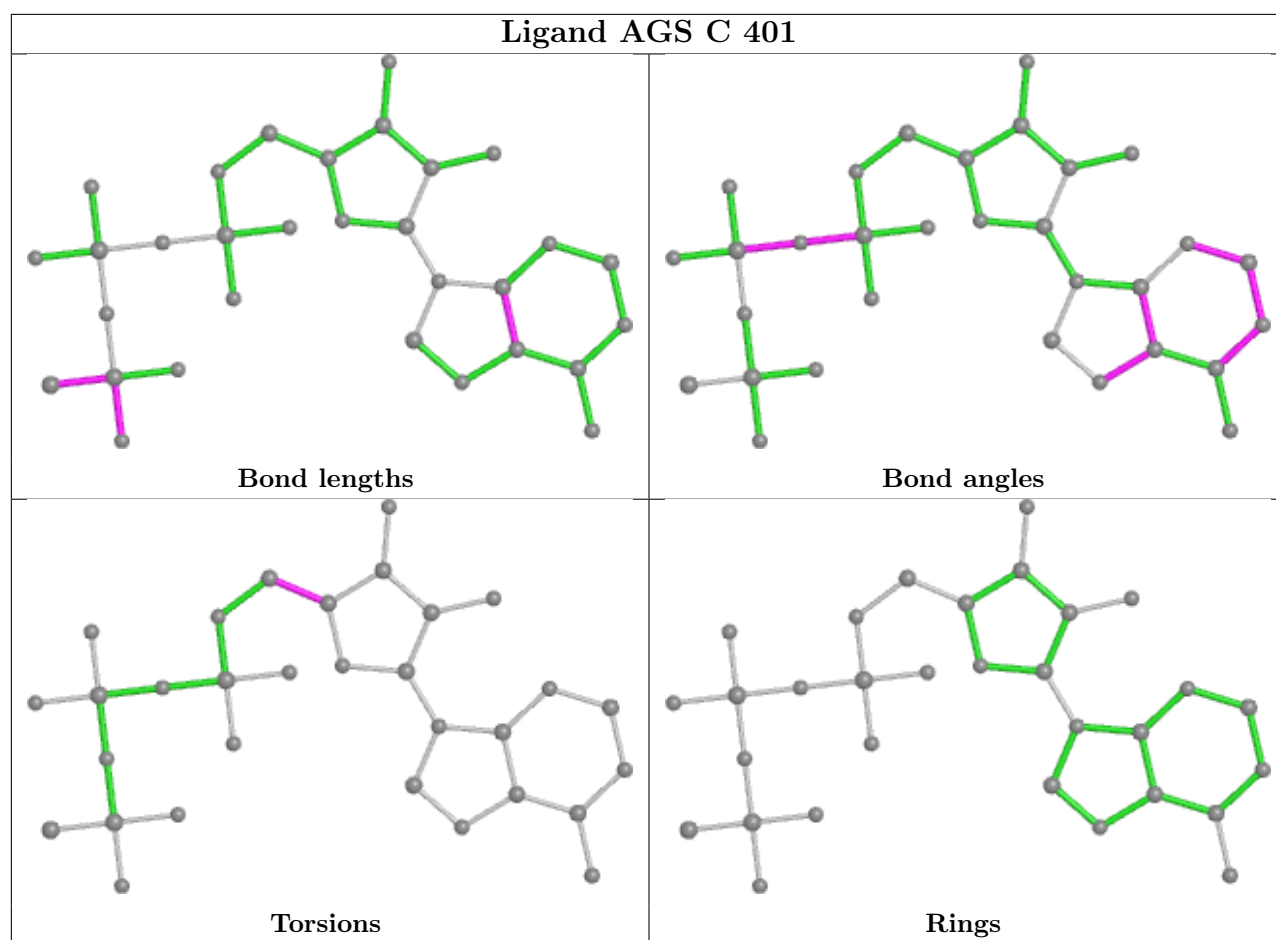


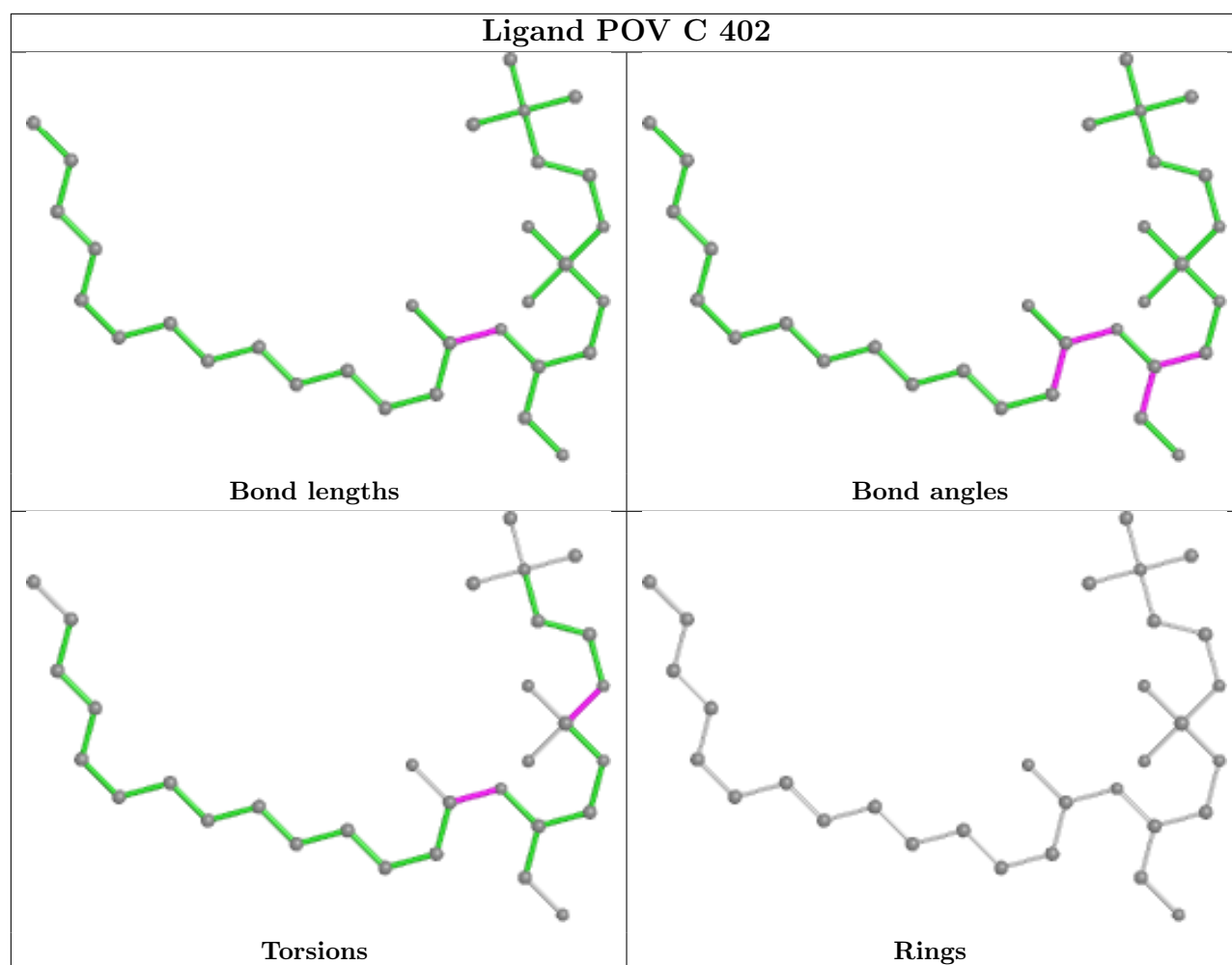


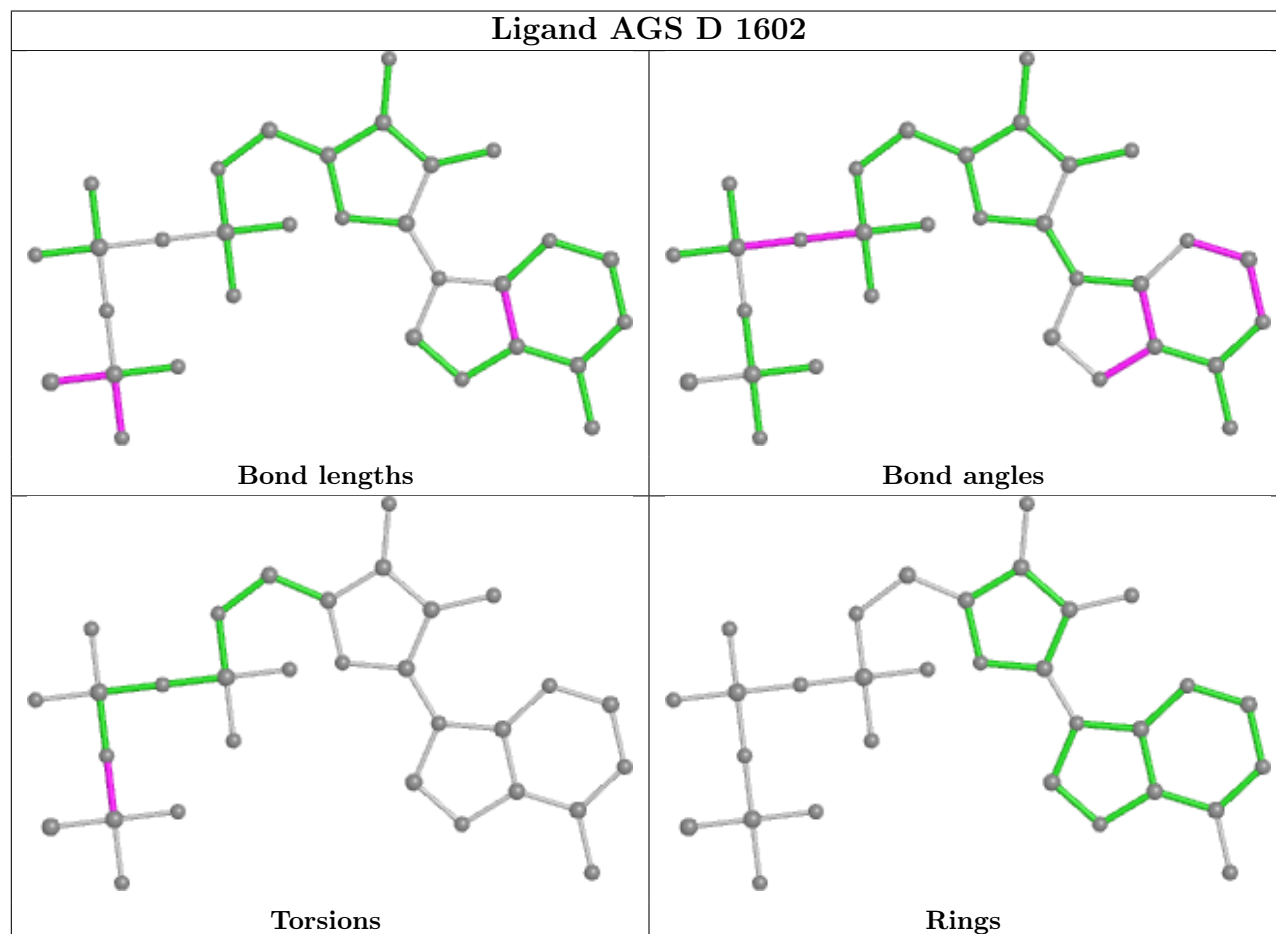
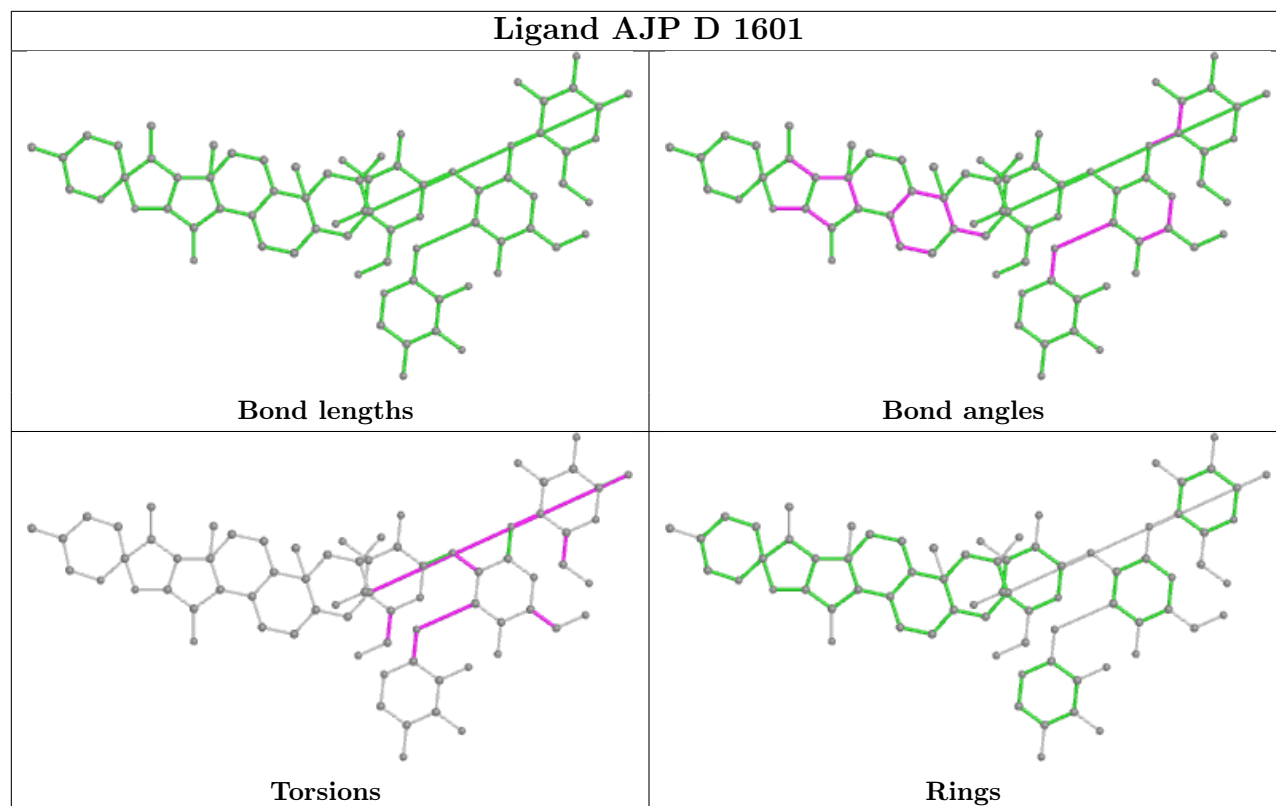
Ligand PTY B 1614



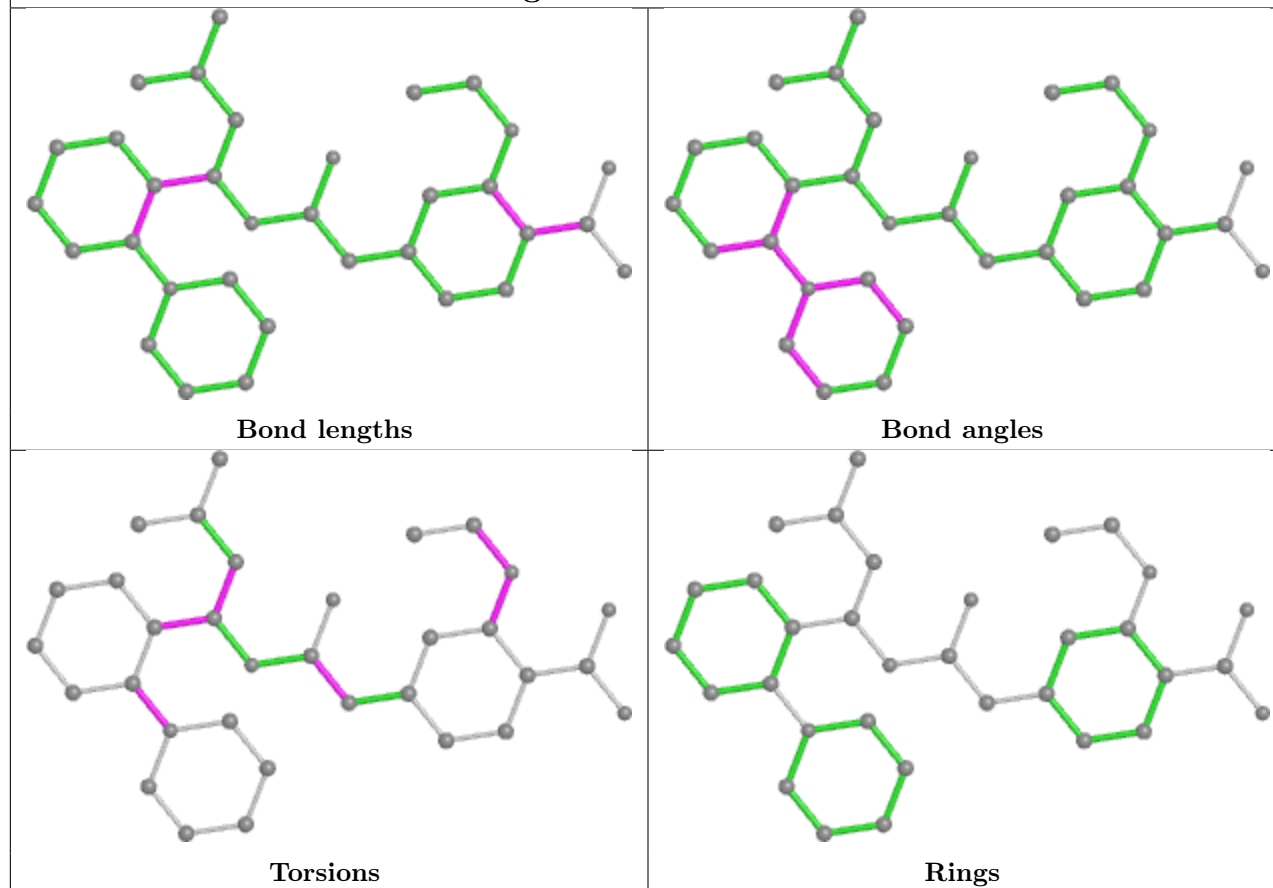




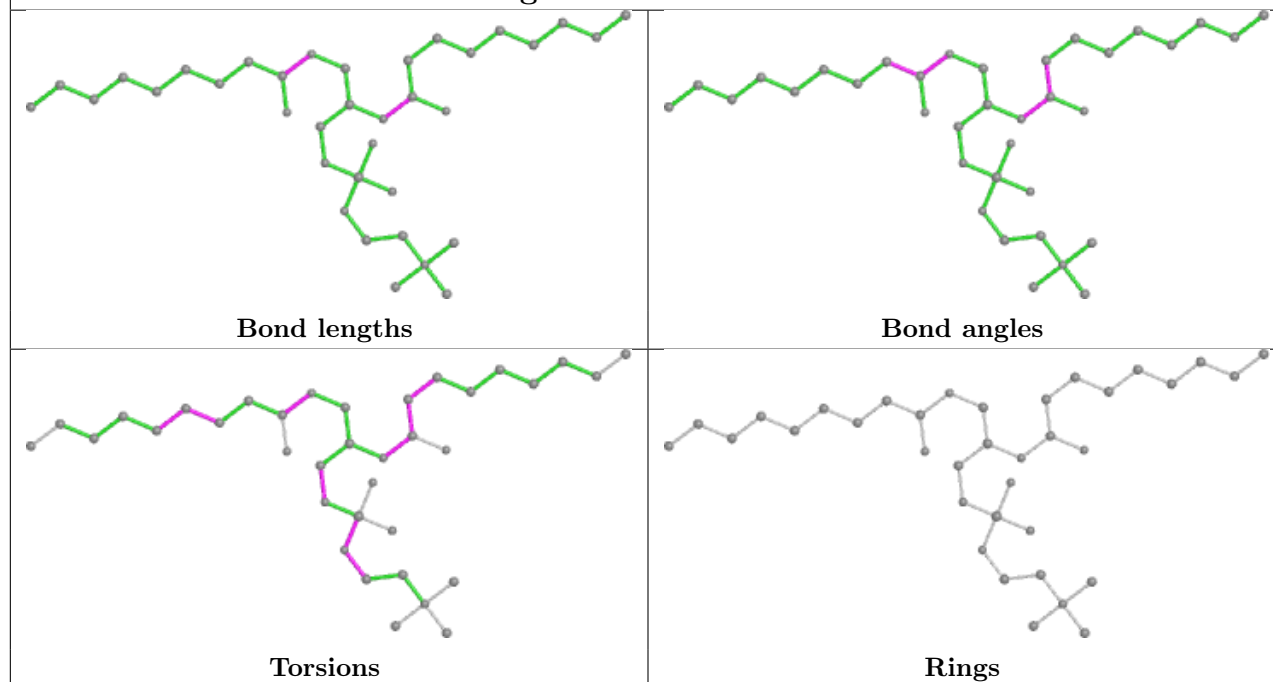


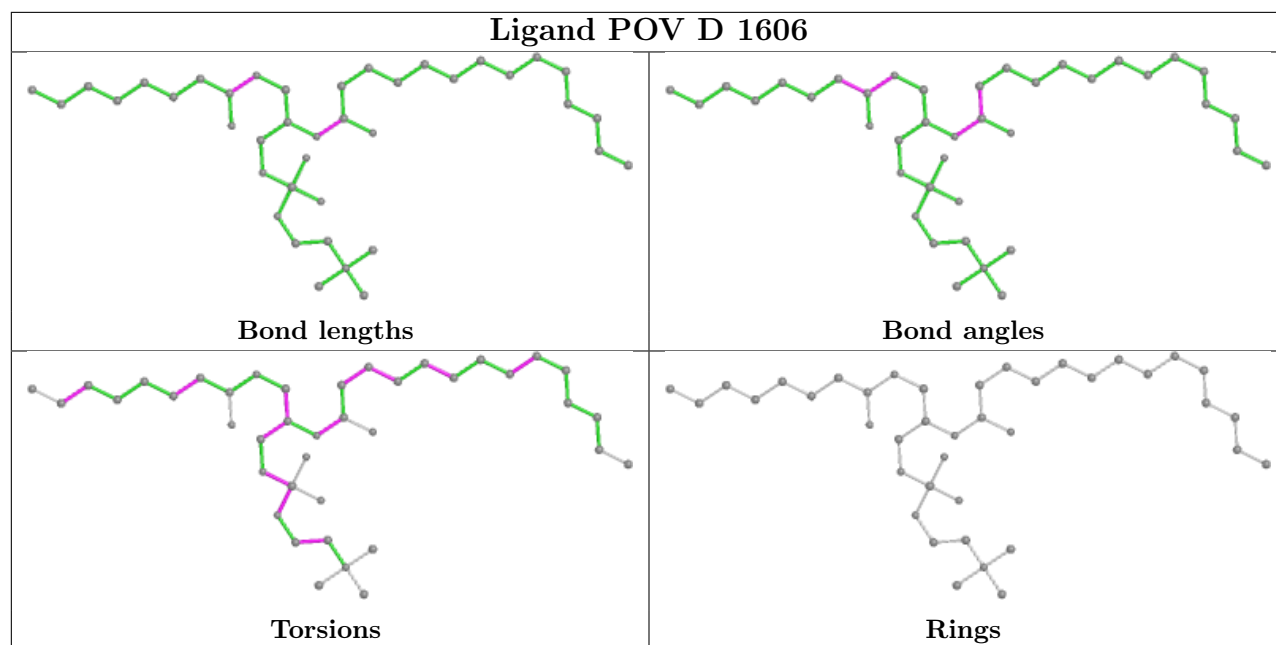
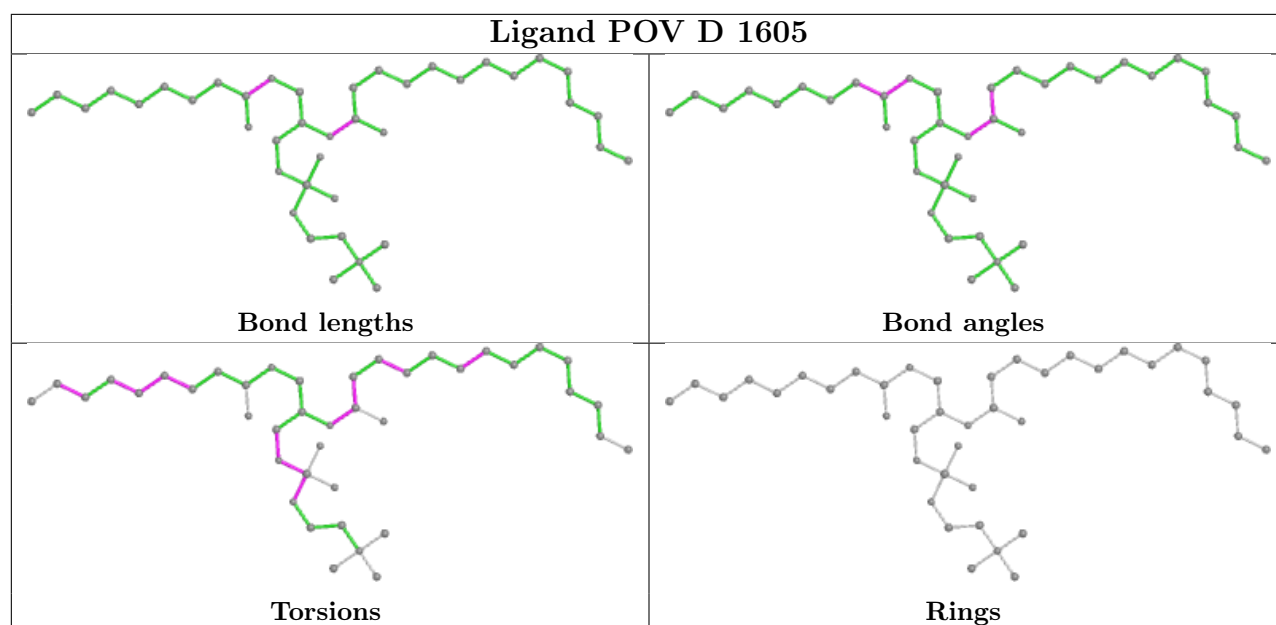


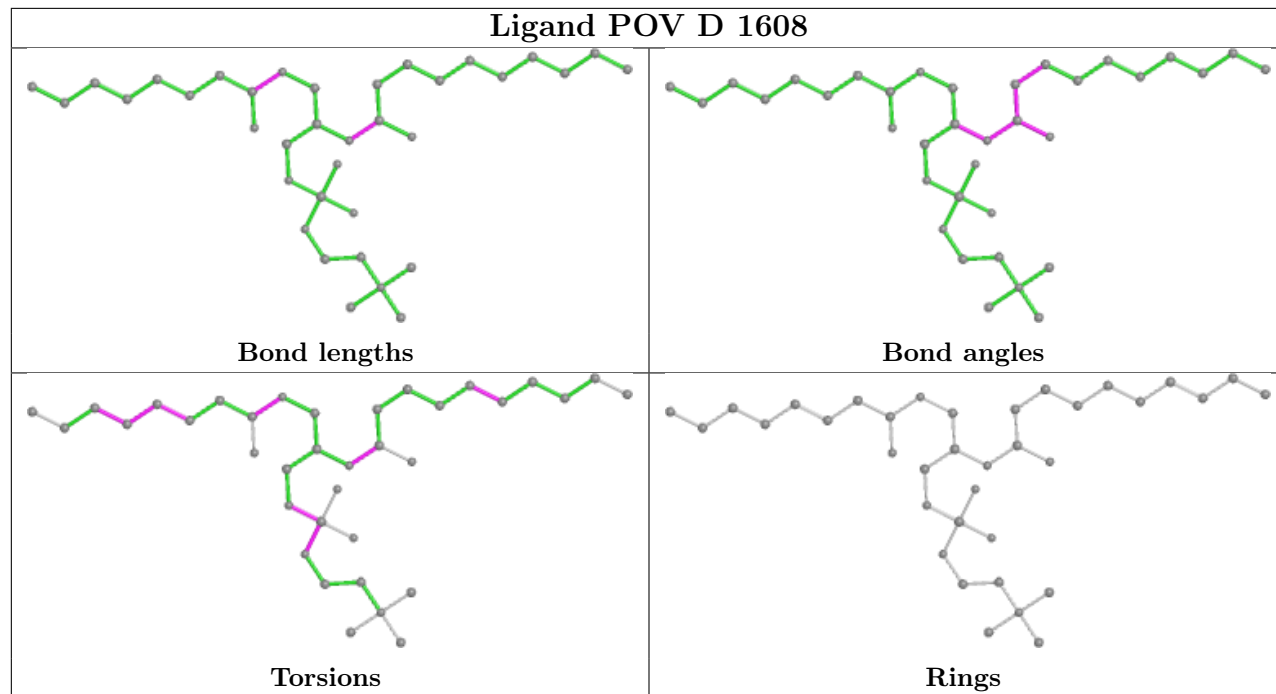
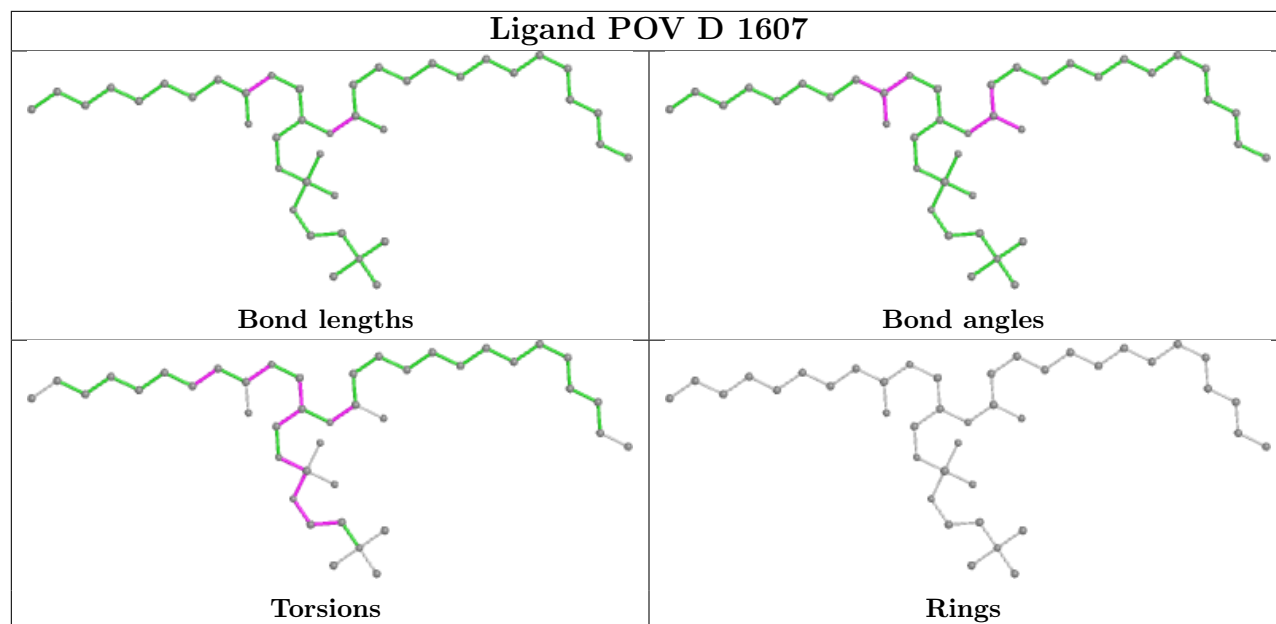
Ligand BJX D 1603

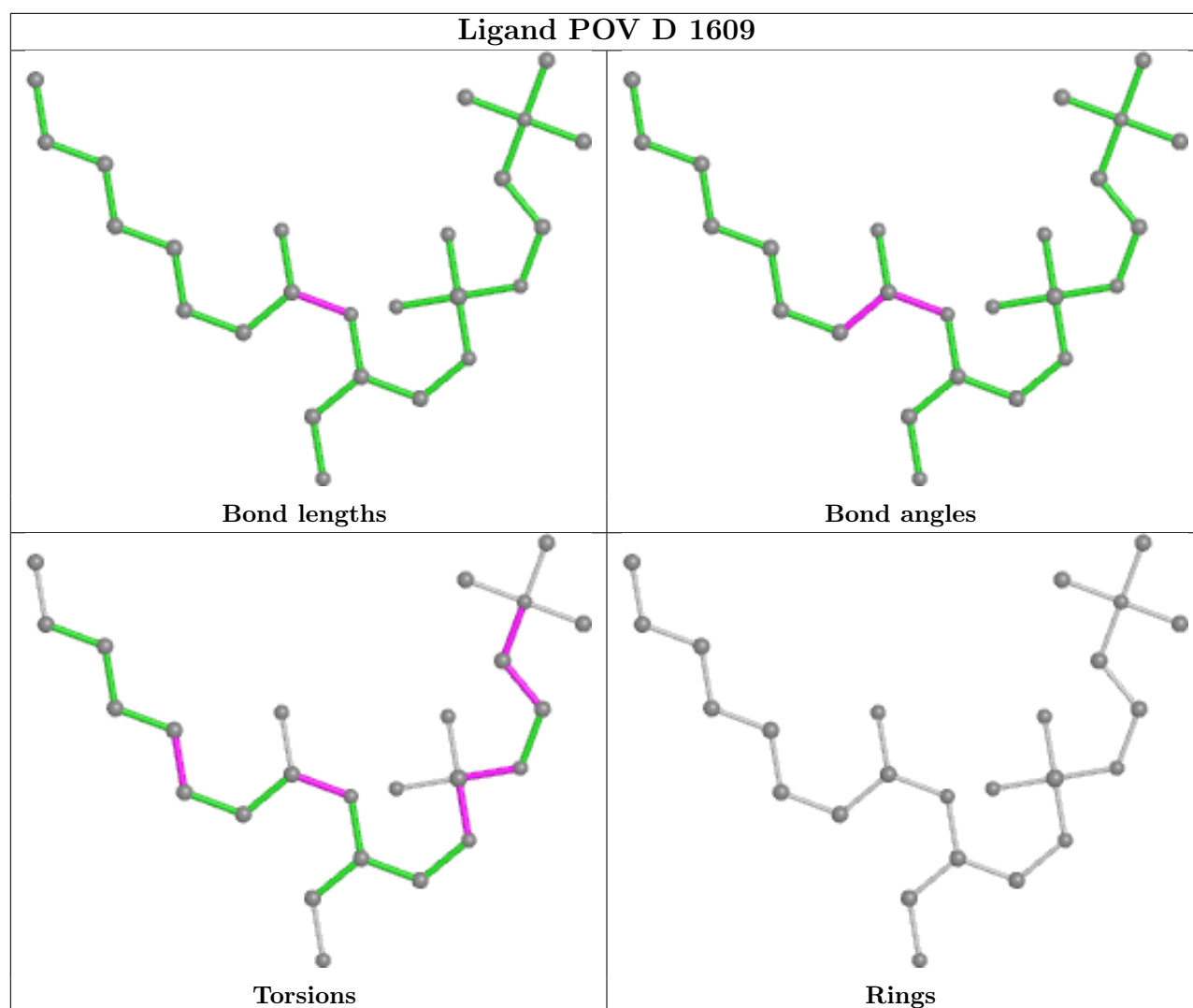


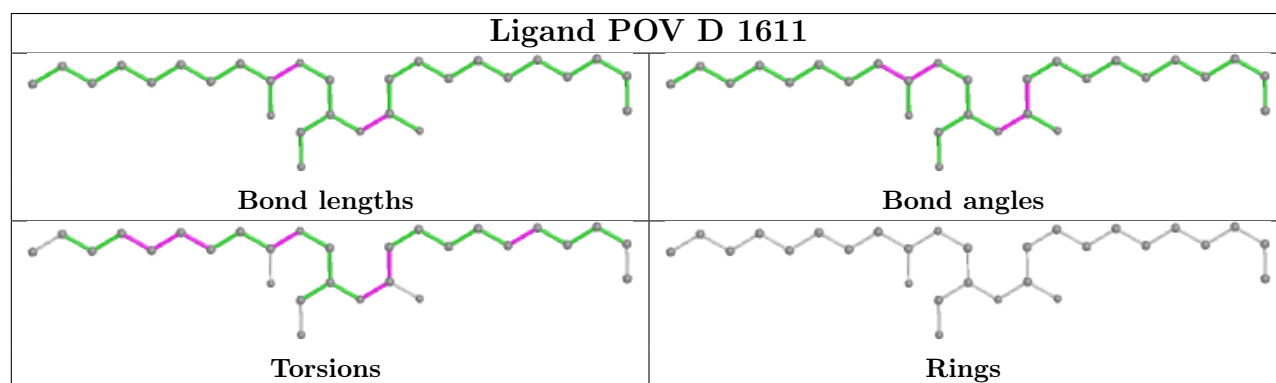
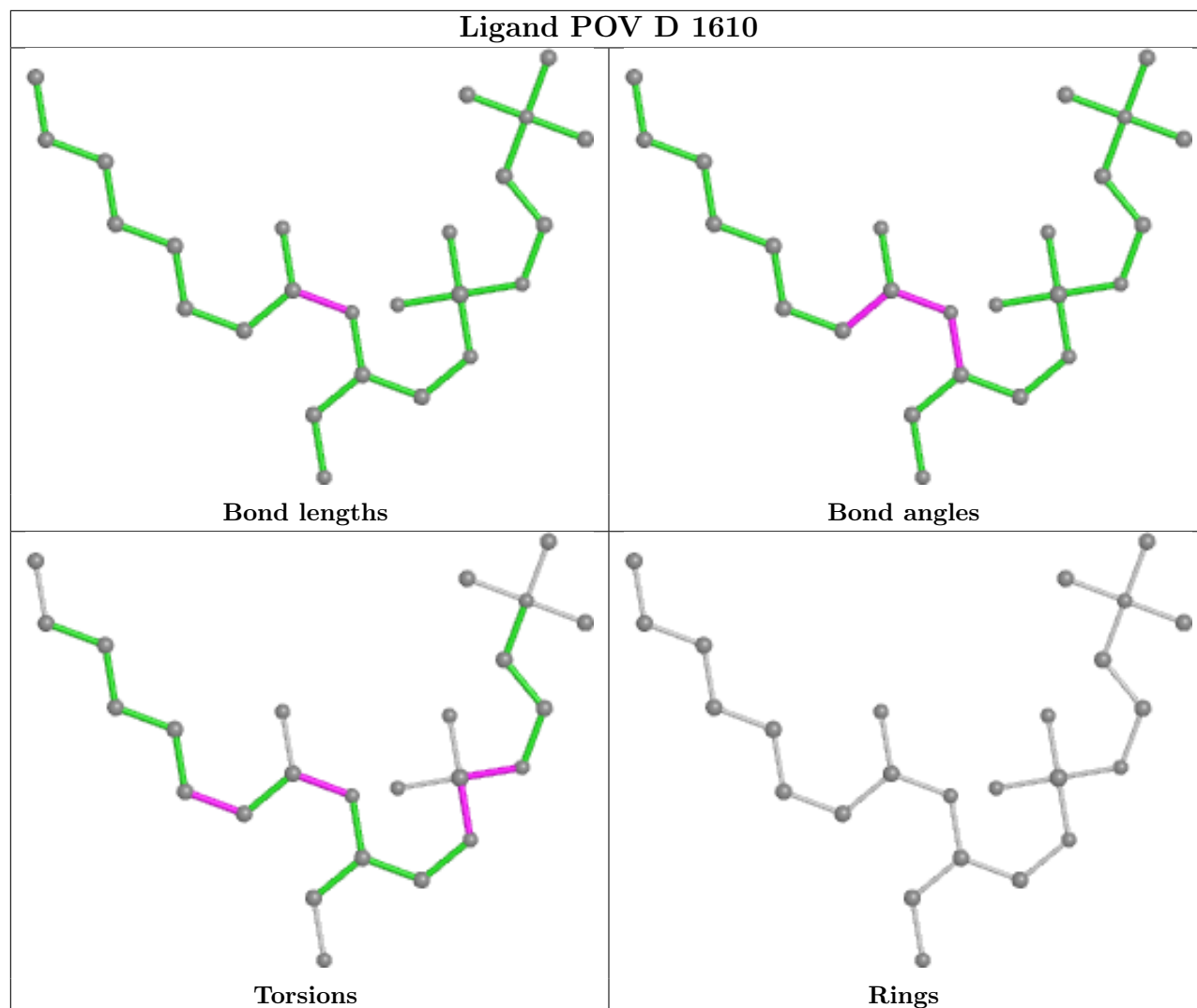
Ligand POV D 1604

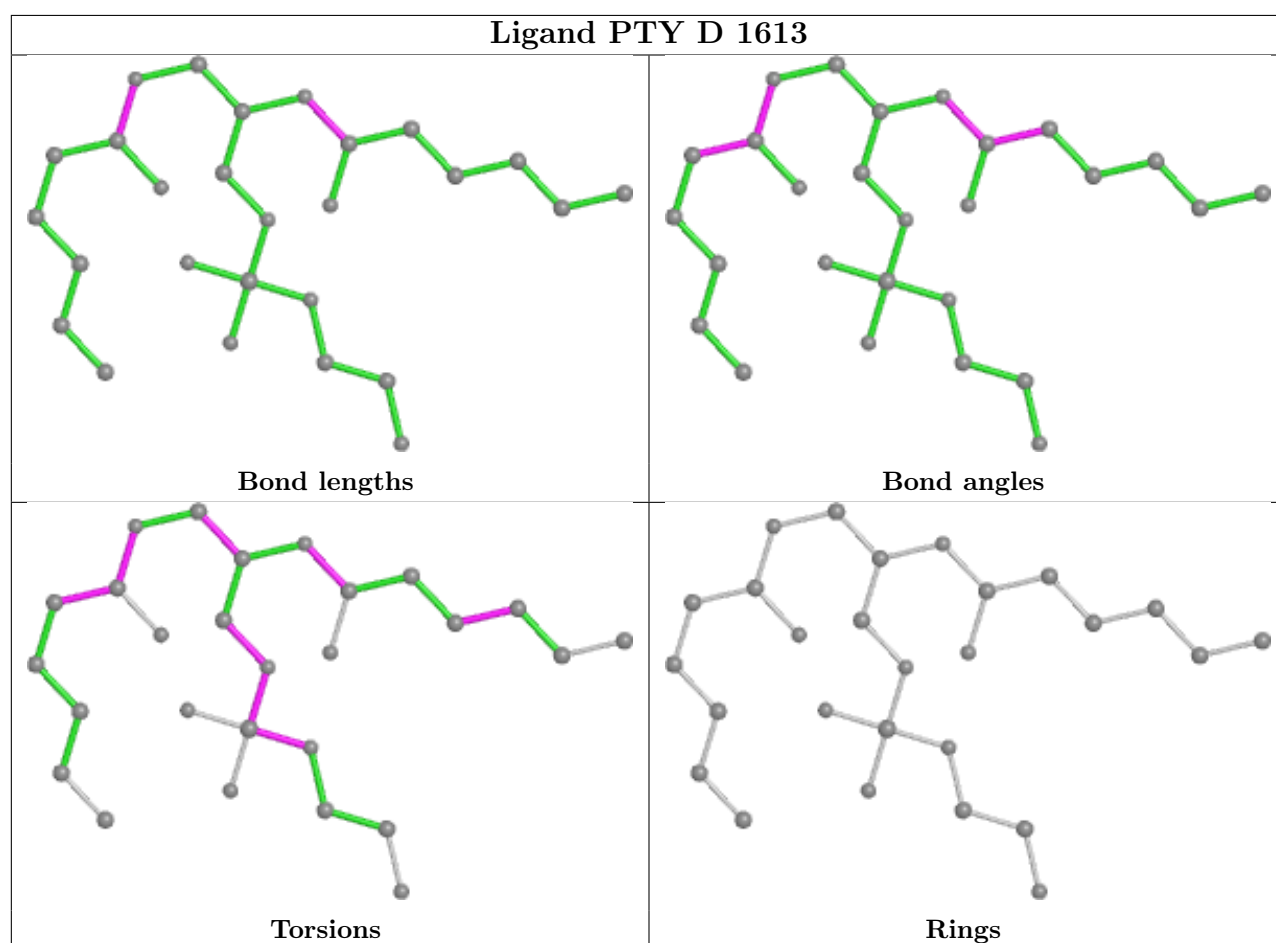
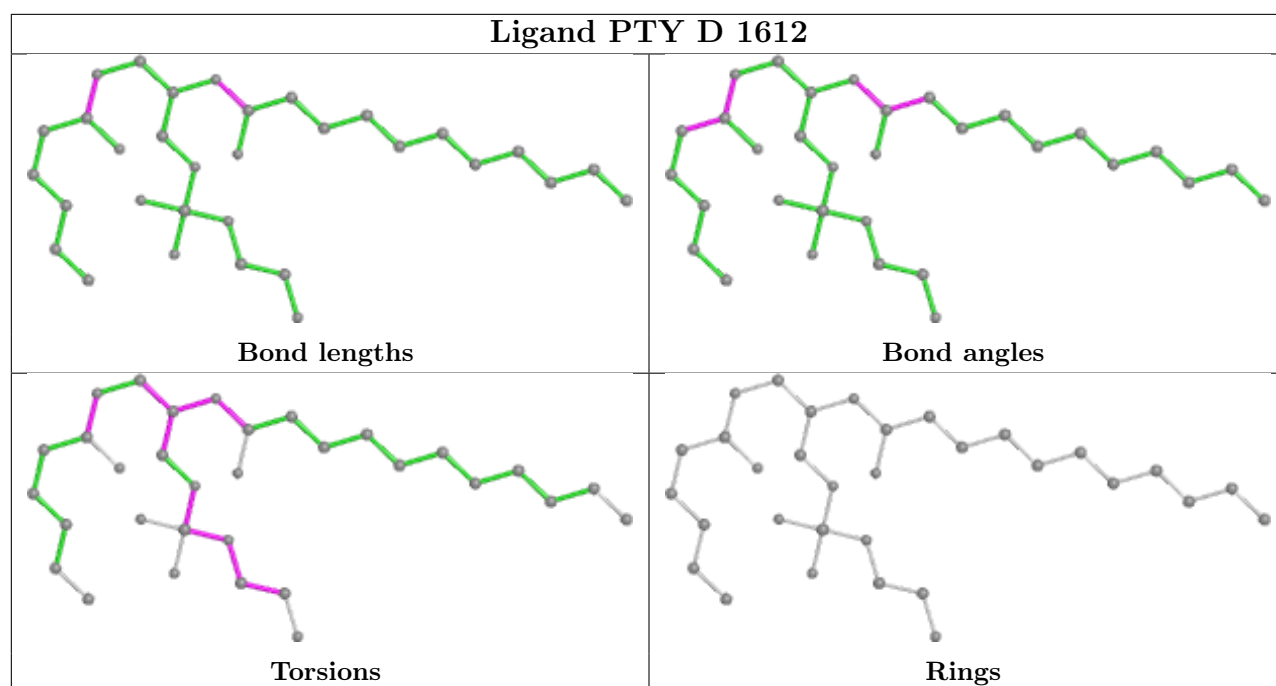


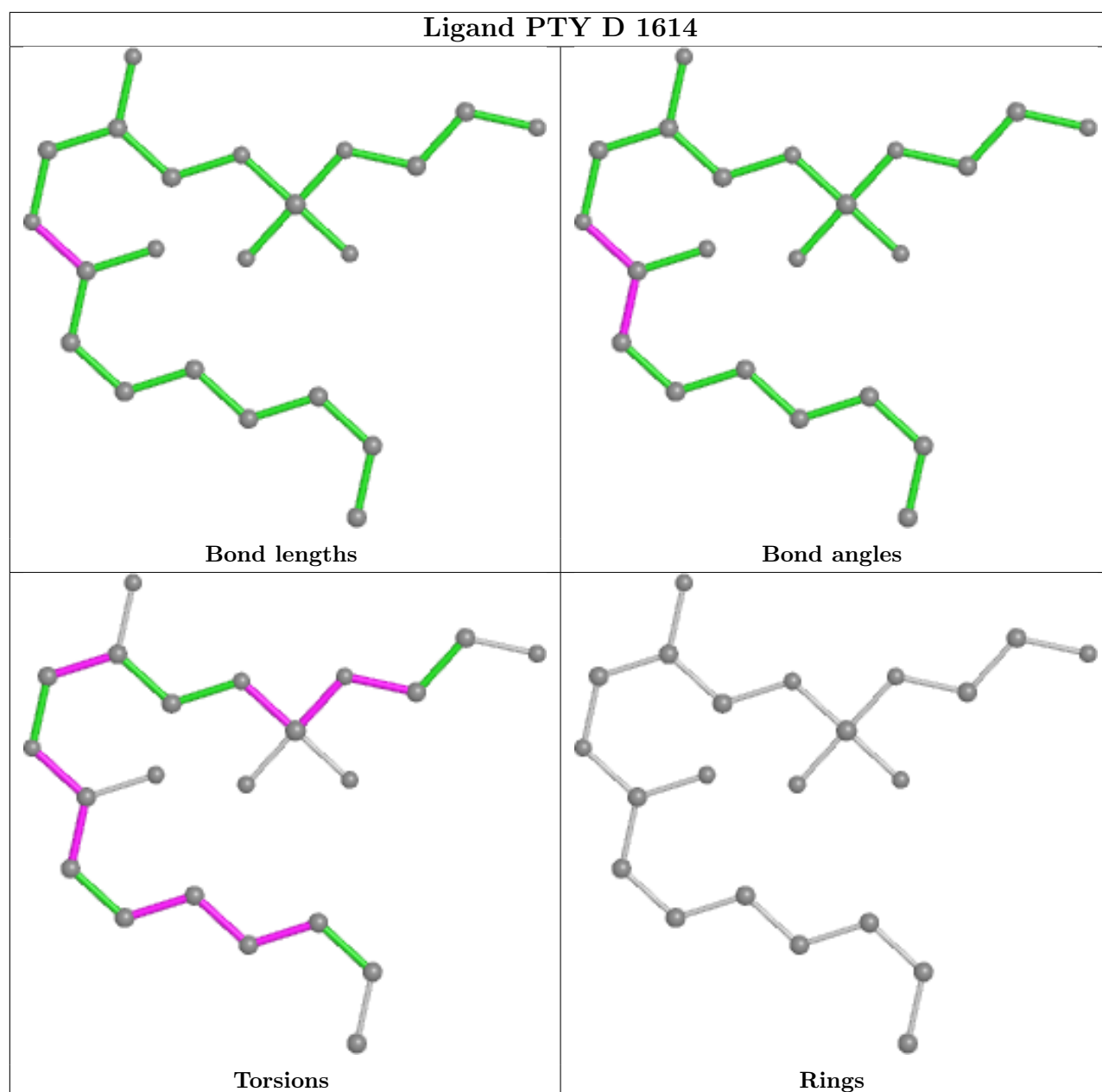


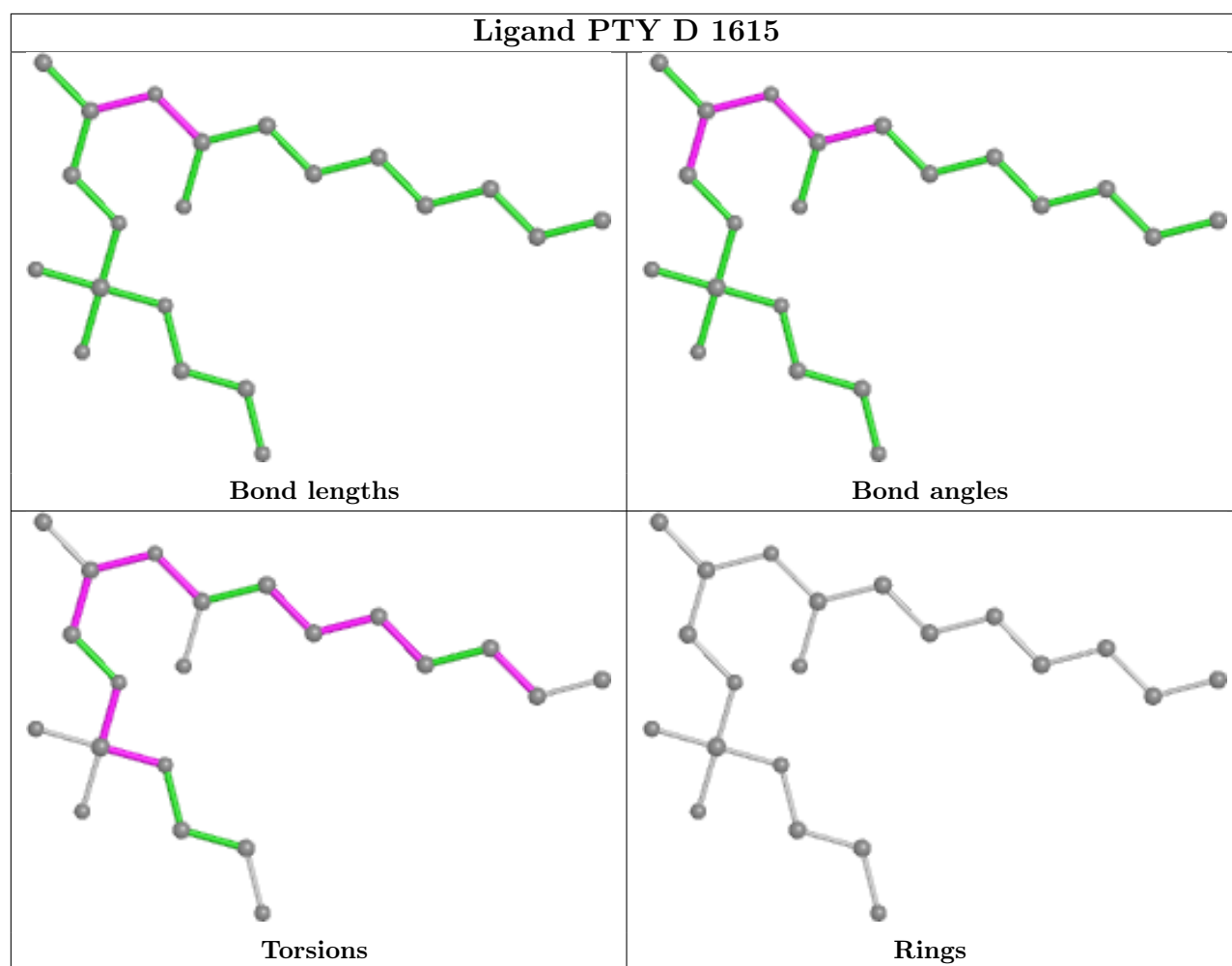


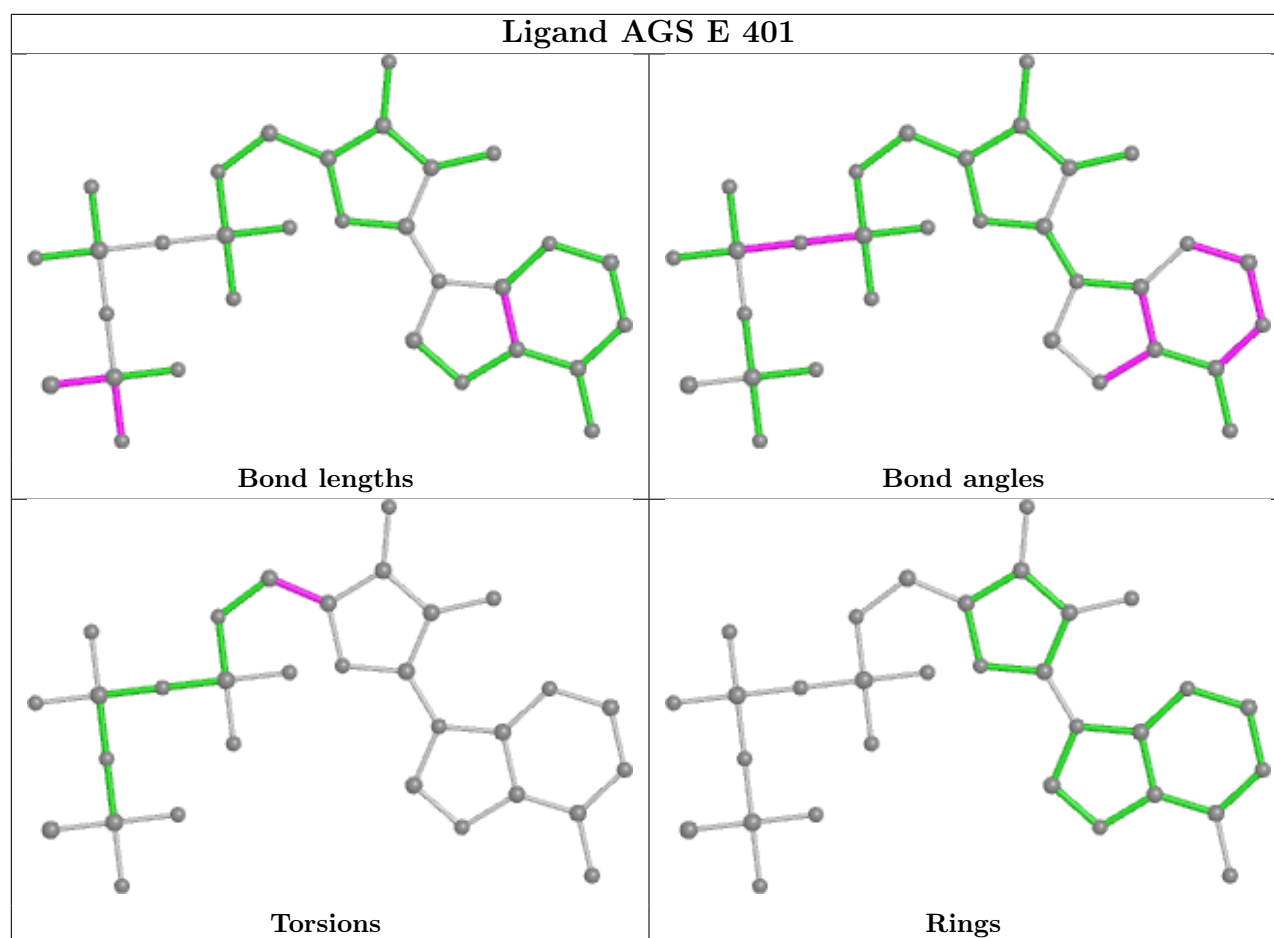


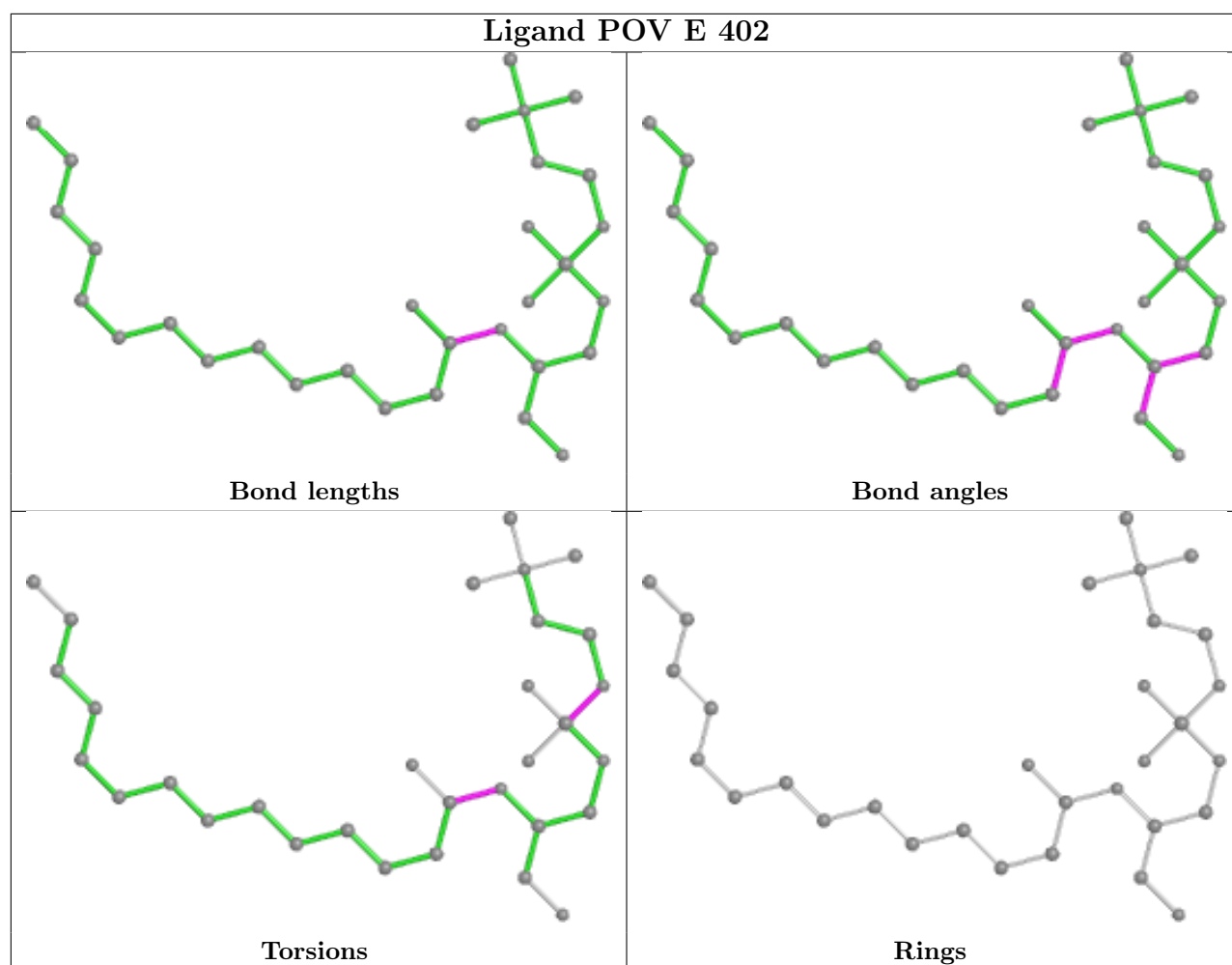


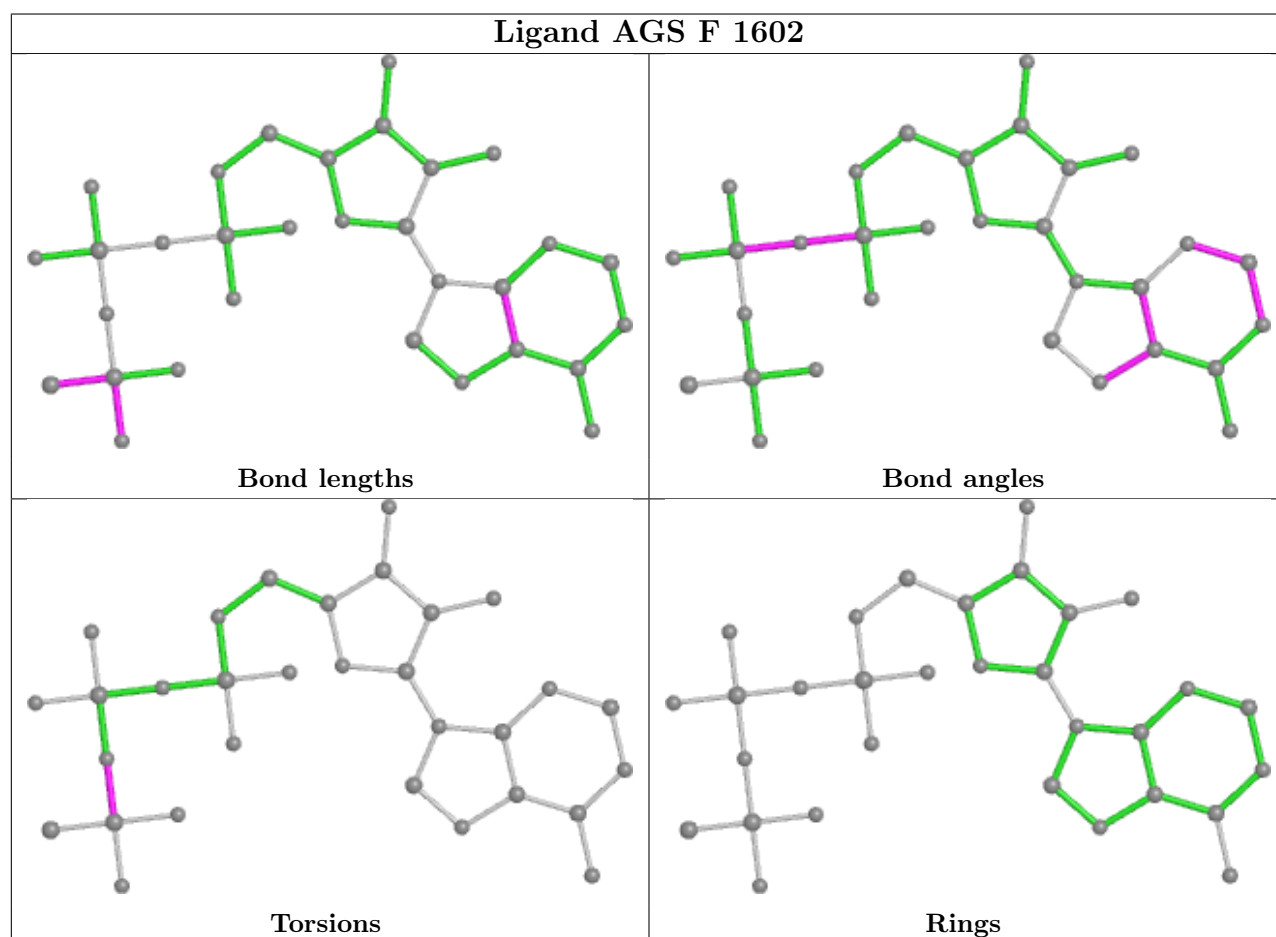
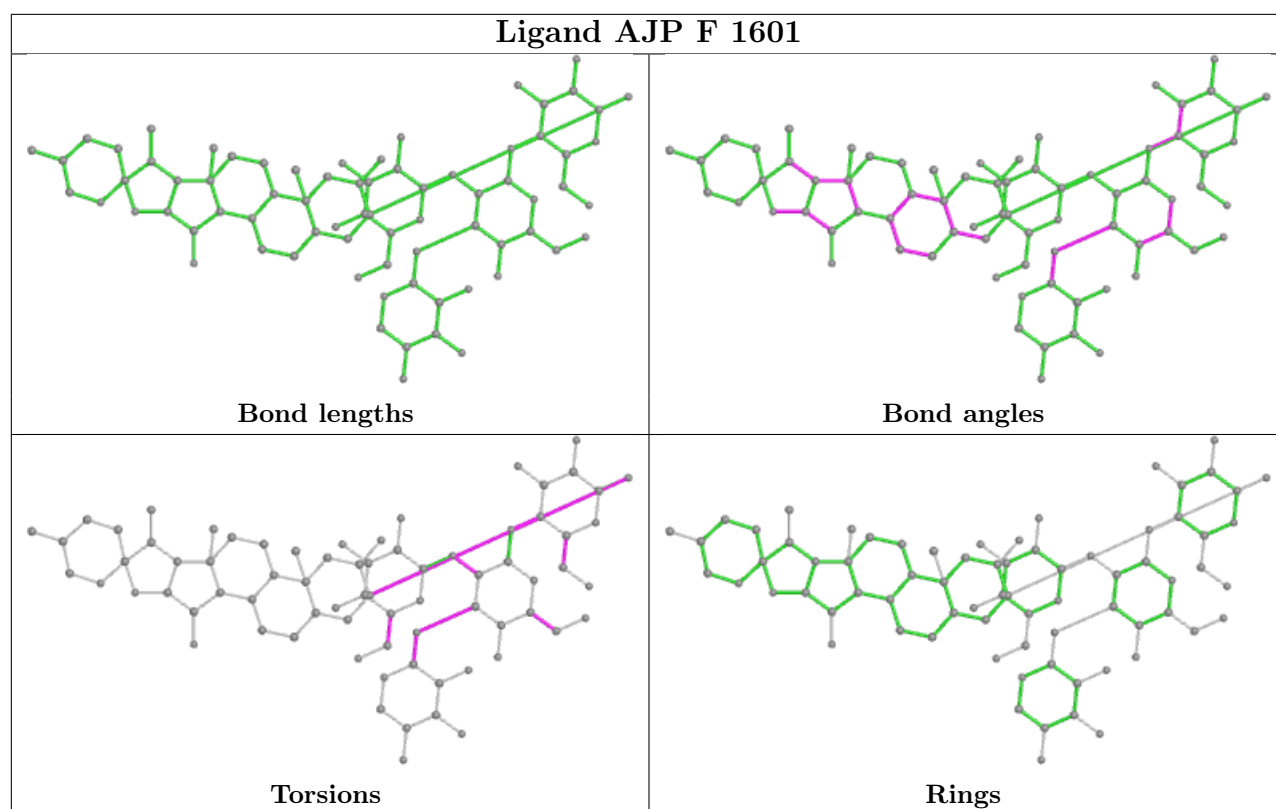


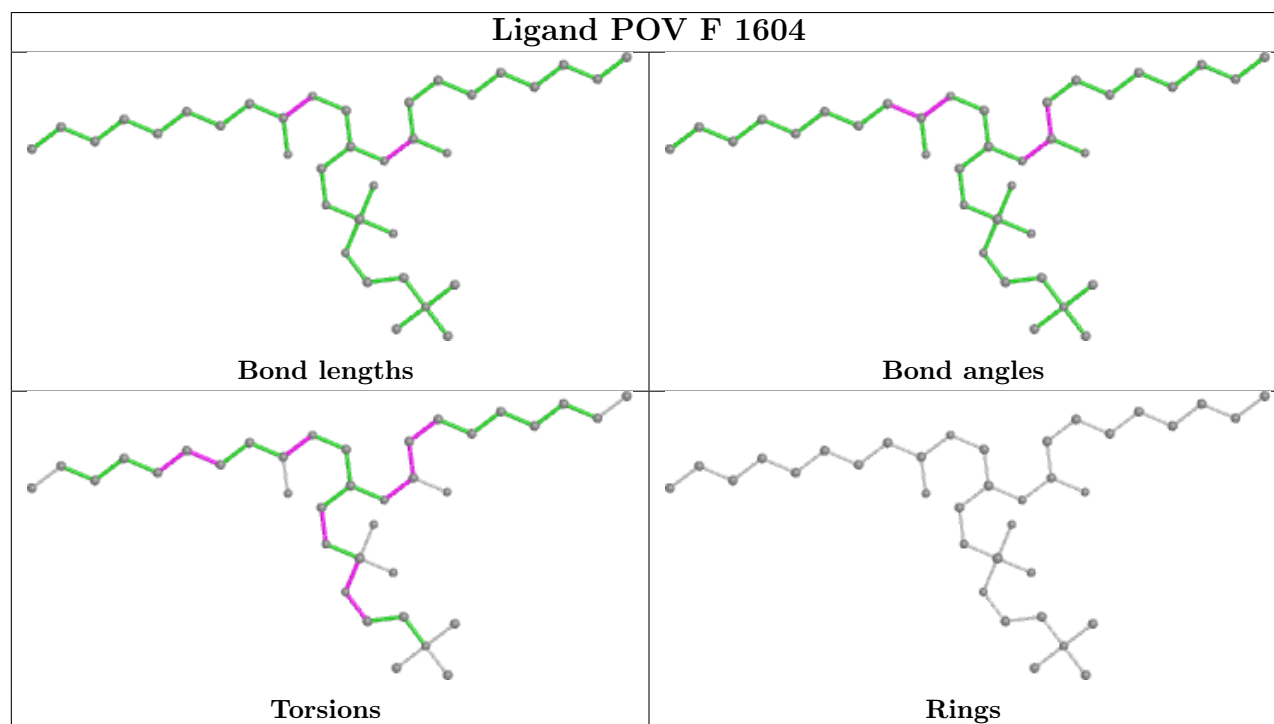
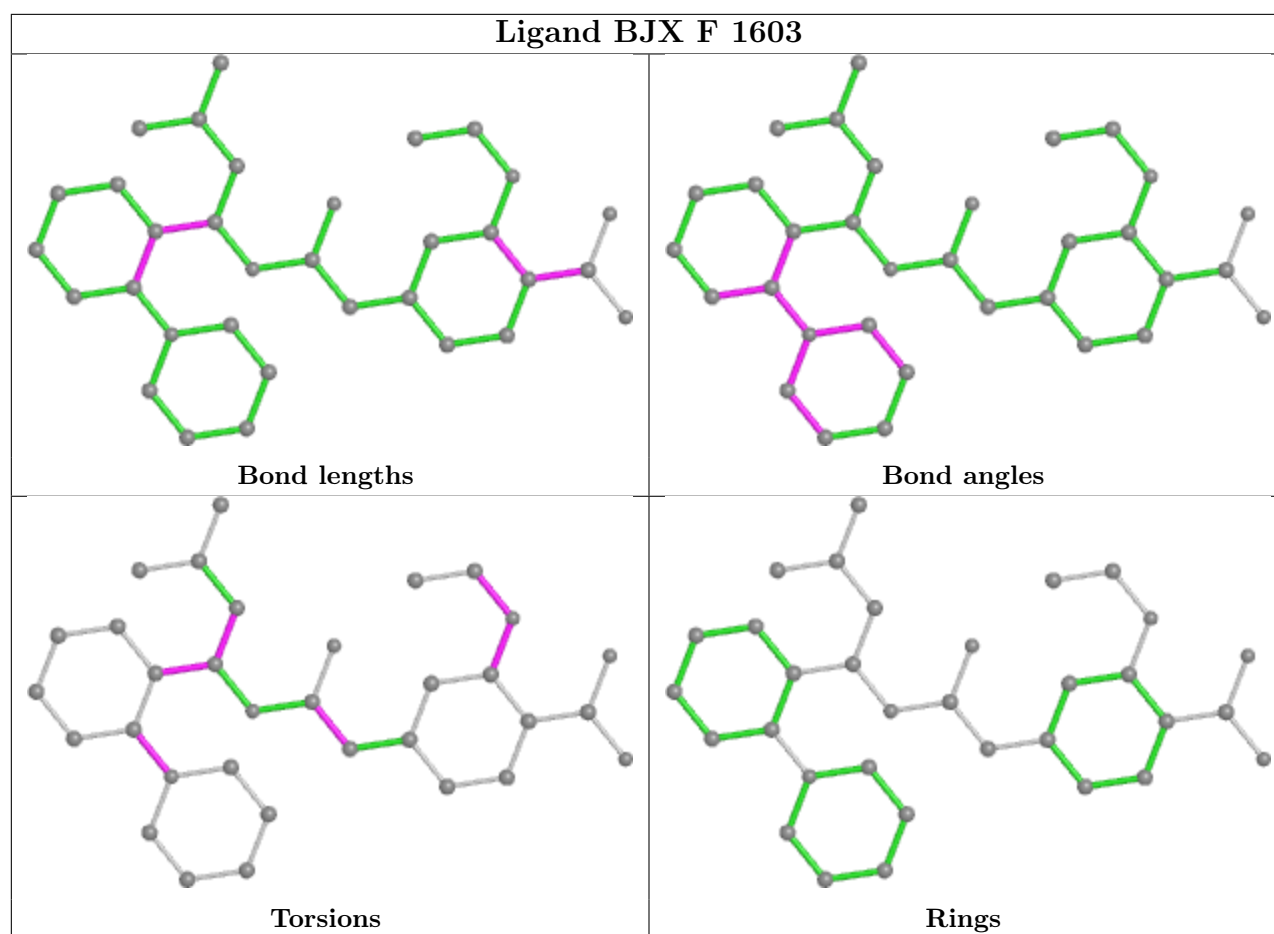


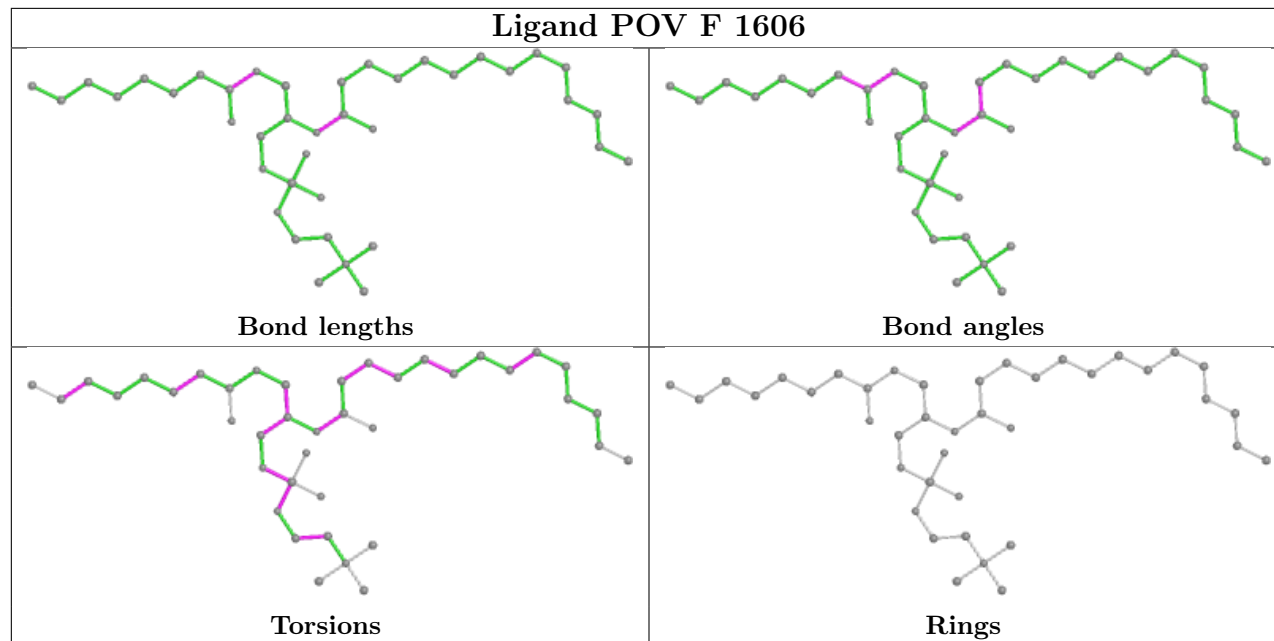
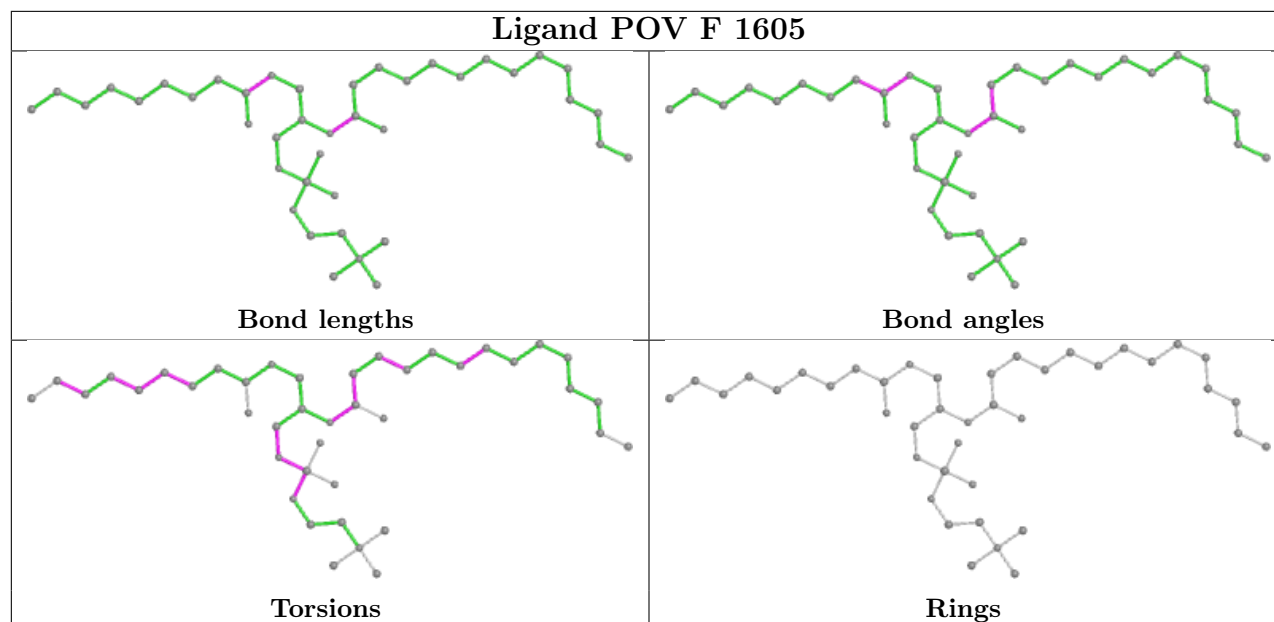


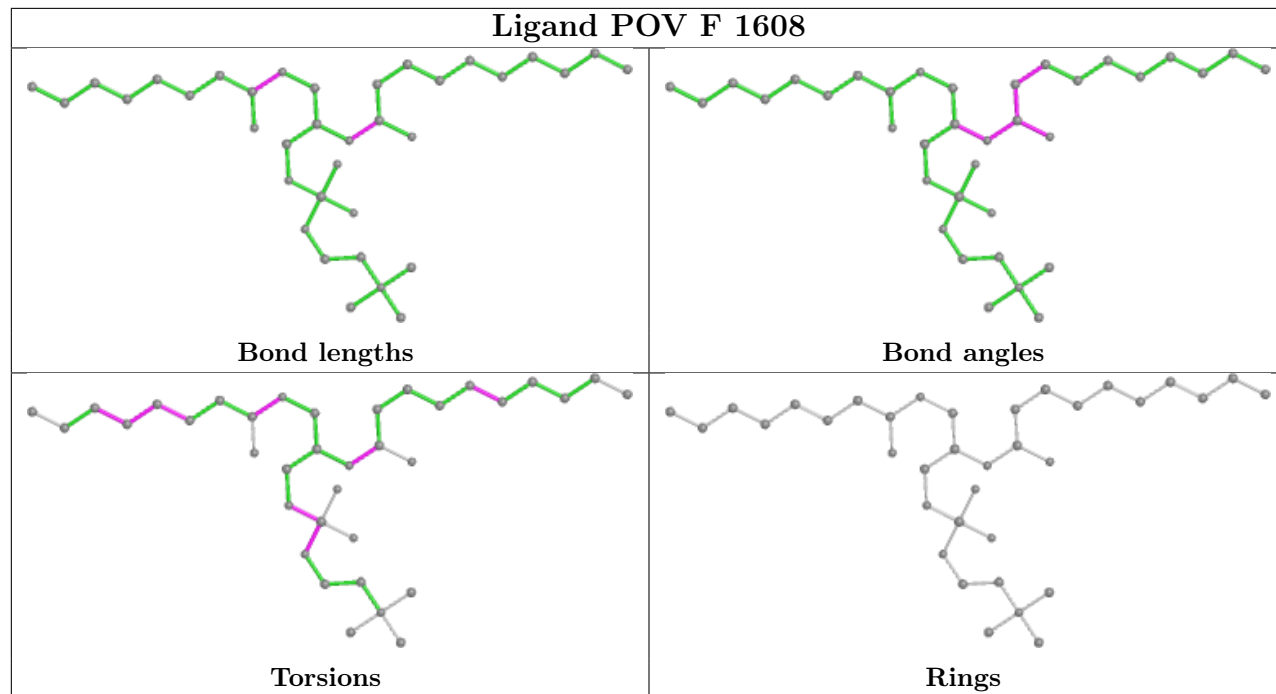
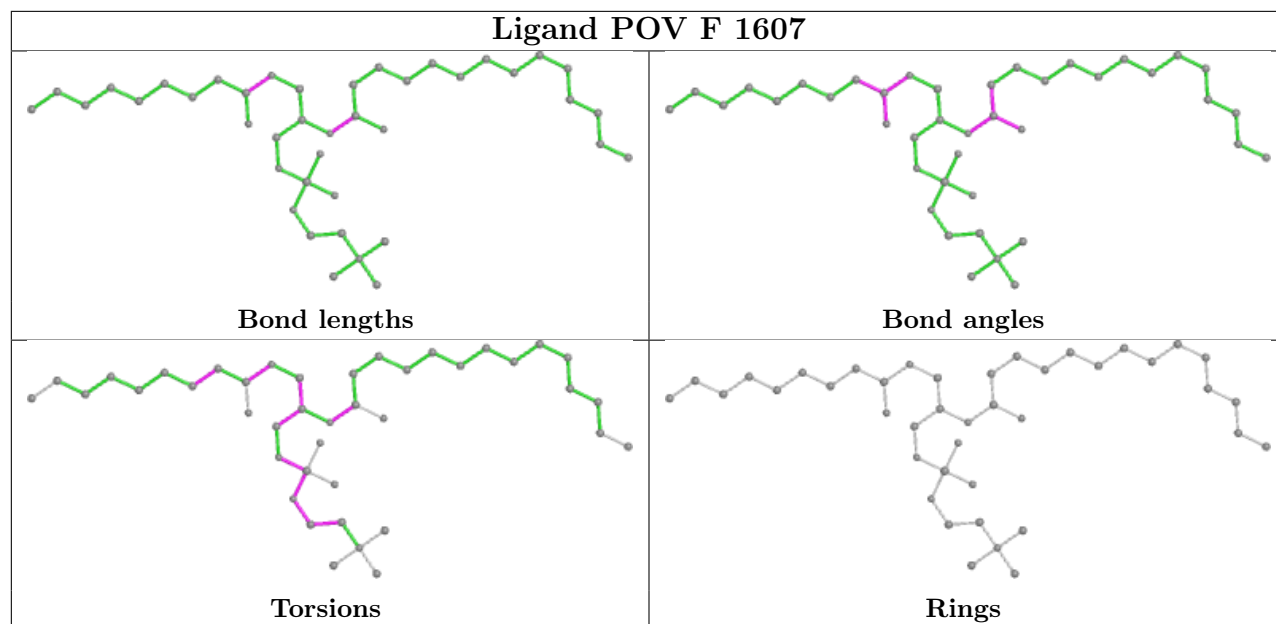


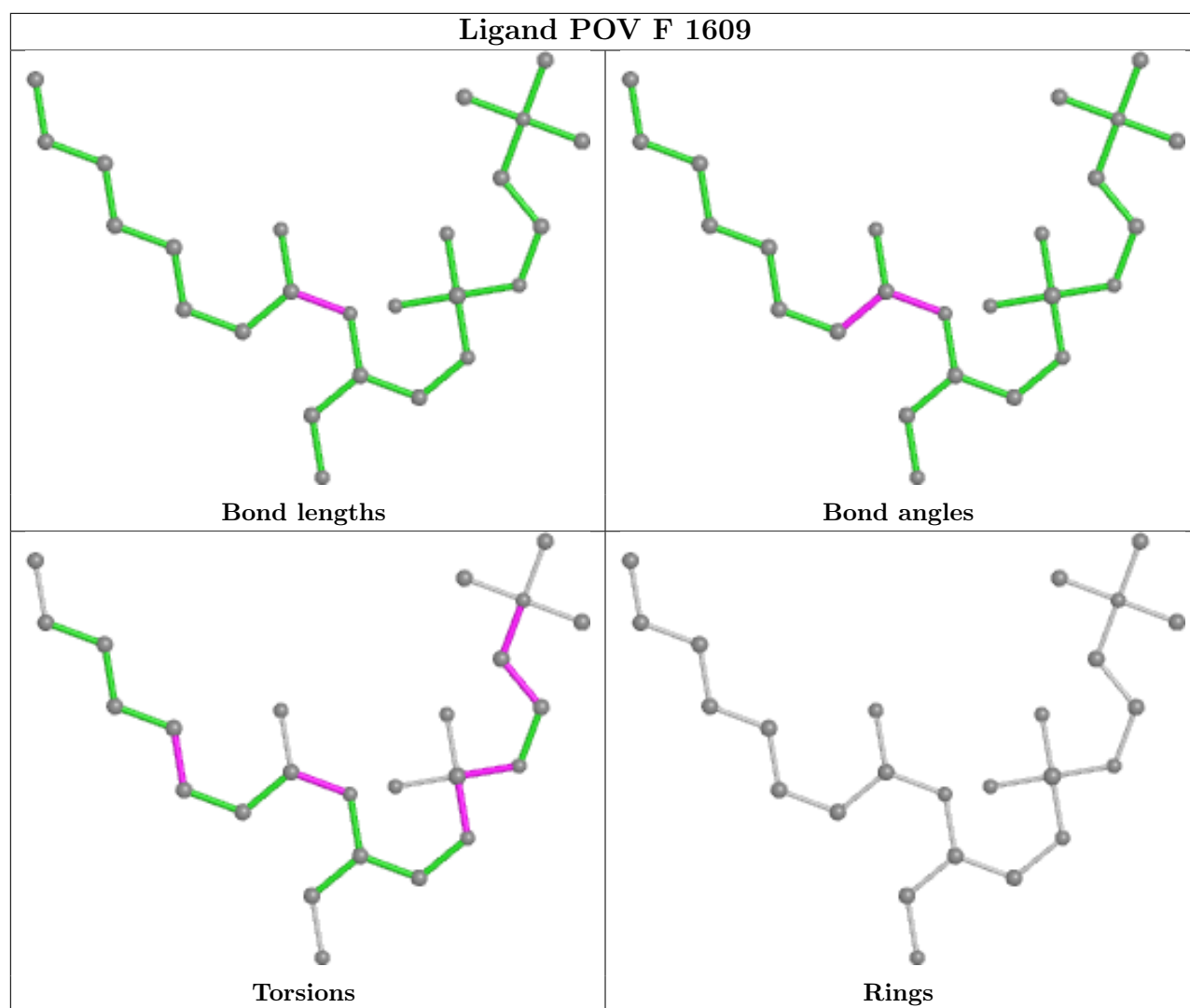


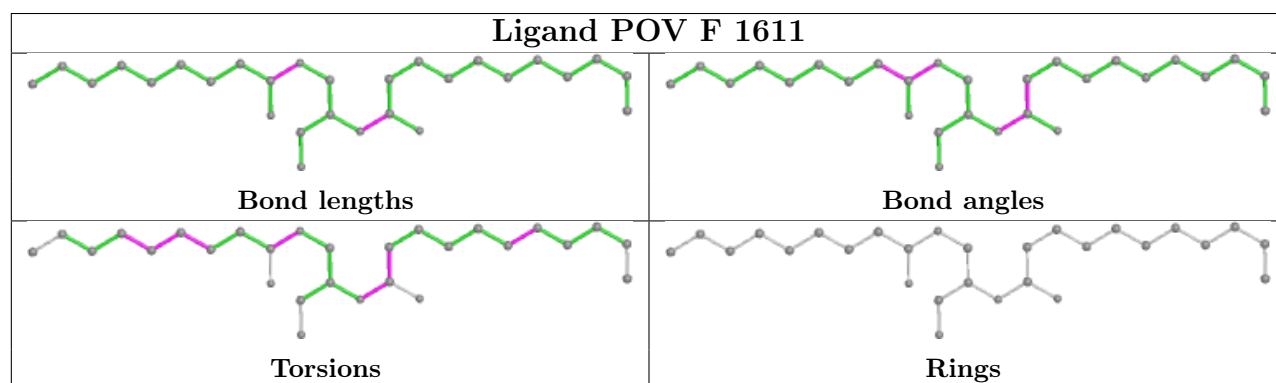
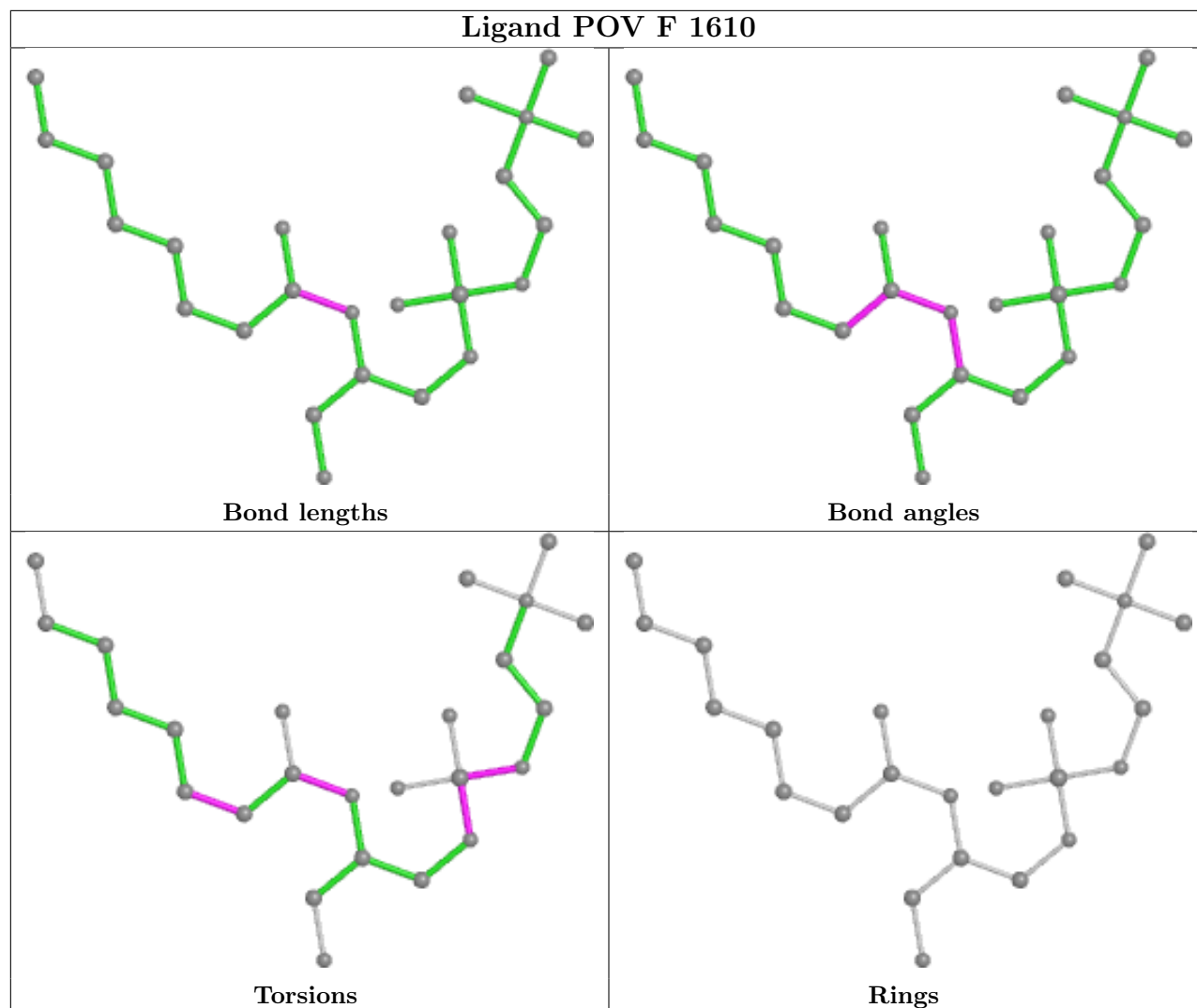


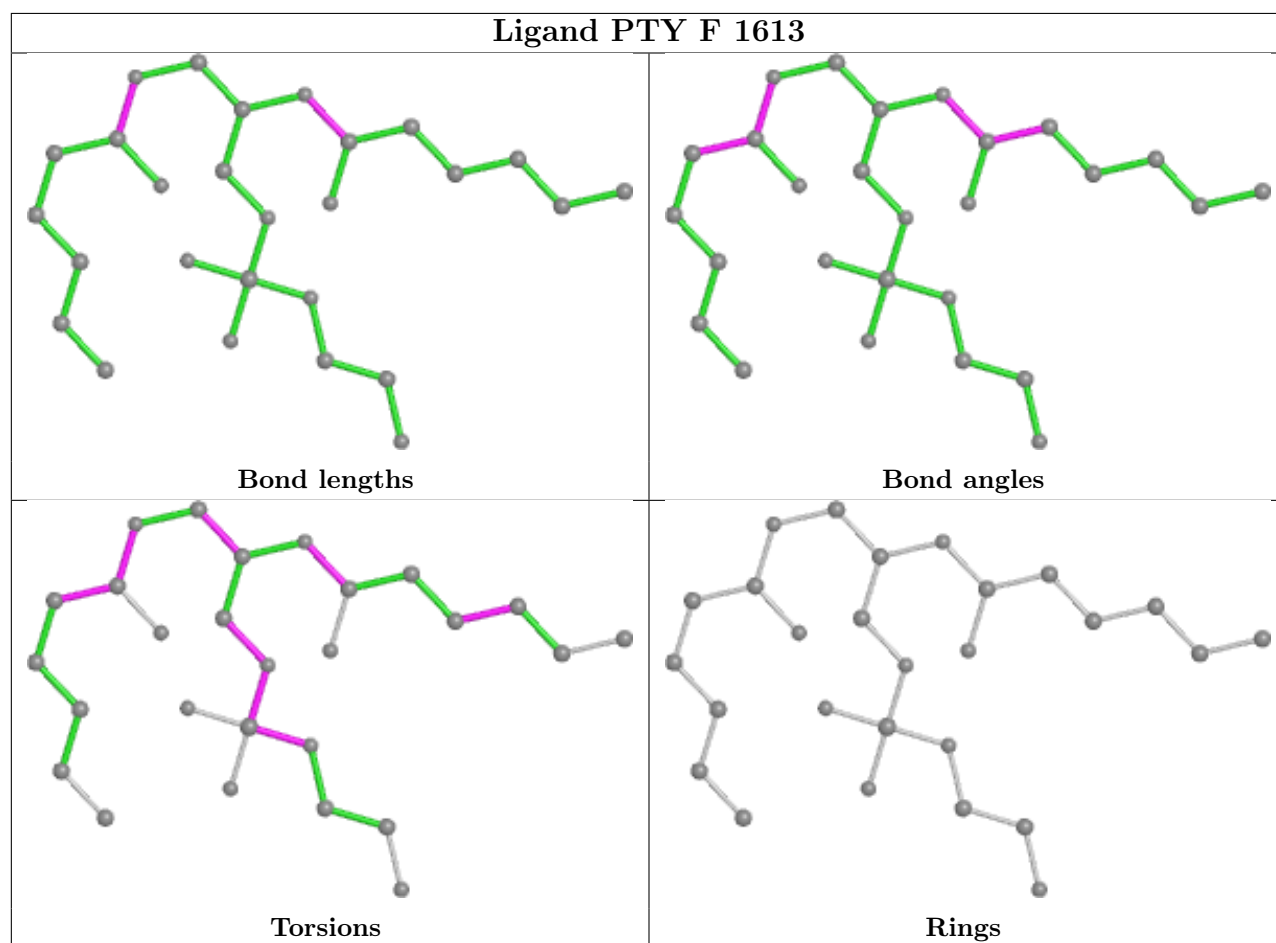
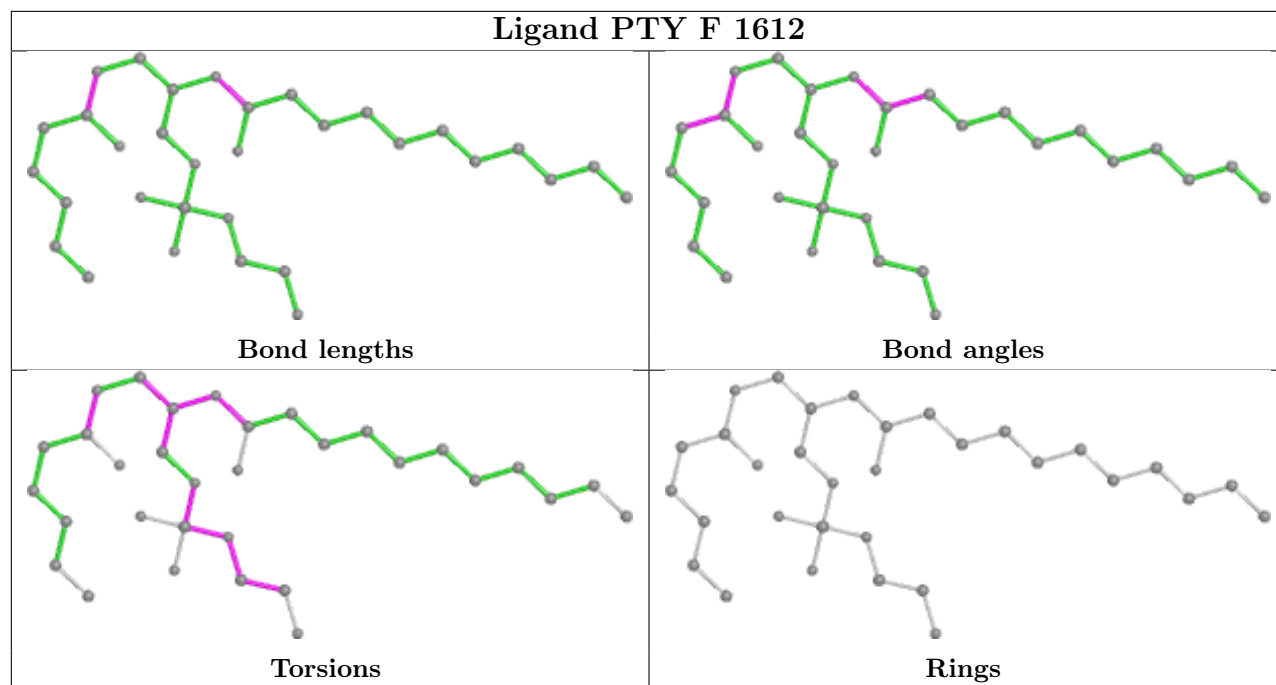


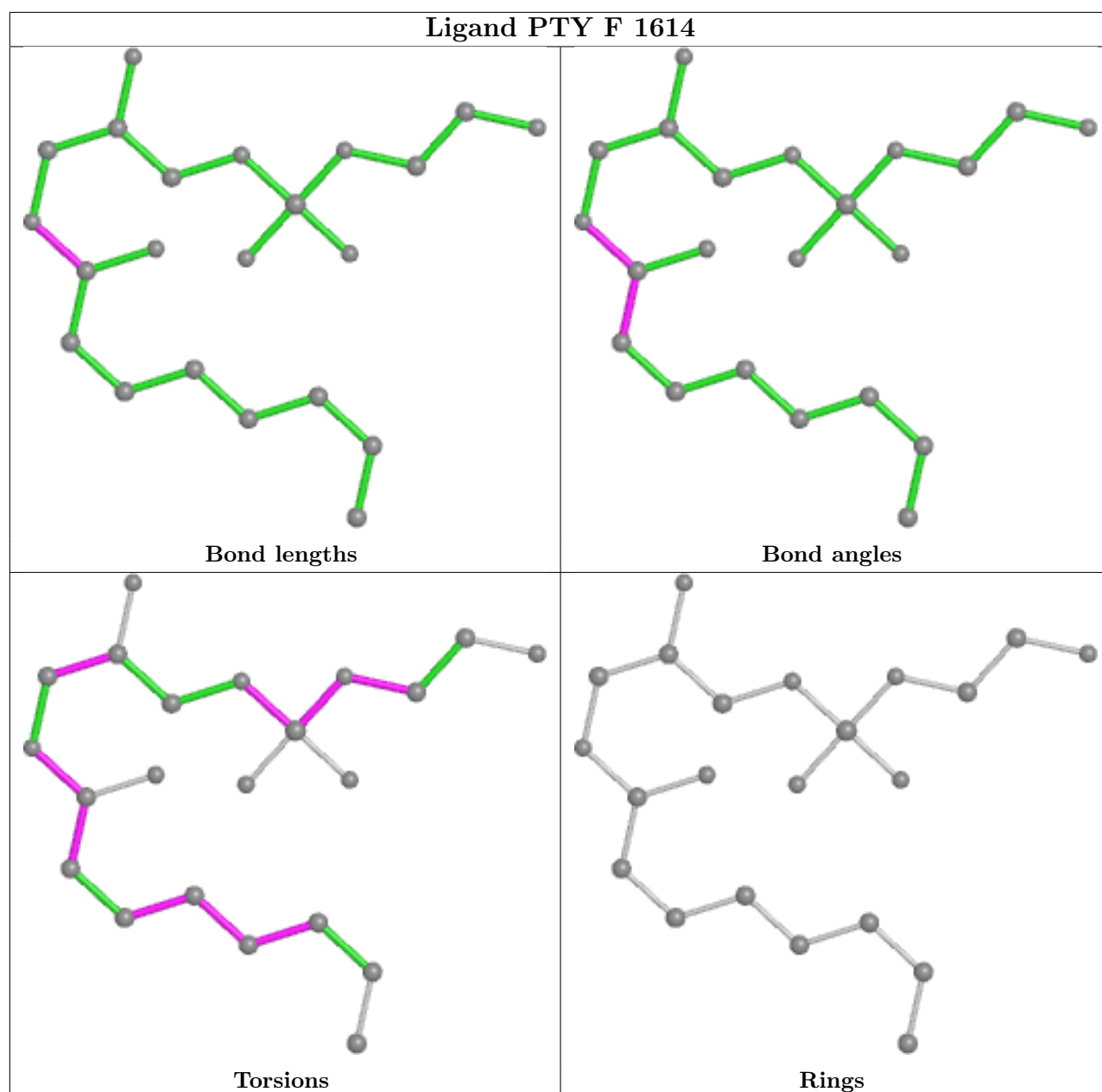


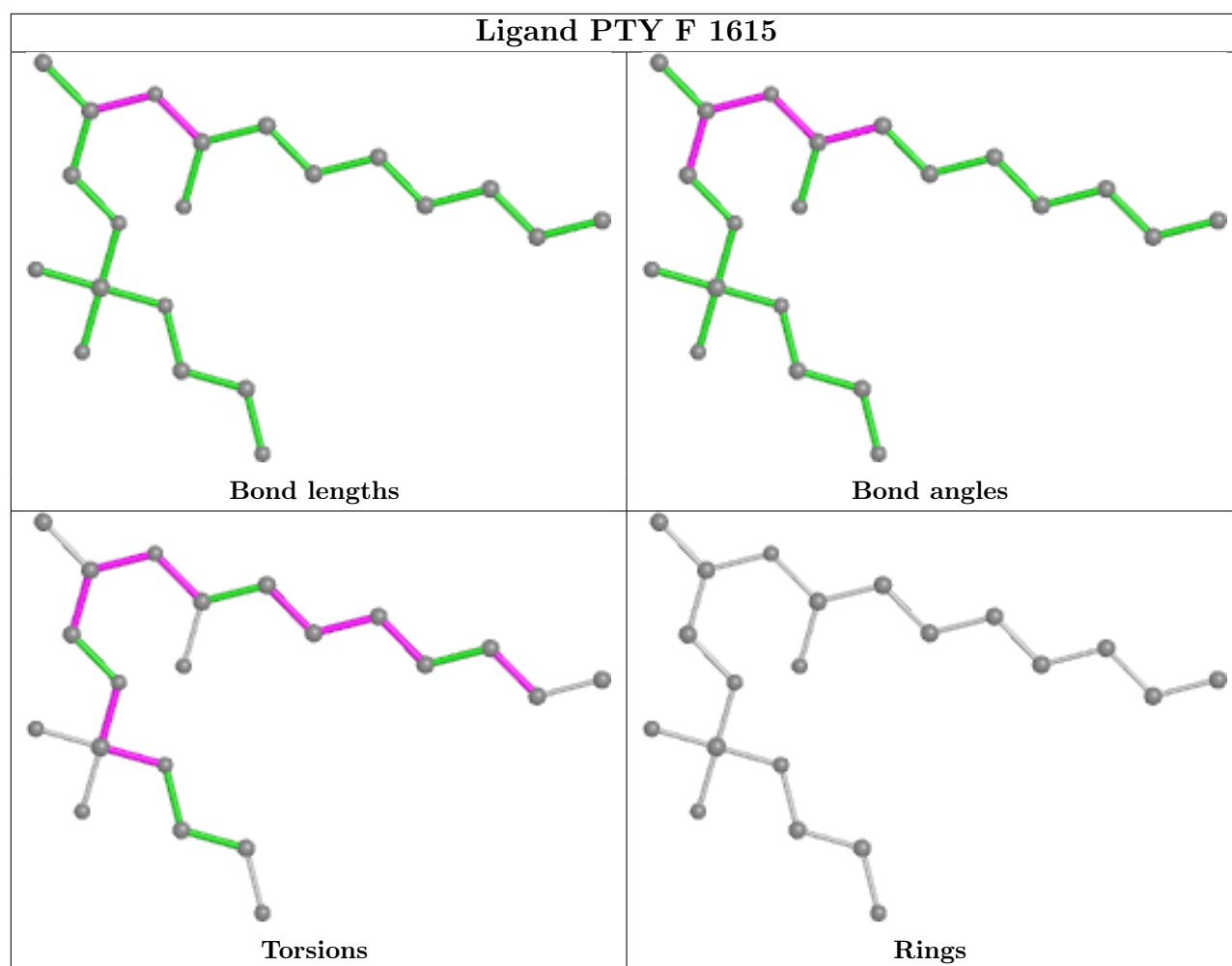


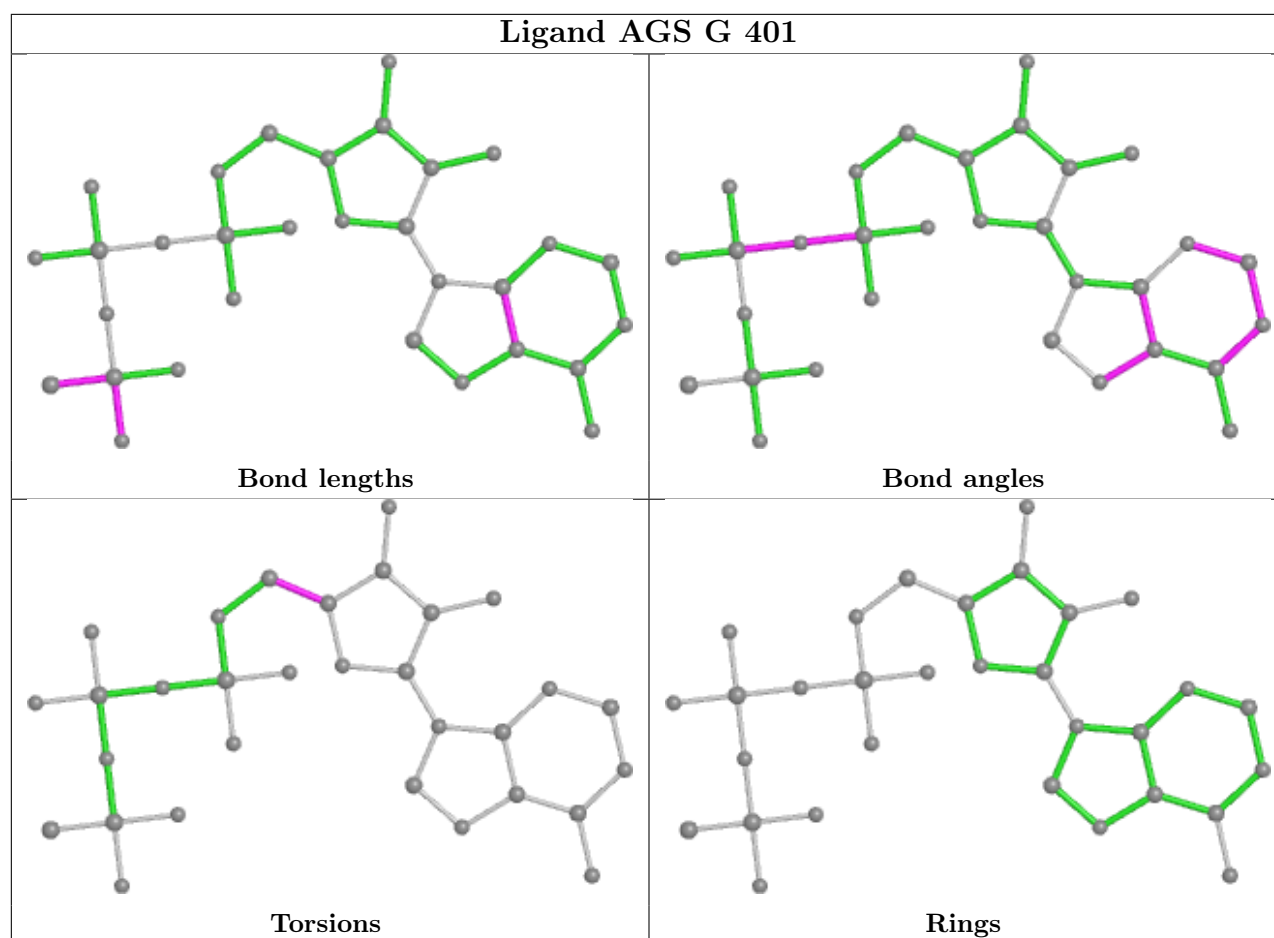


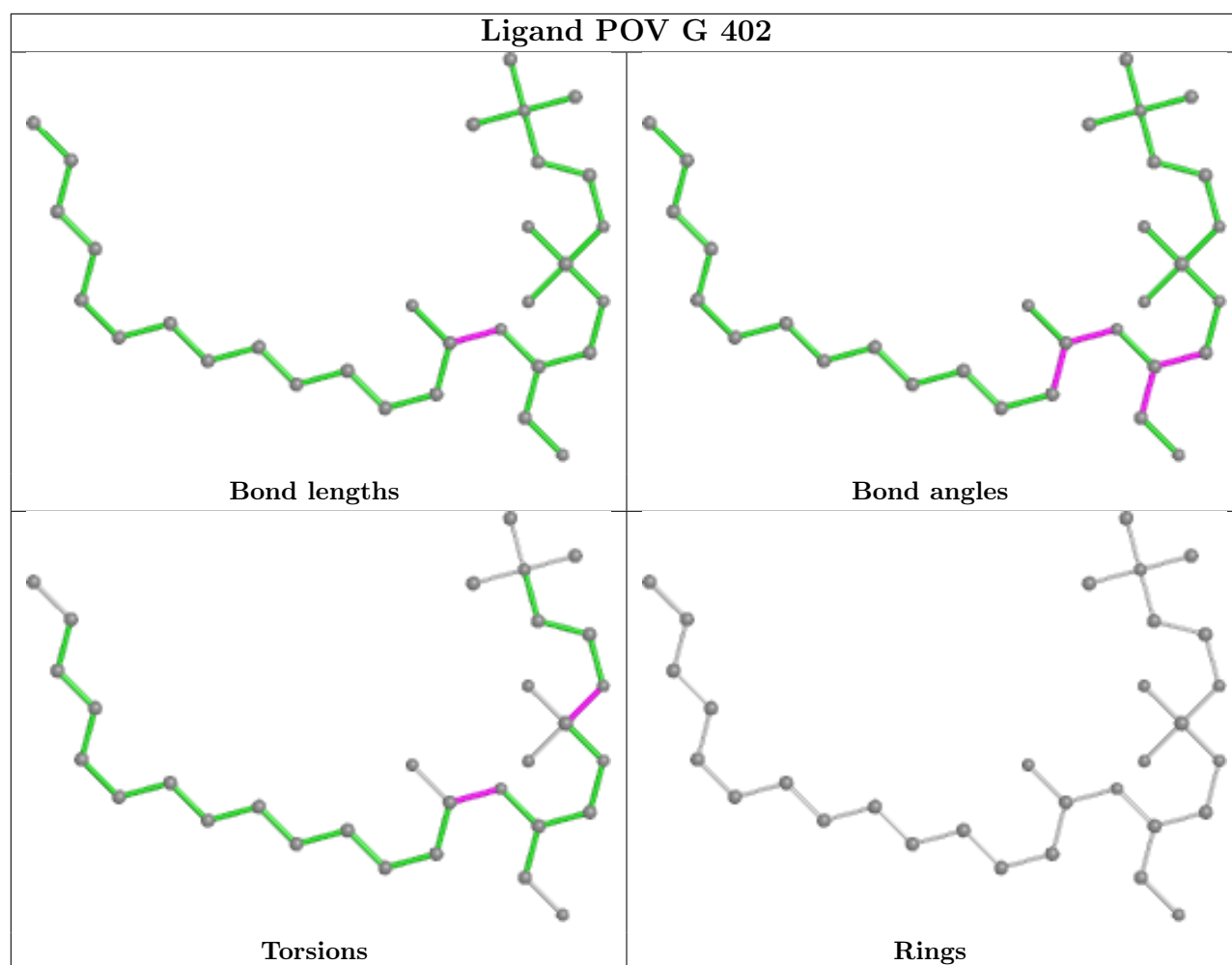


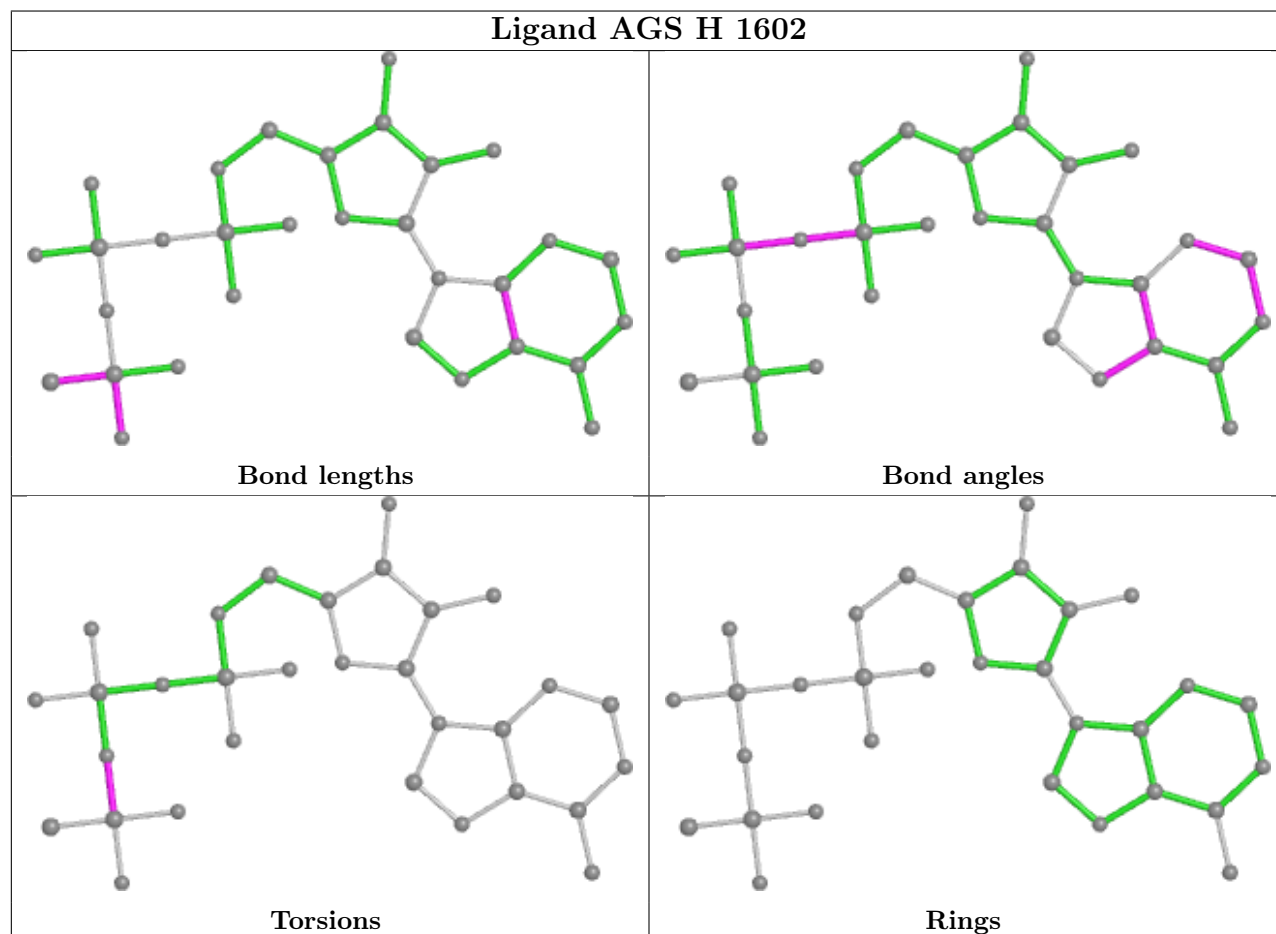
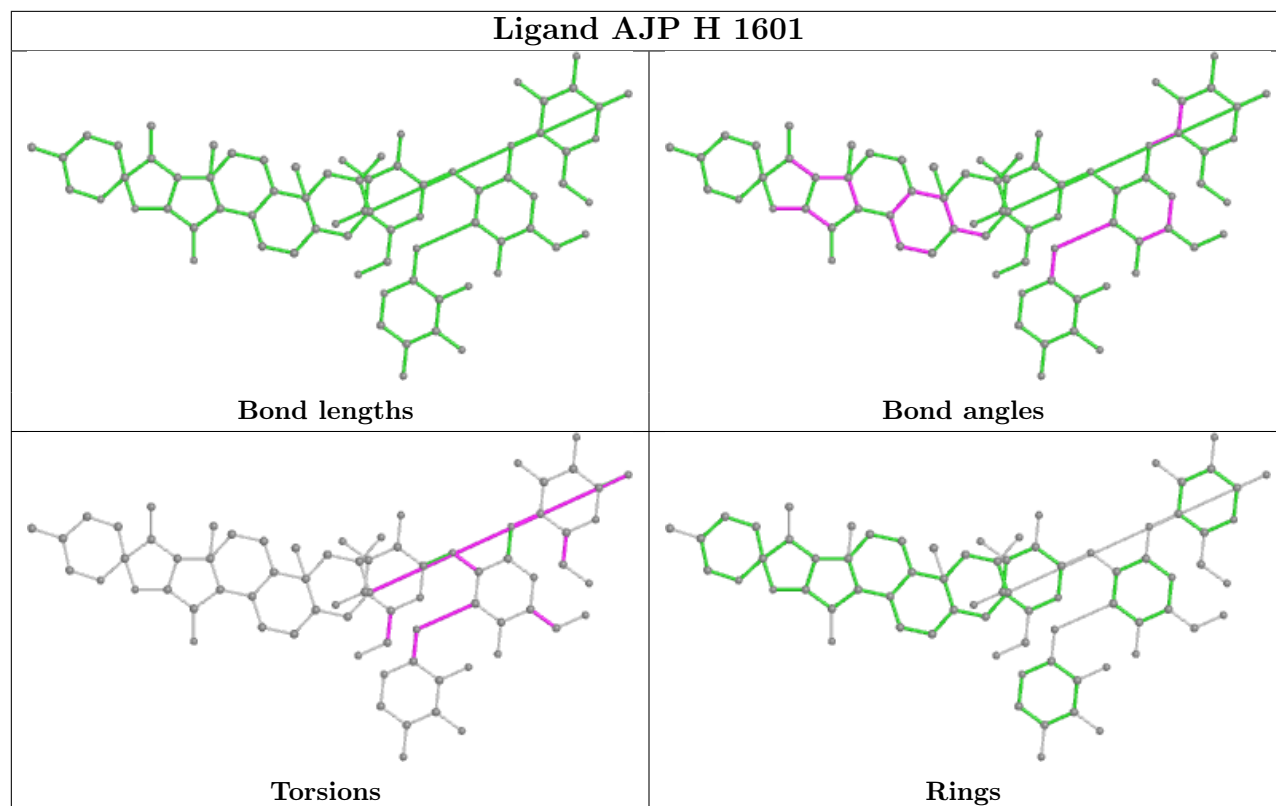




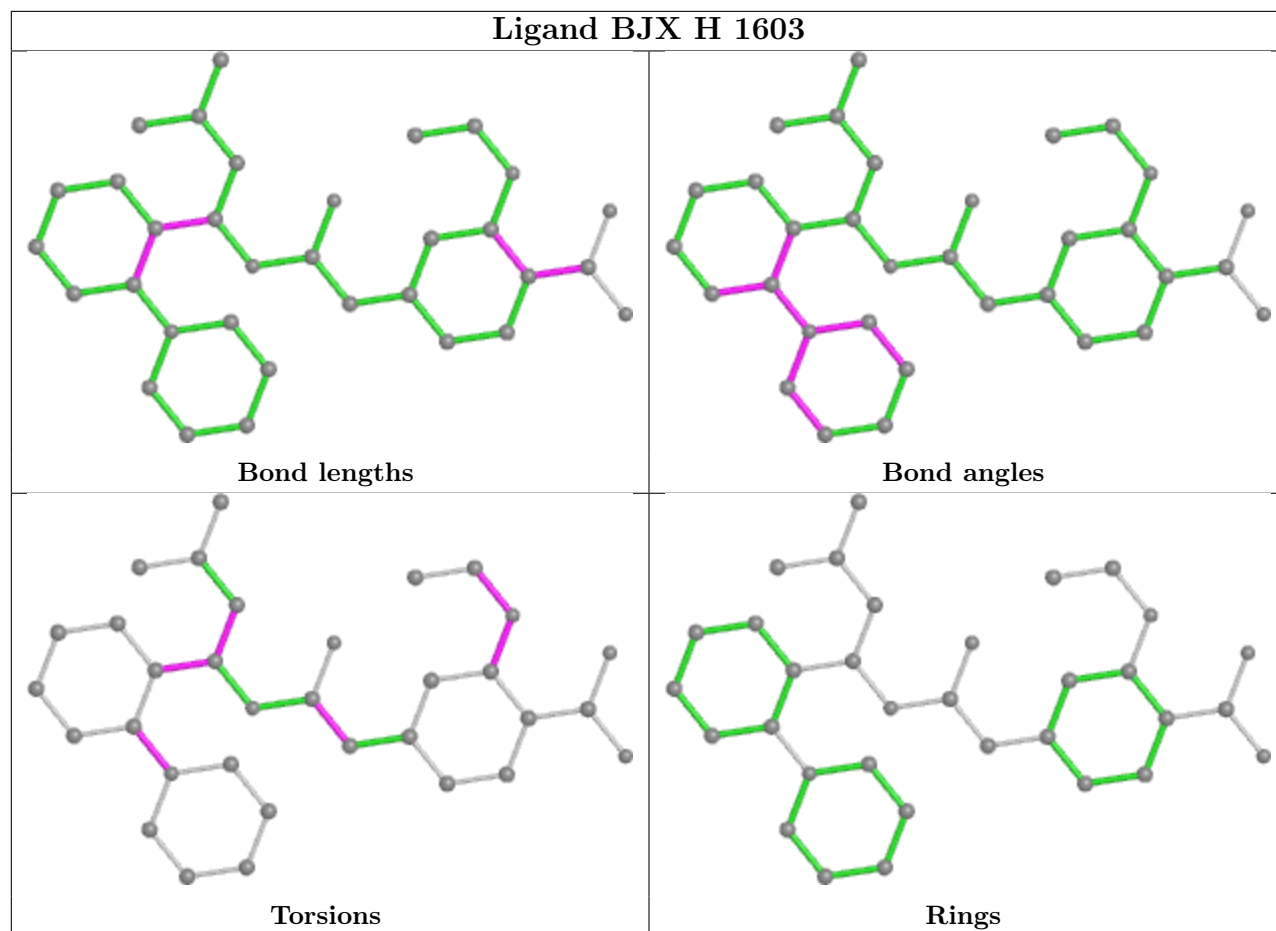




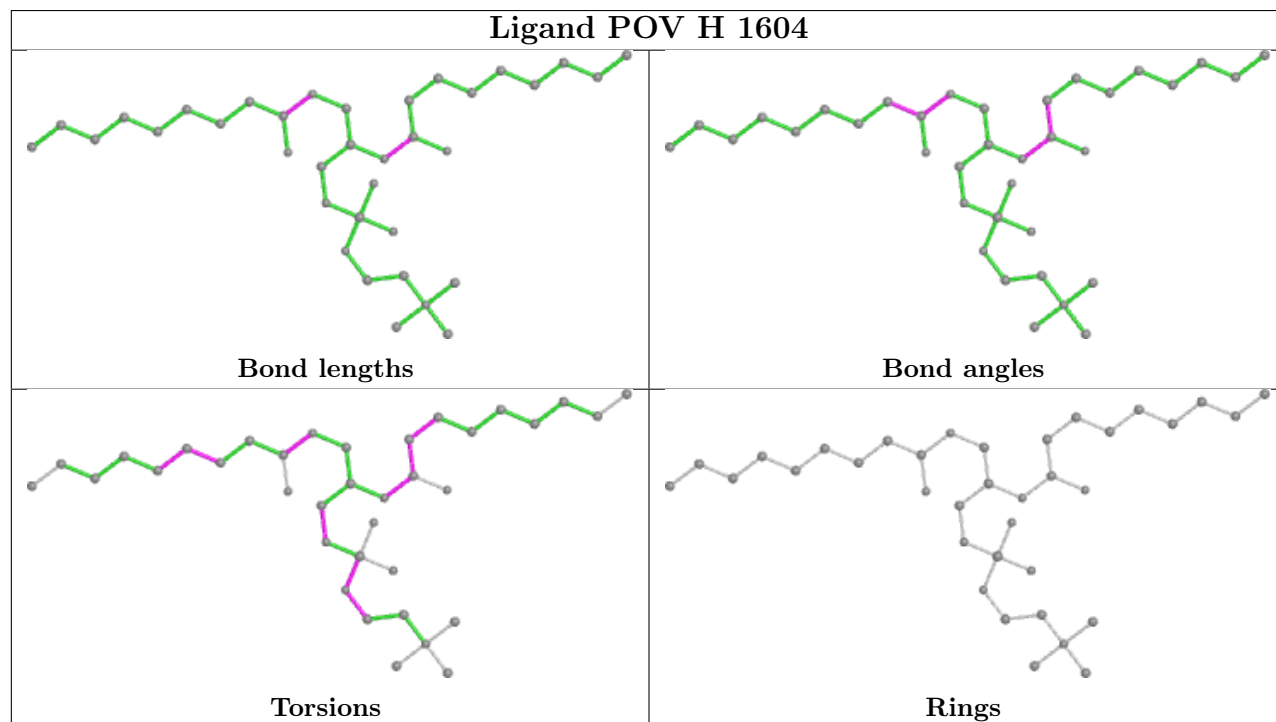


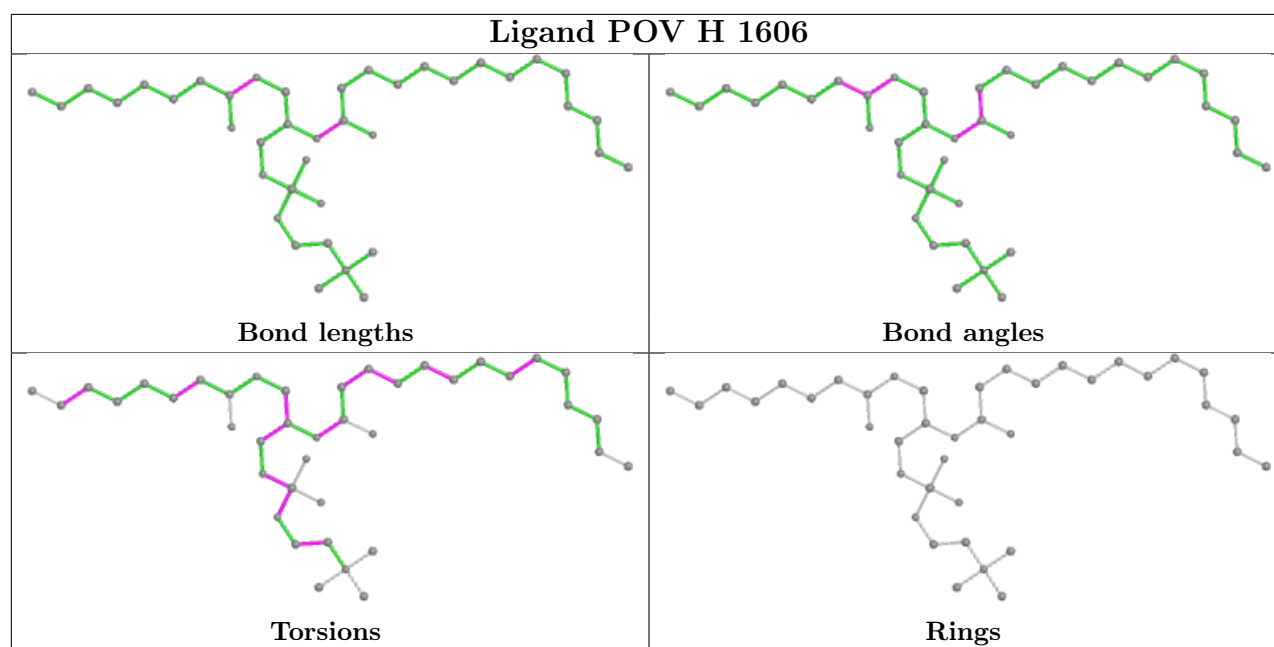
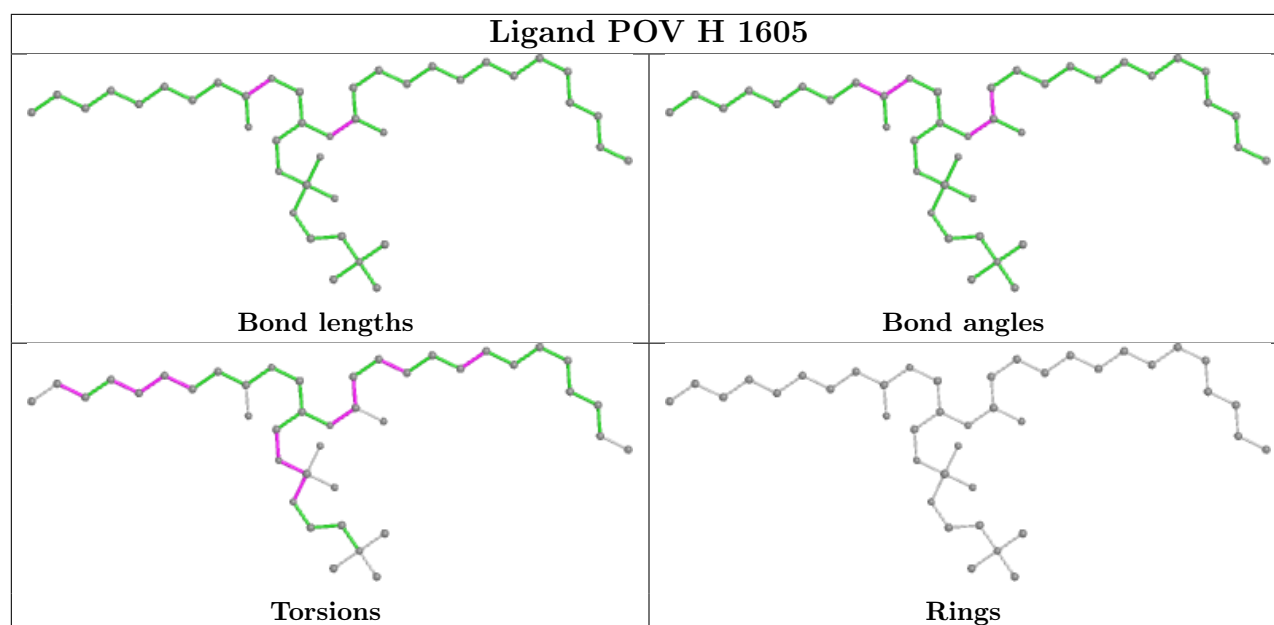


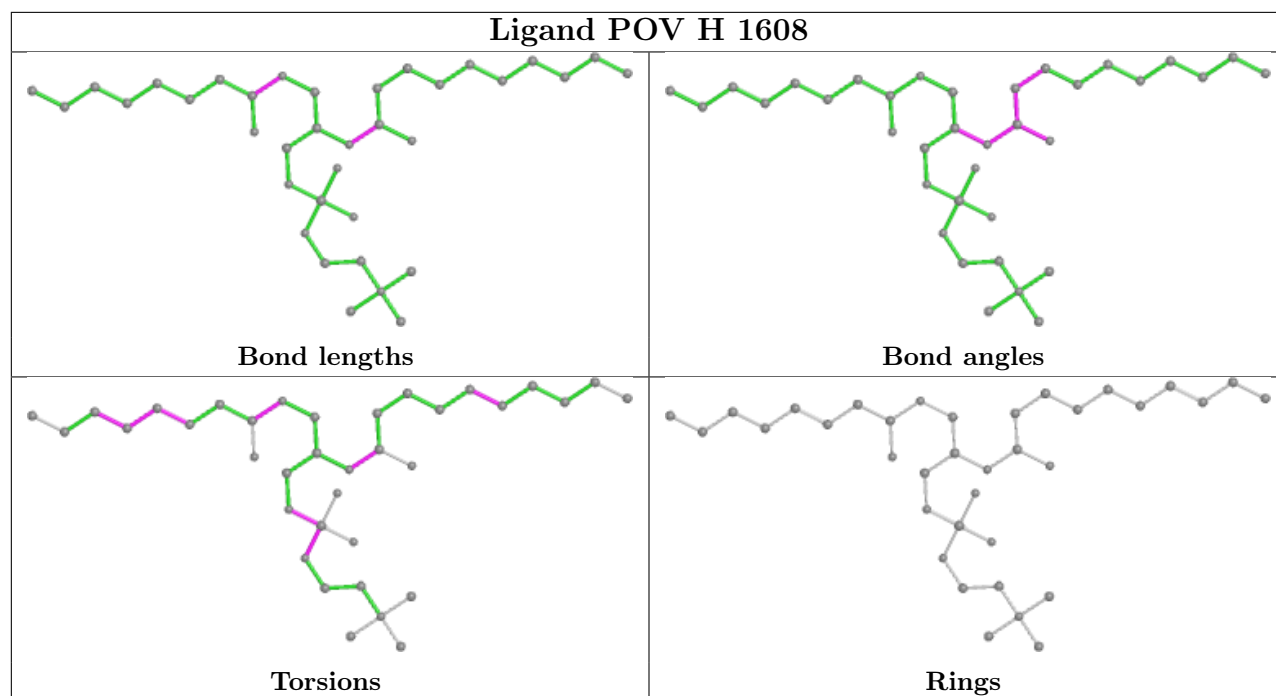
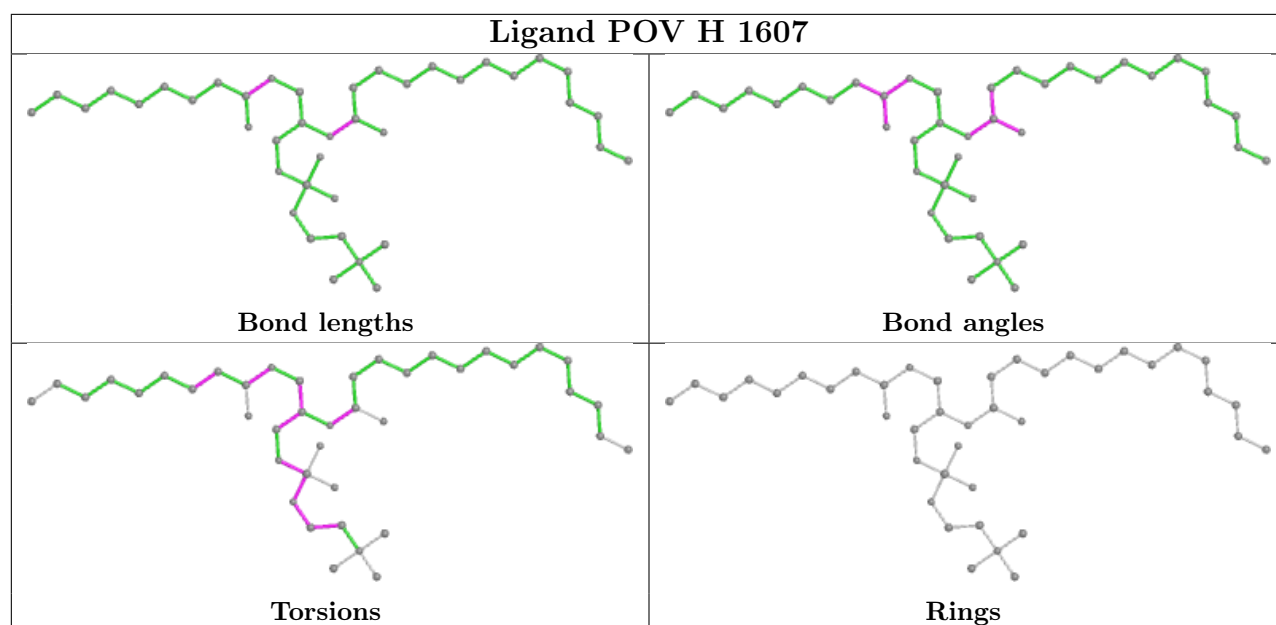
Ligand BJX H 1603

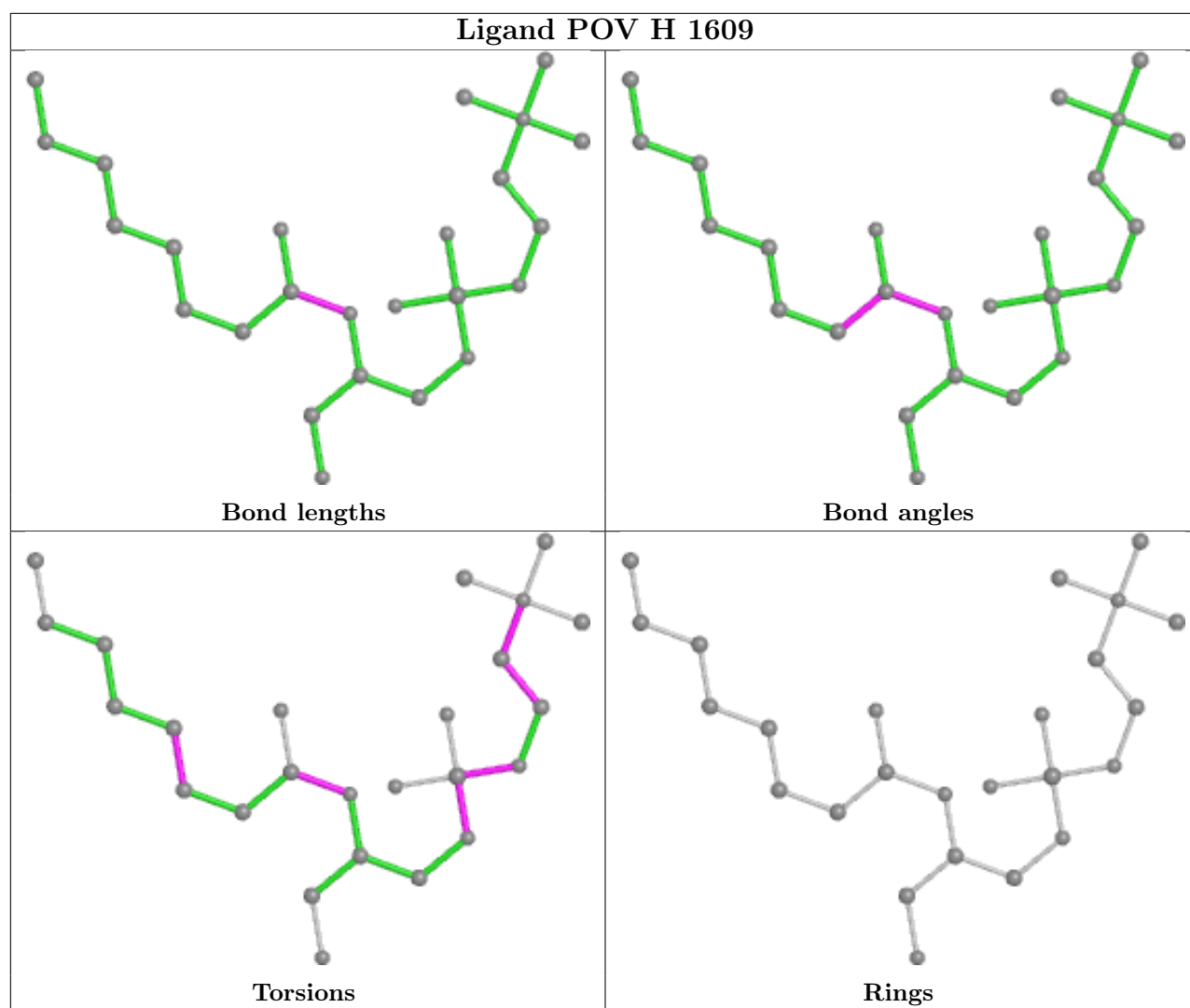


Ligand POV H 1604

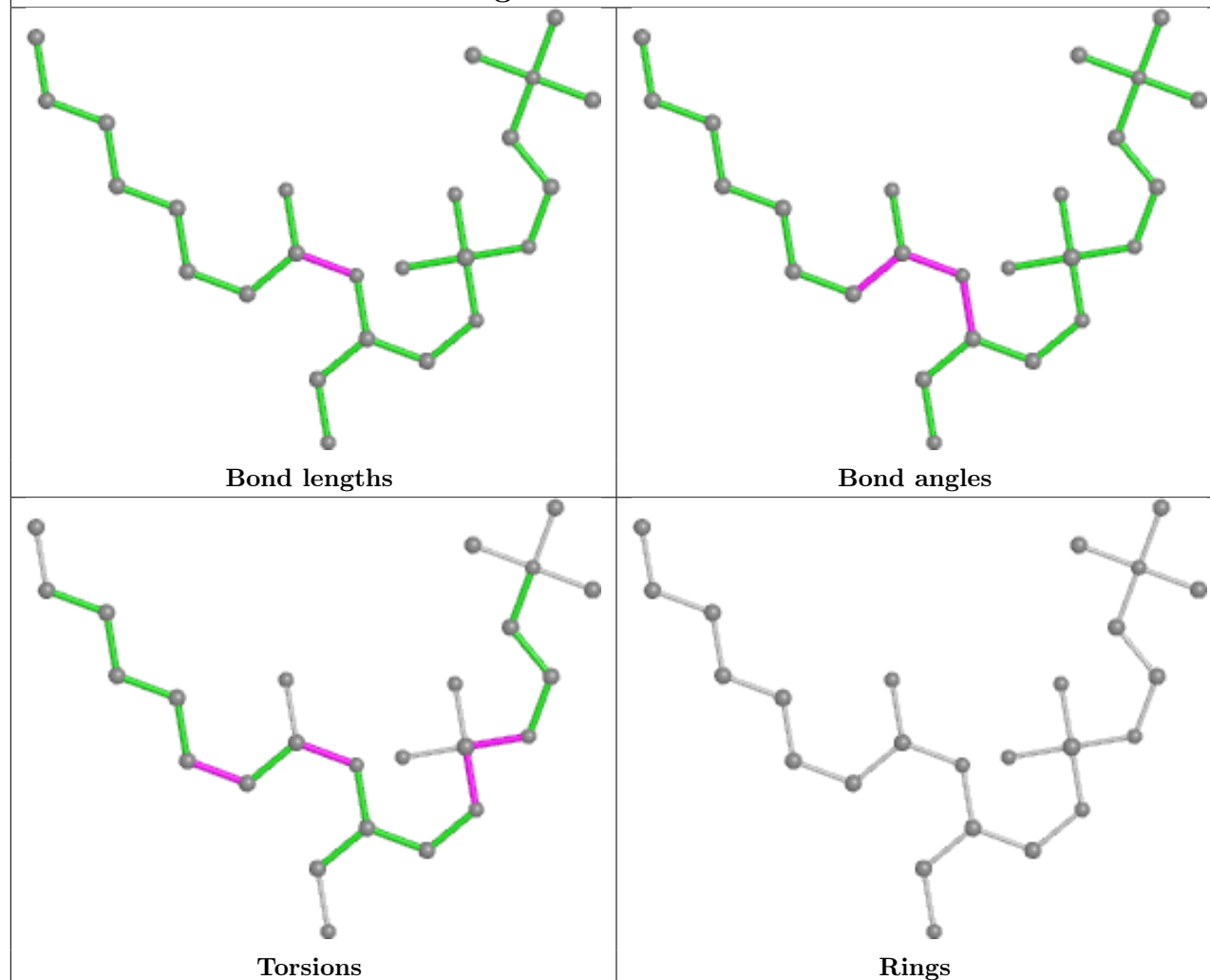




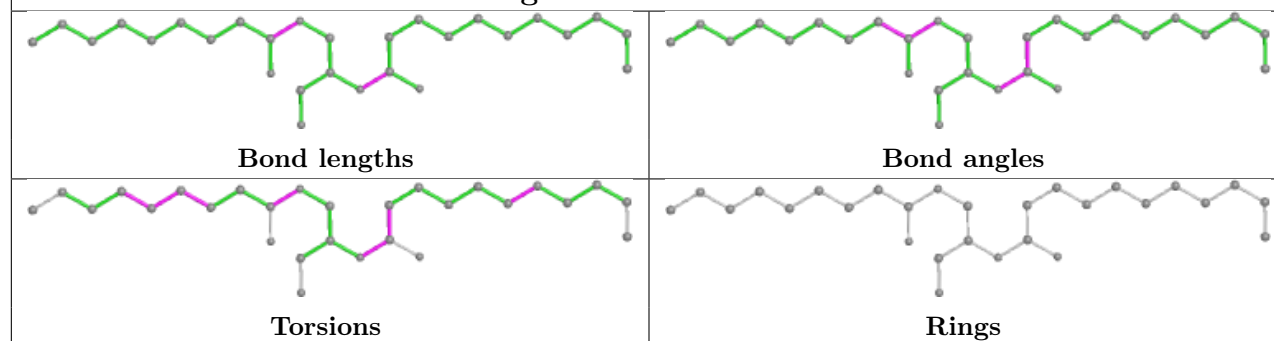


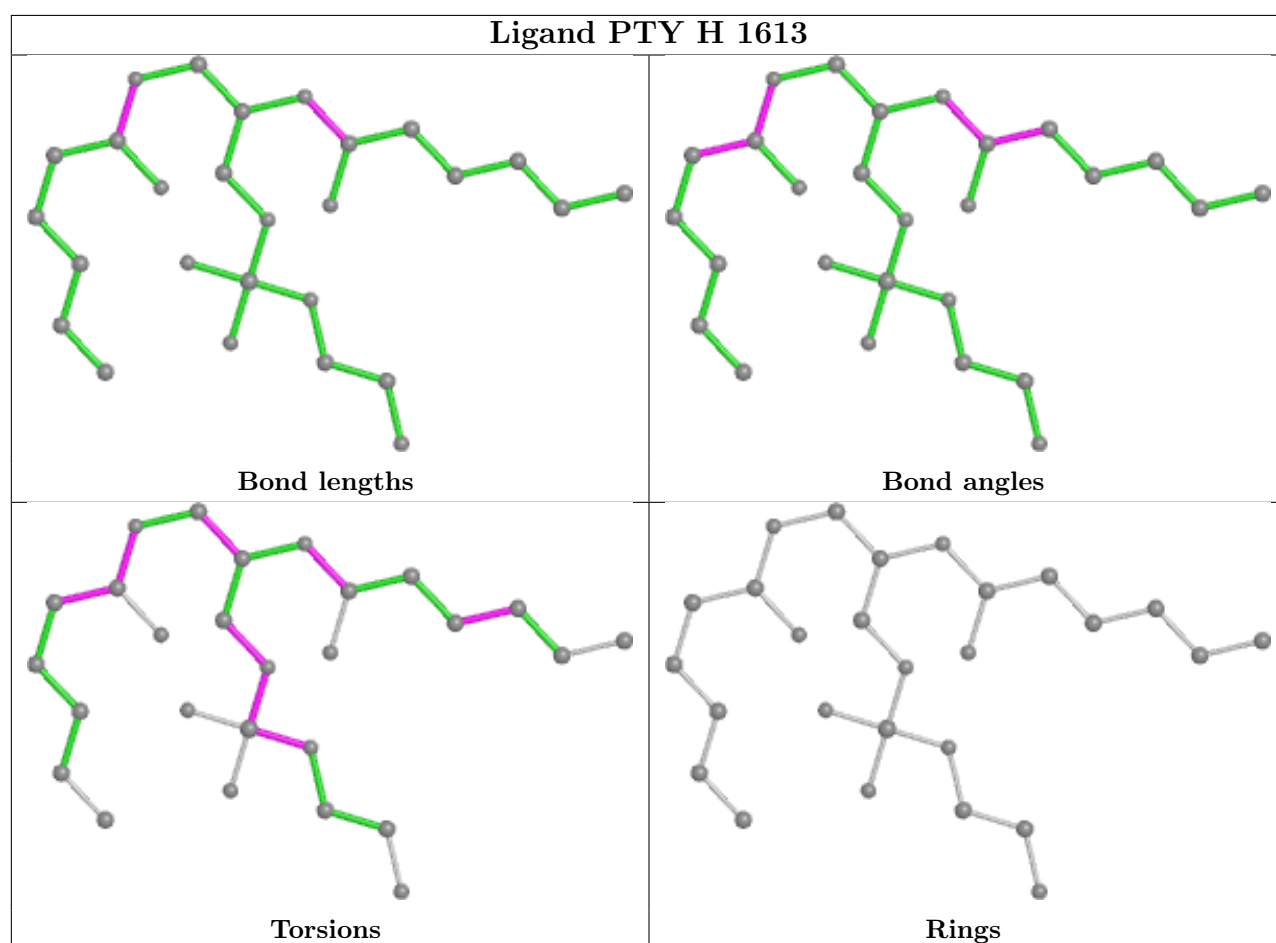
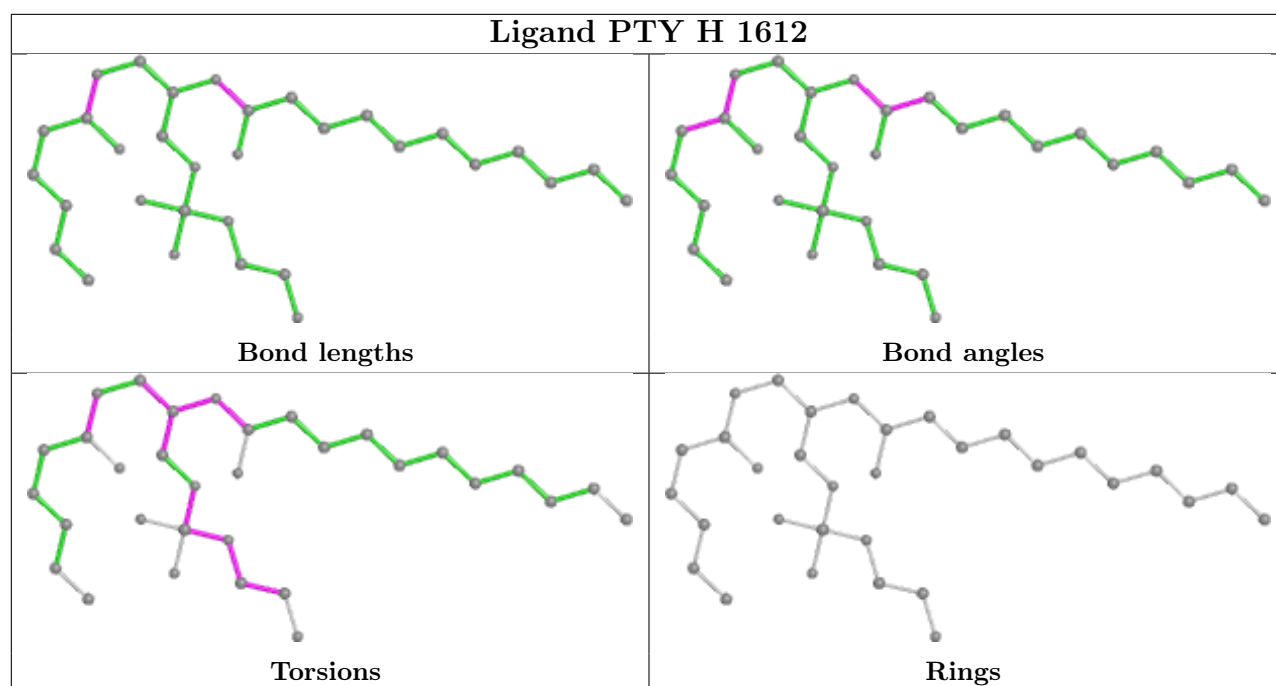


Ligand POV H 1610

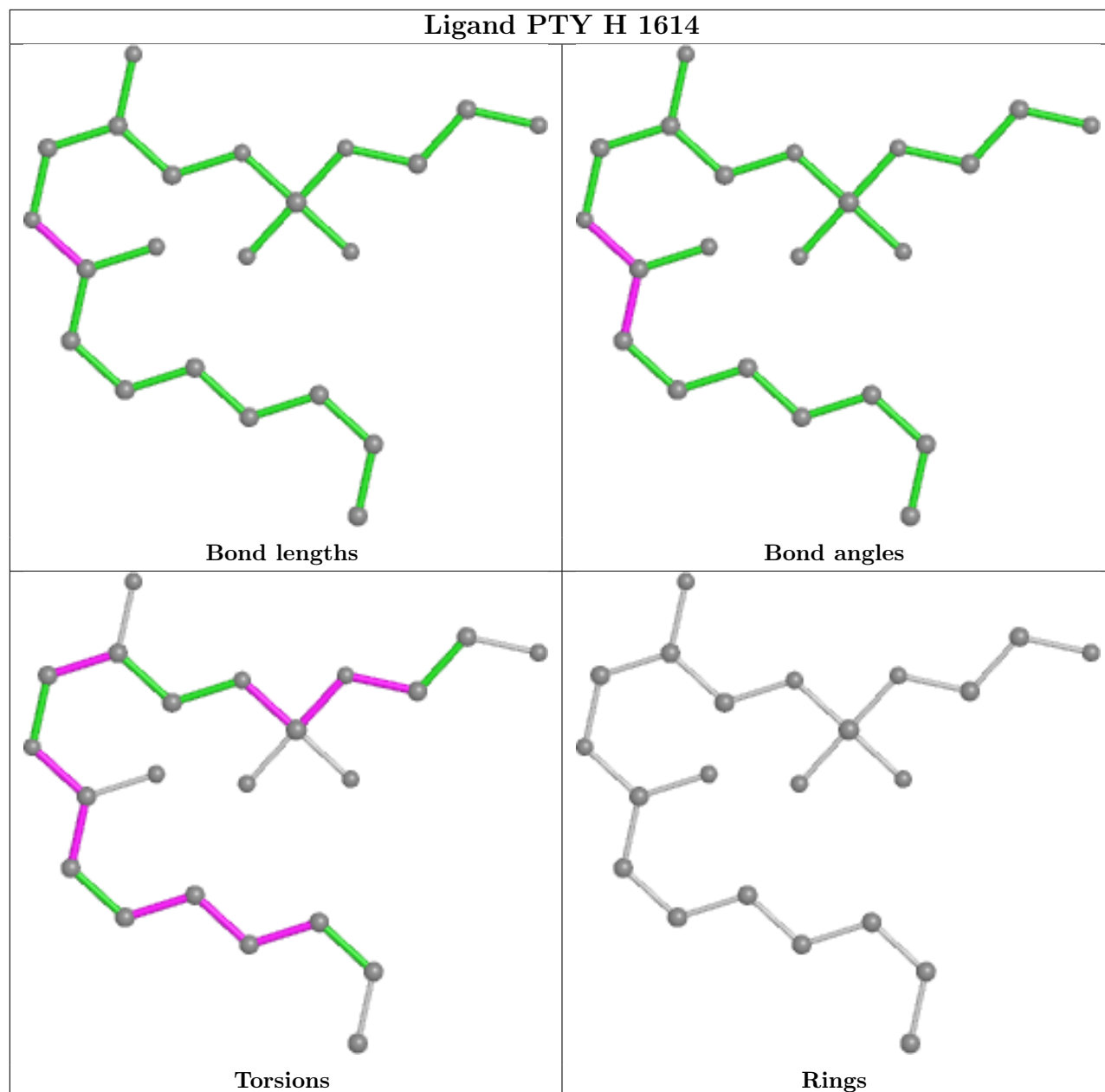


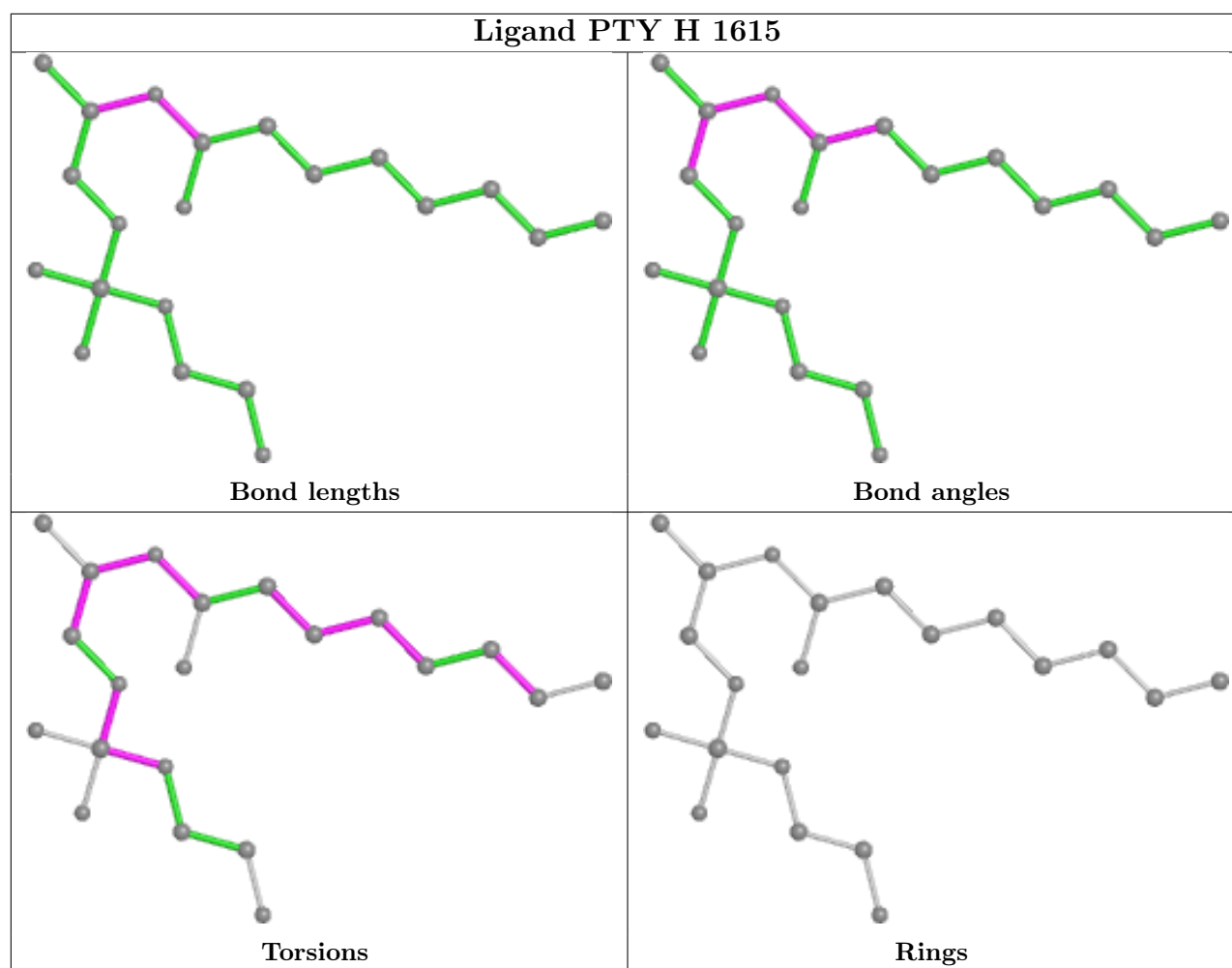
Ligand POV H 1611





Ligand PTY H 1614





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.