



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 27, 2026 – 07:01 PM UTC

PDB ID : 7RSE / pdb_00007rse
BMRB ID : 30734
Title : NMR-driven structure of the KRAS4B-G12D "alpha-beta" dimer on a lipid bilayer nanodisc
Authors : Lee, K.; Enomoto, M.; Gebregiworgis, T.; Gasmi-Seabrook, G.M.; Ikura, M.; Marshall, C.B.
Deposited on : 2021-08-11

This is a wwPDB NMR Structure Validation Summary 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

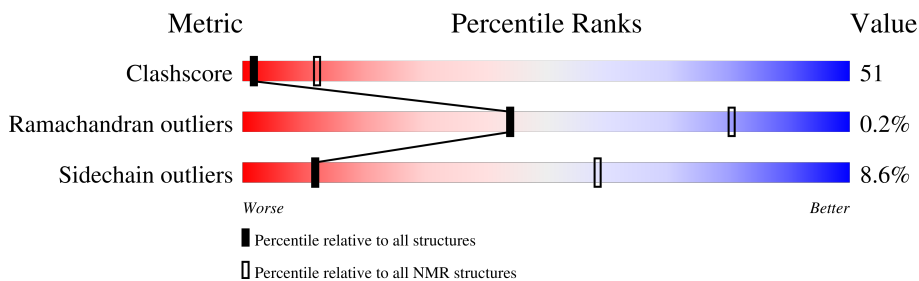
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 1%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	185	83% 10% 6% .
1	B	185	78% 10% 11% .
2	D	200	86% 8% 6%
2	E	200	82% 11% 6%

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:173, B:2-B:28, B:35-B:169 (334)	1.45	20
2	D:255-D:441, E:555-E:741 (374)	0.40	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	2, 4, 6, 9, 10, 11, 12, 14, 15, 17, 18, 19, 20
2	1, 3, 7, 8, 16
Single-model clusters	5; 13

3 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14322 atoms, of which 1540 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
1	A	183	Total	C	H	N	O	S	0
			1822	917	356	255	287	7	
1	B	183	Total	C	H	N	O	S	0
			1822	917	356	255	287	7	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P01116
A	12	ASP	GLY	engineered mutation	UNP P01116
B	1	SER	-	expression tag	UNP P01116
B	12	ASP	GLY	engineered mutation	UNP P01116

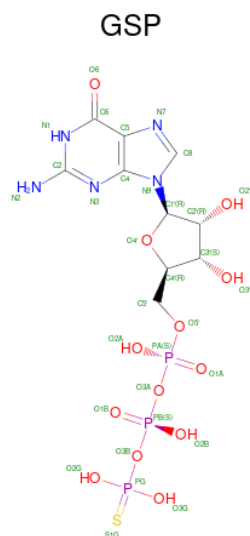
- Molecule 2 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
2	D	187	Total	C	H	N	O	S	0
			1892	960	360	273	296	3	
2	E	187	Total	C	H	N	O	S	0
			1892	960	360	273	296	3	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	242	GLY	-	expression tag	UNP P02647
D	243	PRO	-	expression tag	UNP P02647
E	542	GLY	-	expression tag	UNP P02647
E	543	PRO	-	expression tag	UNP P02647

- Molecule 3 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S) (labeled as "Ligand of Interest" by depositor).

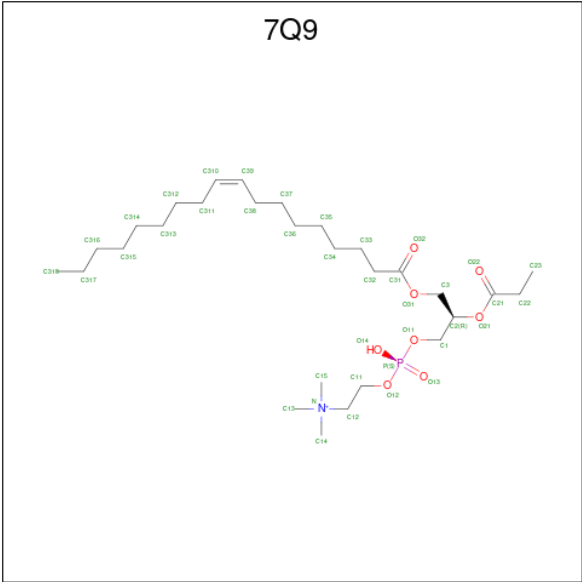


Mol	Chain	Residues	Atoms						
3	A	1	Total 38	C 10	H 6	N 5	O 13	P 3	S 1
3	B	1	Total 38	C 10	H 6	N 5	O 13	P 3	S 1

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	
4	A	1	Total 1	Mg 1
4	B	1	Total 1	Mg 1

- Molecule 5 is [(2 {R})-3-[oxidanyl-2-(trimethyl- $\text{I}^{\{4\}}$ -azanyl)ethoxy]phosphoryl]oxy-2-propionyloxy-propyl] ({Z})-octadec-9-enoate (CCD ID: 7Q9) (formula: $\text{C}_{29}\text{H}_{57}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1
5	D	1	Total	C	N	O	P
			39	29	1	8	1

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
5	D	1	Total 39	29	1	8	1
5	D	1	Total 39	29	1	8	1
5	D	1	Total 39	29	1	8	1
5	D	1	Total 39	29	1	8	1
5	D	1	Total 39	29	1	8	1
5	D	1	Total 39	29	1	8	1
5	D	1	Total 39	29	1	8	1
5	D	1	Total 39	29	1	8	1
5	D	1	Total 39	29	1	8	1
5	D	1	Total 39	29	1	8	1
5	D	1	Total 39	29	1	8	1
5	E	1	Total 39	29	1	8	1
5	E	1	Total 39	29	1	8	1
5	E	1	Total 39	29	1	8	1
5	E	1	Total 39	29	1	8	1
5	E	1	Total 39	29	1	8	1
5	E	1	Total 39	29	1	8	1
5	E	1	Total 39	29	1	8	1
5	E	1	Total 39	29	1	8	1
5	E	1	Total 39	29	1	8	1
5	E	1	Total 39	29	1	8	1
5	E	1	Total 39	29	1	8	1
5	E	1	Total 39	29	1	8	1

Continued on next page...

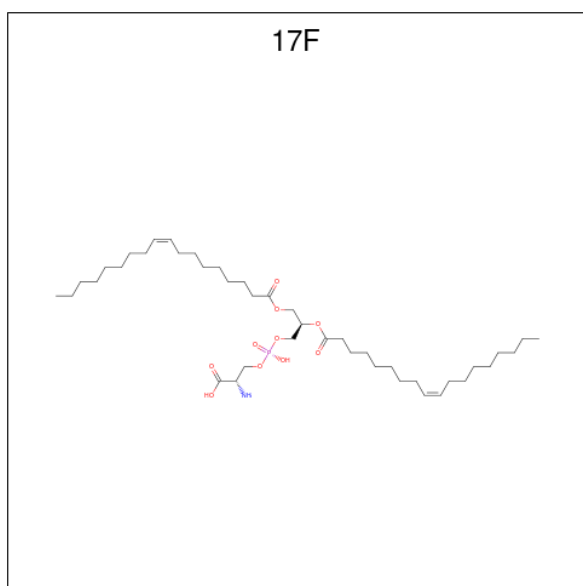
[illegible]

[illegible]

Continued from previous page...

Mol	Chain	Residues	Atoms				
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1

- Molecule 6 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (CCD ID: 17F) (formula: C₄₂H₇₈NO₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					
6	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					
6	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	B	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	B	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	B	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	B	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1

Continued on next page...

Continued from previous page...

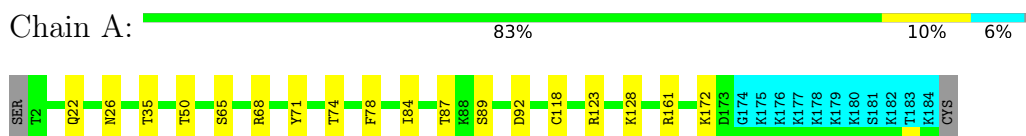
Mol	Chain	Residues	Atoms					
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1

4 Residue-property plots [i](#)

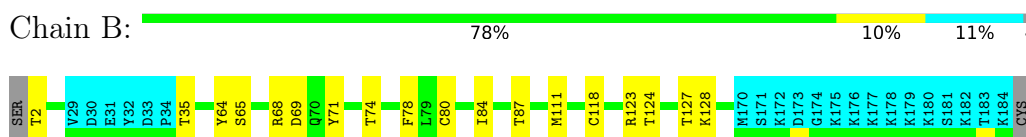
4.1 Average score per residue in the NMR ensemble

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.

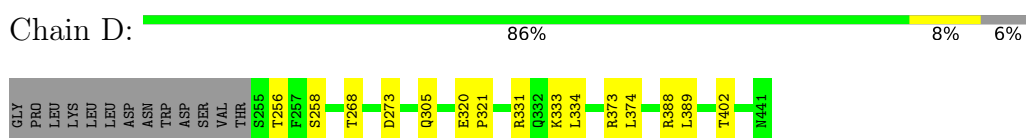
- Molecule 1: GTPase KRas



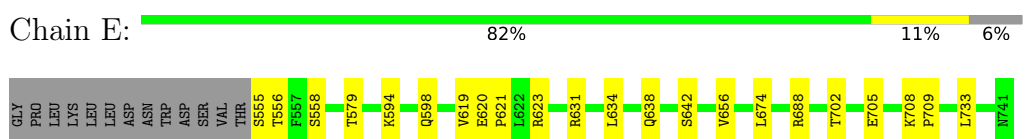
- Molecule 1: GTPase KRas



- Molecule 2: Apolipoprotein A-I



- Molecule 2: Apolipoprotein A-I

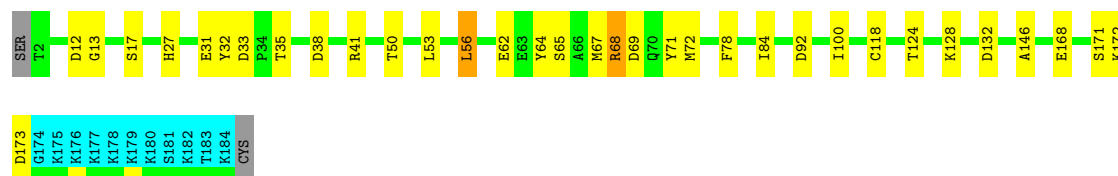


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

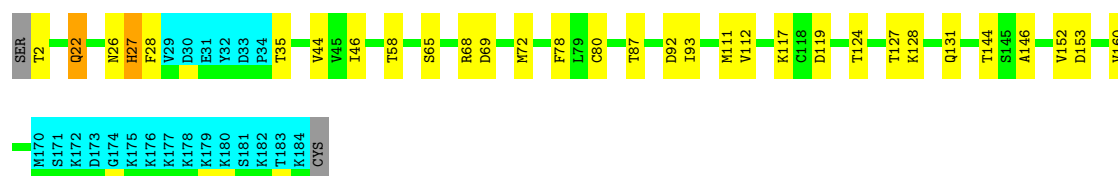
- Molecule 1: GTPase KRas

Chain A:  75% 17% • 6% •



- Molecule 1: GTPase KRas

Chain B:  71% 16% • 11% •



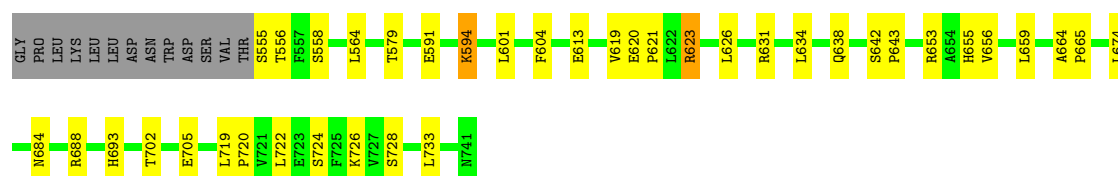
- Molecule 2: Apolipoprotein A-I

Chain D:  80% 12% • 6% •



- Molecule 2: Apolipoprotein A-I

Chain E:  74% 18% • 6% •



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
HADDOCK	refinement	
HADDOCK	structure calculation	

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	154
Number of shifts mapped to atoms	61
Number of unparsed shifts	0
Number of shifts with mapping errors	93
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

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: 7Q9, MG, 17F, GSP

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	0.35±0.01	0±0/1399 (0.0± 0.0%)	0.72±0.01	0±0/1887 (0.0± 0.0%)
1	B	0.35±0.01	0±0/1315 (0.0± 0.0%)	0.71±0.01	0±0/1773 (0.0± 0.0%)
2	D	0.37±0.00	0±0/1557 (0.0± 0.0%)	0.74±0.01	0±0/2090 (0.0± 0.0%)
2	E	0.37±0.01	0±0/1557 (0.0± 0.0%)	0.74±0.01	0±0/2090 (0.0± 0.0%)
All	All	0.36	0/116560 (0.0%)	0.73	1/156800 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	36	ILE	N-CA-C	-5.16	107.54	111.62	19	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
1	A	1377	319	1353	14±4
1	B	1295	305	1282	12±4
2	D	1532	360	1535	19±5
2	E	1532	360	1535	23±5
3	A	32	6	12	6±2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes
3	B	32	6	12	4±3
4	A	1	0	0	1±0
4	B	1	0	0	0±1
5	A	507	0	0	53±8
5	B	546	0	0	74±8
5	D	1521	0	0	172±16
5	E	2418	0	0	294±30
6	A	108	6	152	39±6
6	B	216	12	304	65±9
6	D	540	30	760	213±19
6	E	864	48	1216	253±58
All	All	250440	29040	163227	20932

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 51.

5 of 5875 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:C9	6:D:516:17F:H9	1.24	1.62	17	14
6:D:510:17F:H9A	6:D:516:17F:C9	1.21	1.66	19	15
6:D:510:17F:C9	6:D:516:17F:H8A	1.19	1.67	12	5
6:D:516:17F:H47	6:D:516:17F:C22	1.17	1.68	5	1
6:D:510:17F:H19	6:D:527:17F:C19	1.16	1.70	1	6

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	171/185 (92%)	160±2 (93±1%)	10±2 (6±1%)	1±1 (0±1%)	31	76
1	B	161/185 (87%)	152±2 (95±1%)	9±2 (5±1%)	0±0 (0±0%)	49	83
2	D	185/200 (92%)	181±1 (98±1%)	4±1 (2±1%)	0±0 (0±0%)	44	80
2	E	185/200 (92%)	180±2 (97±1%)	4±2 (2±1%)	0±1 (0±0%)	49	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	14040/15400 (91%)	13467 (96%)	543 (4%)	30 (0%)	44 80

5 of 20 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	36	ILE	4
2	D	419	LEU	3
1	A	173	ASP	2
2	E	598	GLN	2
2	E	718	LEU	2

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	153/165 (93%)	138±3 (90±2%)	15±3 (10±2%)	10 55
1	B	143/165 (87%)	128±2 (90±2%)	15±2 (10±2%)	9 52
2	D	163/175 (93%)	151±3 (93±2%)	12±3 (7±2%)	15 64
2	E	163/175 (93%)	151±2 (93±1%)	12±2 (7±1%)	15 63
All	All	12440/13600 (91%)	11372 (91%)	1068 (9%)	12 58

5 of 260 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)
2	E	556	THR	18
1	B	65	SER	17
1	A	65	SER	16
2	D	258	SER	16
2	D	402	THR	16

6.3.3 RNA ⓘ

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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 164 ligands modelled in this entry, 2 are monoatomic - leaving 162 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
5	7Q9	D	513	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	834	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	866	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	805	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	E	855	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	E	843	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	839	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	831	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	206	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	514	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	862	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	812	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	D	516	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	836	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	213	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	B	214	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	827	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	203	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	523	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	830	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	849	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	B	215	-	52,53,53	0.83±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
5	7Q9	B	220	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	844	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	525	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	539	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	535	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	832	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	825	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	851	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	533	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	D	515	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	544	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	859	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	821	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	D	546	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	815	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	B	211	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	A	214	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	E	856	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	B	210	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	837	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	541	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	835	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	871	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	876	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	816	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	207	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	858	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	A	203	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	503	-	38,38,38	0.80±0.00	0±0 (0±0%)
3	GSP	B	201	4	33,34,34	1.18±0.01	1±0 (3±0%)
5	7Q9	E	813	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	877	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	212	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	861	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	828	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	E	838	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	B	218	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	521	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	A	208	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	869	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	531	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	205	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	A	217	-	38,38,38	0.80±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
5	7Q9	D	518	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	537	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	810	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	D	527	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	854	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	847	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	819	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	519	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	878	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	860	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	505	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	215	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	833	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	536	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	865	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	811	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	845	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	848	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	545	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	210	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	803	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	857	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	868	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	512	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	529	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	526	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	542	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	863	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	501	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	506	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	205	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	549	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	808	-	38,38,38	0.80±0.00	0±0 (0±0%)
3	GSP	A	201	4	33,34,34	1.17±0.01	1±0 (3±0%)
6	17F	E	818	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	540	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	509	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	804	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	508	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	842	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	824	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	809	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	B	208	-	52,53,53	0.83±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
5	7Q9	B	217	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	823	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	204	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	543	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	840	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	213	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	209	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	B	212	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	511	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	A	204	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	D	517	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	A	207	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	507	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	522	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	820	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	817	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	D	520	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	216	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	853	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	A	209	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	873	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	814	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	852	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	864	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	875	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	528	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	538	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	524	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	530	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	872	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	502	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	504	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	867	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	B	216	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	822	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	826	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	806	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	532	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	A	206	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	510	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	547	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	870	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	802	-	38,38,38	0.80±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
6	17F	E	874	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	E	807	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	E	841	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	E	829	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	D	534	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	548	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	B	219	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	846	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	801	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	A	211	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	850	-	38,38,38	0.80±0.00	0±0 (0±0%)

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
5	7Q9	D	513	-	44,46,46	1.02±0.02	4±0 (8±0%)
5	7Q9	E	834	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	E	866	-	44,46,46	0.98±0.02	3±0 (6±0%)
6	17F	E	805	-	54,60,60	1.11±0.04	4±0 (7±0%)
6	17F	E	855	-	54,60,60	1.10±0.02	4±0 (7±0%)
5	7Q9	E	843	-	44,46,46	1.02±0.02	3±0 (7±1%)
5	7Q9	E	839	-	44,46,46	1.00±0.02	3±0 (7±1%)
5	7Q9	E	831	-	44,46,46	1.00±0.02	3±0 (7±1%)
5	7Q9	B	206	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	D	514	-	44,46,46	0.99±0.02	3±0 (7±1%)
5	7Q9	E	862	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	812	-	44,46,46	1.04±0.02	4±0 (9±0%)
6	17F	D	516	-	54,60,60	1.07±0.03	4±0 (7±0%)
5	7Q9	E	836	-	44,46,46	0.99±0.02	3±0 (7±1%)
5	7Q9	A	213	-	44,46,46	1.01±0.03	3±0 (7±0%)
6	17F	B	214	-	54,60,60	1.11±0.05	4±0 (8±0%)
5	7Q9	E	827	-	44,46,46	1.03±0.02	3±0 (7±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
5	7Q9	B	203	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	D	523	-	44,46,46	1.02±0.02	3±0 (6±0%)
5	7Q9	E	830	-	44,46,46	1.01±0.02	3±0 (6±0%)
5	7Q9	E	849	-	44,46,46	1.00±0.01	3±0 (6±0%)
6	17F	B	215	-	54,60,60	1.11±0.02	4±0 (7±0%)
5	7Q9	B	220	-	44,46,46	1.01±0.01	3±0 (6±0%)
5	7Q9	E	844	-	44,46,46	1.01±0.01	3±0 (7±1%)
5	7Q9	D	525	-	44,46,46	0.97±0.02	3±0 (6±0%)
5	7Q9	D	539	-	44,46,46	0.99±0.02	3±0 (7±0%)
5	7Q9	D	535	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	832	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	E	825	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	E	851	-	44,46,46	0.98±0.02	3±0 (6±0%)
6	17F	D	533	-	54,60,60	1.12±0.03	4±0 (7±0%)
5	7Q9	D	515	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	D	544	-	44,46,46	1.01±0.01	3±0 (7±0%)
5	7Q9	E	859	-	44,46,46	1.01±0.02	3±0 (6±0%)
5	7Q9	E	821	-	44,46,46	1.05±0.02	4±0 (9±0%)
6	17F	D	546	-	54,60,60	1.12±0.03	5±0 (8±0%)
5	7Q9	E	815	-	44,46,46	0.97±0.04	3±0 (7±0%)
5	7Q9	B	211	-	44,46,46	0.99±0.03	3±0 (7±0%)
6	17F	A	214	-	54,60,60	1.12±0.02	4±0 (7±0%)
6	17F	E	856	-	54,60,60	1.17±0.05	4±0 (7±0%)
5	7Q9	B	210	-	44,46,46	1.02±0.01	4±0 (8±1%)
5	7Q9	E	837	-	44,46,46	1.03±0.03	4±0 (8±0%)
5	7Q9	D	541	-	44,46,46	0.98±0.02	3±0 (6±0%)
5	7Q9	E	835	-	44,46,46	0.97±0.02	3±0 (6±0%)
5	7Q9	E	871	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	E	876	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	E	816	-	44,46,46	0.98±0.03	3±0 (7±0%)
5	7Q9	B	207	-	44,46,46	0.99±0.02	3±0 (7±1%)
5	7Q9	E	858	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	A	203	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	D	503	-	44,46,46	1.01±0.02	3±0 (7±1%)
3	GSP	B	201	4	47,54,54	1.72±0.03	11±1 (23±1%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
5	7Q9	E	813	-	44,46,46	1.02±0.02	3±0 (7±0%)
5	7Q9	E	877	-	44,46,46	1.00±0.02	4±0 (8±1%)
5	7Q9	A	212	-	44,46,46	0.99±0.02	3±0 (7±0%)
5	7Q9	E	861	-	44,46,46	0.99±0.02	3±0 (7±1%)
6	17F	E	828	-	54,60,60	1.09±0.02	4±0 (7±0%)
6	17F	E	838	-	54,60,60	1.12±0.04	5±0 (8±0%)
5	7Q9	B	218	-	44,46,46	0.98±0.03	3±0 (7±0%)
5	7Q9	D	521	-	44,46,46	1.00±0.02	3±0 (7±0%)
6	17F	A	208	-	54,60,60	1.09±0.03	4±0 (7±0%)
5	7Q9	E	869	-	44,46,46	1.01±0.01	4±0 (8±0%)
5	7Q9	D	531	-	44,46,46	1.00±0.03	4±0 (8±1%)
5	7Q9	A	205	-	44,46,46	1.02±0.03	3±0 (7±0%)
5	7Q9	A	217	-	44,46,46	1.00±0.01	3±0 (6±0%)
5	7Q9	D	518	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	D	537	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	E	810	-	44,46,46	1.01±0.02	3±0 (7±0%)
6	17F	D	527	-	54,60,60	1.14±0.03	4±0 (8±0%)
5	7Q9	E	854	-	44,46,46	0.99±0.01	3±0 (6±0%)
5	7Q9	E	847	-	44,46,46	1.01±0.01	3±0 (6±0%)
6	17F	E	819	-	54,60,60	1.07±0.05	4±0 (7±0%)
5	7Q9	D	519	-	44,46,46	1.01±0.02	3±1 (7±1%)
5	7Q9	E	878	-	44,46,46	1.01±0.01	3±0 (7±0%)
5	7Q9	E	860	-	44,46,46	1.02±0.02	3±0 (7±0%)
5	7Q9	D	505	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	A	215	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	E	833	-	44,46,46	0.99±0.02	4±0 (7±1%)
5	7Q9	D	536	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	E	865	-	44,46,46	1.00±0.02	3±0 (6±0%)
6	17F	E	811	-	54,60,60	1.08±0.03	4±0 (7±0%)
5	7Q9	E	845	-	44,46,46	1.02±0.02	4±0 (8±1%)
5	7Q9	E	848	-	44,46,46	1.00±0.01	3±0 (7±0%)
5	7Q9	D	545	-	44,46,46	1.02±0.02	4±0 (8±0%)
5	7Q9	A	210	-	44,46,46	0.99±0.02	3±0 (7±0%)
5	7Q9	E	803	-	44,46,46	0.99±0.03	3±0 (7±1%)
5	7Q9	E	857	-	44,46,46	0.99±0.02	3±0 (6±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
5	7Q9	E	868	-	44,46,46	1.01±0.02	4±0 (7±1%)
5	7Q9	D	512	-	44,46,46	1.01±0.02	3±0 (6±0%)
5	7Q9	D	529	-	44,46,46	1.01±0.02	4±0 (8±1%)
5	7Q9	D	526	-	44,46,46	1.09±0.02	4±0 (9±0%)
5	7Q9	D	542	-	44,46,46	1.02±0.02	4±0 (8±0%)
5	7Q9	E	863	-	44,46,46	1.01±0.02	3±0 (7±1%)
6	17F	D	501	-	54,60,60	1.11±0.07	5±0 (8±0%)
5	7Q9	D	506	-	44,46,46	1.04±0.03	4±0 (8±1%)
5	7Q9	B	205	-	44,46,46	0.97±0.02	3±0 (7±0%)
5	7Q9	D	549	-	44,46,46	1.01±0.01	3±0 (6±0%)
5	7Q9	E	808	-	44,46,46	0.96±0.02	3±0 (6±0%)
3	GSP	A	201	4	47,54,54	1.72±0.02	11±1 (24±1%)
6	17F	E	818	-	54,60,60	1.06±0.04	4±0 (7±0%)
5	7Q9	D	540	-	44,46,46	1.03±0.01	4±0 (8±0%)
5	7Q9	D	509	-	44,46,46	1.03±0.03	4±0 (8±0%)
5	7Q9	E	804	-	44,46,46	1.01±0.02	4±0 (8±1%)
5	7Q9	D	508	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	E	842	-	44,46,46	0.98±0.02	3±0 (7±0%)
5	7Q9	E	824	-	44,46,46	0.98±0.03	3±0 (7±0%)
6	17F	E	809	-	54,60,60	1.17±0.03	5±0 (9±0%)
6	17F	B	208	-	54,60,60	1.07±0.03	4±0 (7±0%)
5	7Q9	B	217	-	44,46,46	1.02±0.02	3±0 (7±1%)
5	7Q9	E	823	-	44,46,46	1.01±0.01	3±0 (7±0%)
5	7Q9	B	204	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	D	543	-	44,46,46	1.00±0.02	3±0 (7±1%)
5	7Q9	E	840	-	44,46,46	0.96±0.03	3±0 (7±0%)
5	7Q9	B	213	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	B	209	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	B	212	-	44,46,46	1.01±0.02	4±0 (8±1%)
6	17F	D	511	-	54,60,60	1.10±0.03	4±0 (8±0%)
5	7Q9	A	204	-	44,46,46	1.01±0.03	4±0 (8±1%)
6	17F	D	517	-	54,60,60	1.12±0.03	4±0 (7±0%)
5	7Q9	A	207	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	D	507	-	44,46,46	1.02±0.02	3±0 (6±0%)
5	7Q9	D	522	-	44,46,46	1.02±0.01	4±0 (8±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
5	7Q9	E	820	-	44,46,46	1.00±0.02	3±0 (7±1%)
6	17F	E	817	-	54,60,60	1.10±0.03	4±0 (7±0%)
5	7Q9	D	520	-	44,46,46	1.04±0.02	4±0 (9±0%)
5	7Q9	A	216	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	E	853	-	44,46,46	1.01±0.01	3±0 (6±0%)
5	7Q9	A	209	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	873	-	44,46,46	0.99±0.01	3±0 (6±0%)
5	7Q9	E	814	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	852	-	44,46,46	1.03±0.02	4±0 (8±0%)
5	7Q9	E	864	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	875	-	44,46,46	0.99±0.02	3±0 (7±0%)
6	17F	D	528	-	54,60,60	1.11±0.02	5±0 (9±0%)
5	7Q9	D	538	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	D	524	-	44,46,46	0.97±0.02	3±0 (7±0%)
5	7Q9	D	530	-	44,46,46	1.00±0.02	3±0 (7±1%)
6	17F	E	872	-	54,60,60	1.16±0.02	4±0 (8±0%)
5	7Q9	D	502	-	44,46,46	1.00±0.01	3±0 (6±0%)
5	7Q9	D	504	-	44,46,46	1.01±0.03	3±0 (7±0%)
5	7Q9	E	867	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	B	216	-	44,46,46	1.01±0.03	3±0 (7±1%)
5	7Q9	E	822	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	E	826	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	E	806	-	44,46,46	1.05±0.02	4±0 (8±0%)
5	7Q9	D	532	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	A	206	-	44,46,46	1.00±0.01	3±0 (7±0%)
6	17F	D	510	-	54,60,60	1.06±0.07	4±1 (6±1%)
5	7Q9	D	547	-	44,46,46	1.01±0.03	3±0 (7±1%)
6	17F	E	870	-	54,60,60	1.13±0.02	4±0 (7±0%)
5	7Q9	E	802	-	44,46,46	1.03±0.02	3±0 (7±0%)
6	17F	E	874	-	54,60,60	1.12±0.02	5±0 (8±0%)
6	17F	E	807	-	54,60,60	1.10±0.02	4±0 (8±0%)
6	17F	E	841	-	54,60,60	1.11±0.02	4±0 (7±0%)
5	7Q9	E	829	-	44,46,46	0.99±0.02	4±0 (7±1%)
6	17F	D	534	-	54,60,60	1.14±0.02	4±0 (8±0%)
5	7Q9	D	548	-	44,46,46	0.99±0.03	3±0 (6±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
6	17F	B	219	-	54,60,60	1.15±0.04	5±0 (8±0%)
5	7Q9	E	846	-	44,46,46	1.03±0.01	4±0 (8±1%)
6	17F	E	801	-	54,60,60	1.13±0.04	4±0 (7±0%)
5	7Q9	A	211	-	44,46,46	1.03±0.02	4±0 (8±1%)
5	7Q9	E	850	-	44,46,46	1.00±0.02	3±0 (7±1%)

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
6	17F	E	855	-	-	0±0,59,59,59	-
5	7Q9	E	843	-	-	0±0,42,42,42	-
5	7Q9	B	203	-	-	0±0,42,42,42	-
5	7Q9	B	206	-	-	0±0,42,42,42	-
5	7Q9	B	218	-	-	0±0,42,42,42	-
5	7Q9	D	521	-	-	0±0,42,42,42	-
5	7Q9	D	519	-	-	0±0,42,42,42	-
6	17F	E	838	-	-	0±0,59,59,59	-
5	7Q9	D	545	-	-	0±0,42,42,42	-
6	17F	D	516	-	-	0±0,59,59,59	-
5	7Q9	B	209	-	-	0±0,42,42,42	-
5	7Q9	E	853	-	-	0±0,42,42,42	-
5	7Q9	A	209	-	-	0±0,42,42,42	-
5	7Q9	A	216	-	-	0±0,42,42,42	-
5	7Q9	E	849	-	-	0±0,42,42,42	-
6	17F	B	214	-	-	0±0,59,59,59	-
6	17F	D	546	-	-	0±0,59,59,59	-
5	7Q9	E	822	-	-	0±0,42,42,42	-
5	7Q9	B	220	-	-	0±0,42,42,42	-
5	7Q9	E	804	-	-	0±0,42,42,42	-
6	17F	D	527	-	-	0±0,59,59,59	-
5	7Q9	D	532	-	-	0±0,42,42,42	-
6	17F	D	501	-	-	0±0,59,59,59	-
5	7Q9	E	842	-	-	0±0,42,42,42	-
5	7Q9	B	210	-	-	0±0,42,42,42	-
5	7Q9	A	207	-	-	0±0,42,42,42	-
5	7Q9	E	861	-	-	0±0,42,42,42	-
5	7Q9	D	505	-	-	0±0,42,42,42	-
5	7Q9	D	504	-	-	0±0,42,42,42	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	17F	E	807	-	-	0±0,59,59,59	-
5	7Q9	E	831	-	-	0±0,42,42,42	-
6	17F	D	528	-	-	0±0,59,59,59	-
5	7Q9	D	518	-	-	0±0,42,42,42	-
5	7Q9	E	824	-	-	0±0,42,42,42	-
5	7Q9	B	212	-	-	0±0,42,42,42	-
5	7Q9	B	217	-	-	0±0,42,42,42	-
5	7Q9	D	544	-	-	0±0,42,42,42	-
6	17F	E	819	-	-	0±0,59,59,59	-
5	7Q9	E	810	-	-	0±0,42,42,42	-
5	7Q9	E	866	-	-	0±0,42,42,42	-
5	7Q9	E	846	-	-	0±0,42,42,42	-
5	7Q9	E	878	-	-	0±0,42,42,42	-
6	17F	E	805	-	-	0±0,59,59,59	-
5	7Q9	A	204	-	-	0±0,42,42,42	-
5	7Q9	E	813	-	-	0±0,42,42,42	-
5	7Q9	E	834	-	-	0±0,42,42,42	-
5	7Q9	E	875	-	-	0±0,42,42,42	-
5	7Q9	D	507	-	-	0±0,42,42,42	-
5	7Q9	D	548	-	-	0±0,42,42,42	-
6	17F	E	809	-	-	0±0,59,59,59	-
5	7Q9	D	524	-	-	0±0,42,42,42	-
5	7Q9	D	537	-	-	0±0,42,42,42	-
5	7Q9	D	522	-	-	0±0,42,42,42	-
6	17F	E	817	-	-	0±0,59,59,59	-
5	7Q9	E	868	-	-	0±0,42,42,42	-
5	7Q9	E	871	-	-	0±0,42,42,42	-
5	7Q9	E	847	-	-	0±0,42,42,42	-
3	GSP	B	201	4	-	0±0,21,38,38	0±0,3,3,3
5	7Q9	E	820	-	-	0±0,42,42,42	-
5	7Q9	E	806	-	-	0±0,42,42,42	-
6	17F	A	208	-	-	0±0,59,59,59	-
5	7Q9	E	827	-	-	0±0,42,42,42	-
5	7Q9	B	207	-	-	0±0,42,42,42	-
6	17F	D	517	-	-	0±0,59,59,59	-
6	17F	E	841	-	-	0±0,59,59,59	-
5	7Q9	D	520	-	-	0±0,42,42,42	-
6	17F	E	811	-	-	0±0,59,59,59	-
5	7Q9	A	203	-	-	0±0,42,42,42	-
6	17F	E	870	-	-	0±0,59,59,59	-
5	7Q9	D	543	-	-	0±0,42,42,42	-
6	17F	E	801	-	-	0±0,59,59,59	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	7Q9	E	877	-	-	0±0,42,42,42	-
5	7Q9	D	542	-	-	0±0,42,42,42	-
6	17F	D	534	-	-	0±0,59,59,59	-
6	17F	E	874	-	-	0±0,59,59,59	-
5	7Q9	D	525	-	-	0±0,42,42,42	-
5	7Q9	D	514	-	-	0±0,42,42,42	-
5	7Q9	E	862	-	-	0±0,42,42,42	-
5	7Q9	D	526	-	-	0±0,42,42,42	-
5	7Q9	D	549	-	-	0±0,42,42,42	-
6	17F	E	872	-	-	0±0,59,59,59	-
5	7Q9	E	823	-	-	0±0,42,42,42	-
5	7Q9	E	852	-	-	0±0,42,42,42	-
5	7Q9	E	844	-	-	0±0,42,42,42	-
6	17F	E	856	-	-	0±0,59,59,59	-
5	7Q9	D	538	-	-	0±0,42,42,42	-
6	17F	E	818	-	-	0±0,59,59,59	-
5	7Q9	E	815	-	-	0±0,42,42,42	-
6	17F	D	511	-	-	0±0,59,59,59	-
5	7Q9	E	832	-	-	0±0,42,42,42	-
5	7Q9	D	502	-	-	0±0,42,42,42	-
3	GSP	A	201	4	-	0±0,21,38,38	0±0,3,3,3
5	7Q9	E	863	-	-	0±0,42,42,42	-
5	7Q9	D	513	-	-	0±0,42,42,42	-
5	7Q9	D	530	-	-	0±0,42,42,42	-
5	7Q9	E	851	-	-	0±0,42,42,42	-
5	7Q9	E	869	-	-	0±0,42,42,42	-
5	7Q9	E	833	-	-	0±0,42,42,42	-
5	7Q9	D	503	-	-	0±0,42,42,42	-
5	7Q9	E	835	-	-	0±0,42,42,42	-
5	7Q9	E	873	-	-	0±0,42,42,42	-
5	7Q9	E	865	-	-	0±0,42,42,42	-
6	17F	D	533	-	-	0±0,59,59,59	-
5	7Q9	E	808	-	-	0±0,42,42,42	-
5	7Q9	B	205	-	-	0±0,42,42,42	-
5	7Q9	E	816	-	-	0±0,42,42,42	-
5	7Q9	E	840	-	-	0±0,42,42,42	-
5	7Q9	D	512	-	-	0±0,42,42,42	-
5	7Q9	D	536	-	-	0±0,42,42,42	-
6	17F	D	510	-	-	0±0,59,59,59	-
5	7Q9	A	211	-	-	0±0,42,42,42	-
5	7Q9	E	830	-	-	0±0,42,42,42	-
5	7Q9	E	857	-	-	0±0,42,42,42	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	17F	B	215	-	-	0±0,59,59,59	-
5	7Q9	D	508	-	-	0±0,42,42,42	-
5	7Q9	B	216	-	-	0±0,42,42,42	-
5	7Q9	E	876	-	-	0±0,42,42,42	-
5	7Q9	B	204	-	-	0±0,42,42,42	-
5	7Q9	D	539	-	-	0±0,42,42,42	-
5	7Q9	A	217	-	-	0±0,42,42,42	-
5	7Q9	E	867	-	-	0±0,42,42,42	-
5	7Q9	A	206	-	-	0±0,42,42,42	-
5	7Q9	E	837	-	-	0±0,42,42,42	-
5	7Q9	E	845	-	-	0±0,42,42,42	-
5	7Q9	A	213	-	-	0±0,42,42,42	-
5	7Q9	E	860	-	-	0±0,42,42,42	-
5	7Q9	D	515	-	-	0±0,42,42,42	-
6	17F	B	219	-	-	0±0,59,59,59	-
5	7Q9	D	509	-	-	0±0,42,42,42	-
5	7Q9	E	839	-	-	0±0,42,42,42	-
6	17F	A	214	-	-	0±0,59,59,59	-
5	7Q9	D	535	-	-	0±0,42,42,42	-
5	7Q9	D	547	-	-	0±0,42,42,42	-
5	7Q9	A	205	-	-	0±0,42,42,42	-
5	7Q9	A	210	-	-	0±0,42,42,42	-
5	7Q9	B	213	-	-	0±0,42,42,42	-
6	17F	B	208	-	-	0±0,59,59,59	-
5	7Q9	E	859	-	-	0±0,42,42,42	-
5	7Q9	D	523	-	-	0±0,42,42,42	-
5	7Q9	E	829	-	-	0±0,42,42,42	-
5	7Q9	D	506	-	-	0±0,42,42,42	-
5	7Q9	D	529	-	-	0±0,42,42,42	-
5	7Q9	E	826	-	-	0±0,42,42,42	-
5	7Q9	E	850	-	-	0±0,42,42,42	-
5	7Q9	E	812	-	-	0±0,42,42,42	-
5	7Q9	E	825	-	-	0±0,42,42,42	-
5	7Q9	D	541	-	-	0±0,42,42,42	-
5	7Q9	E	854	-	-	0±0,42,42,42	-
5	7Q9	E	821	-	-	0±0,42,42,42	-
5	7Q9	E	858	-	-	0±0,42,42,42	-
5	7Q9	B	211	-	-	0±0,42,42,42	-
5	7Q9	A	212	-	-	0±0,42,42,42	-
5	7Q9	D	531	-	-	0±0,42,42,42	-
5	7Q9	A	215	-	-	0±0,42,42,42	-
5	7Q9	E	803	-	-	0±0,42,42,42	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	7Q9	E	836	-	-	0±0,42,42,42	-
5	7Q9	E	848	-	-	0±0,42,42,42	-
5	7Q9	E	864	-	-	0±0,42,42,42	-
5	7Q9	E	814	-	-	0±0,42,42,42	-
6	17F	E	828	-	-	0±0,59,59,59	-
5	7Q9	D	540	-	-	0±0,42,42,42	-
5	7Q9	E	802	-	-	0±0,42,42,42	-

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	B	201	GSP	C5-N7	2.99	1.33	1.39	8	20
3	A	201	GSP	C5-N7	2.98	1.33	1.39	6	20
3	B	201	GSP	PB-O3A	2.02	1.61	1.59	17	1
3	A	201	GSP	PB-O3B	2.01	1.61	1.59	15	1
3	B	201	GSP	PG-O2G	2.00	1.48	1.54	7	1

5 of 677 unique angle 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(°)	Ideal(°)	Models	
								Worst	Total
3	A	201	GSP	C2-N3-C4	5.36	121.53	112.30	14	20
3	B	201	GSP	C2-N3-C4	5.34	121.50	112.30	14	20
6	E	805	17F	O3-C1-C2	5.20	112.59	108.06	6	20
6	E	856	17F	O3-C1-C2	5.08	112.49	108.06	20	20
3	A	201	GSP	C5-C4-N3	5.01	120.42	128.39	2	20

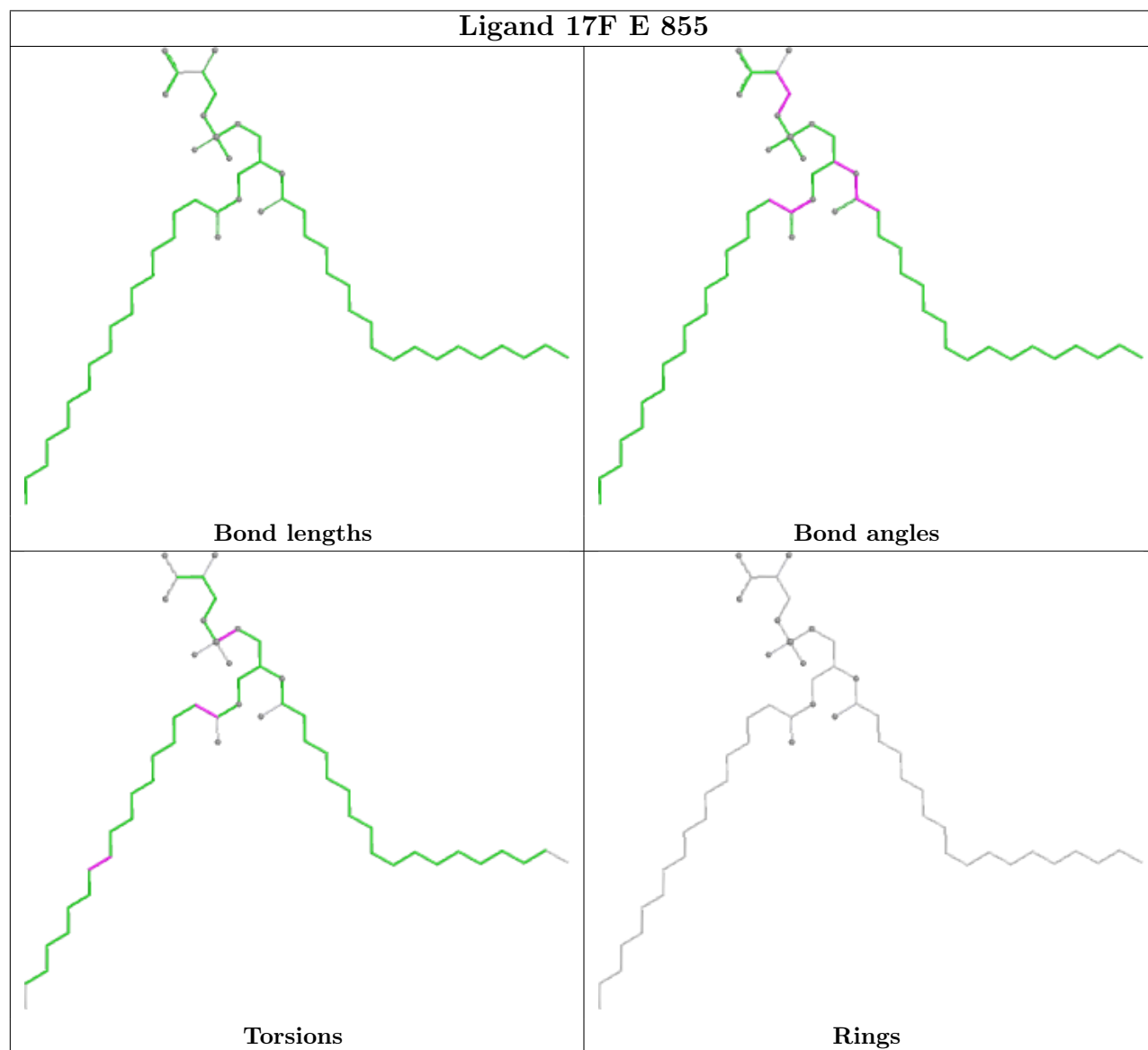
There are no chirality outliers.

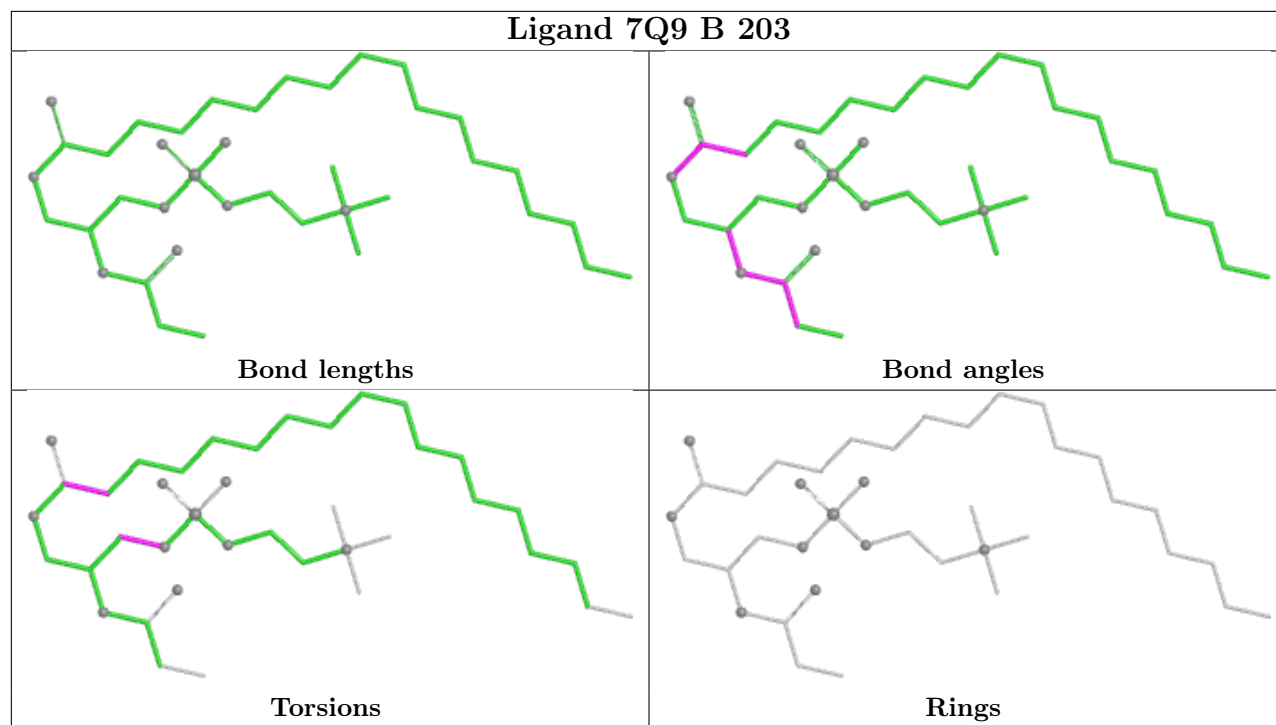
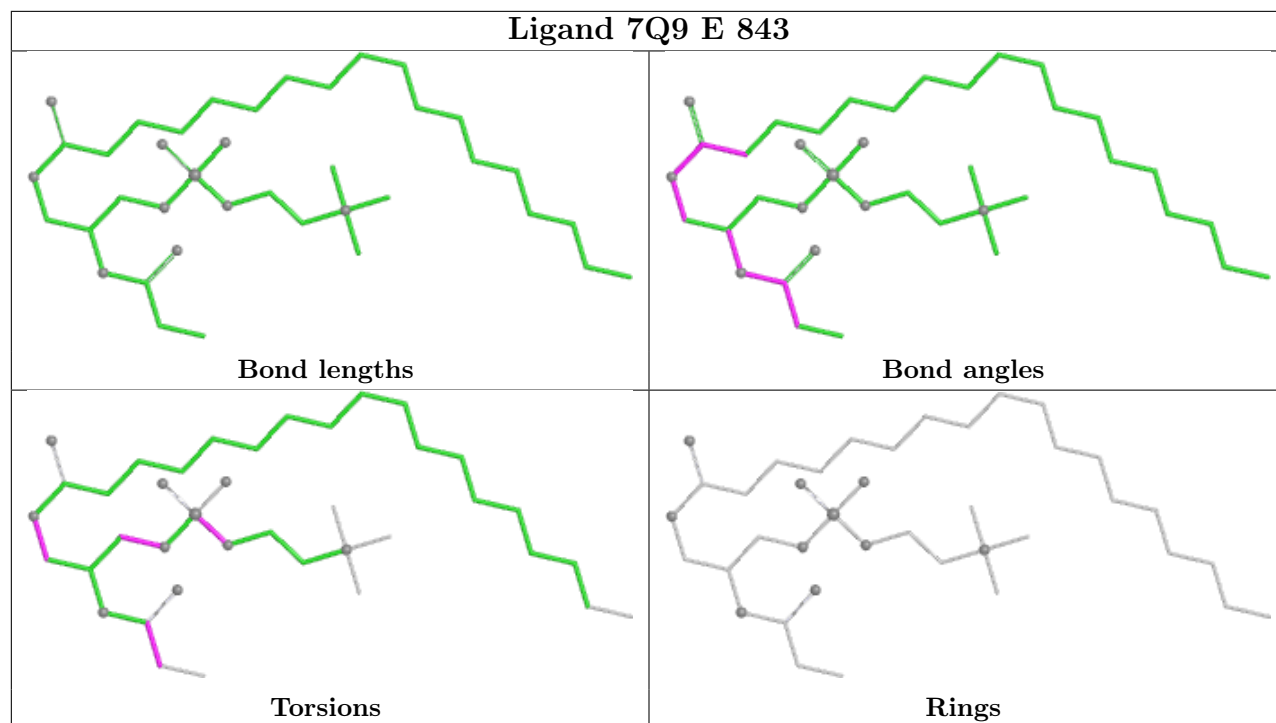
There are no torsion outliers.

There are no ring outliers.

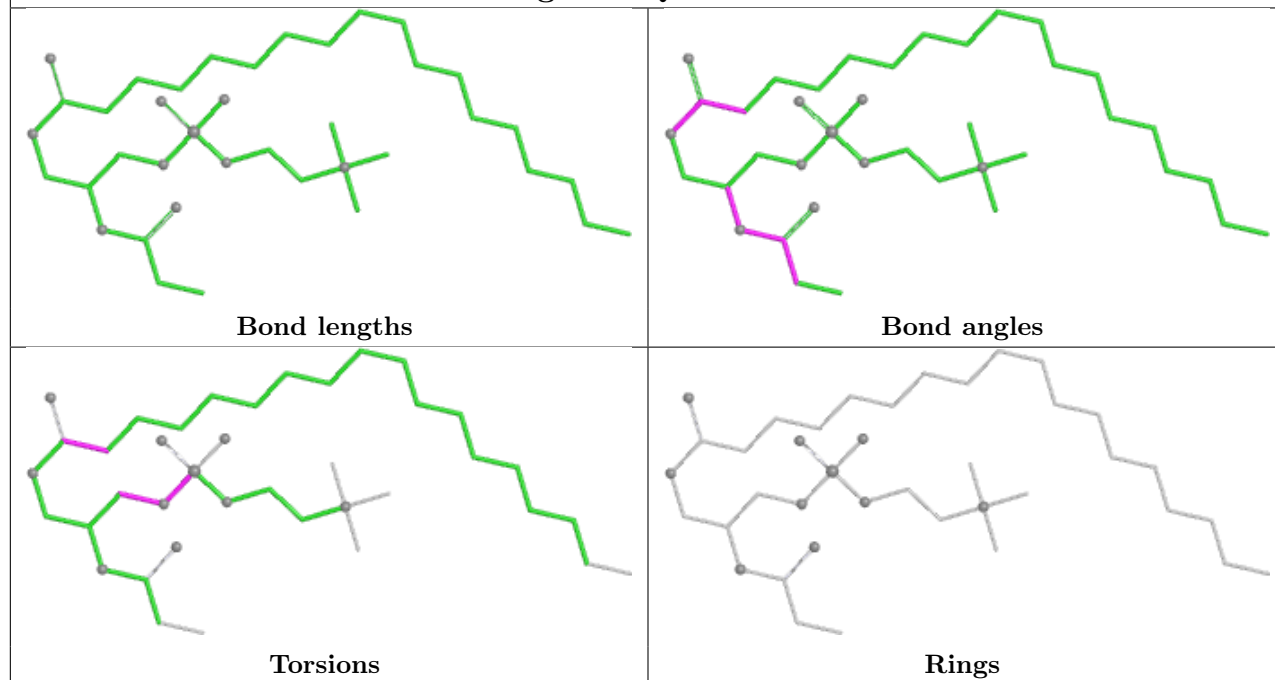
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

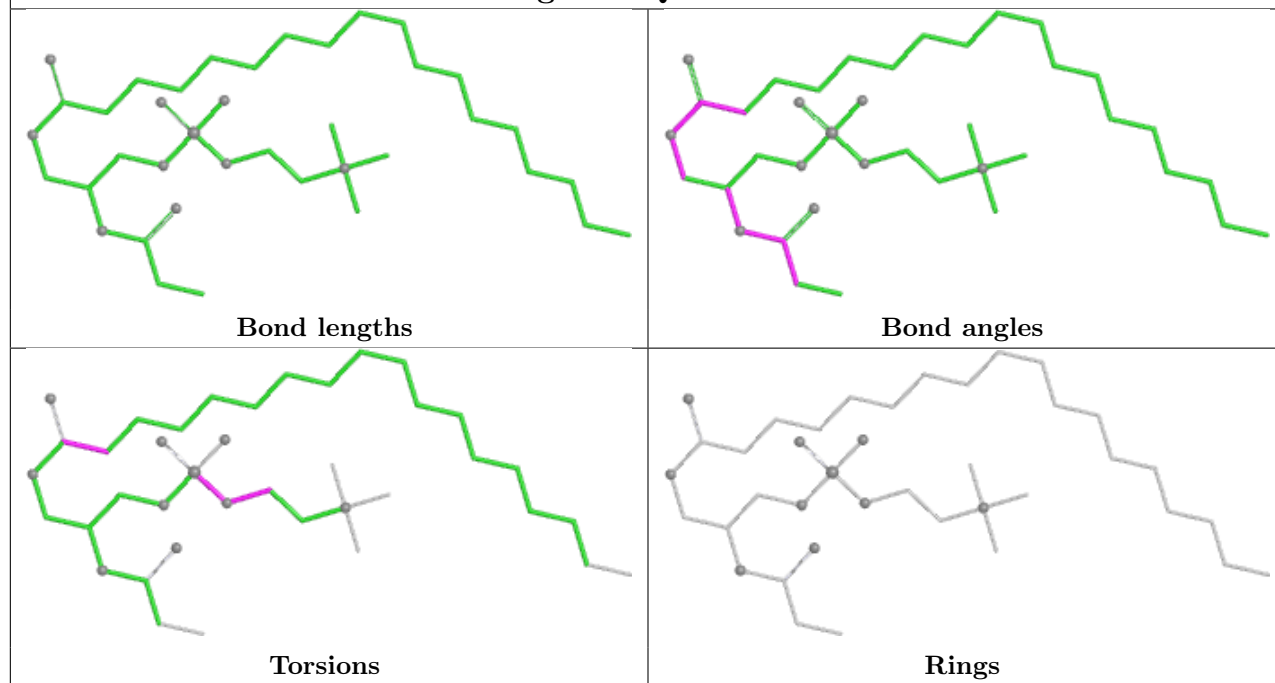


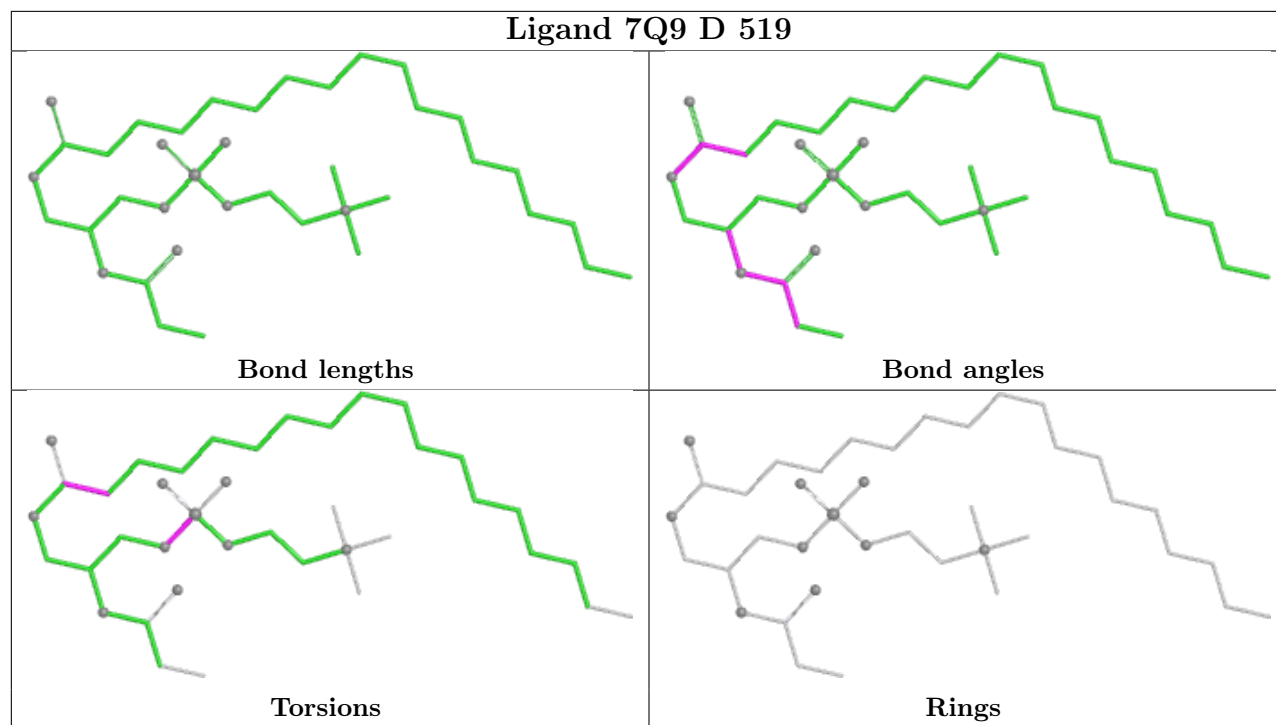
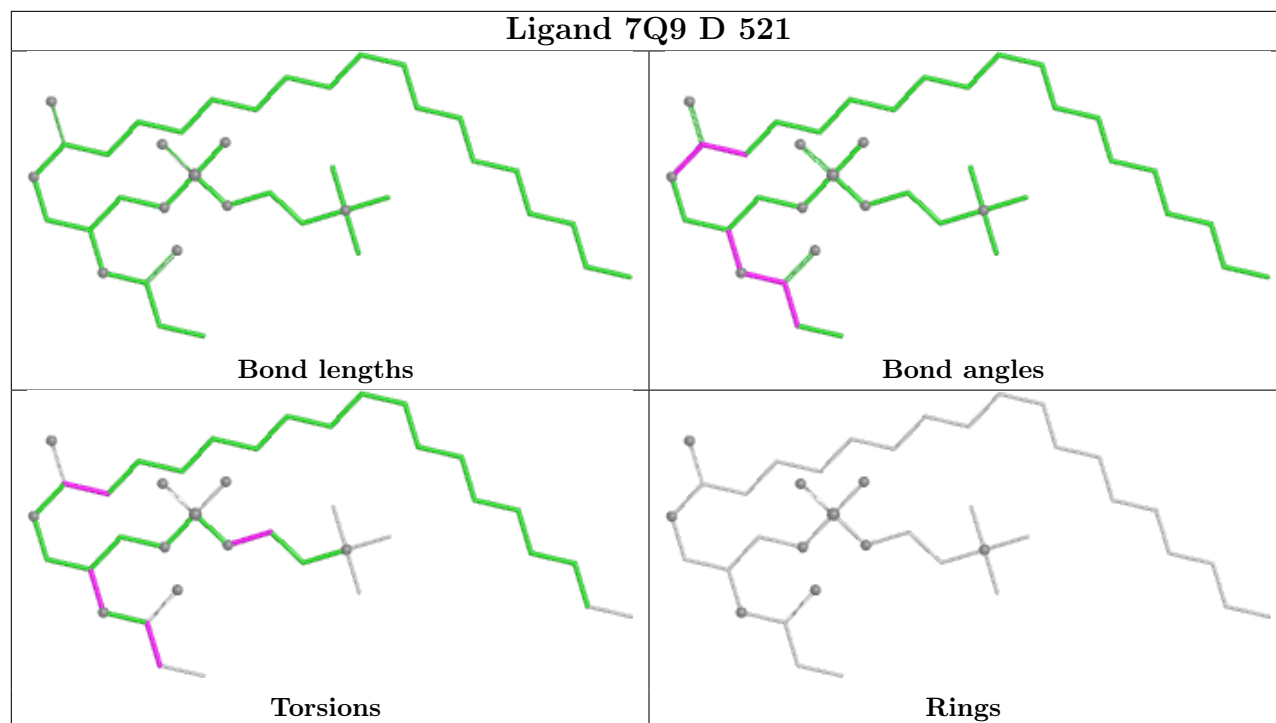


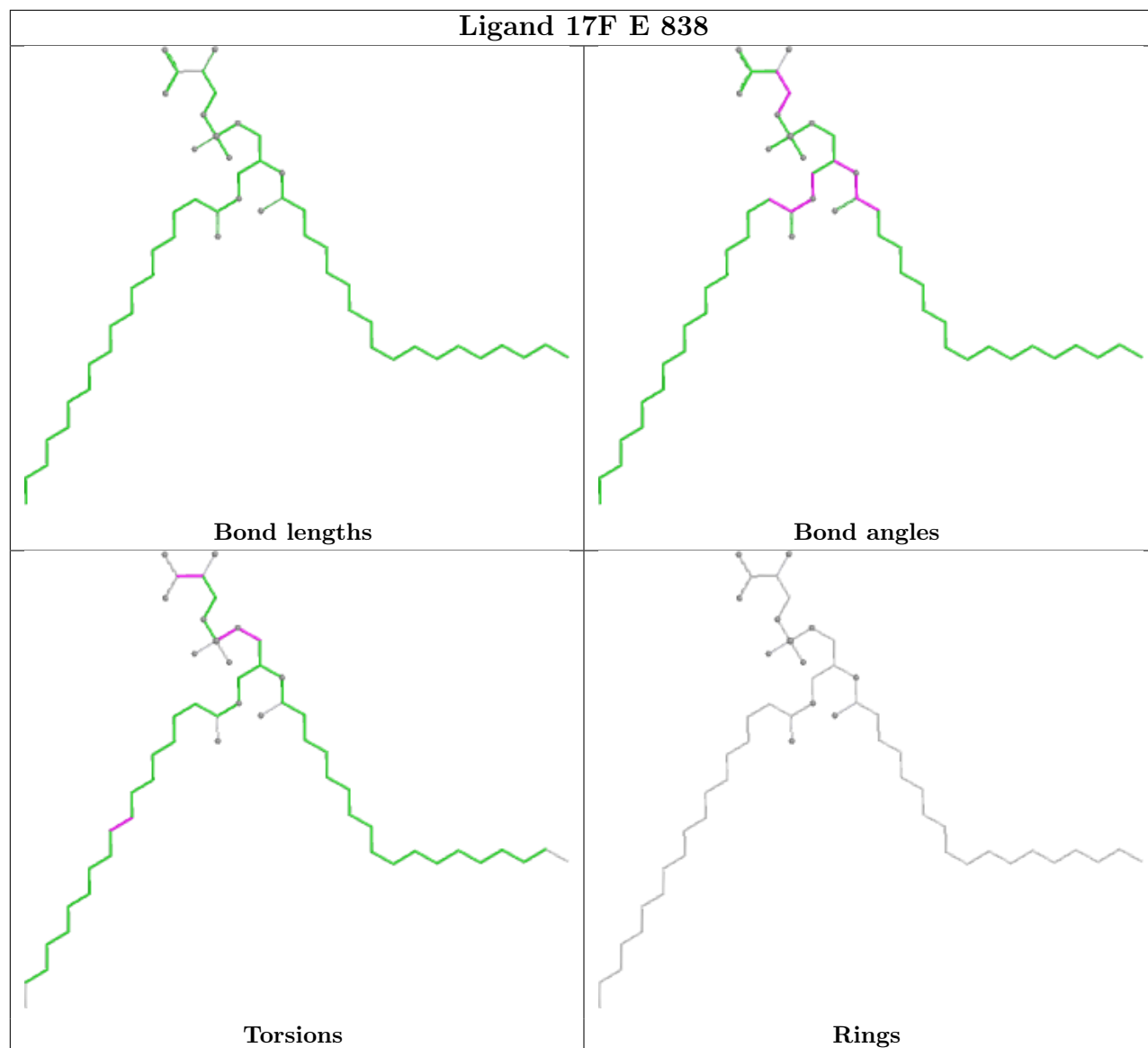
Ligand 7Q9 B 206

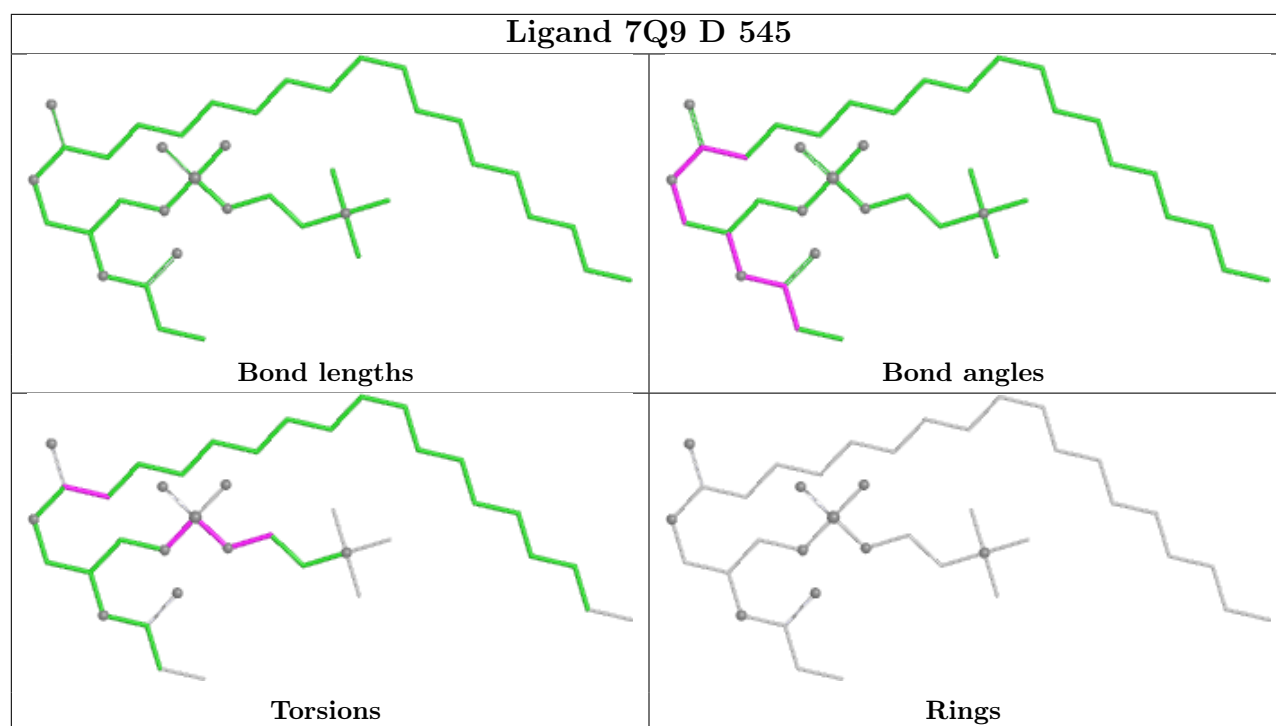


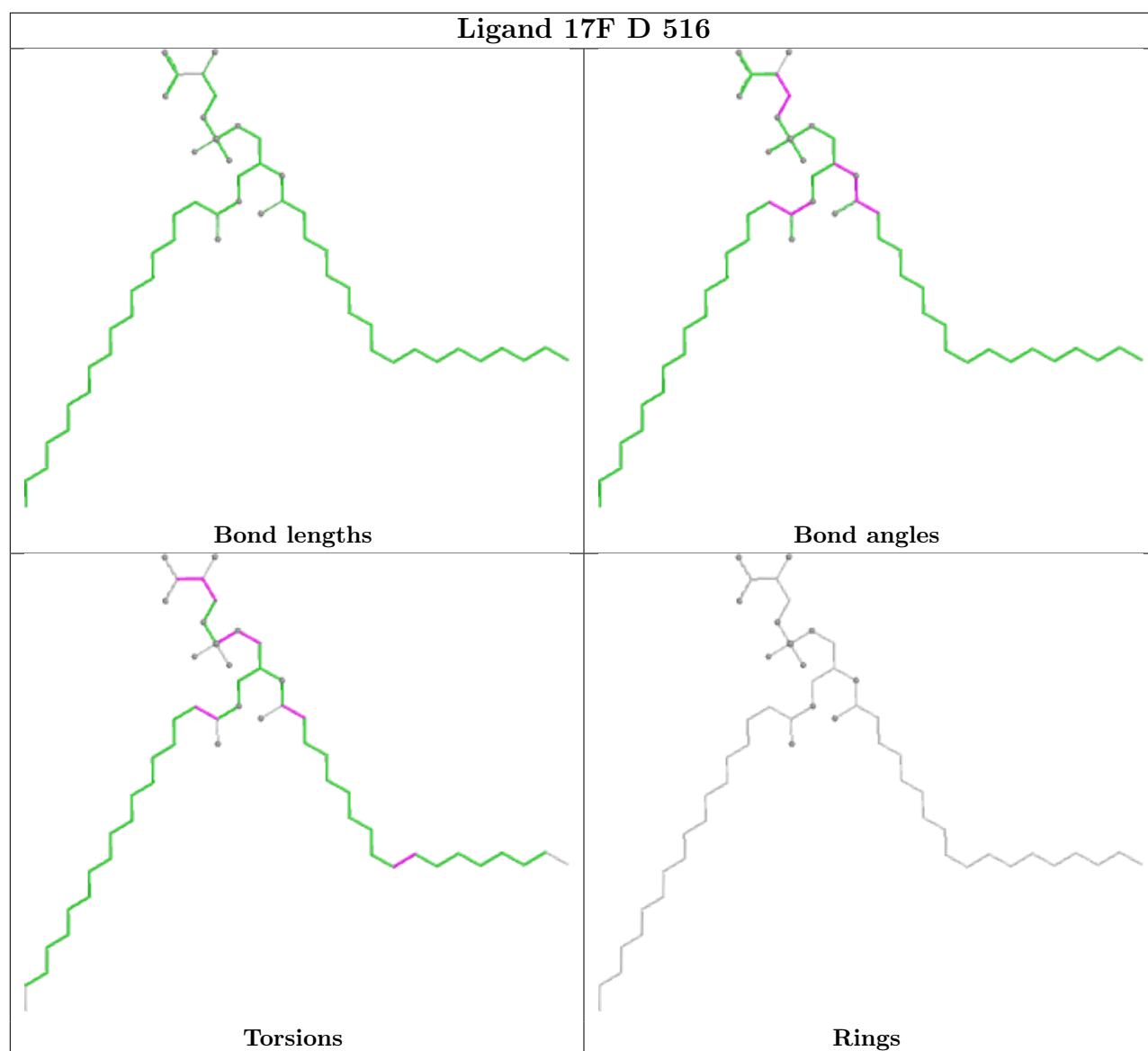
Ligand 7Q9 B 218

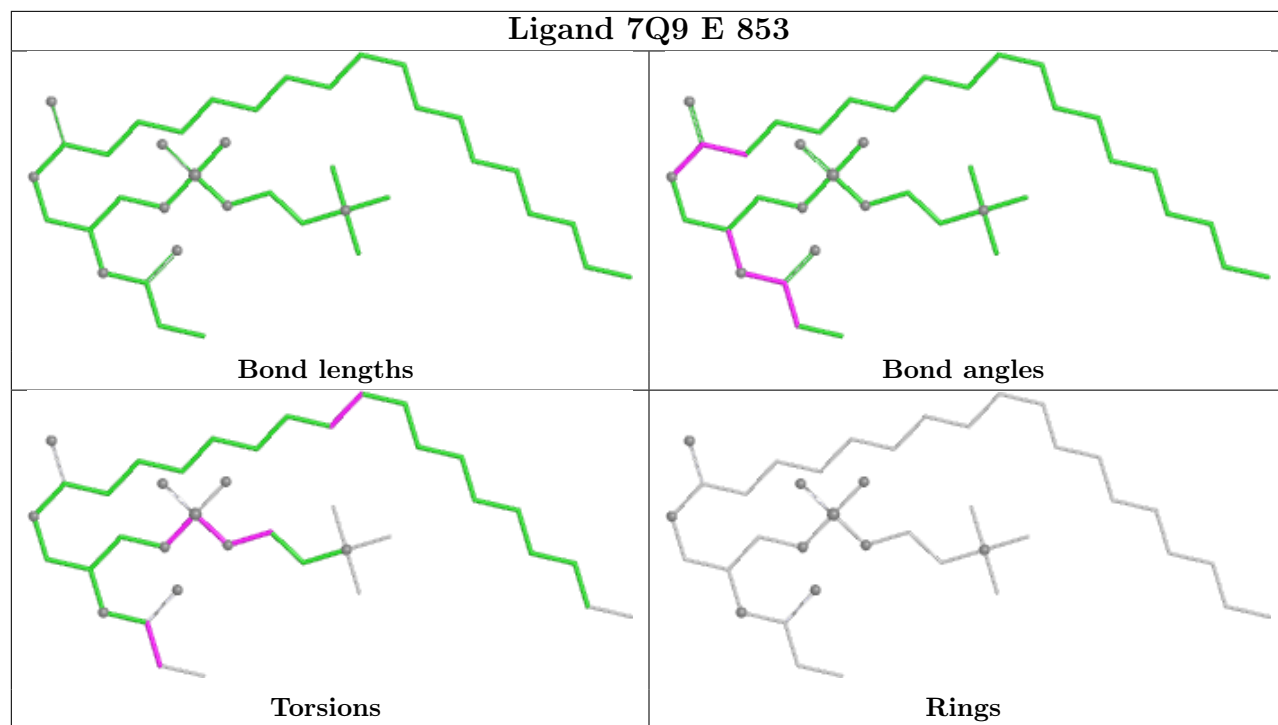
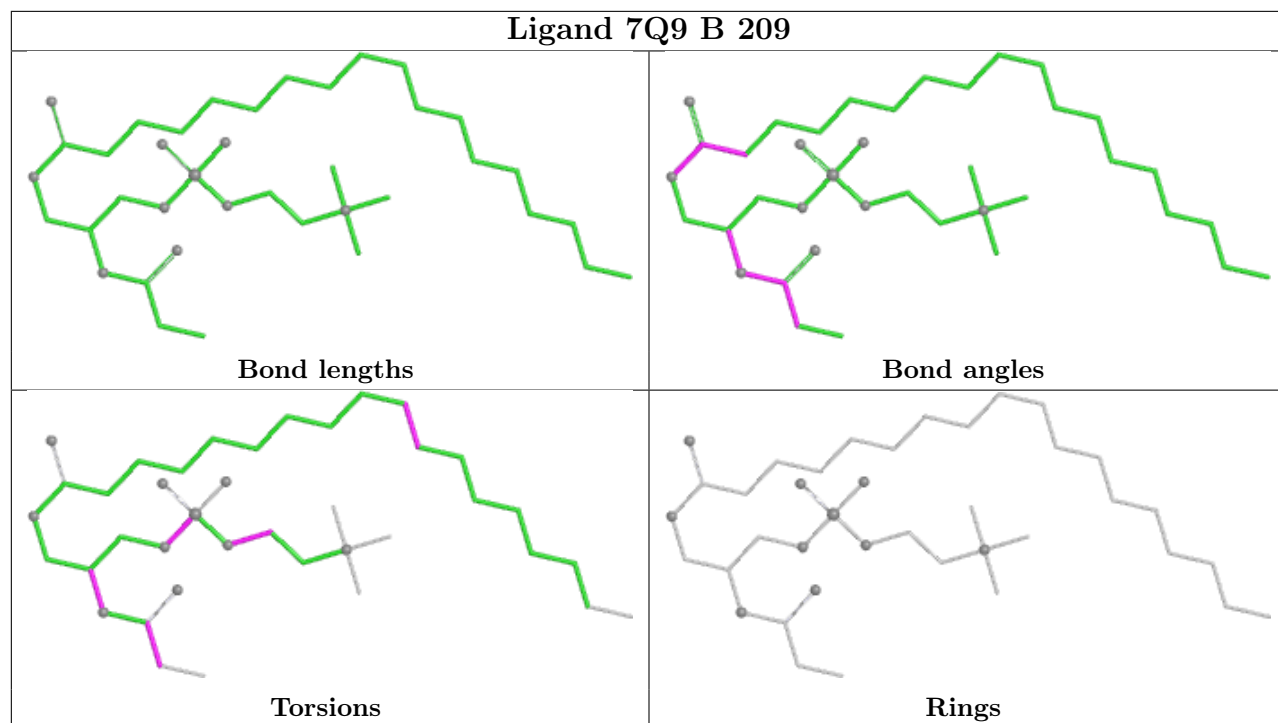


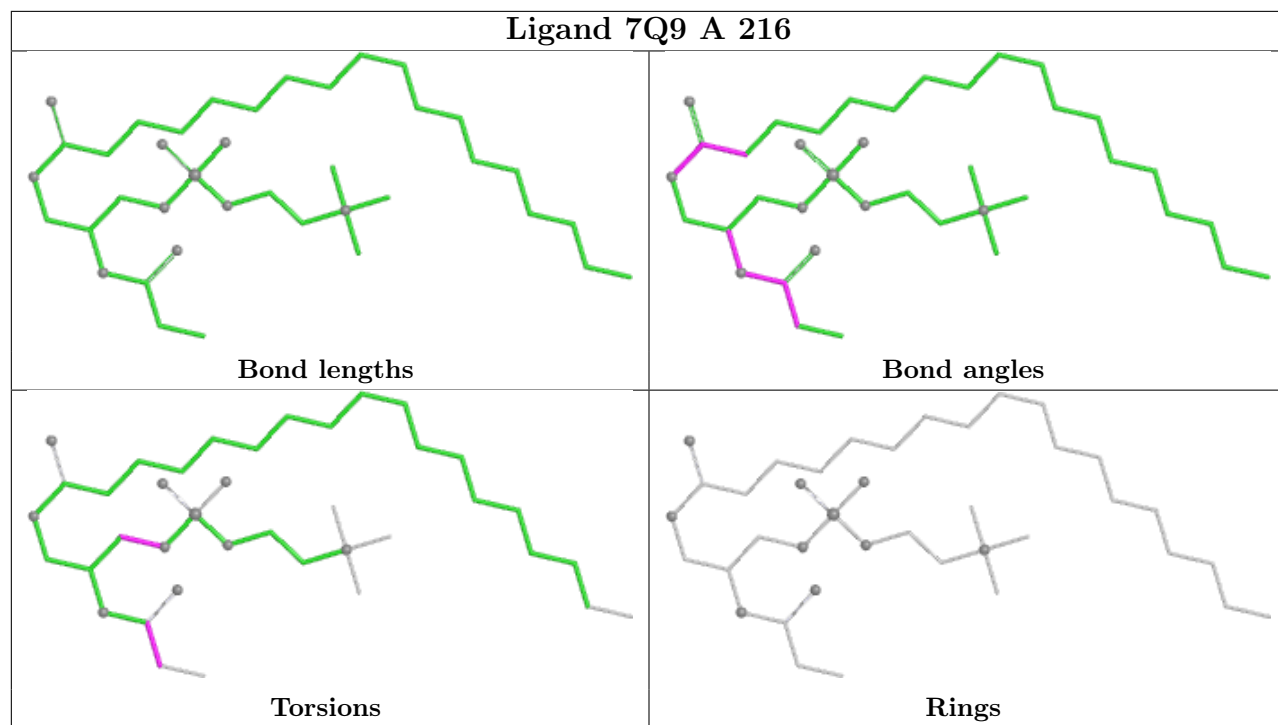
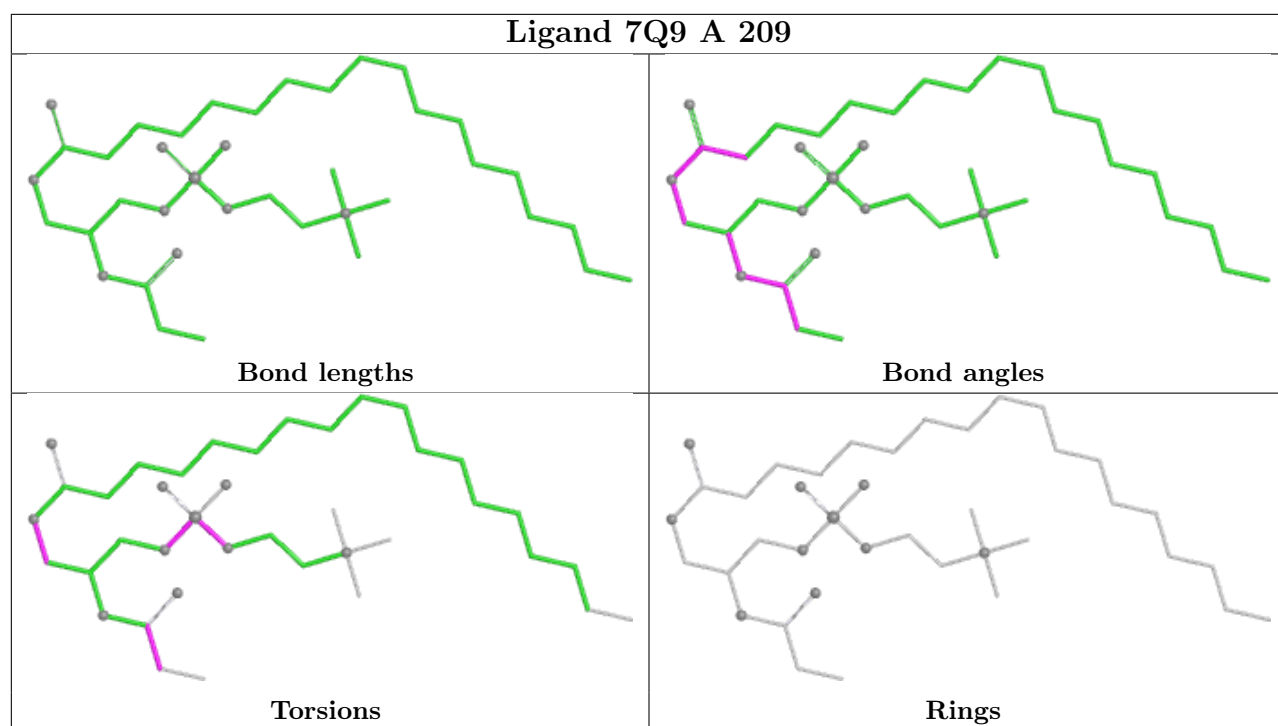


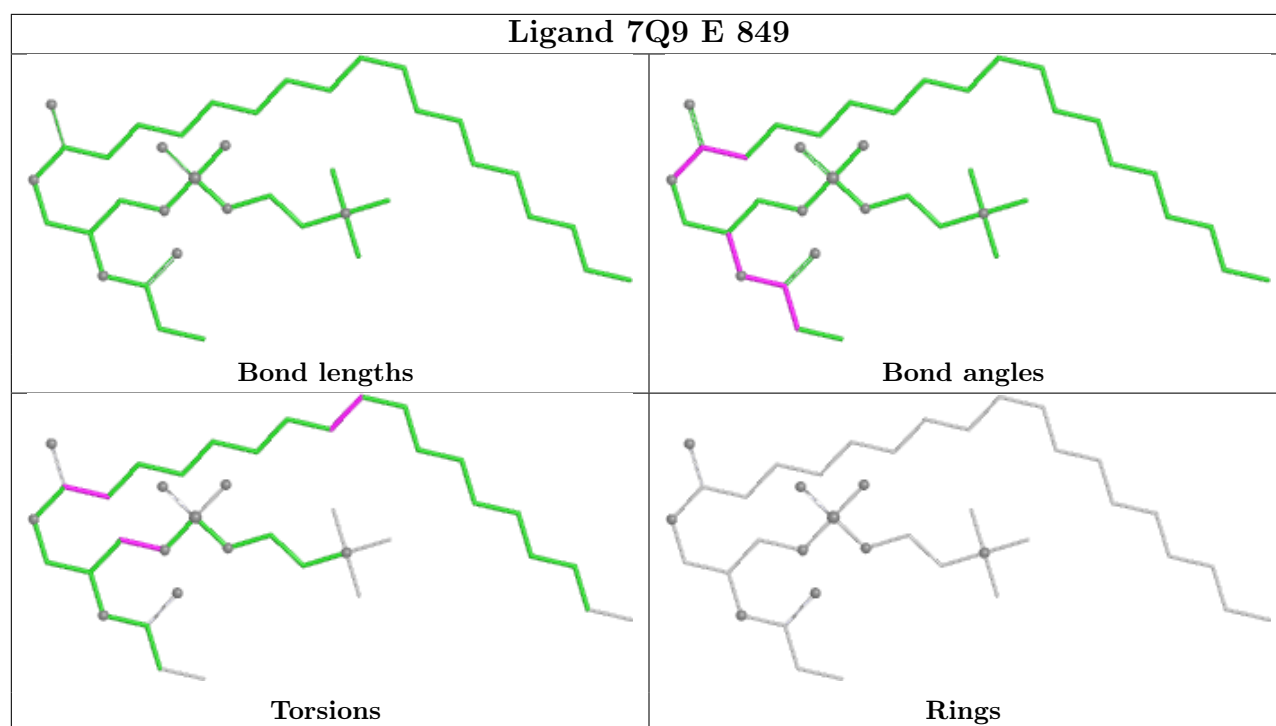




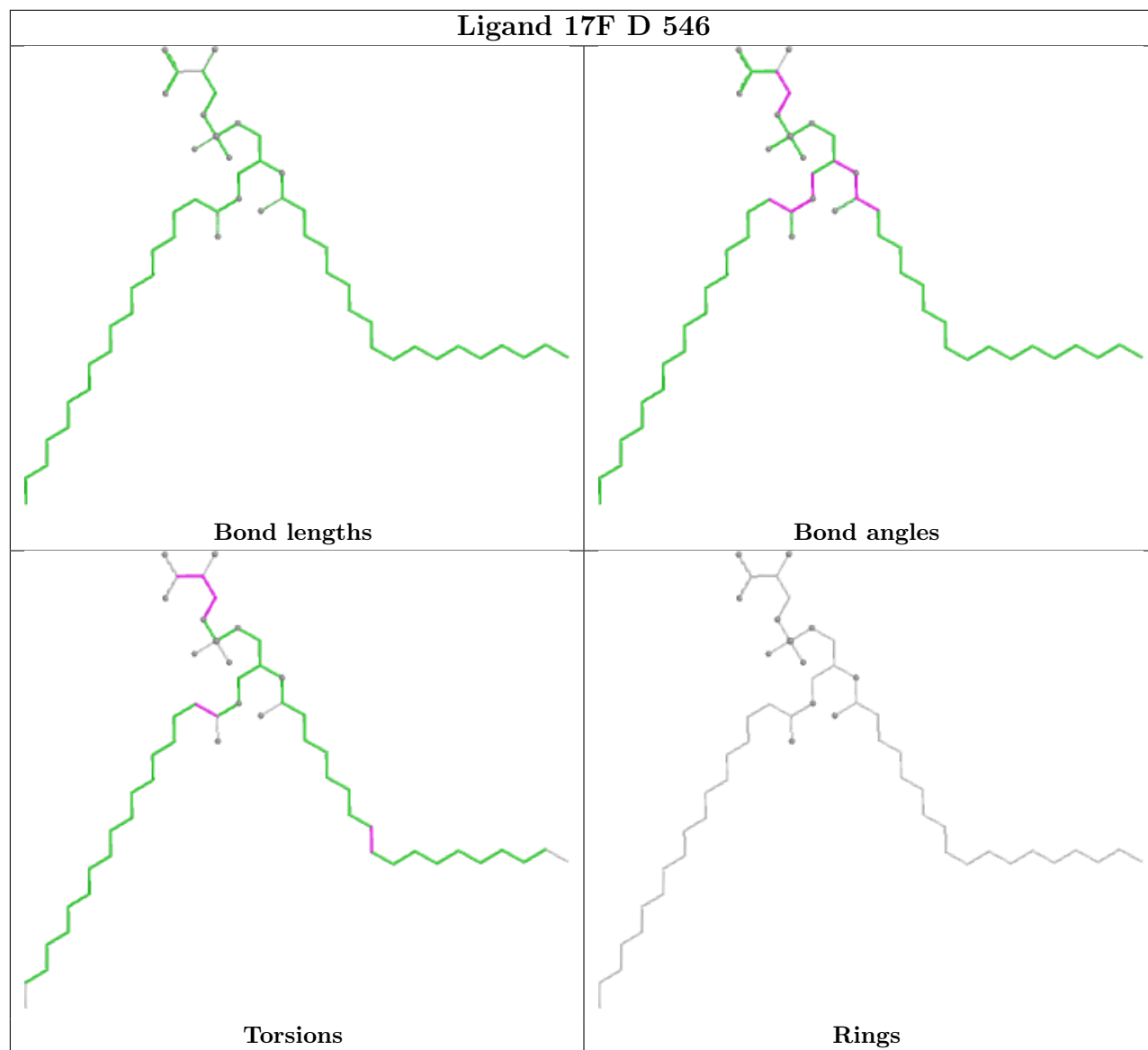


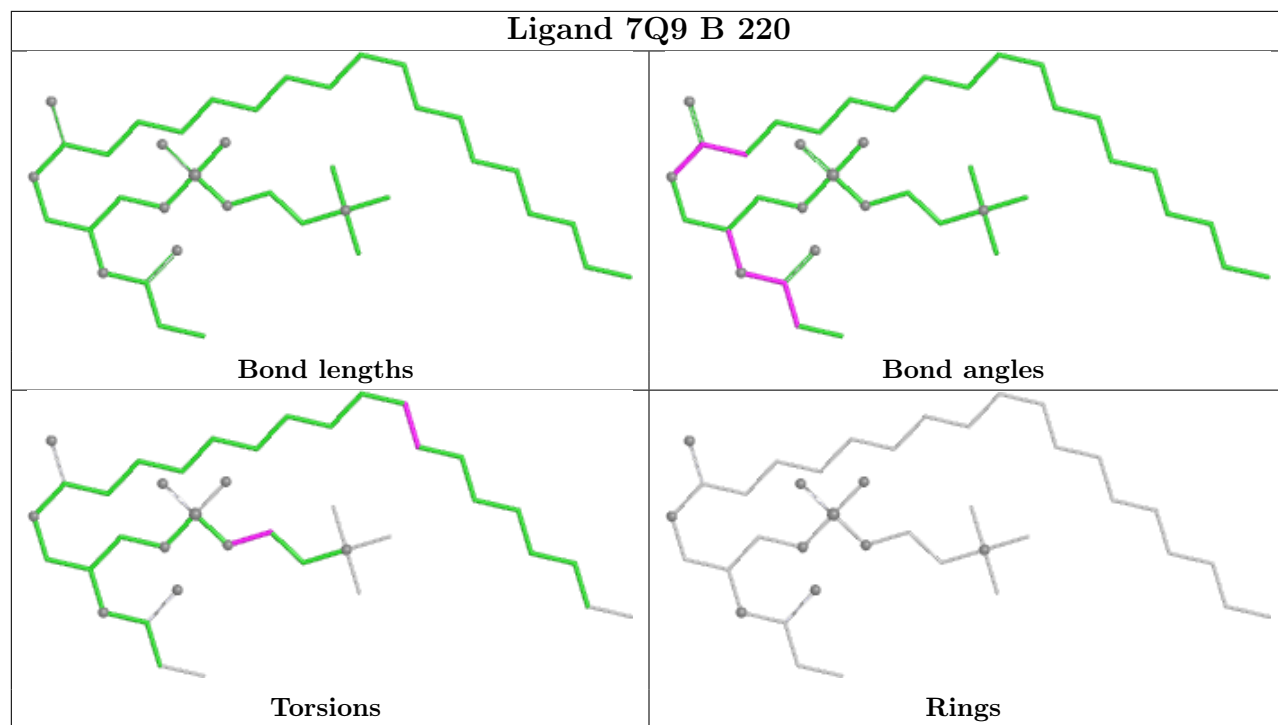
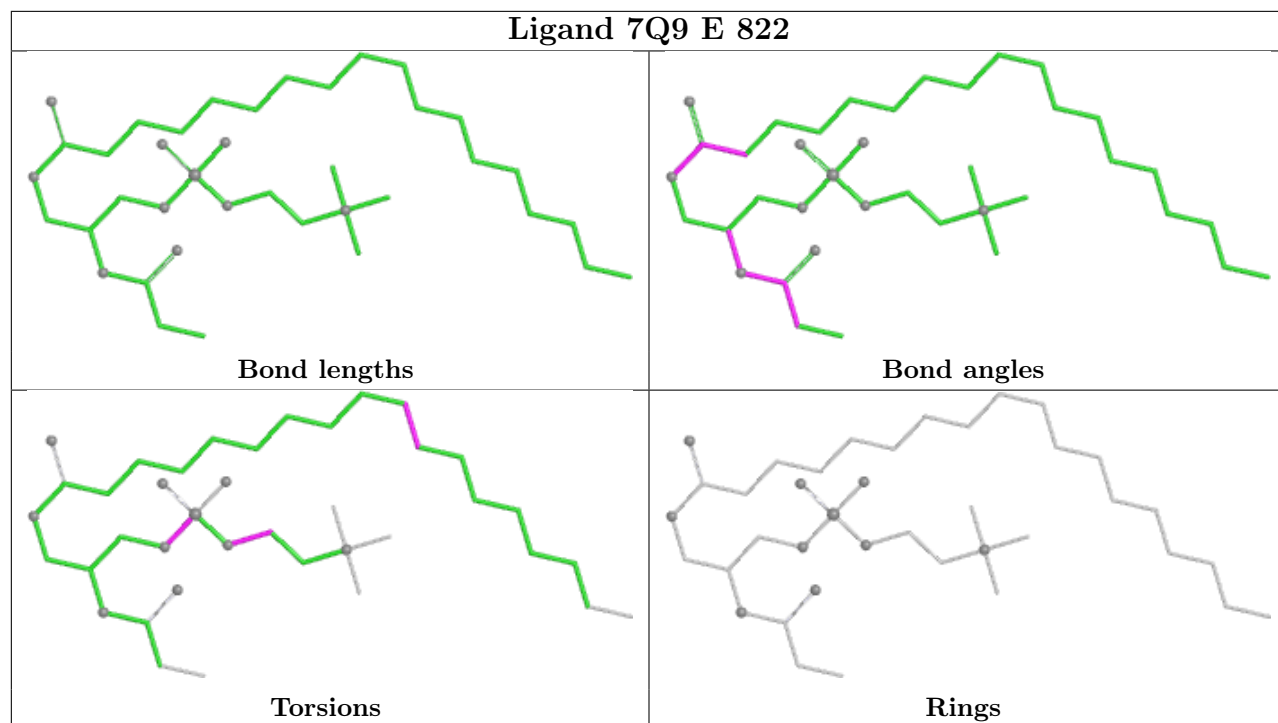


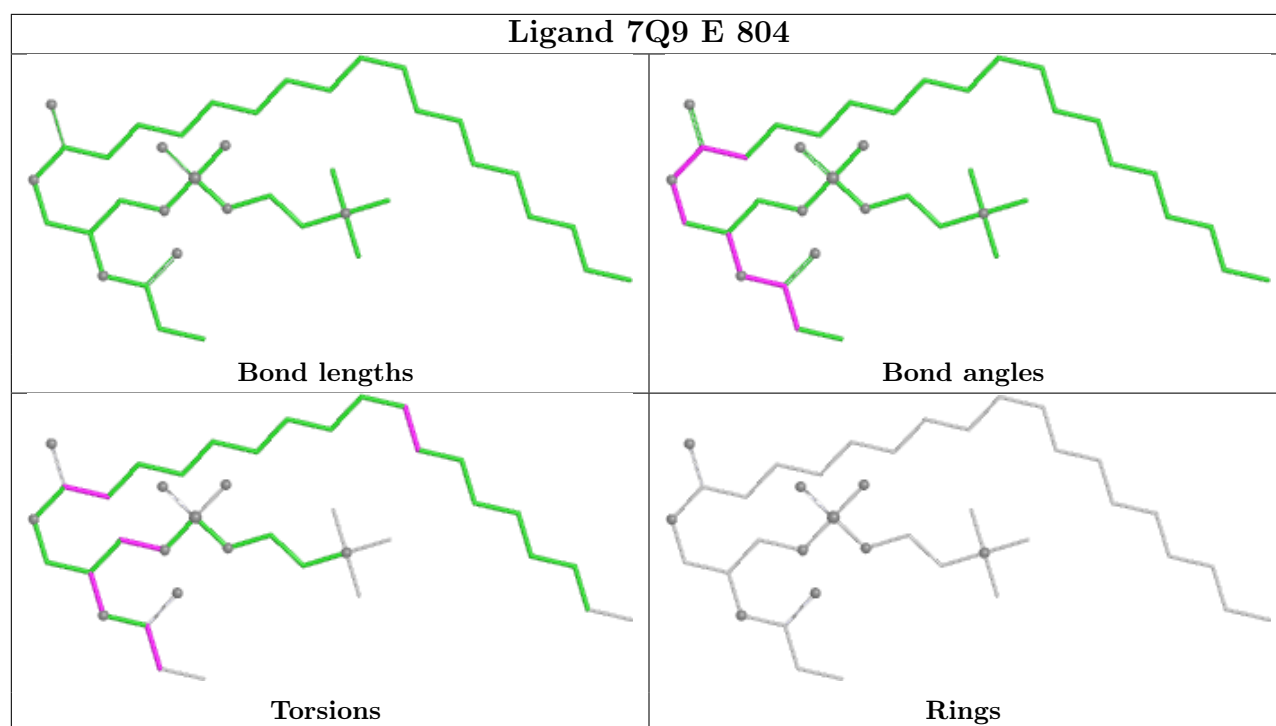


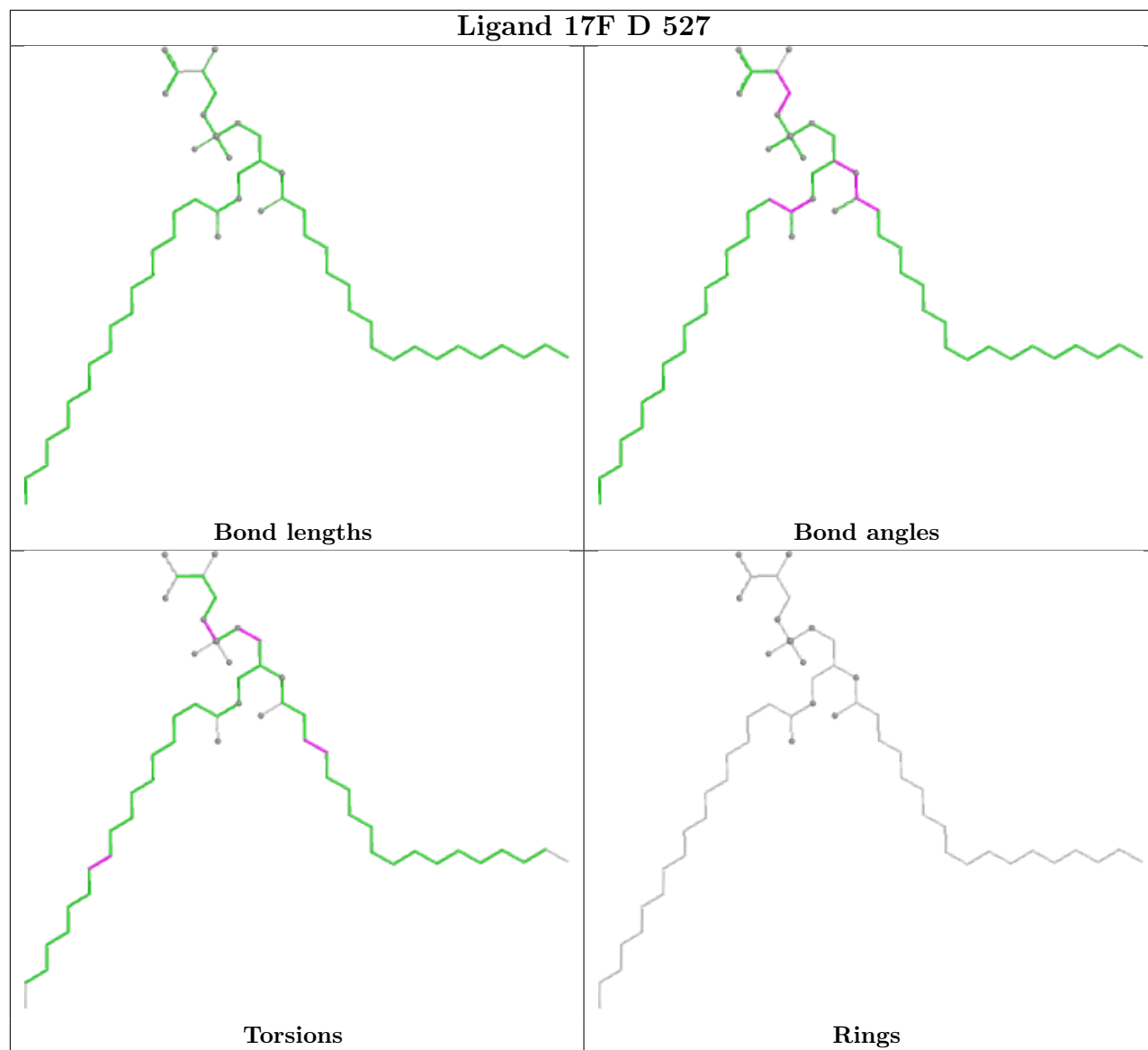


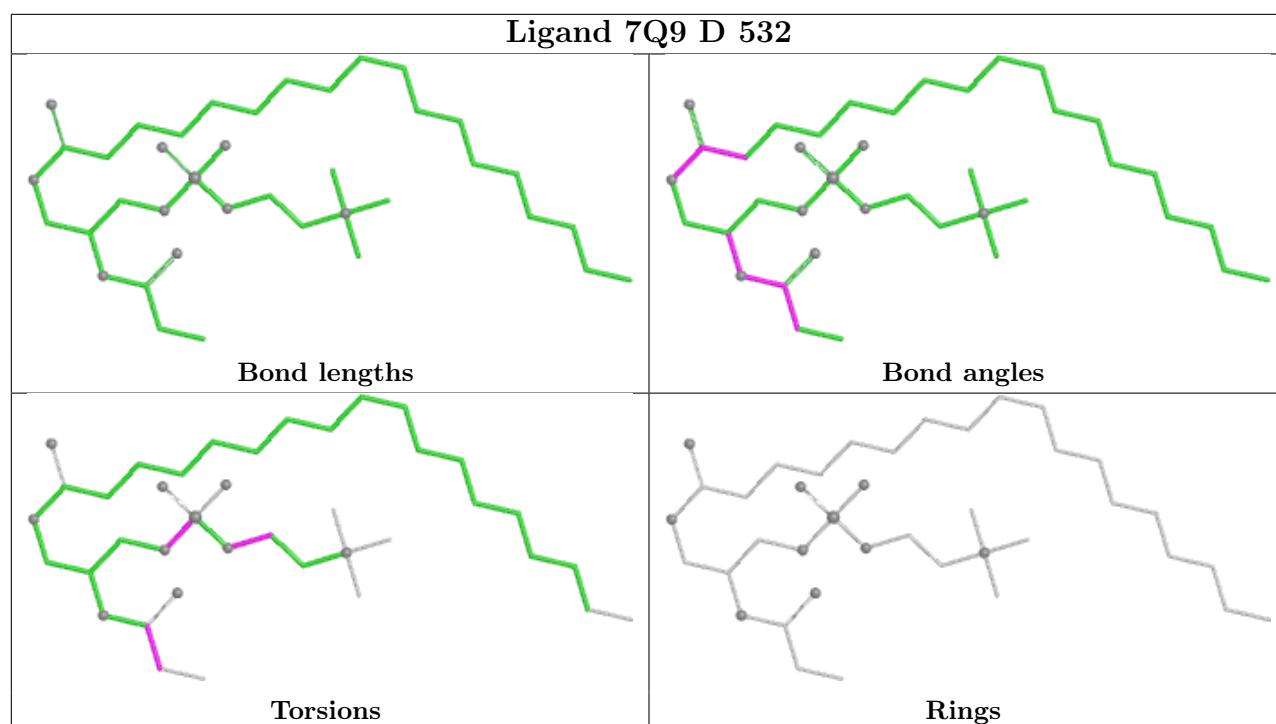


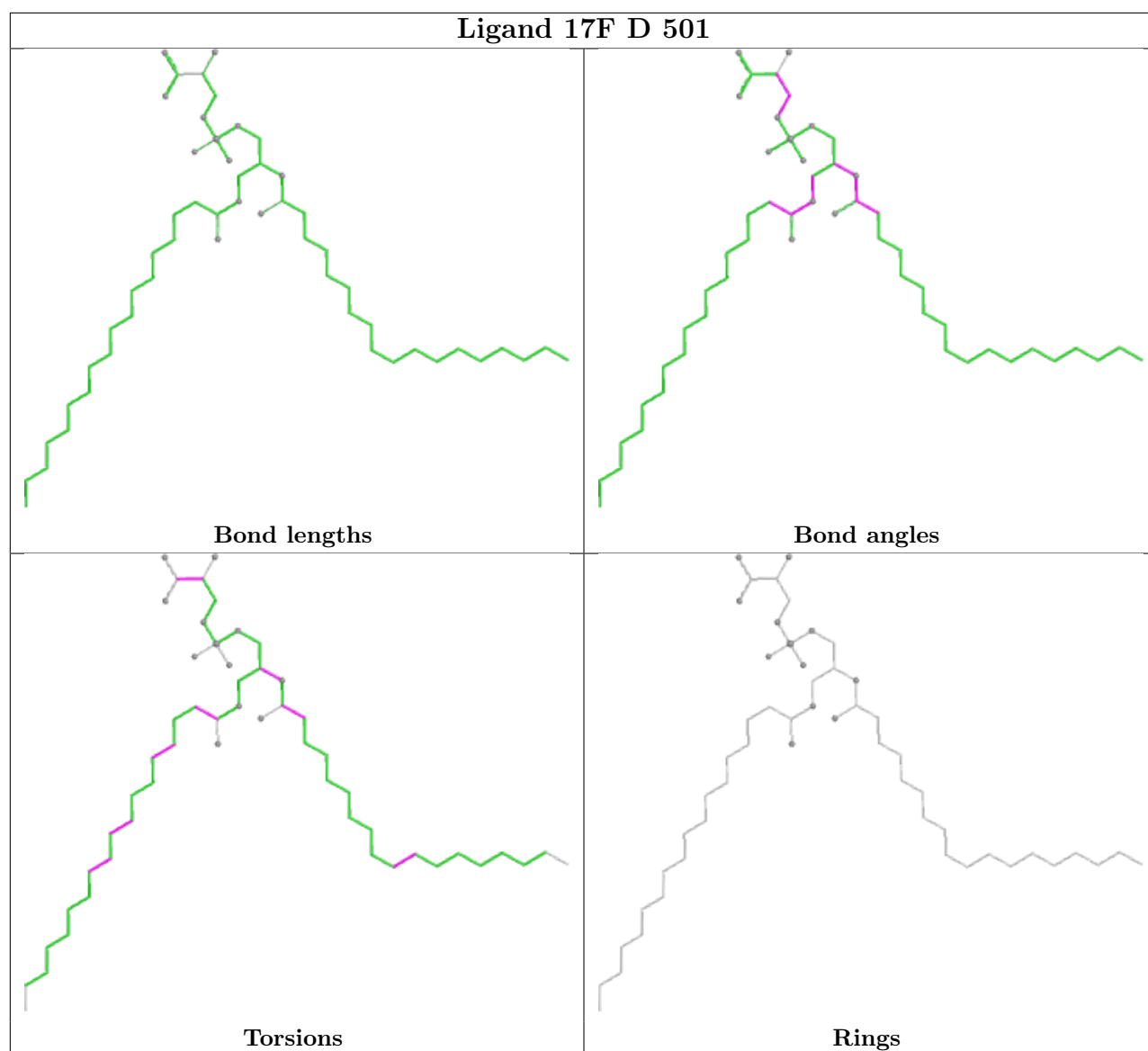


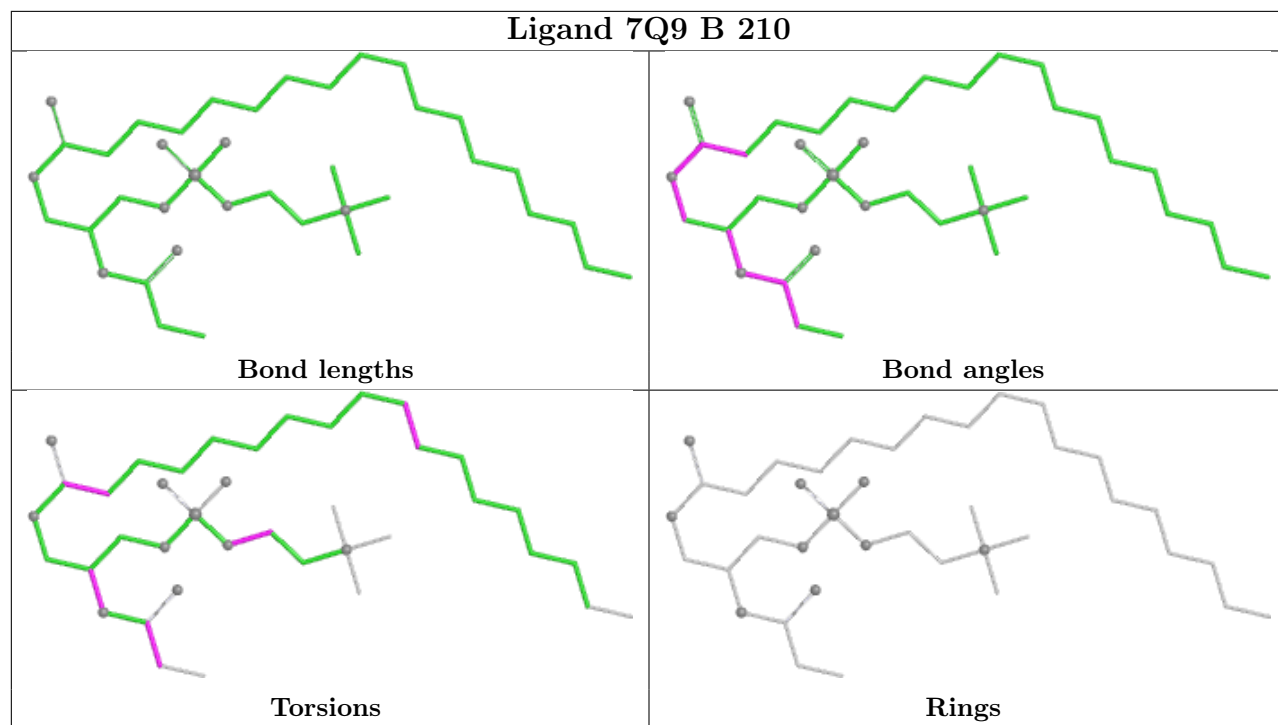
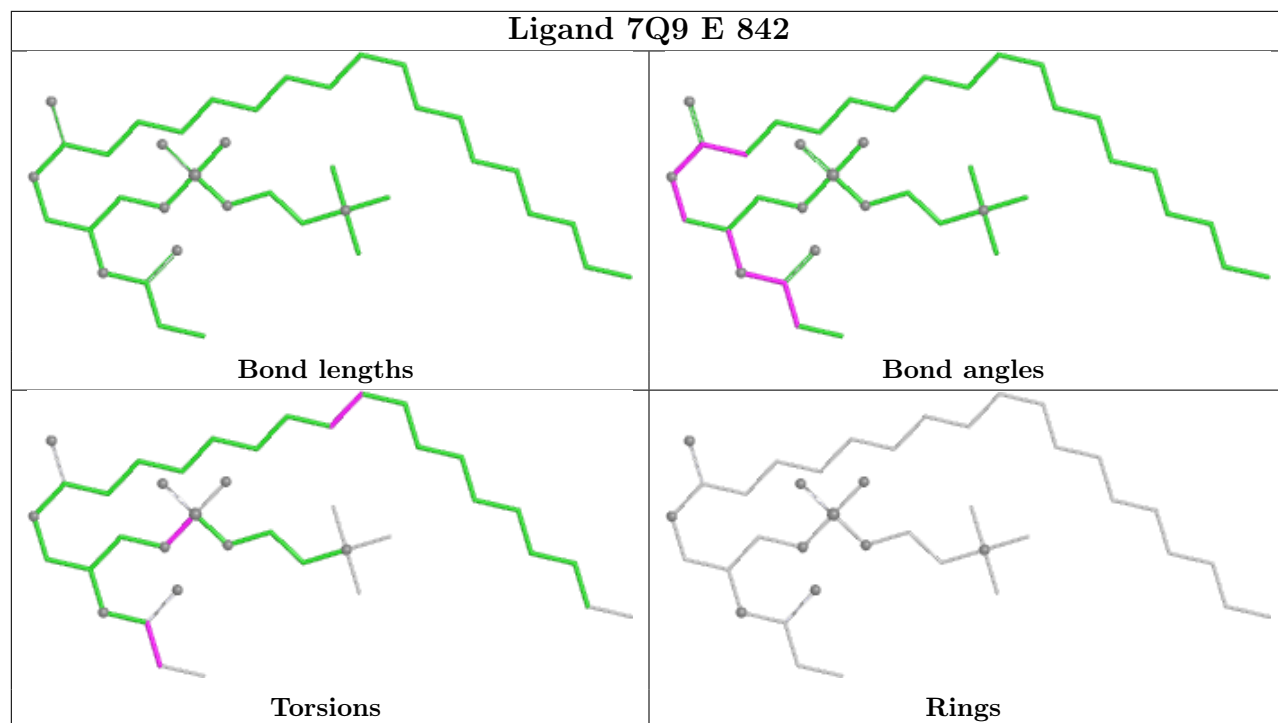


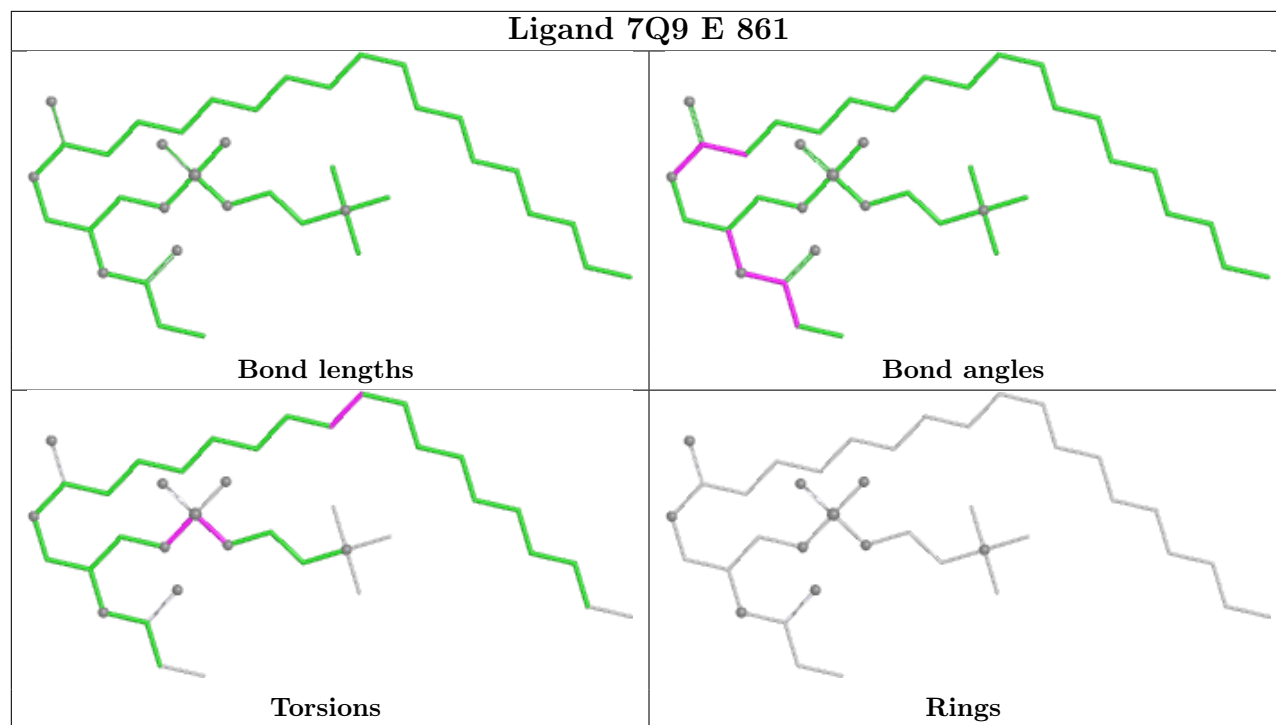
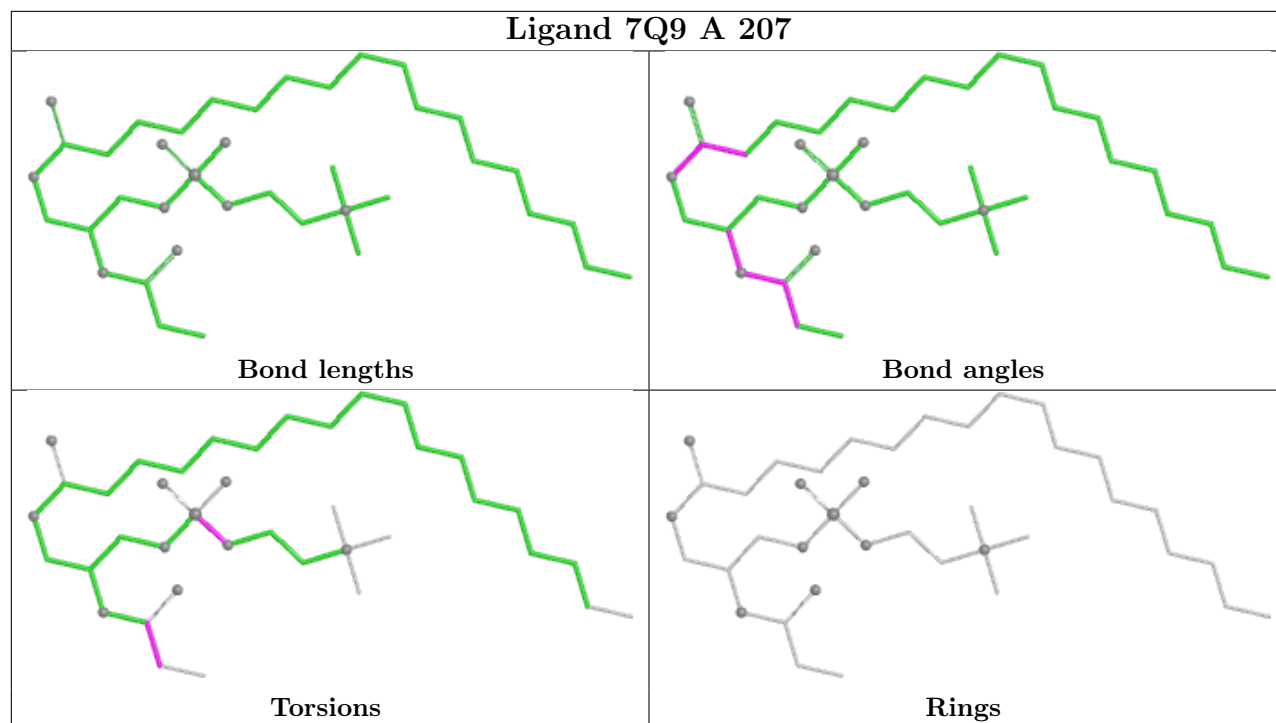


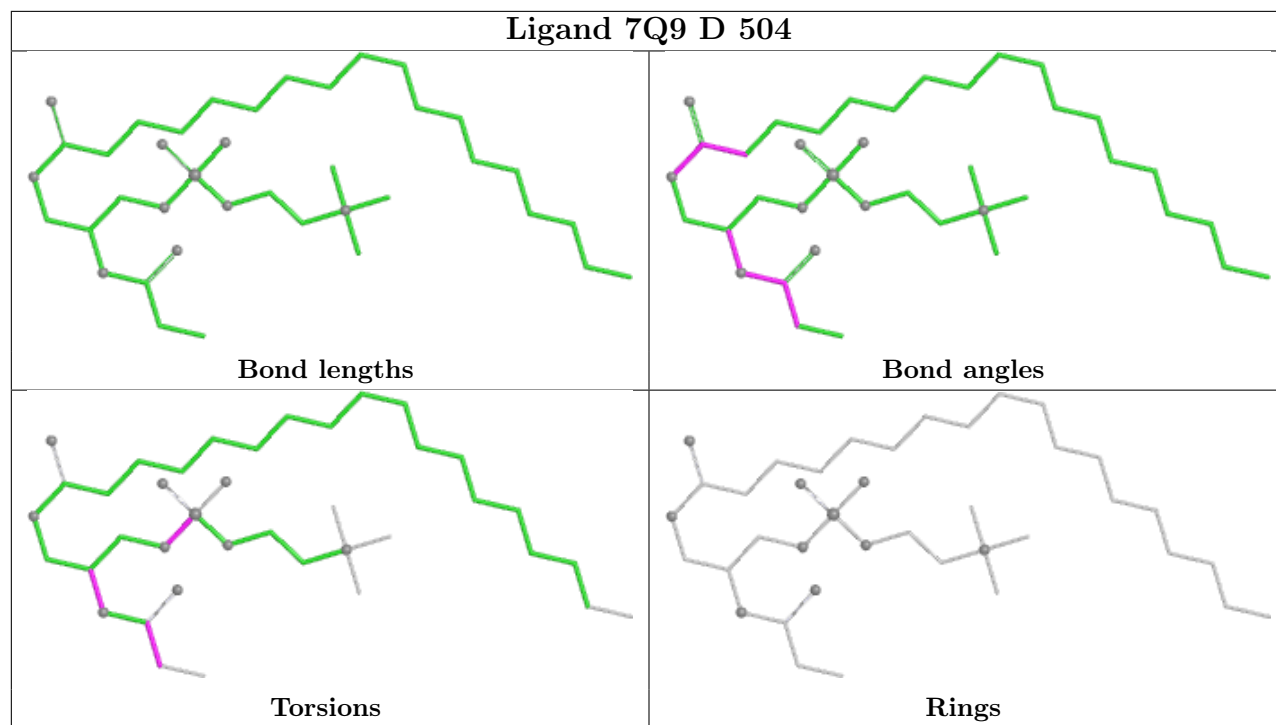
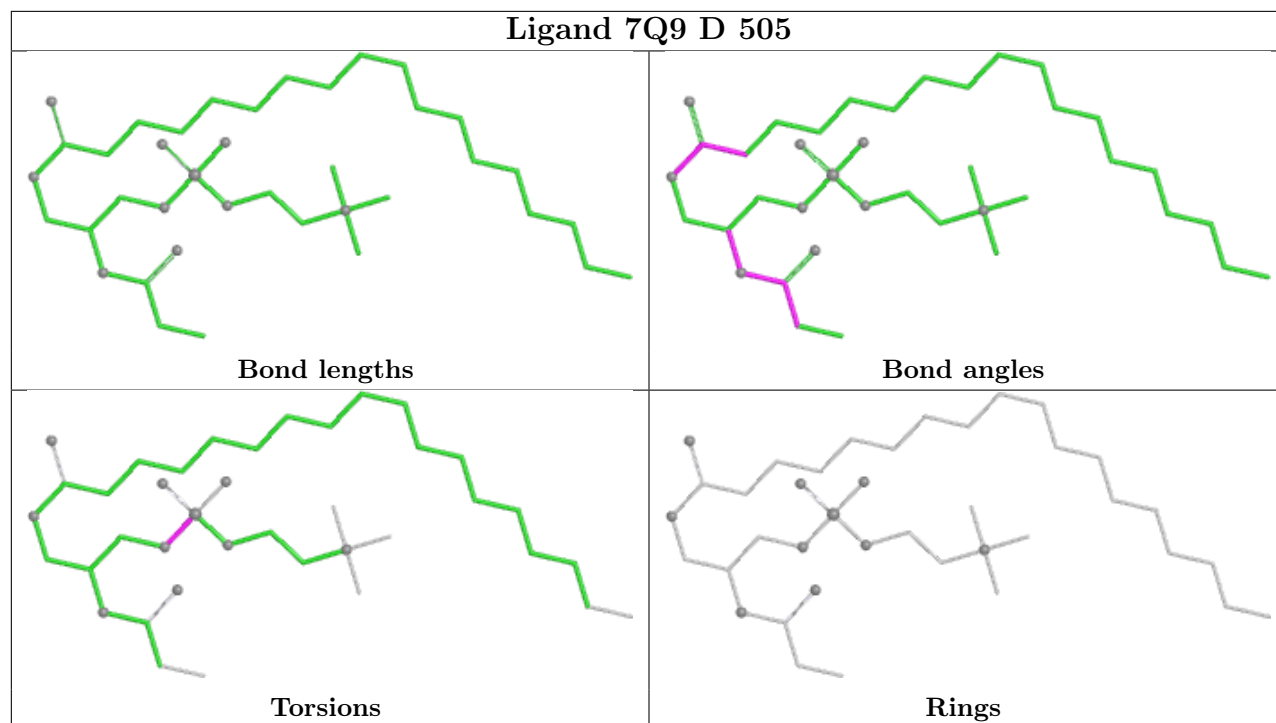


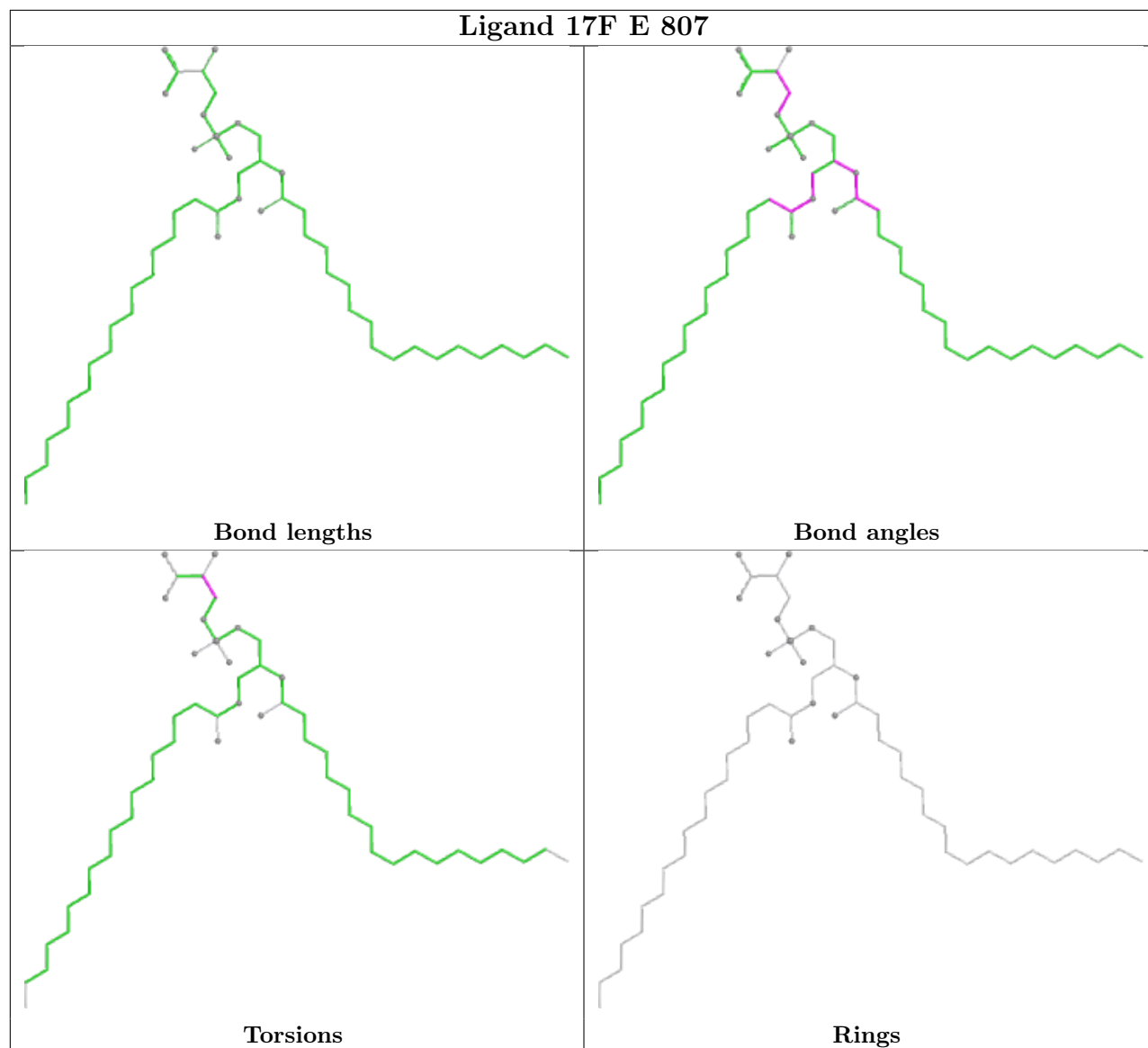


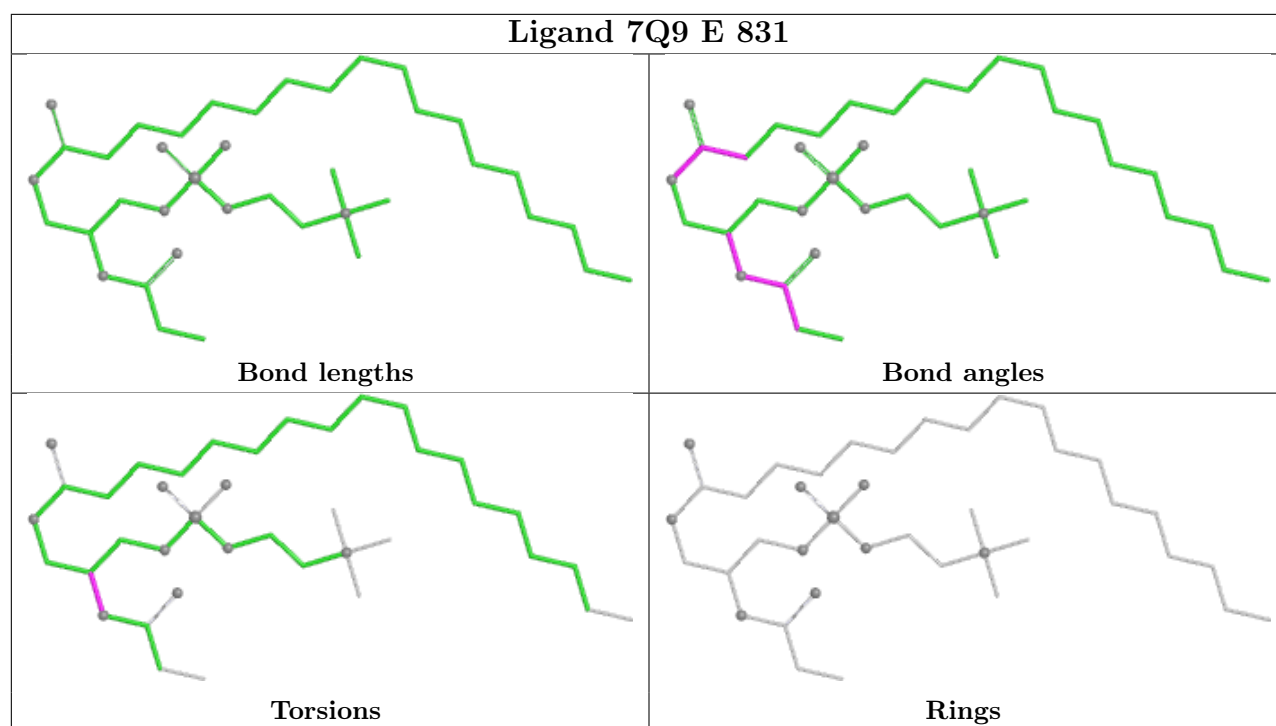


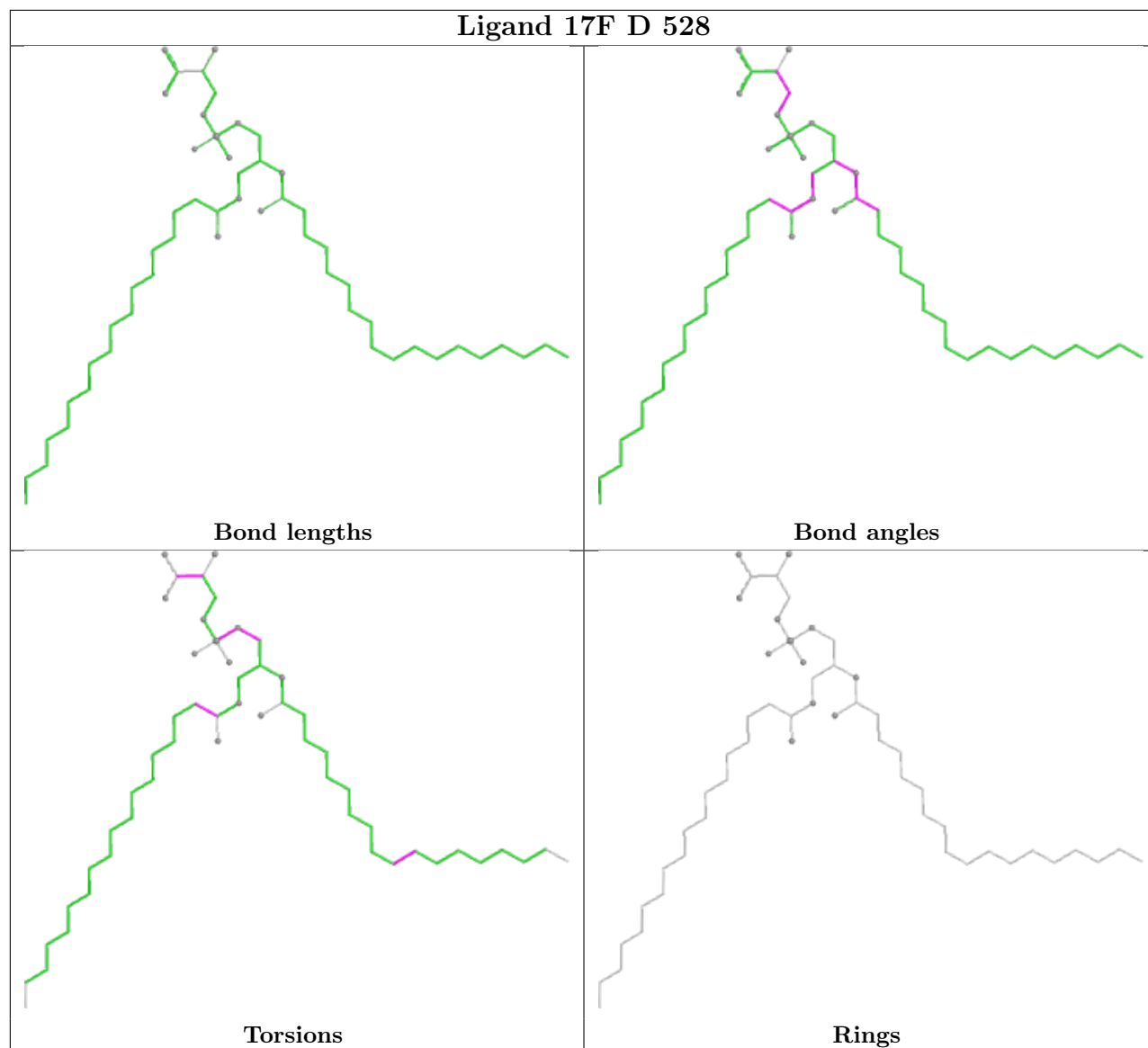


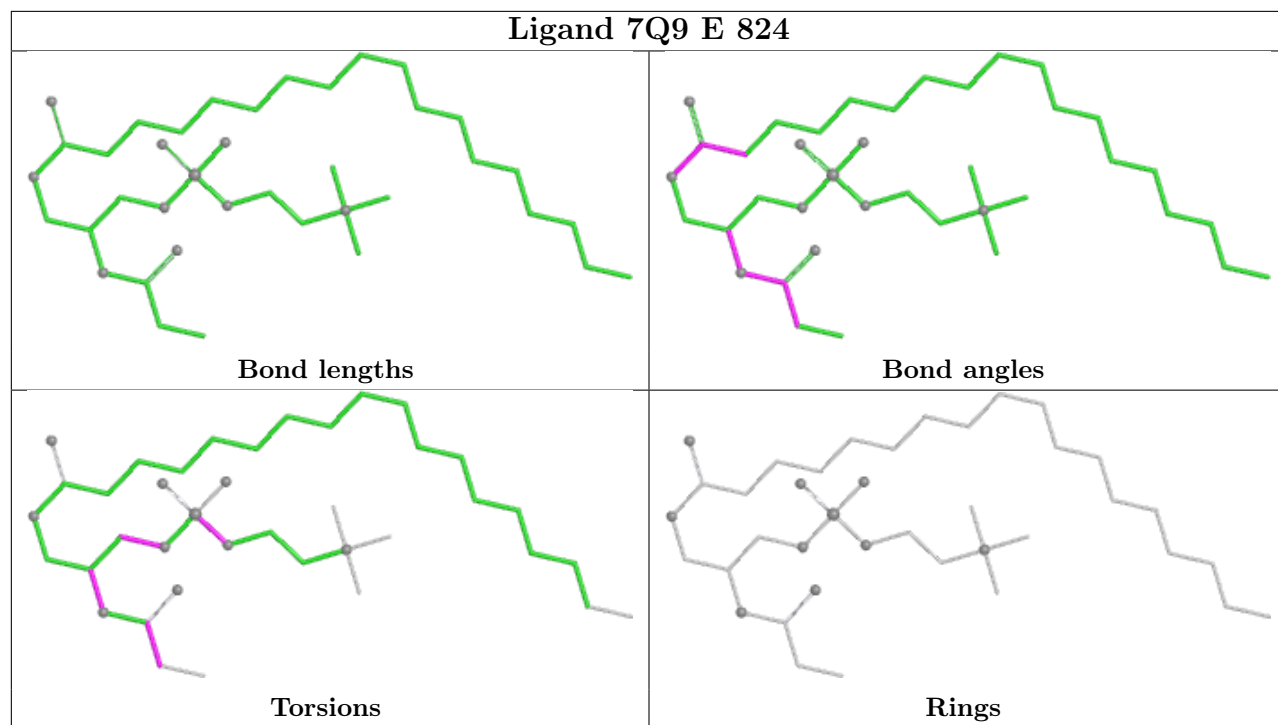
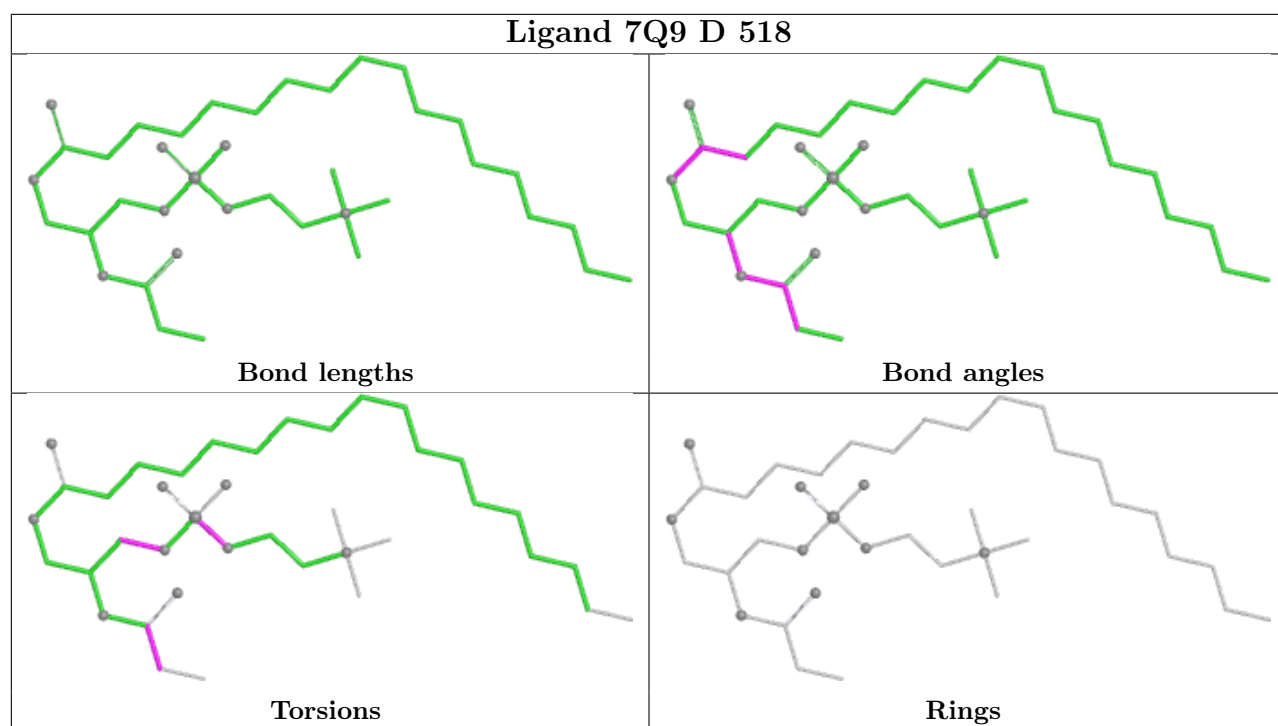


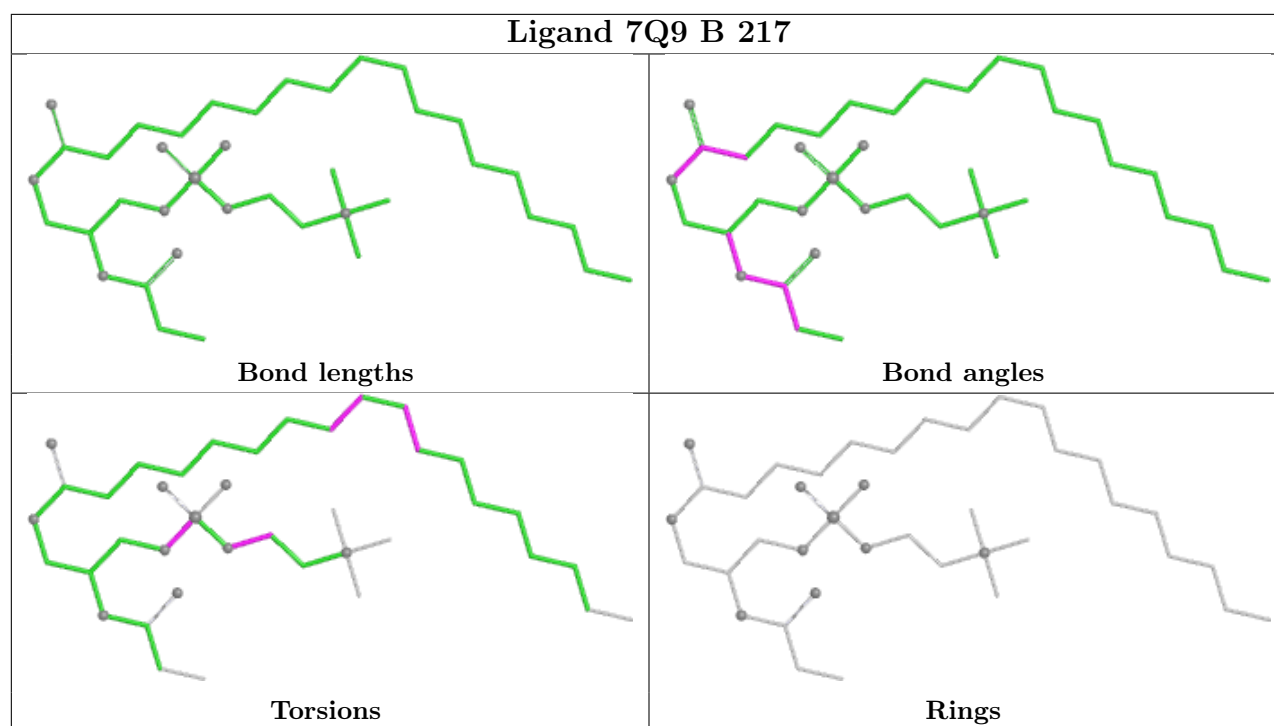
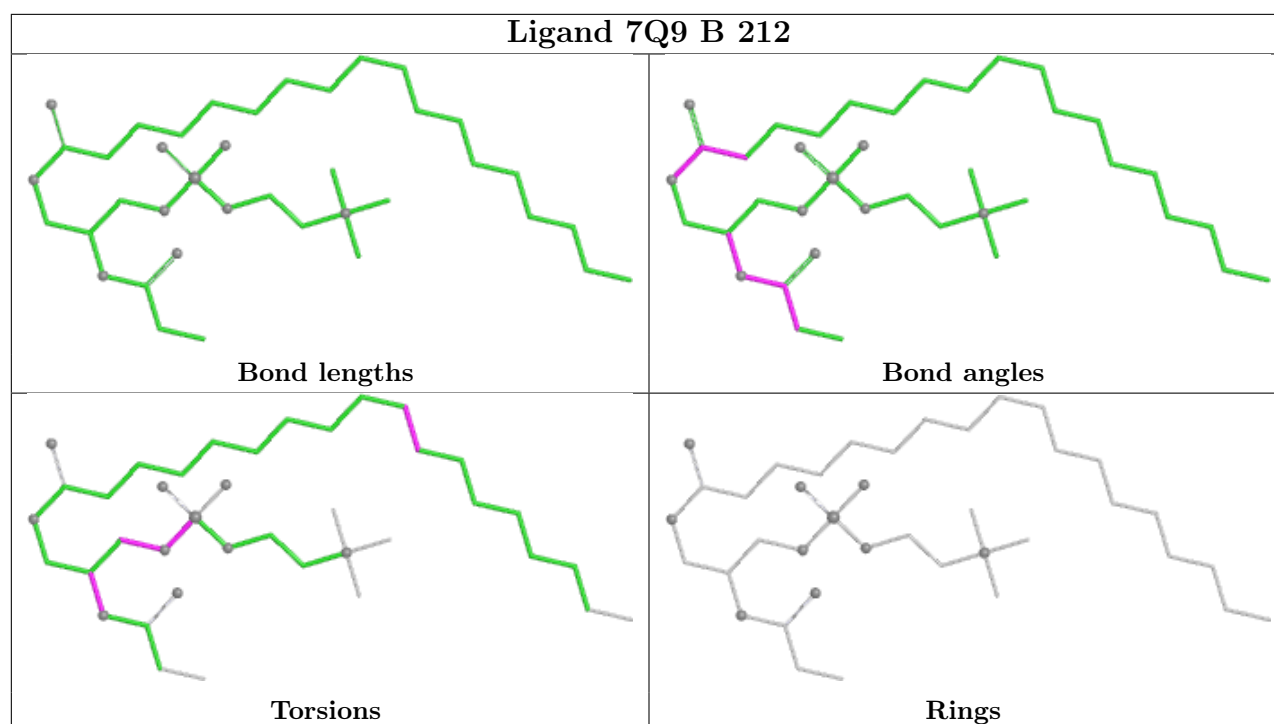


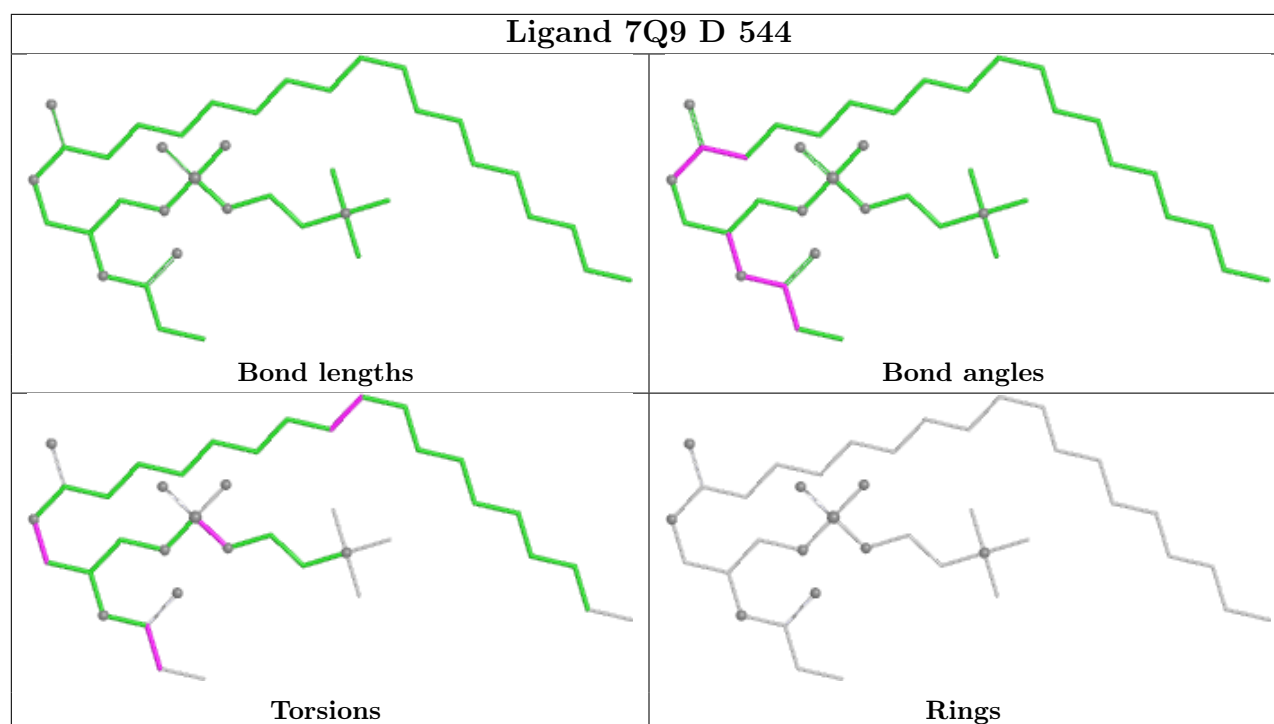


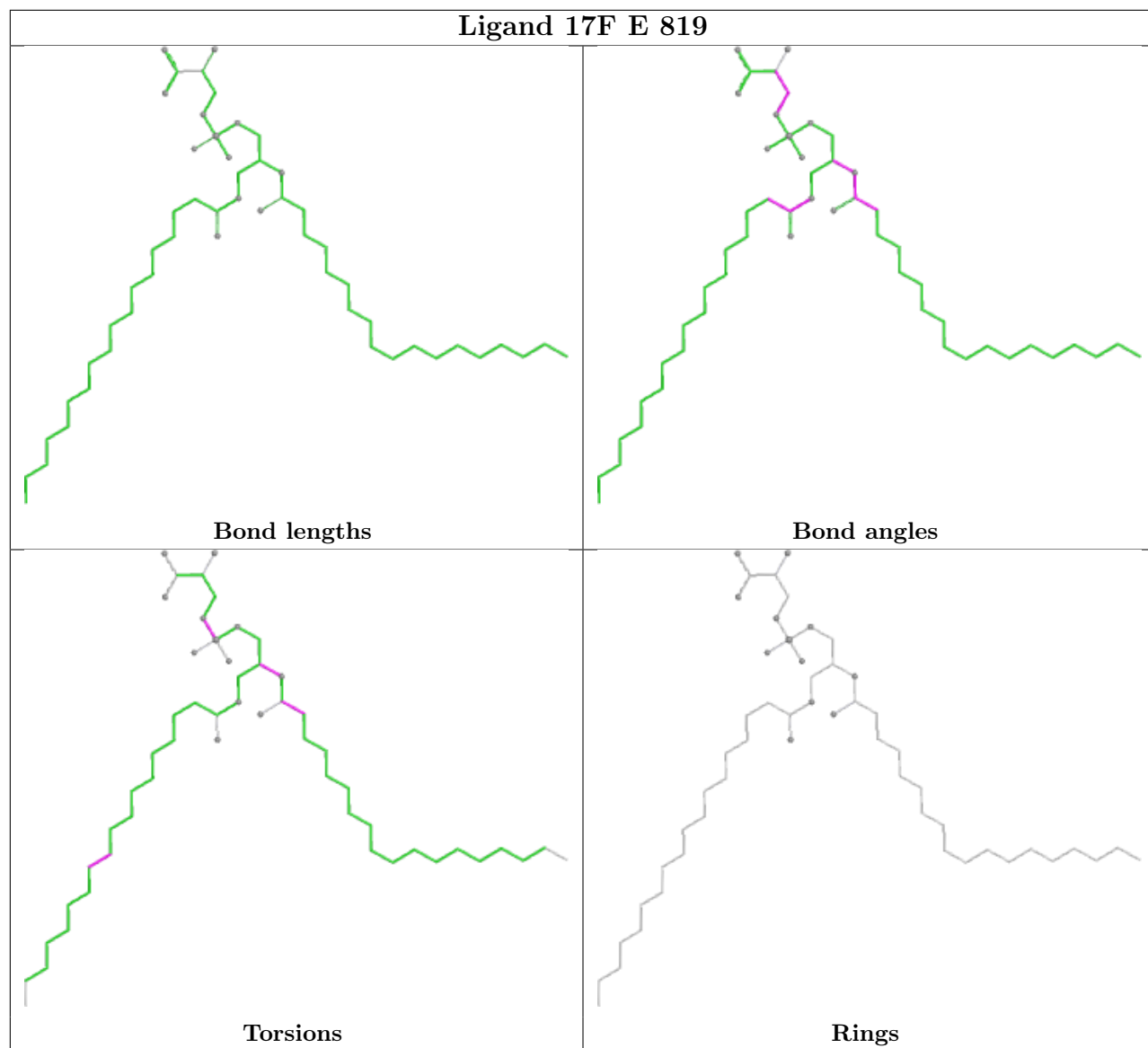


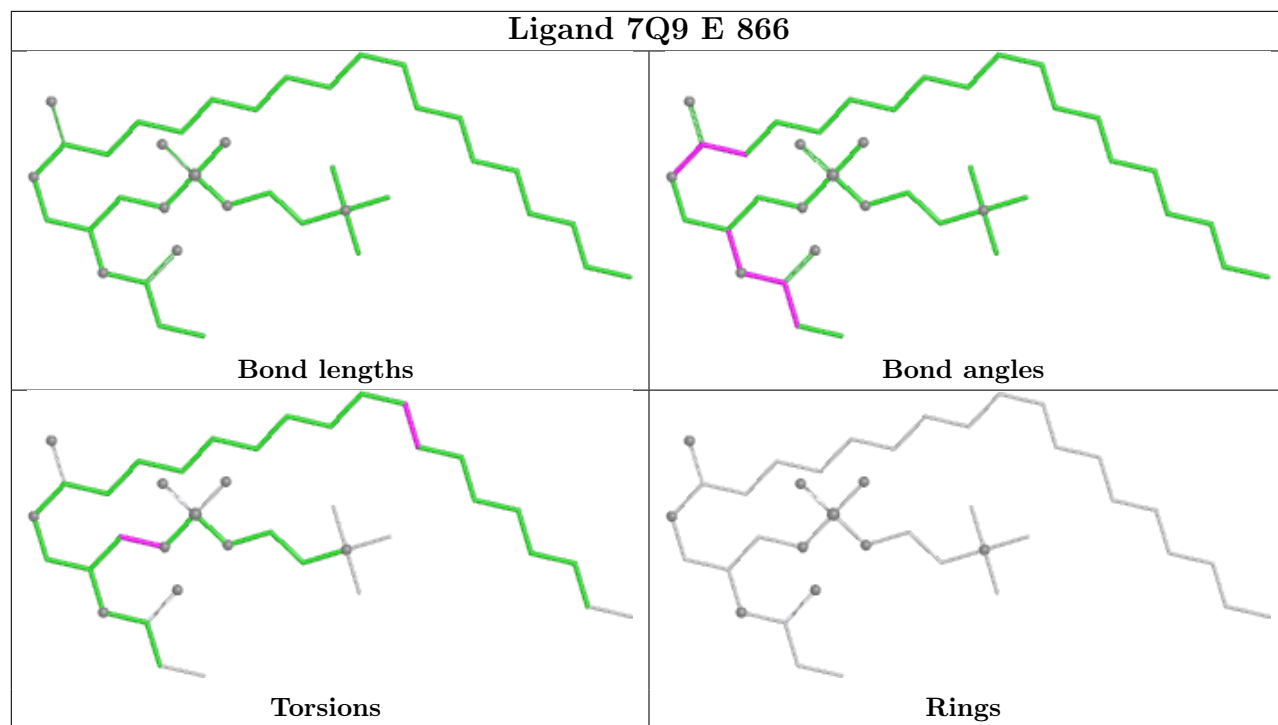
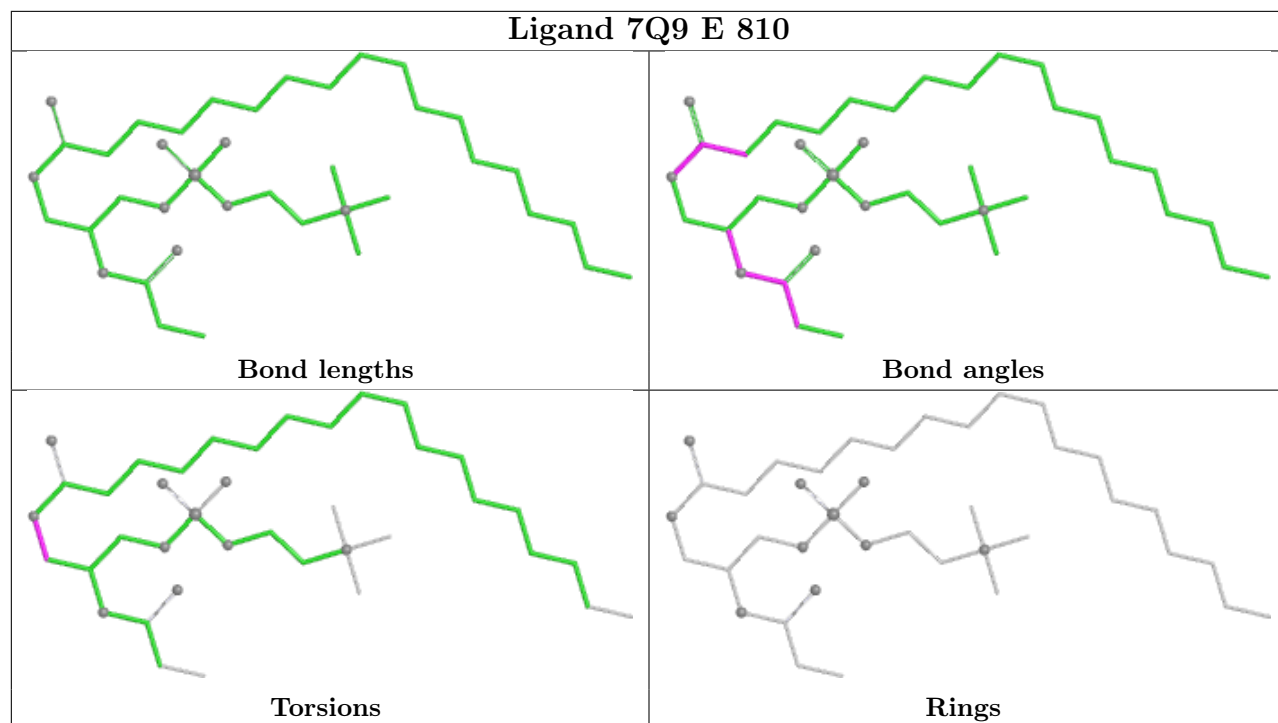


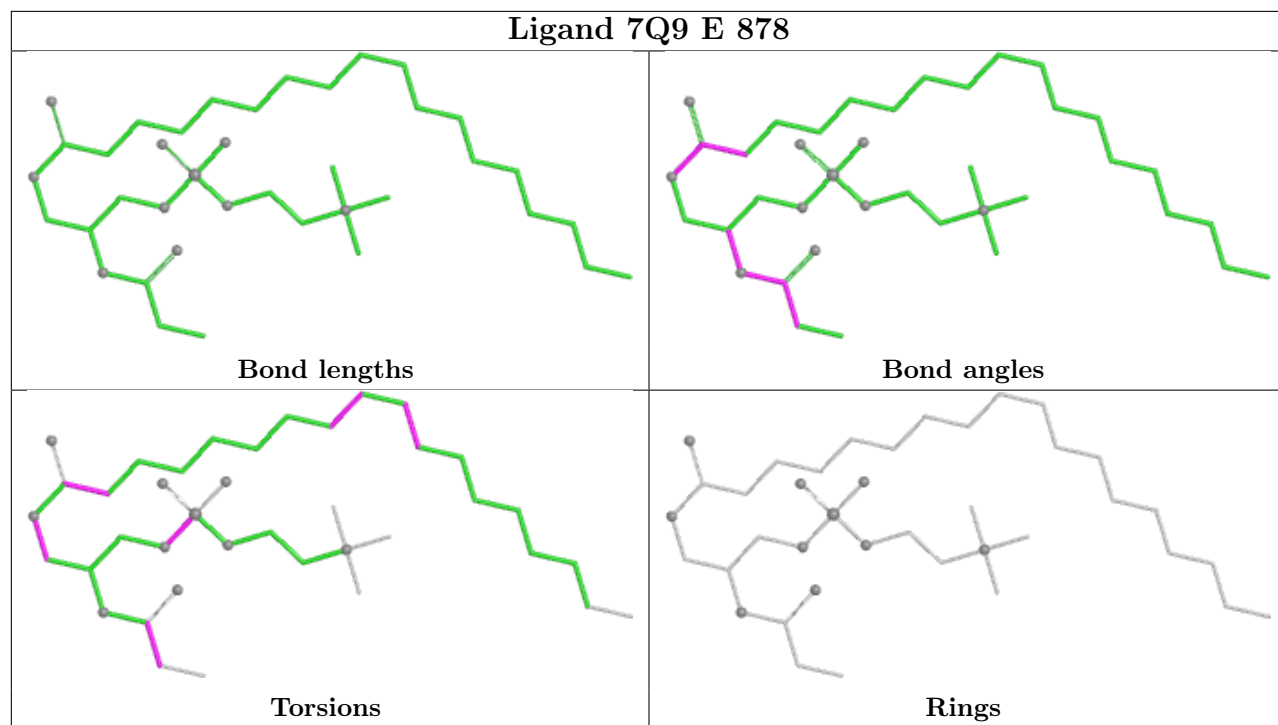
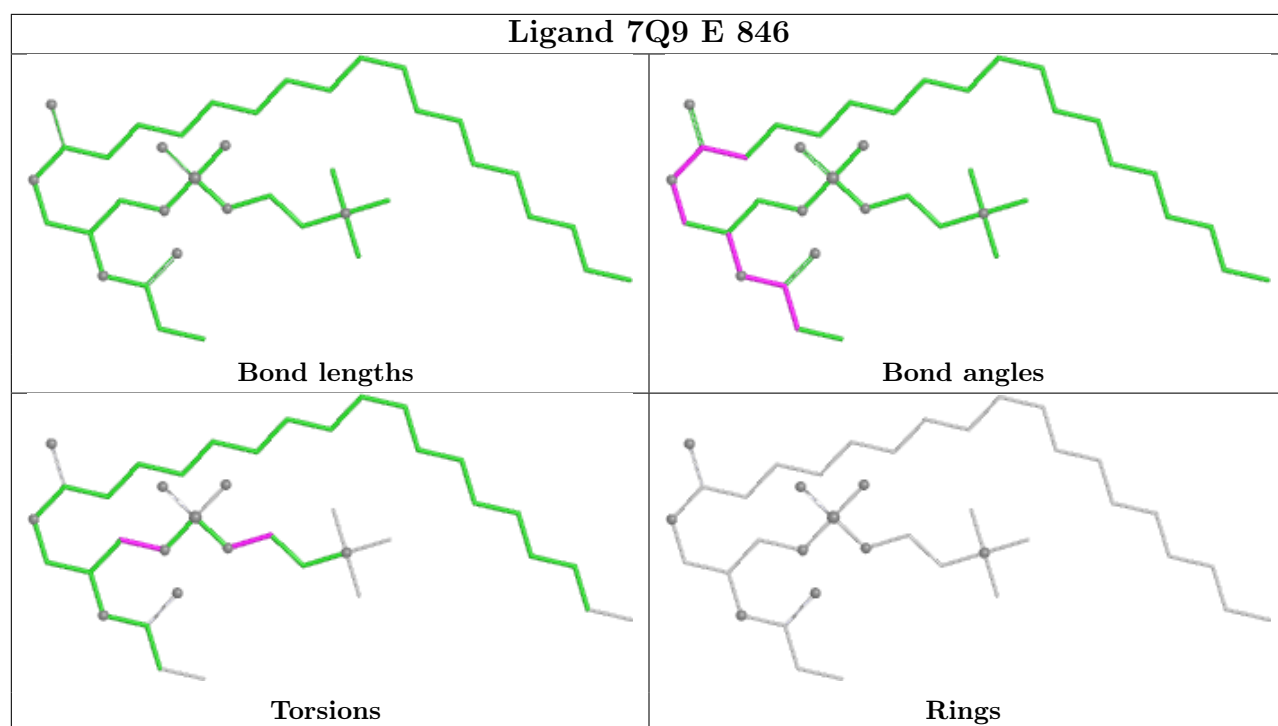


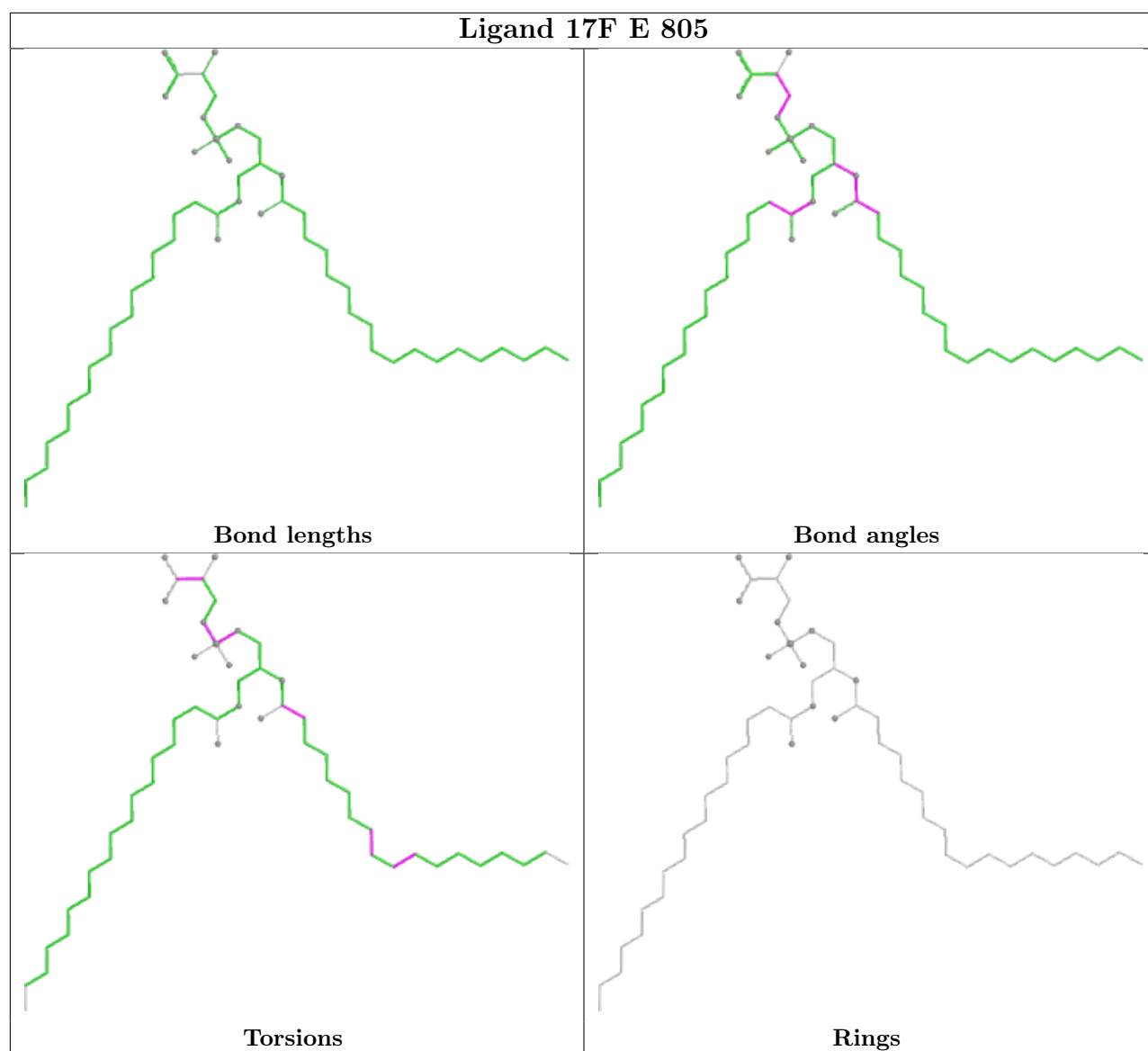


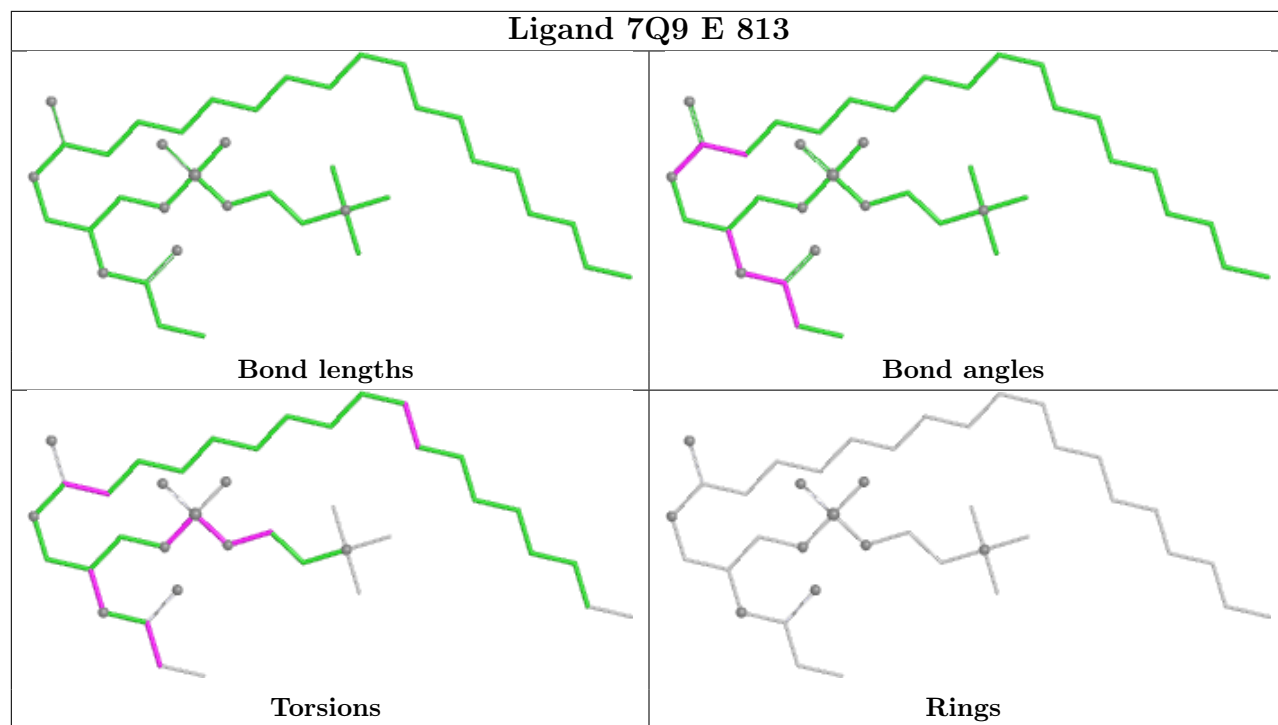
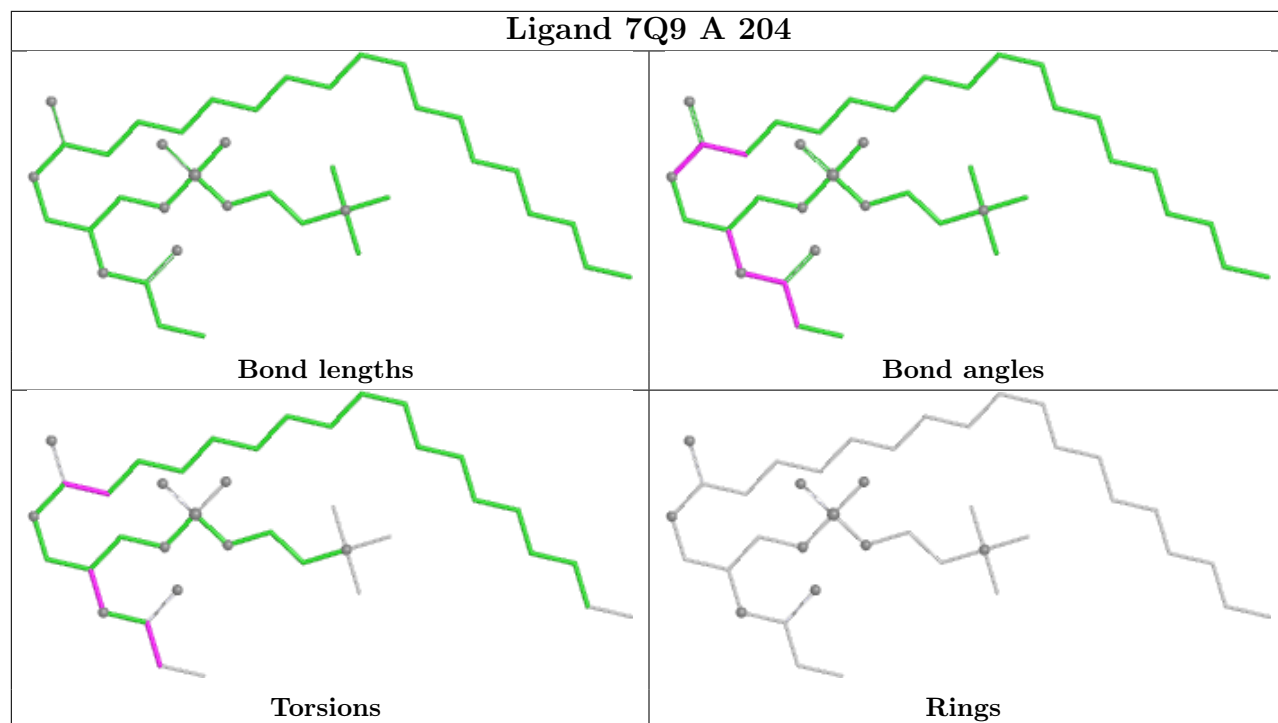


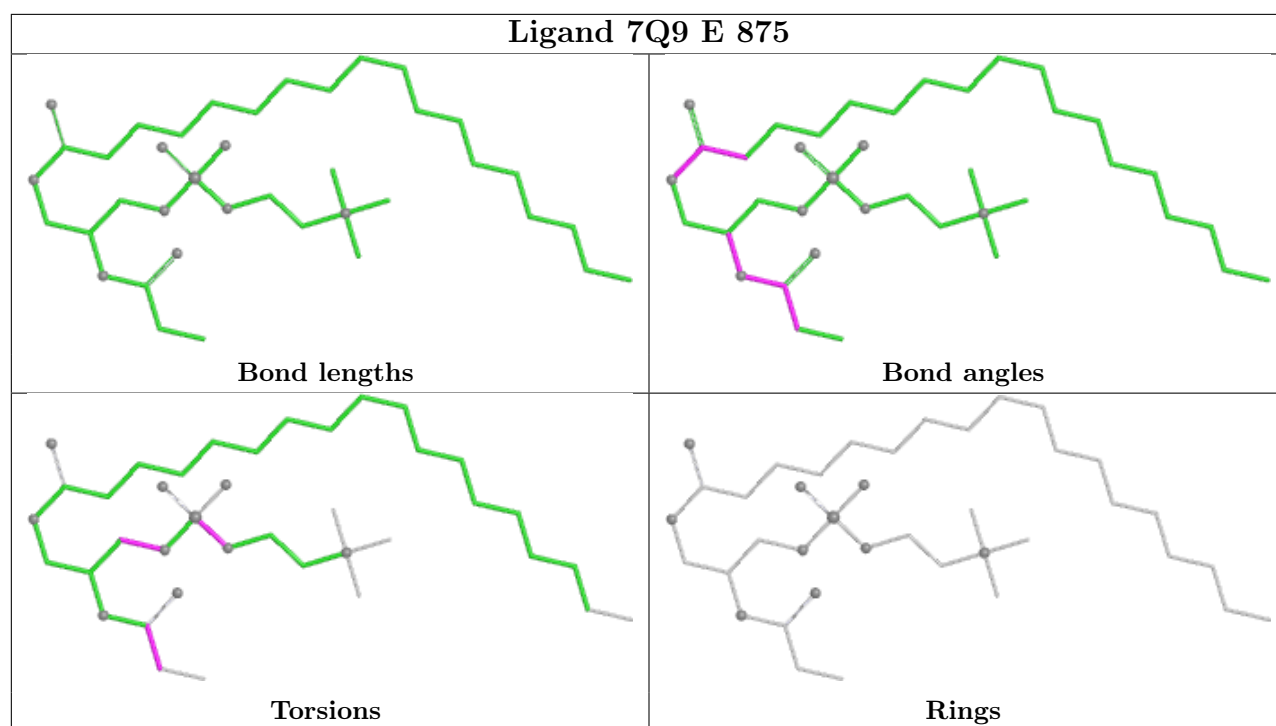
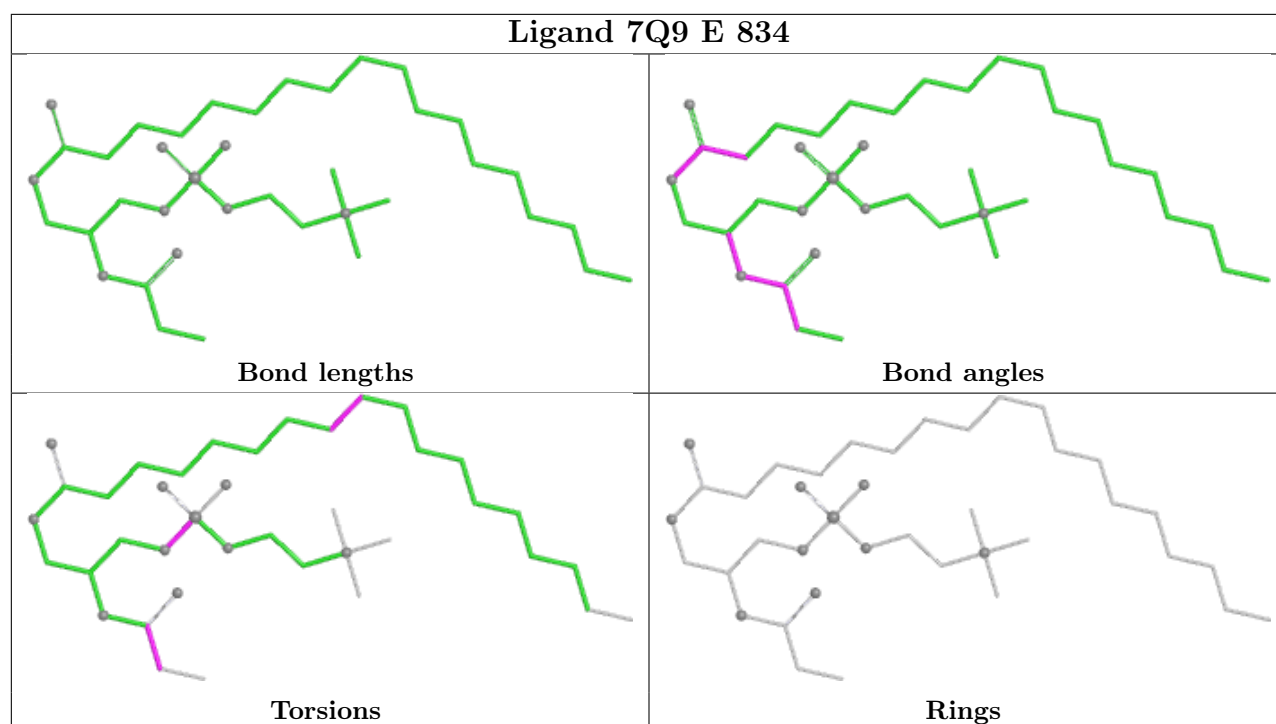


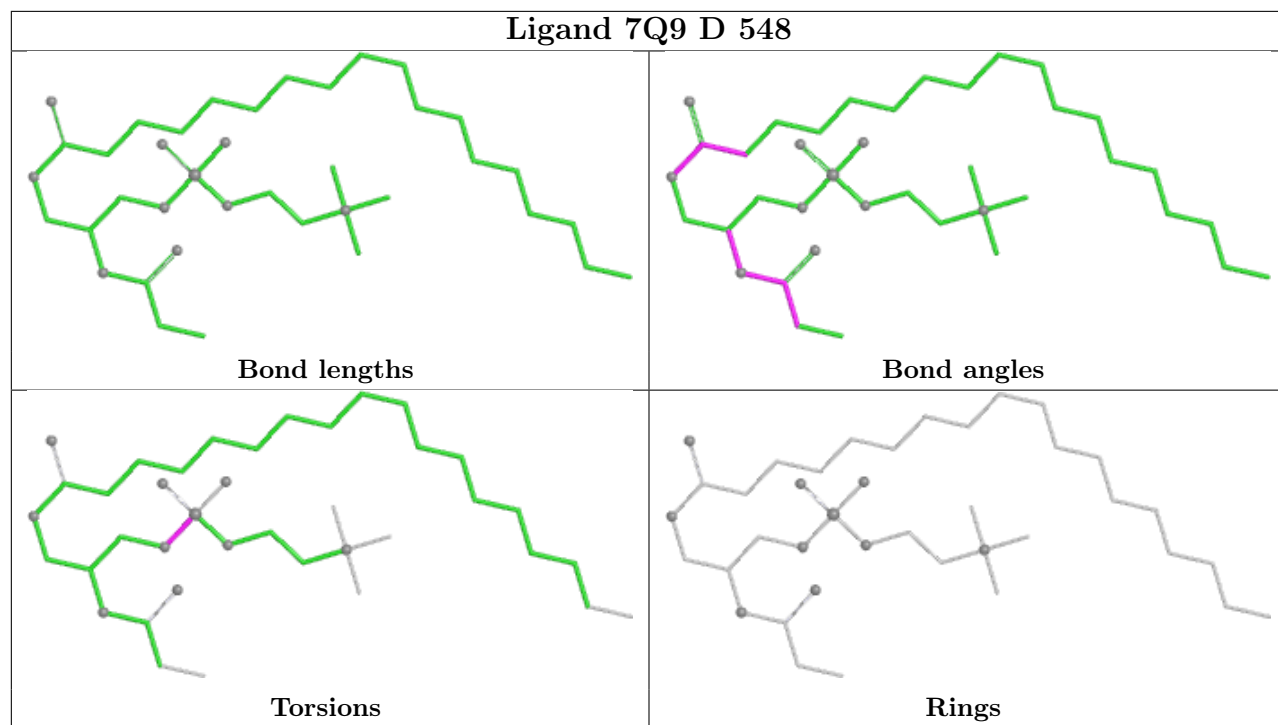
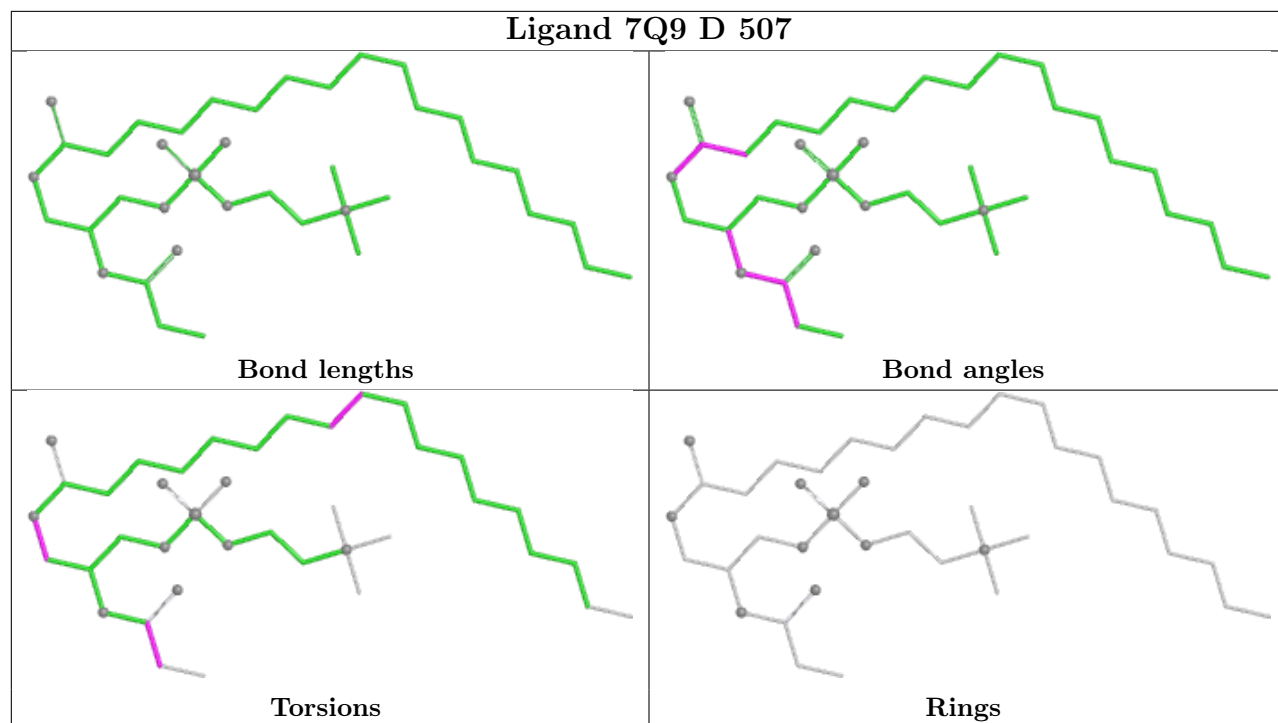


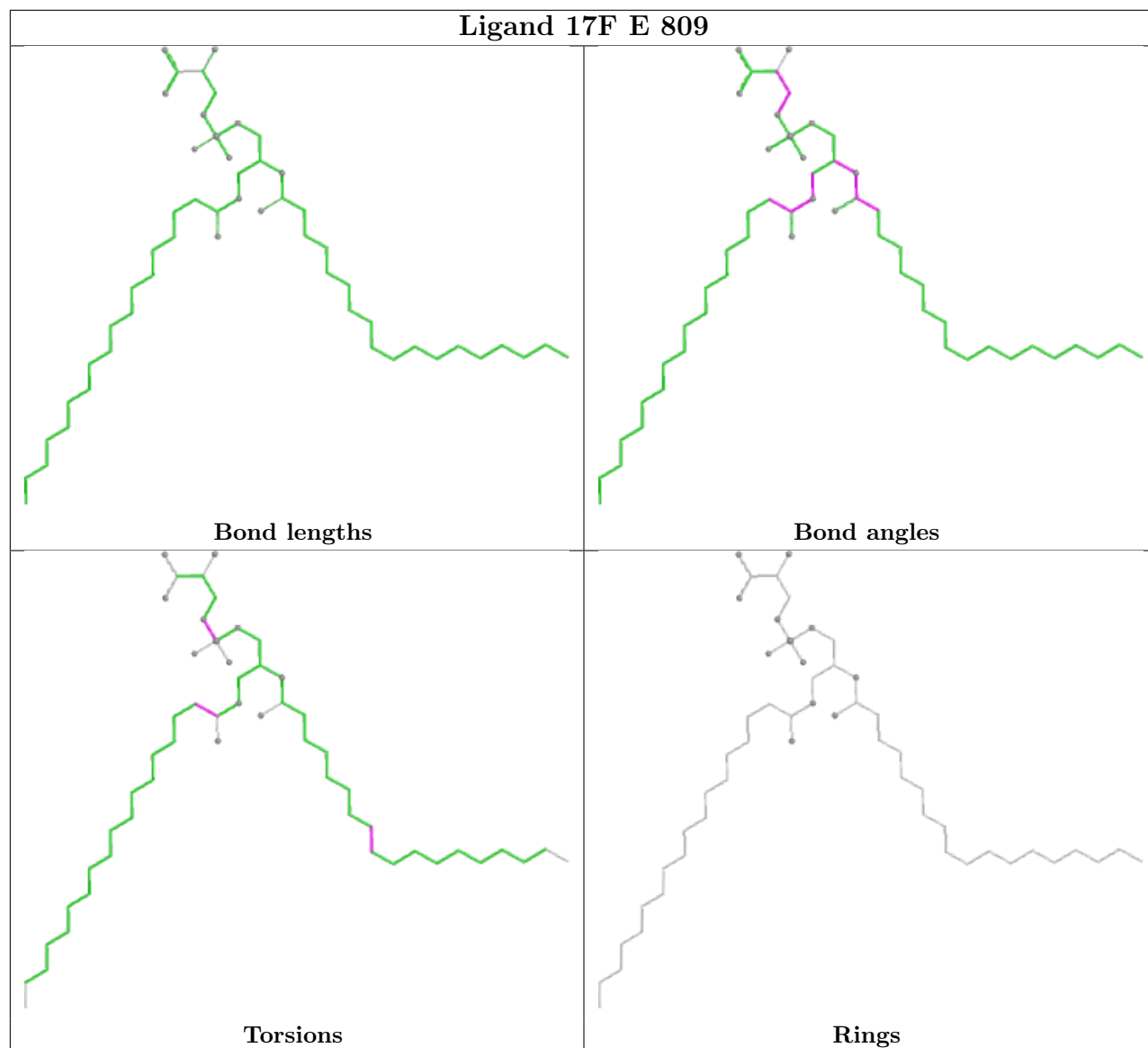


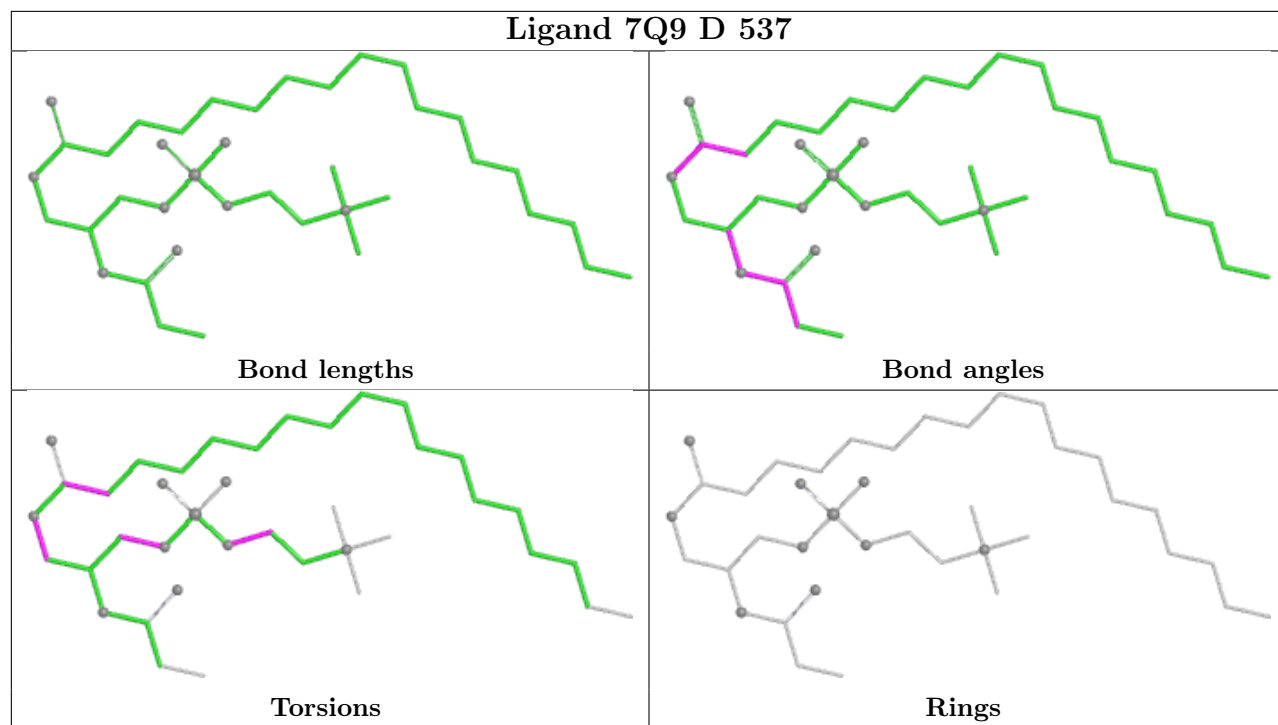
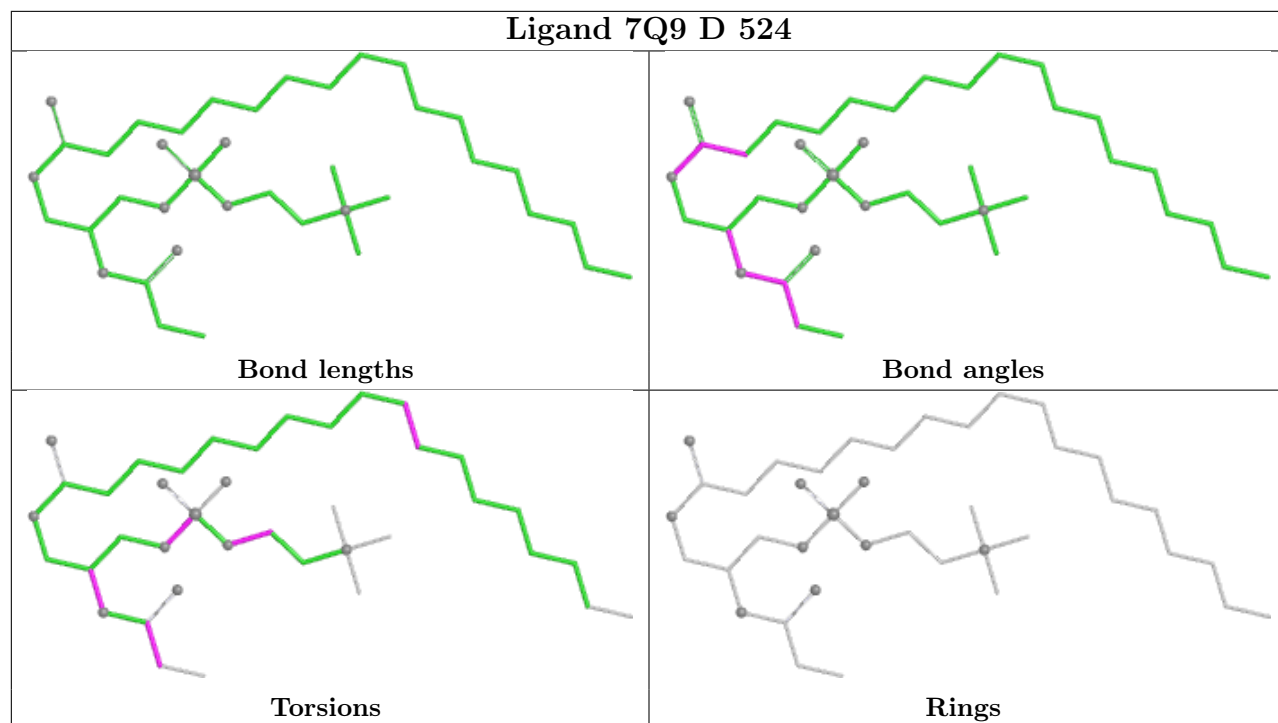


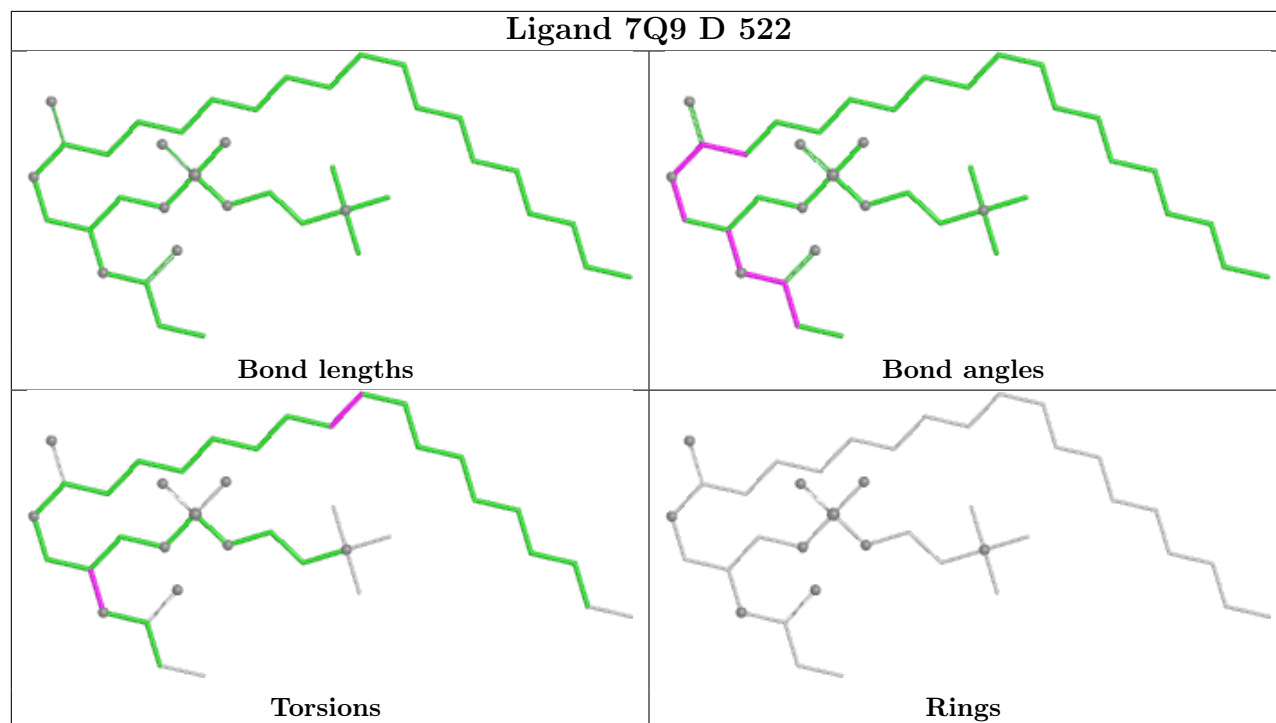


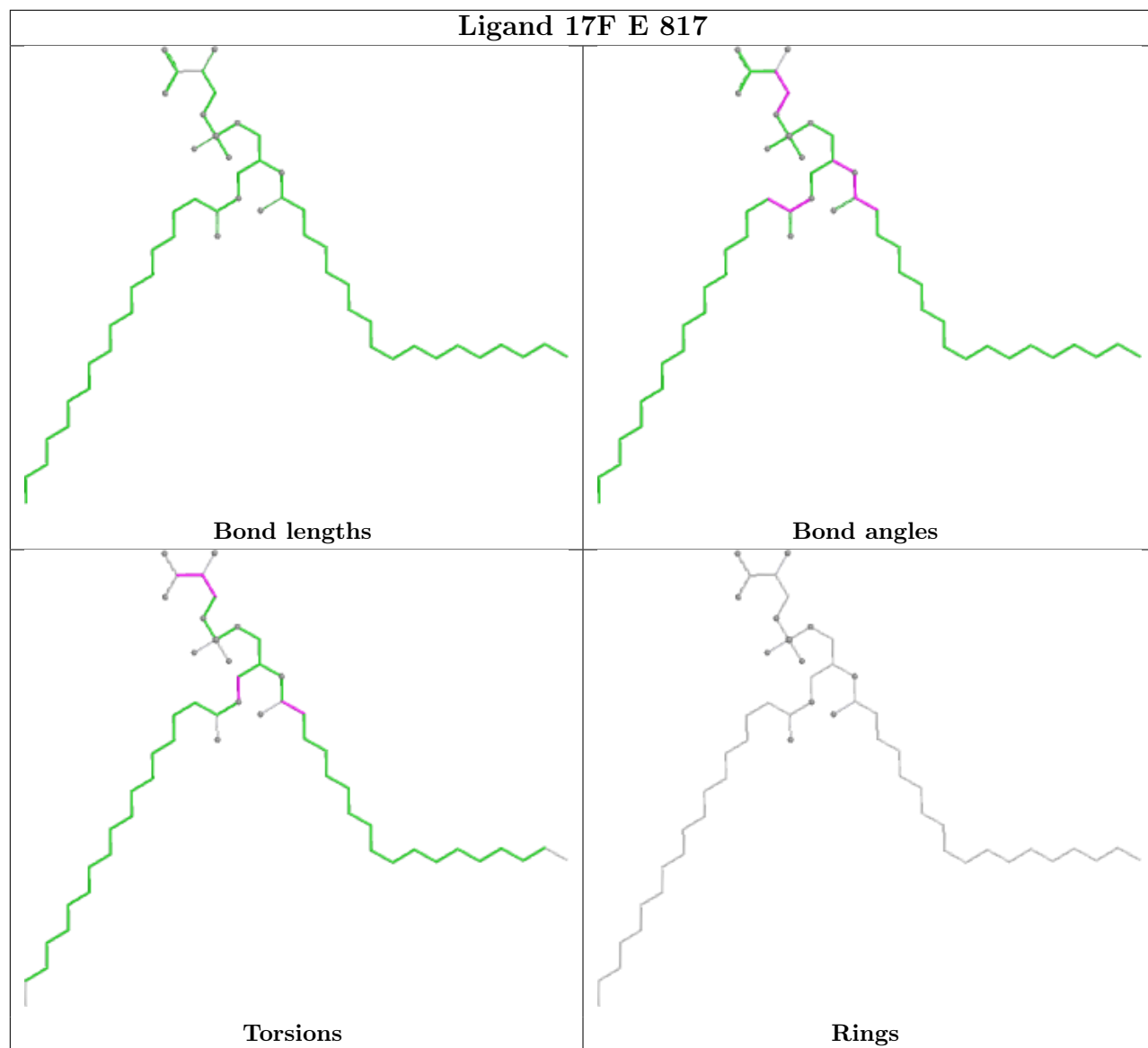


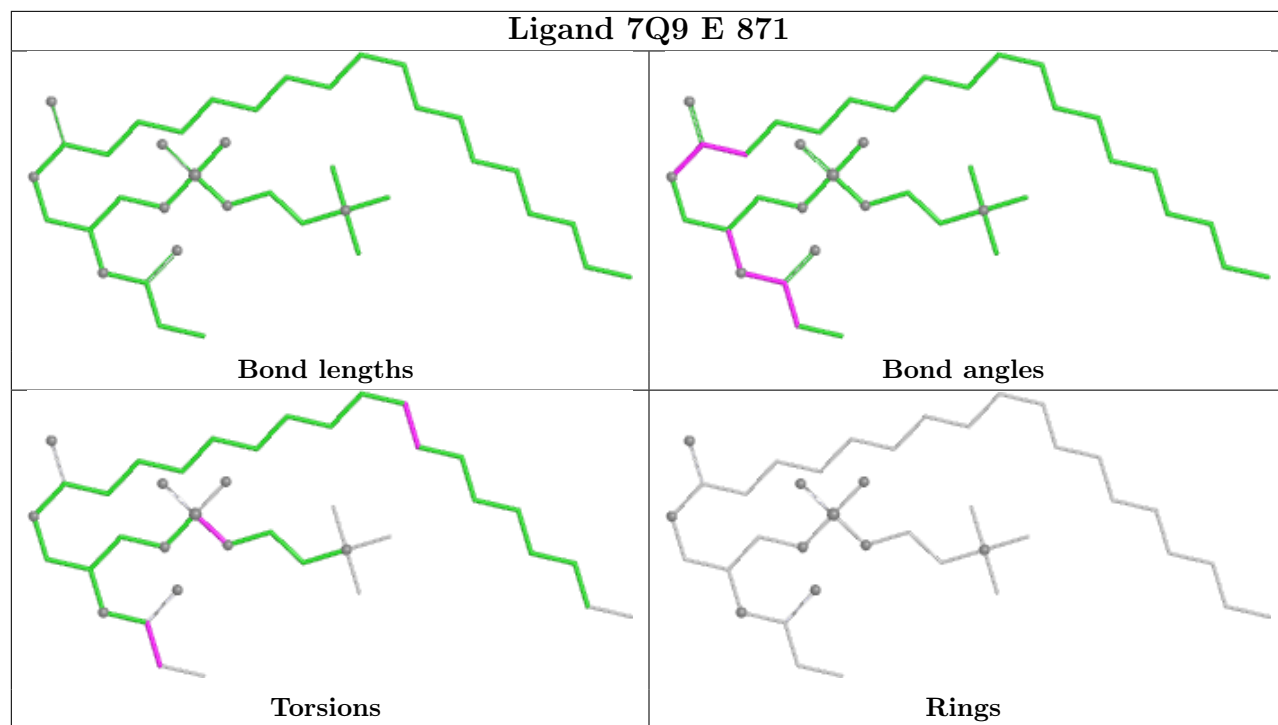
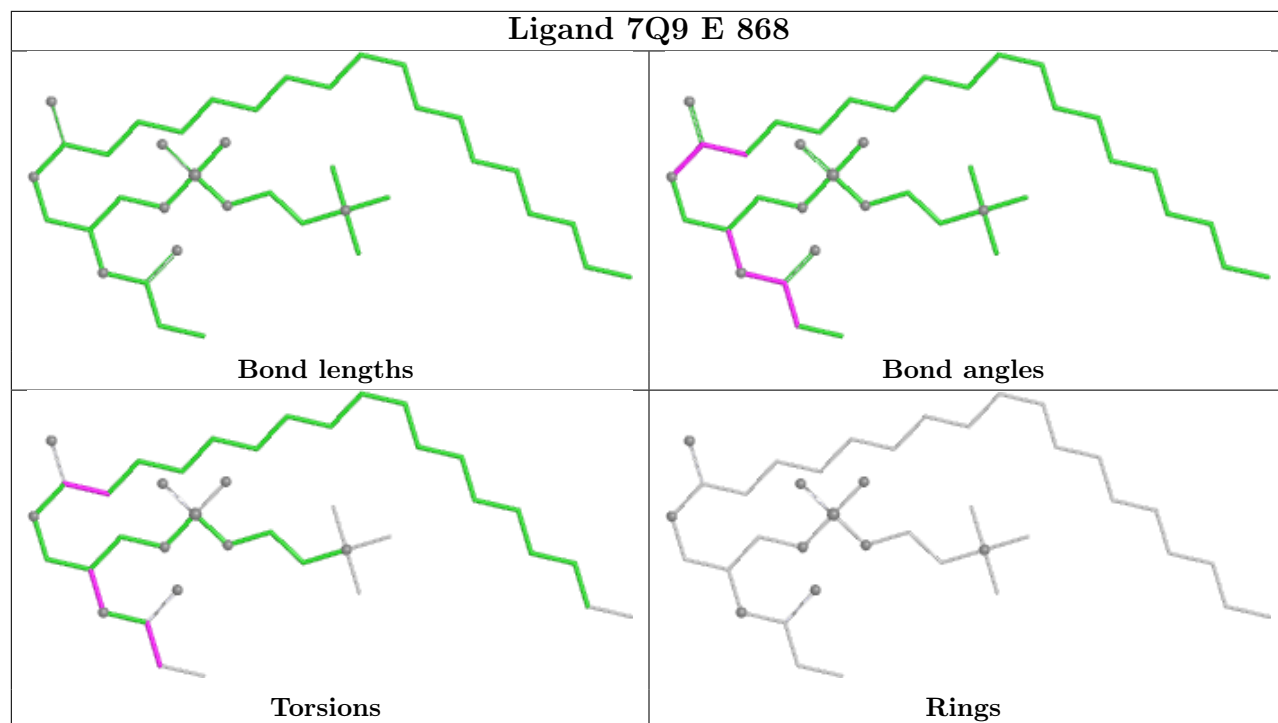


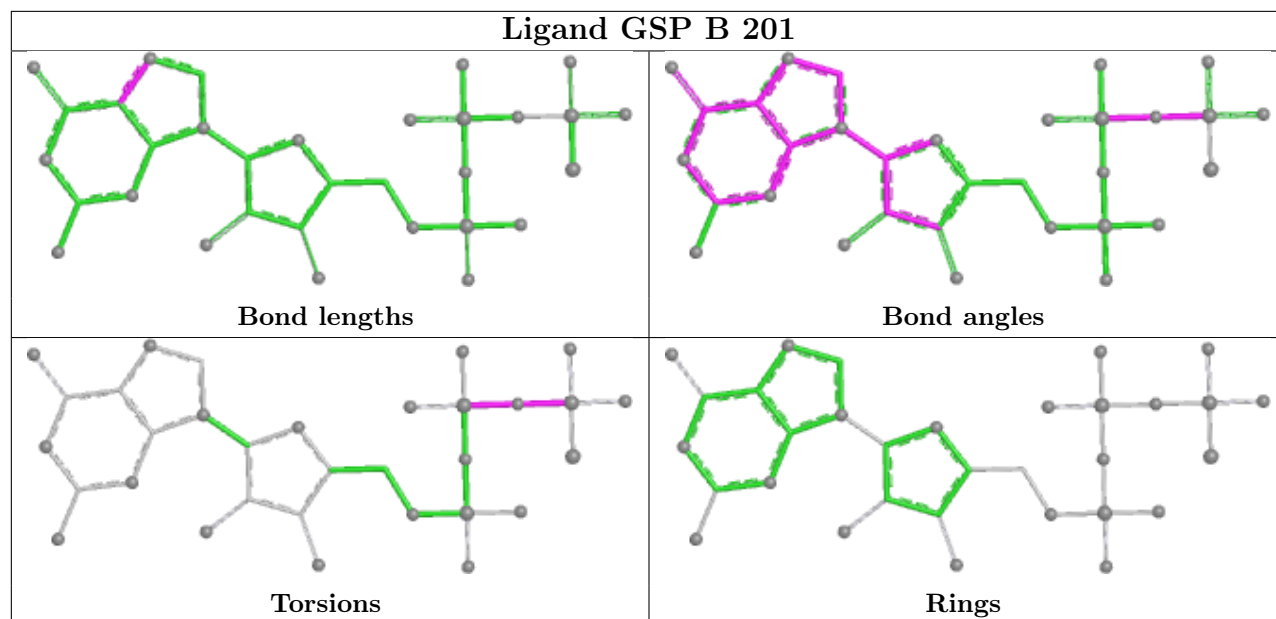
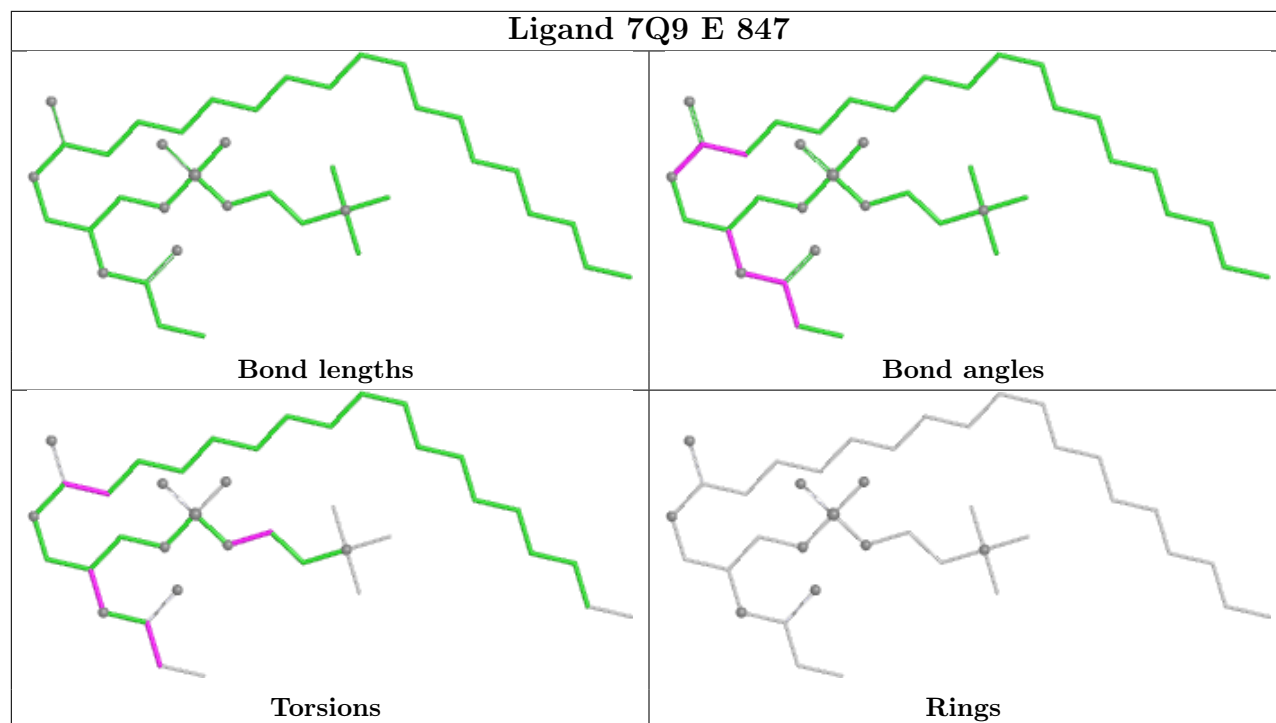


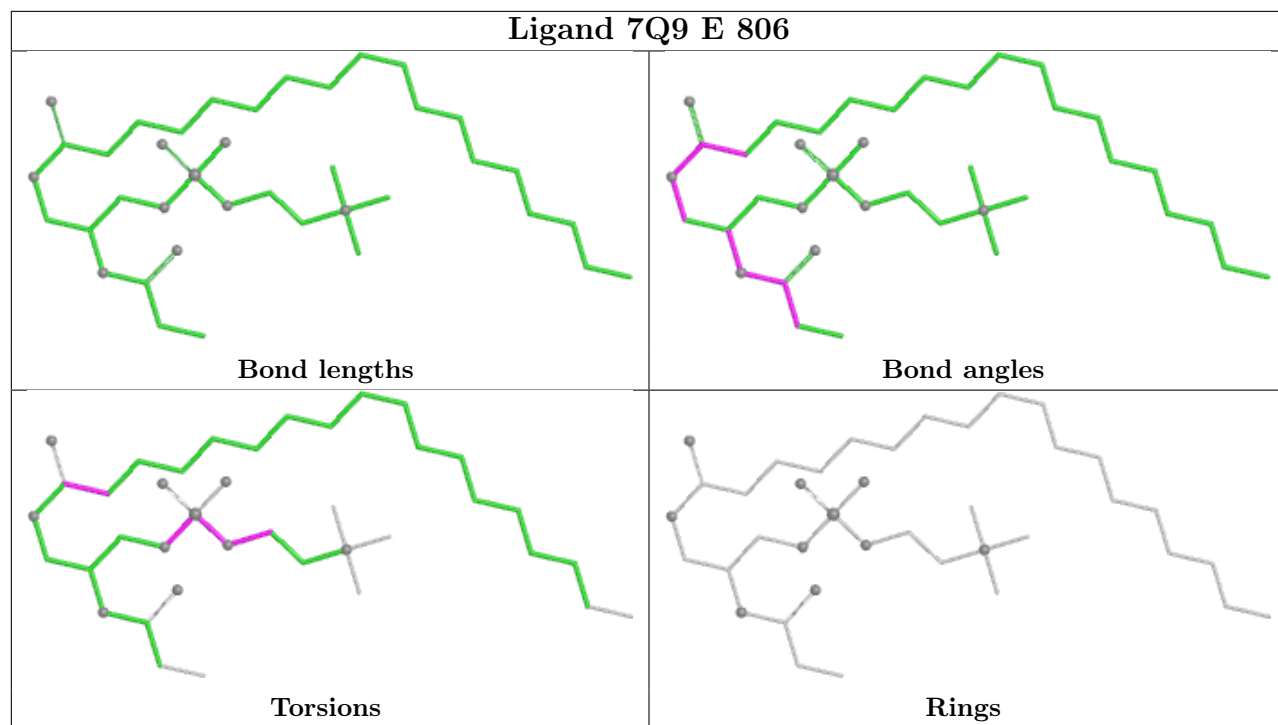
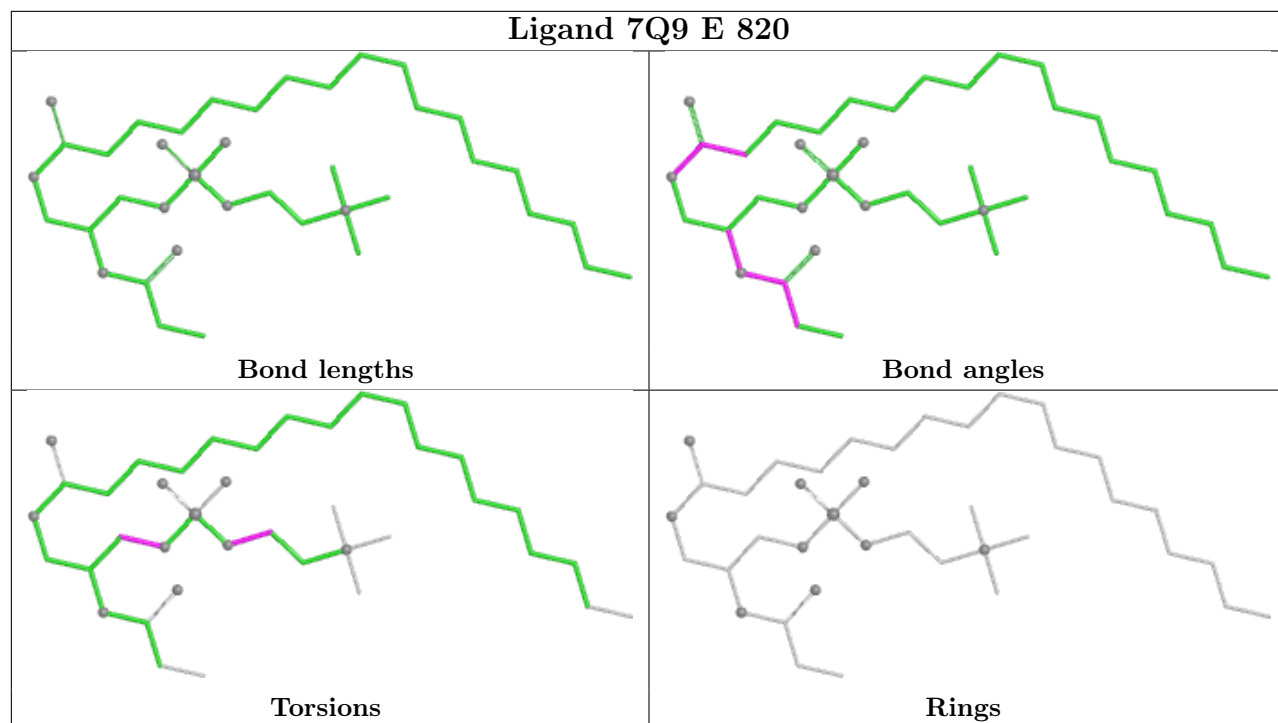


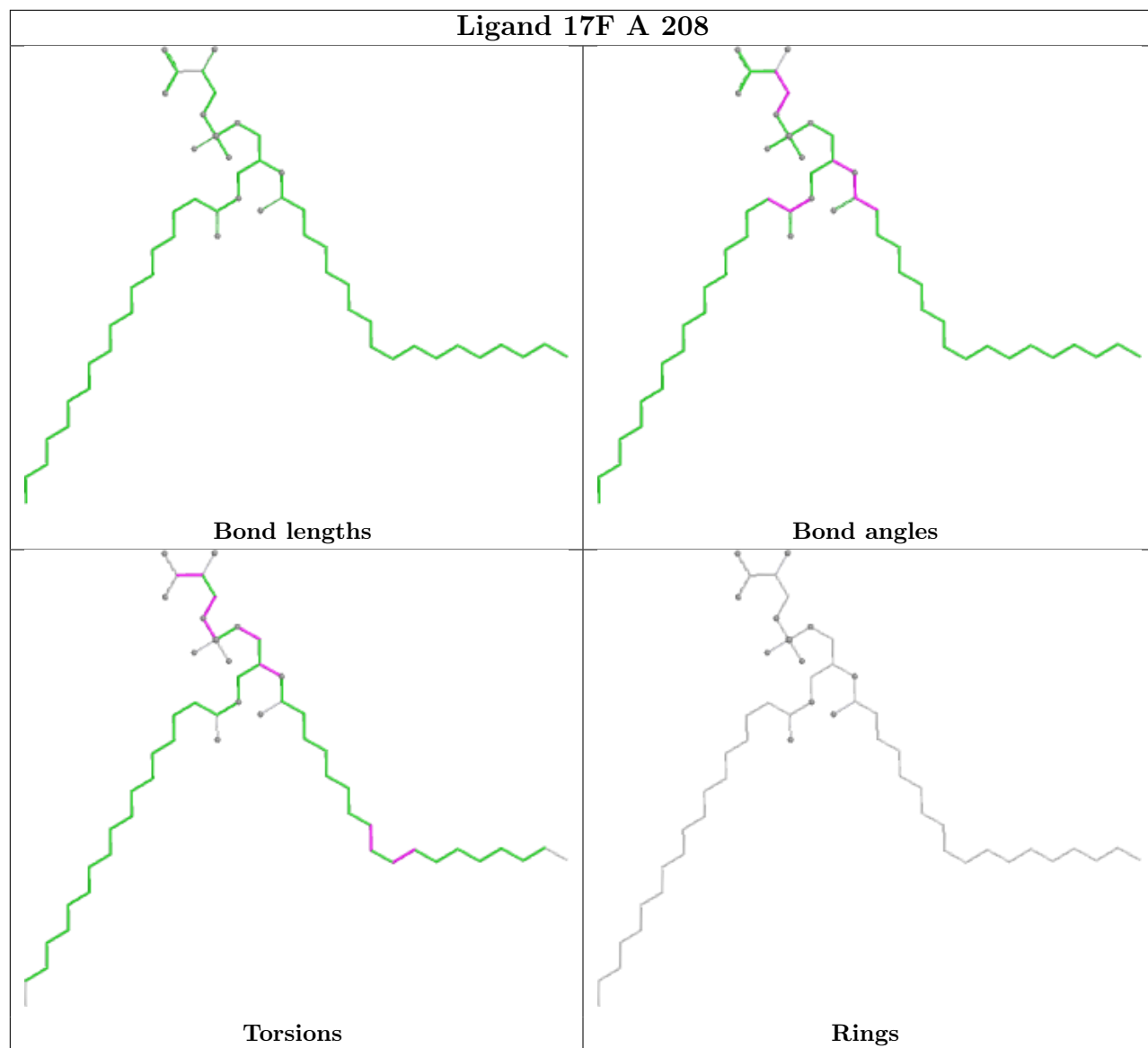


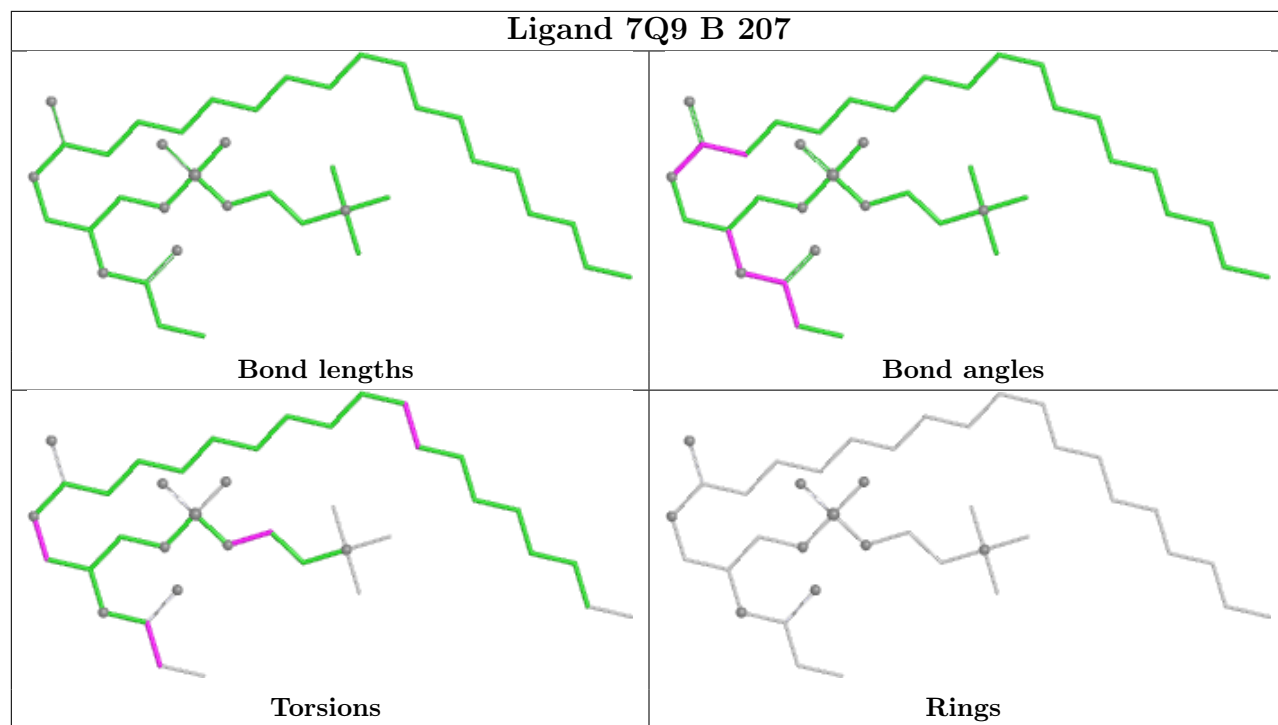
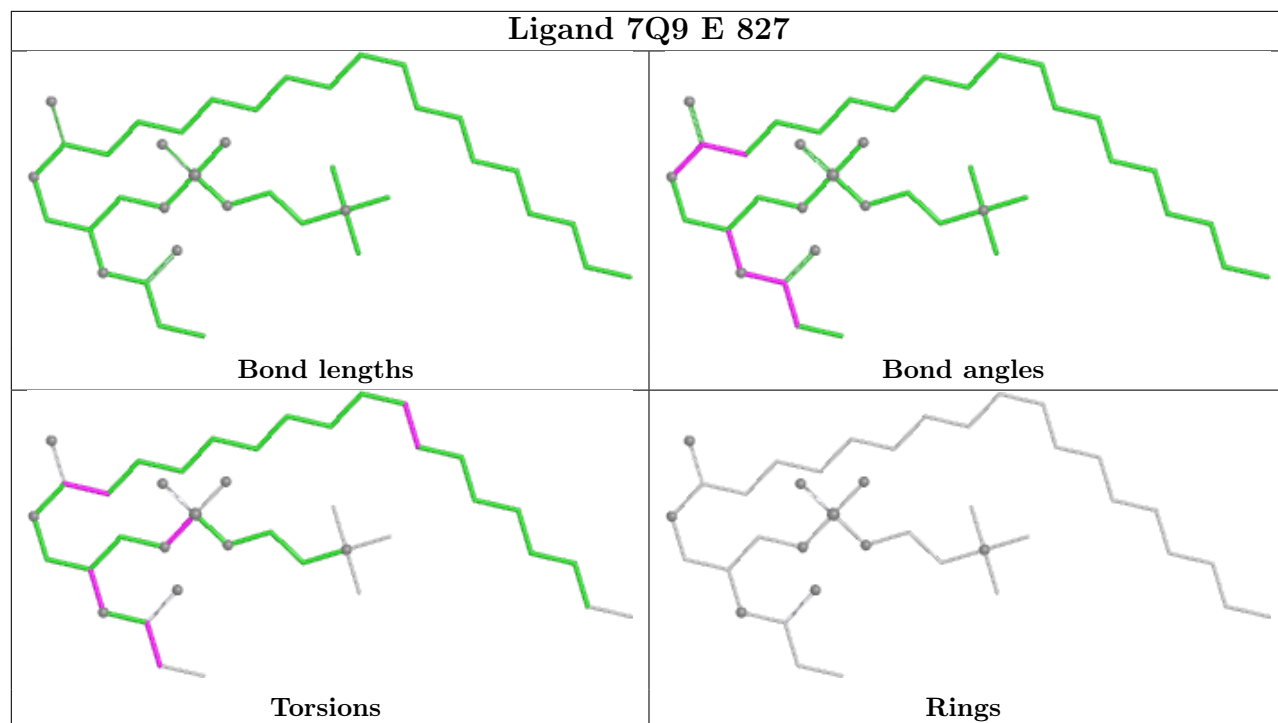


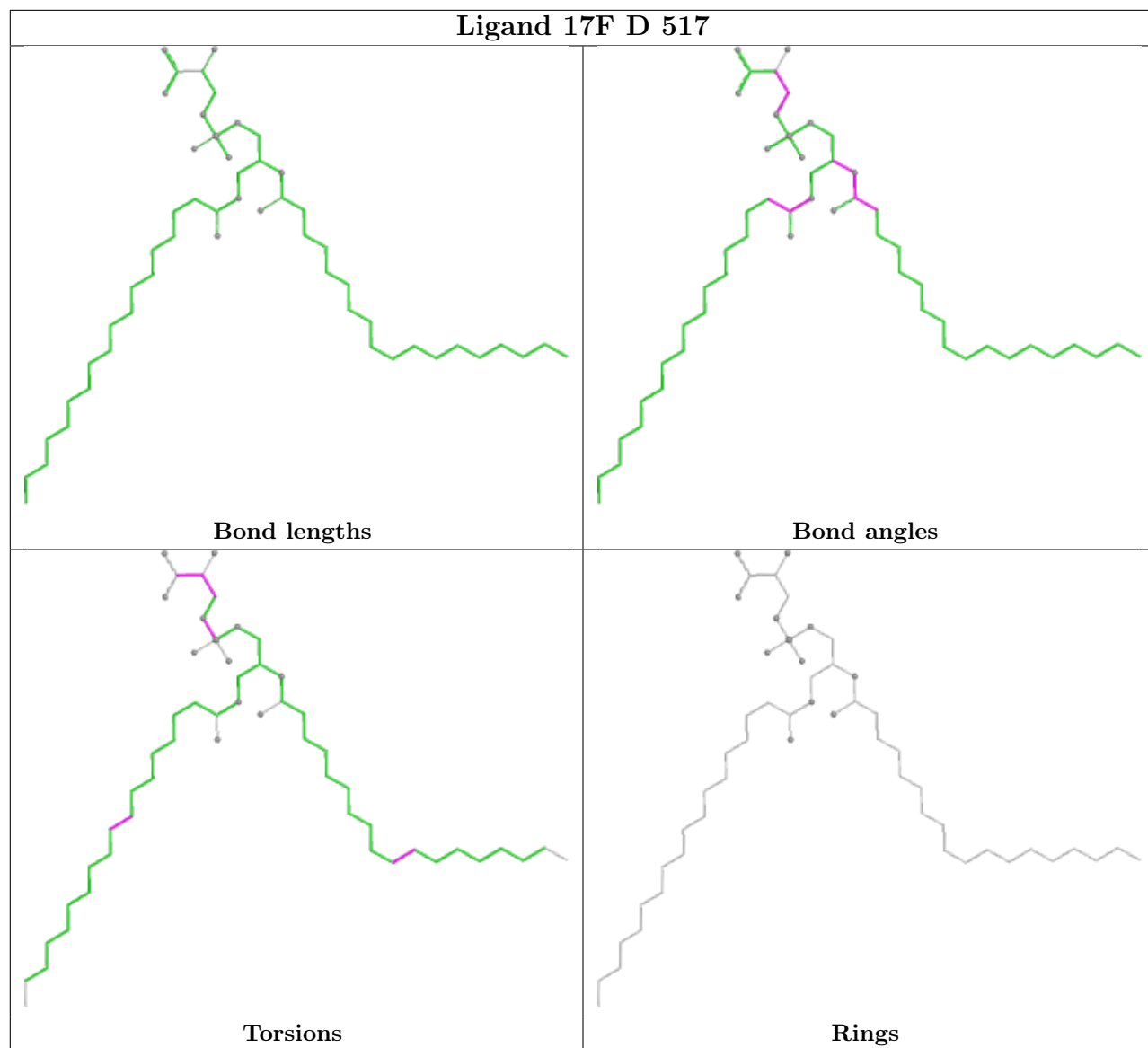


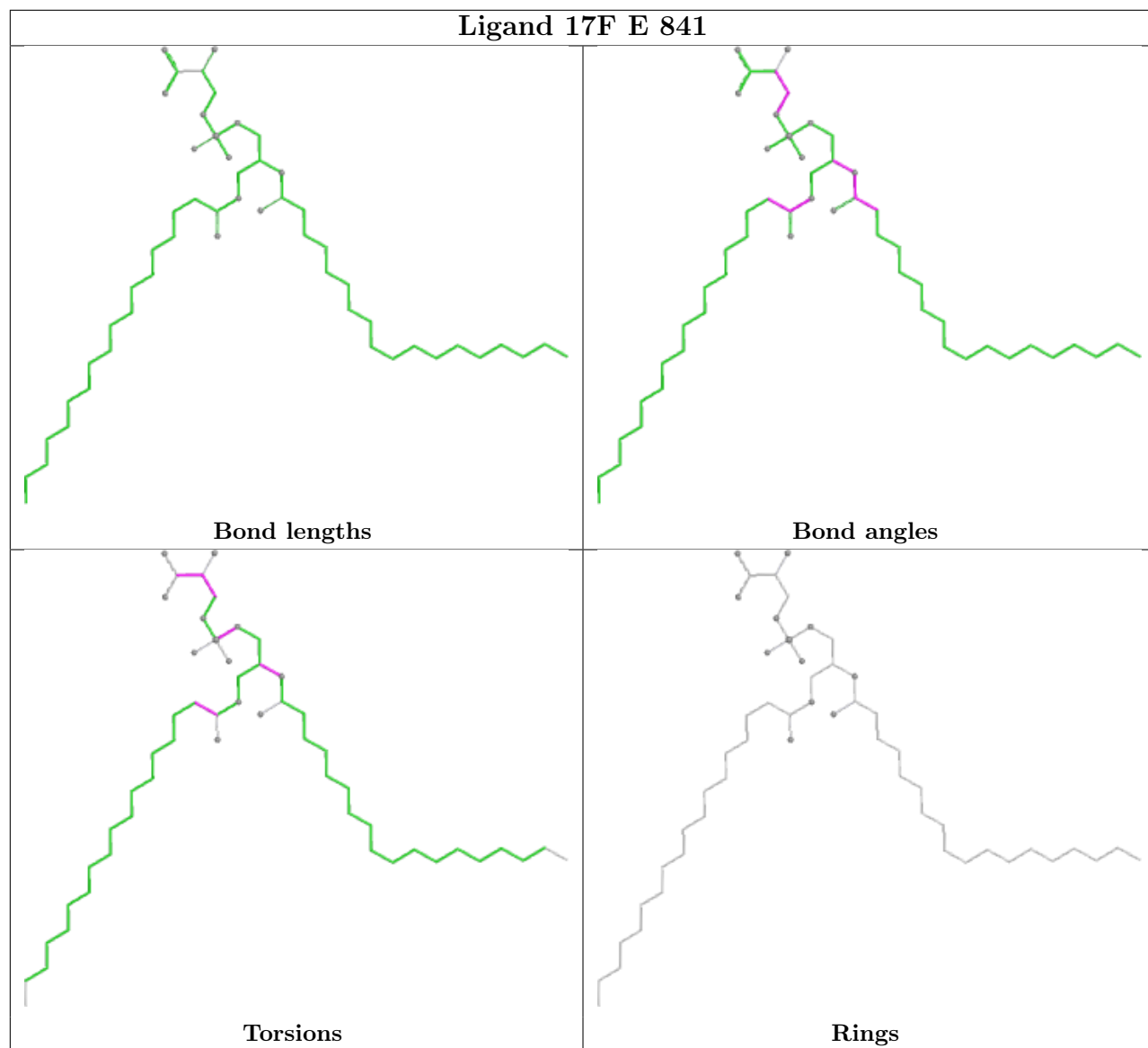


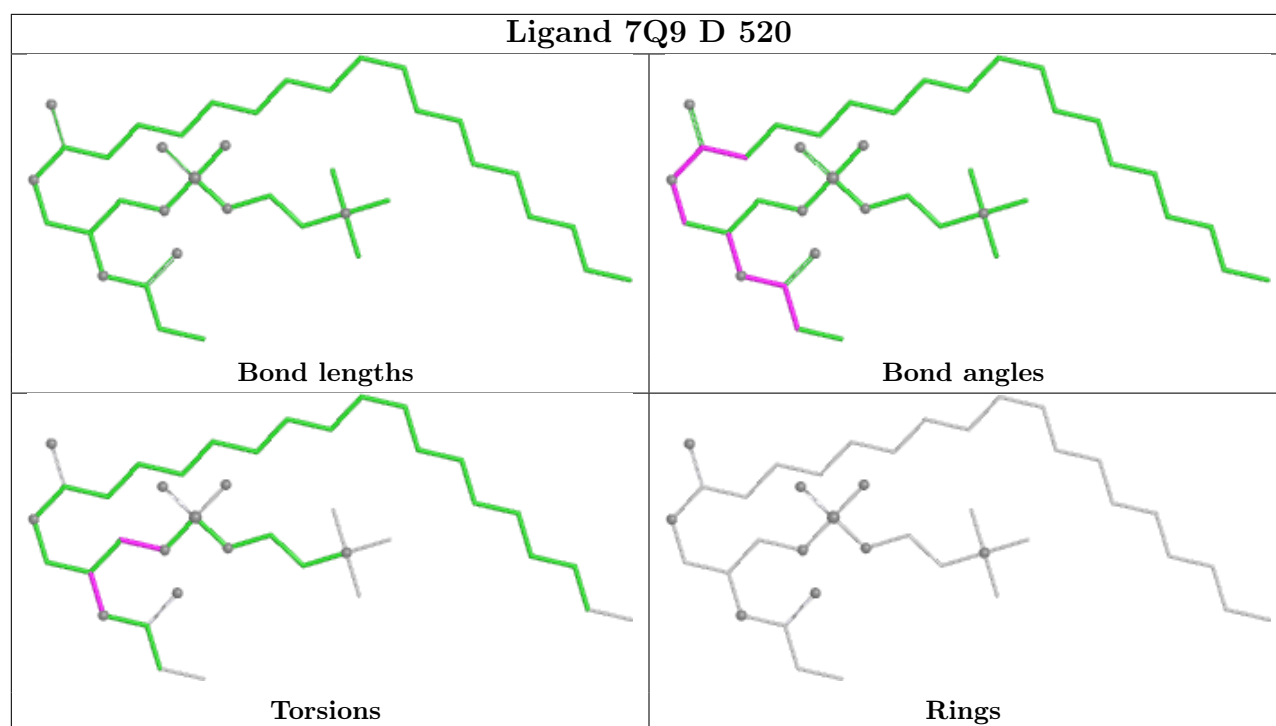


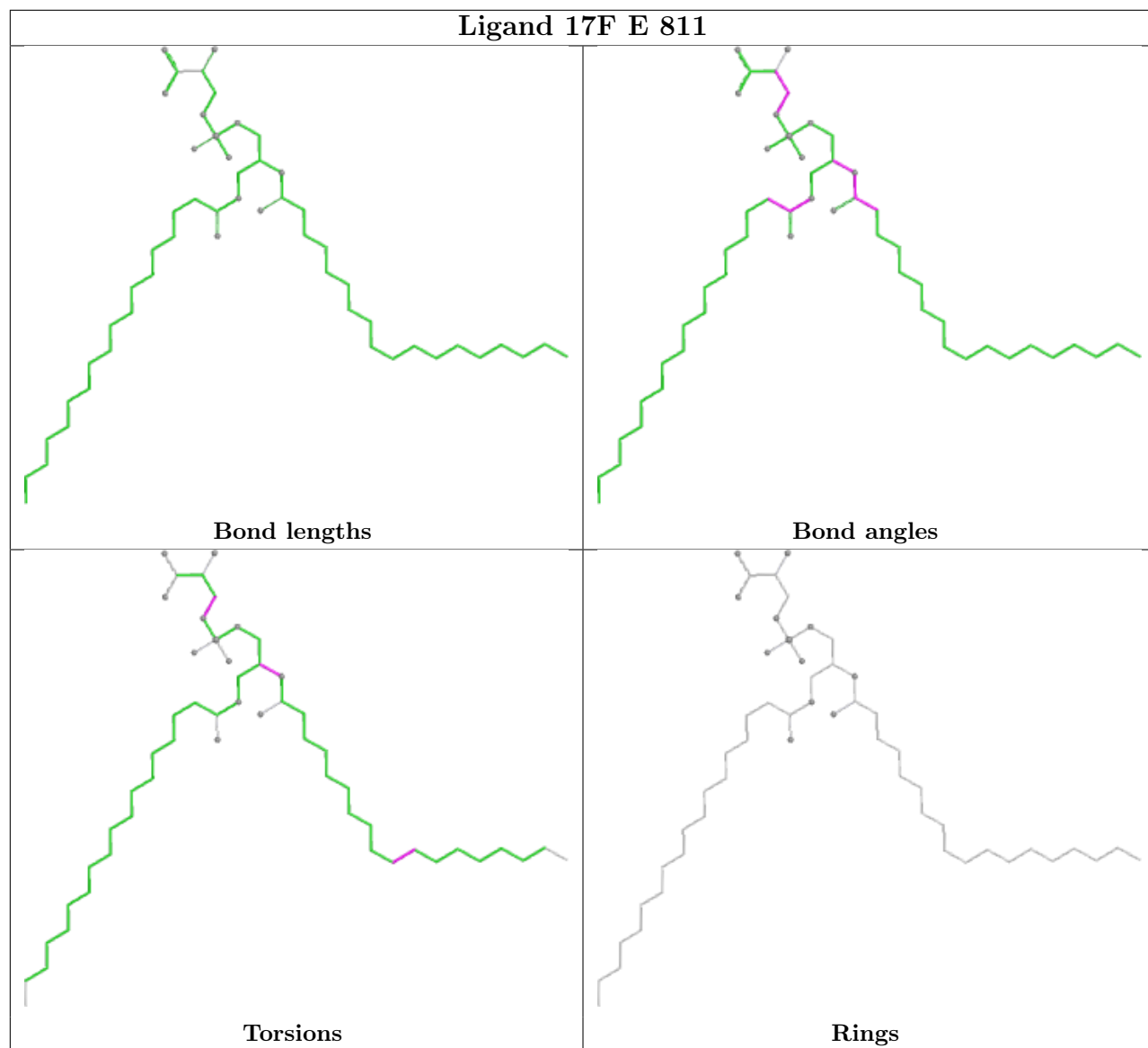


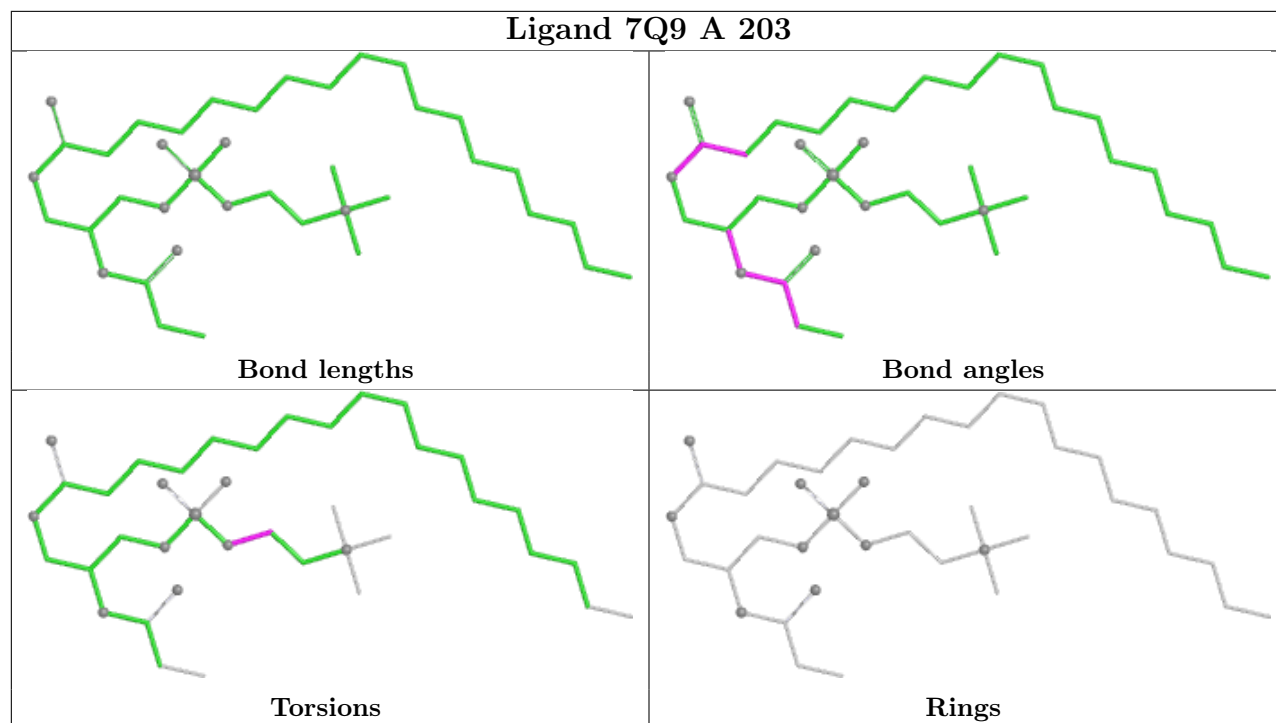


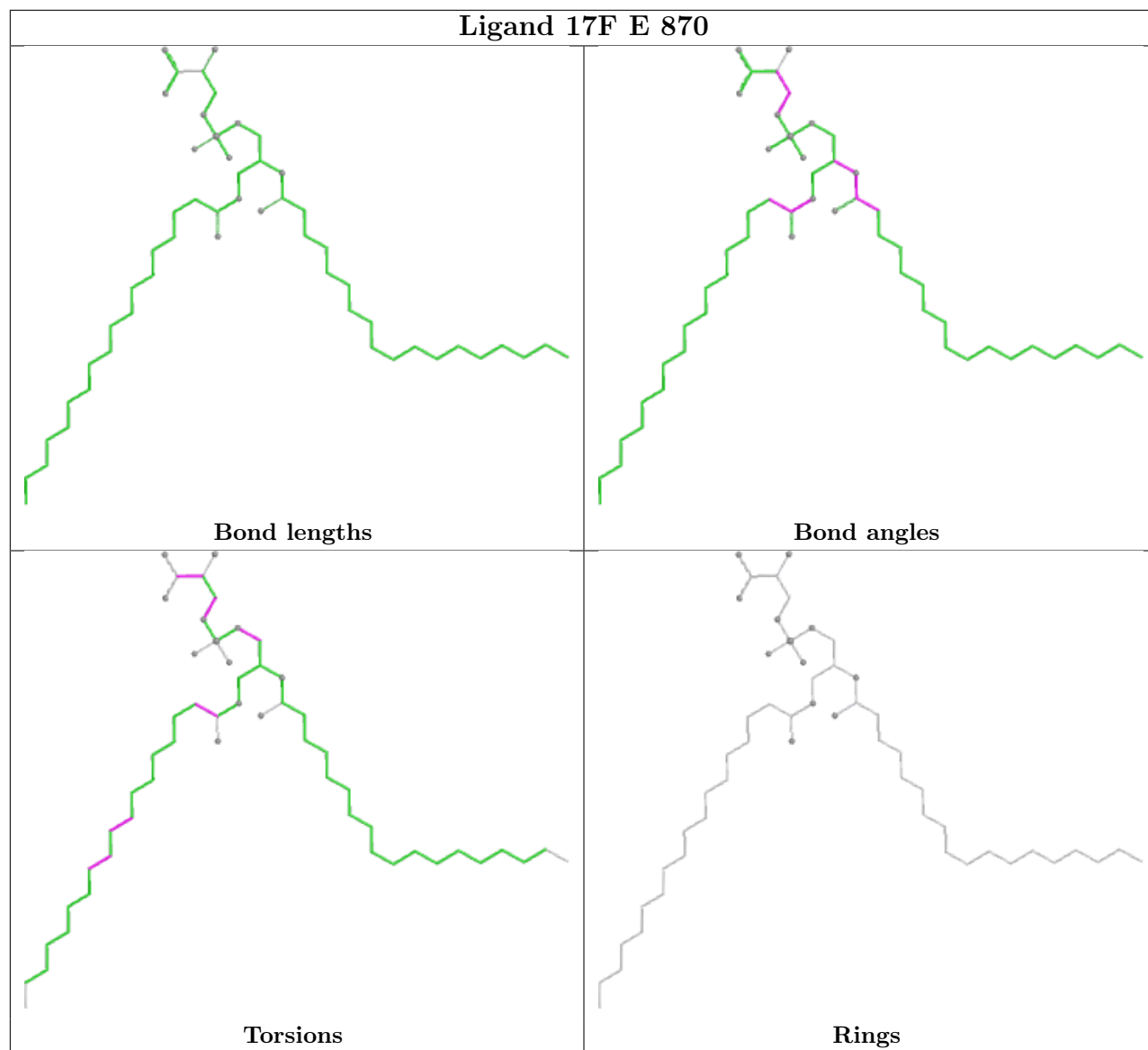


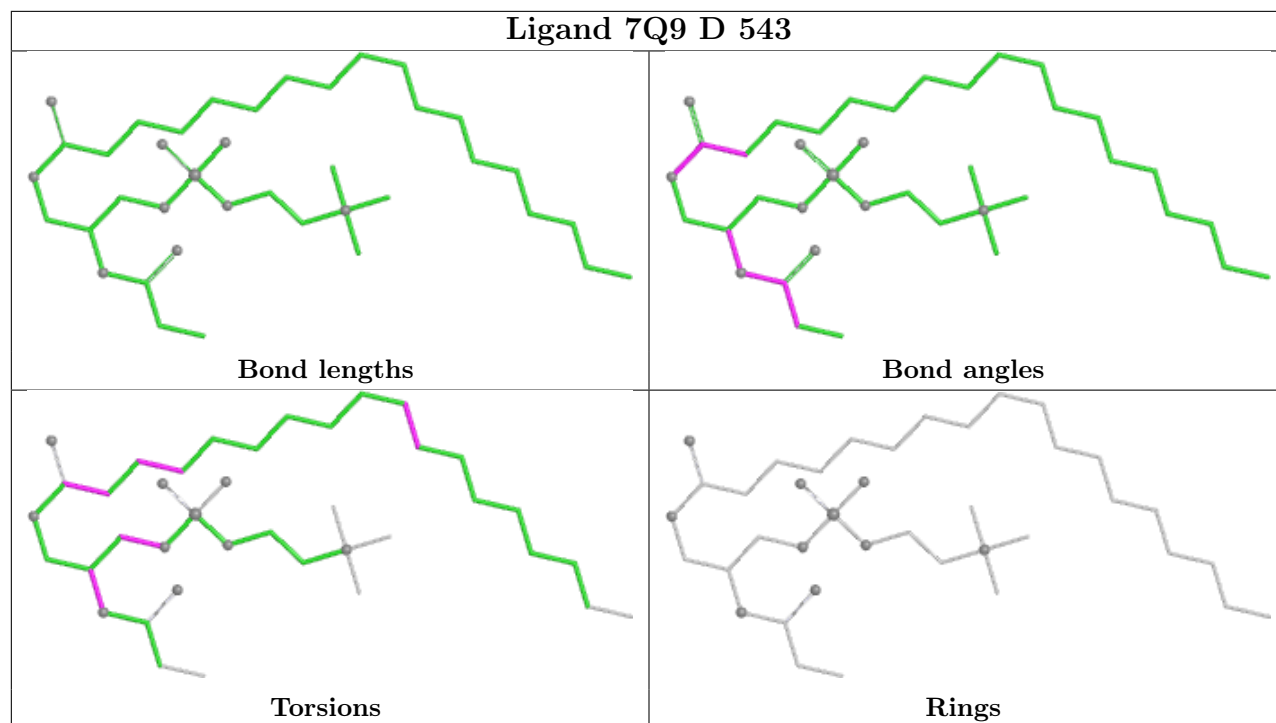






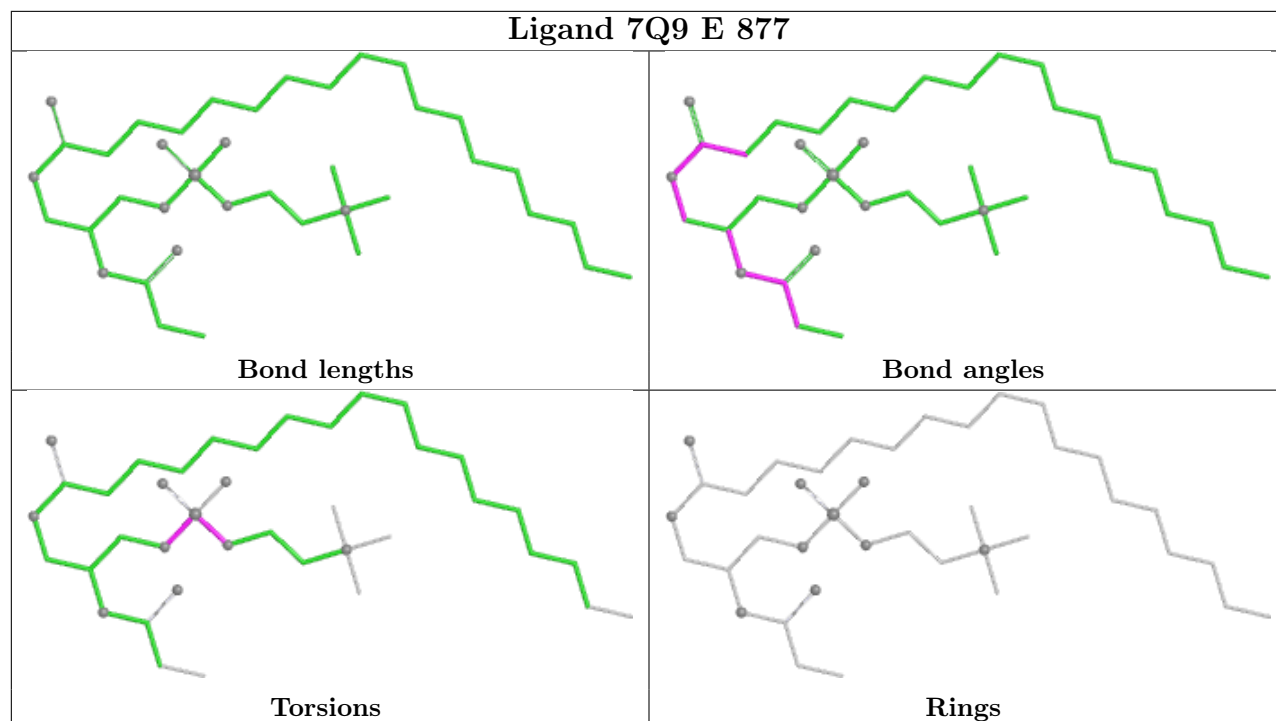




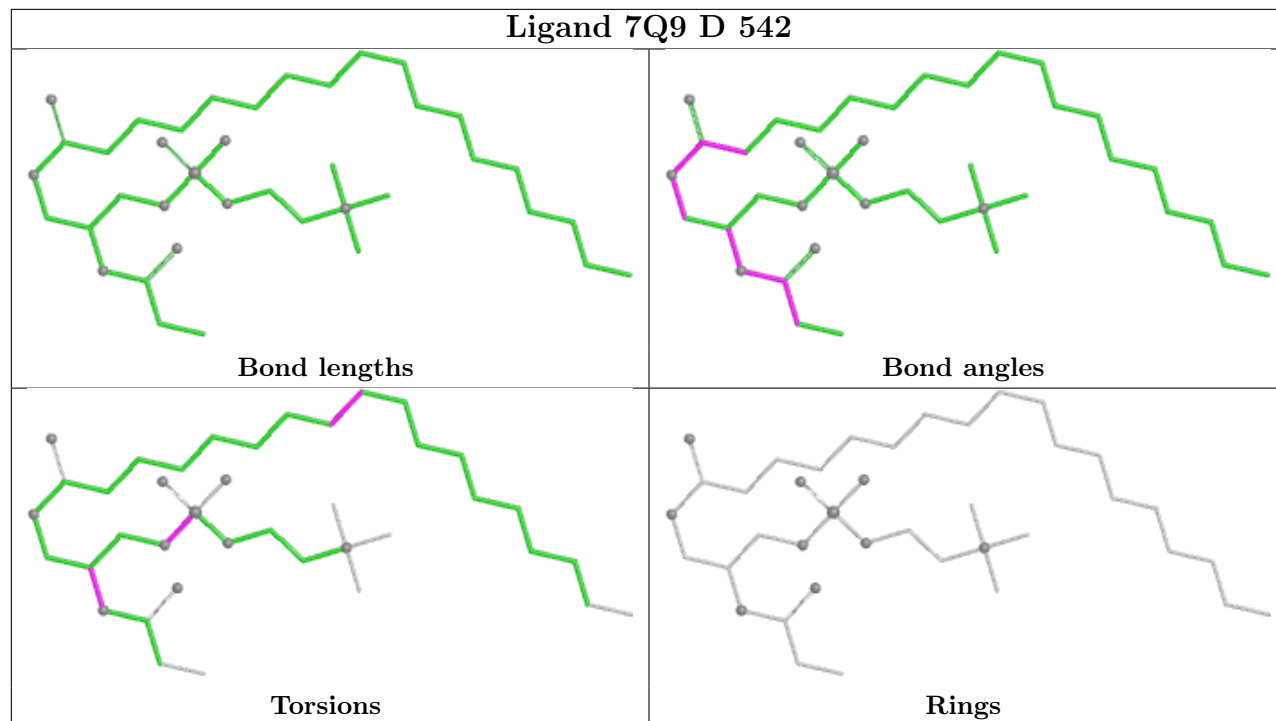


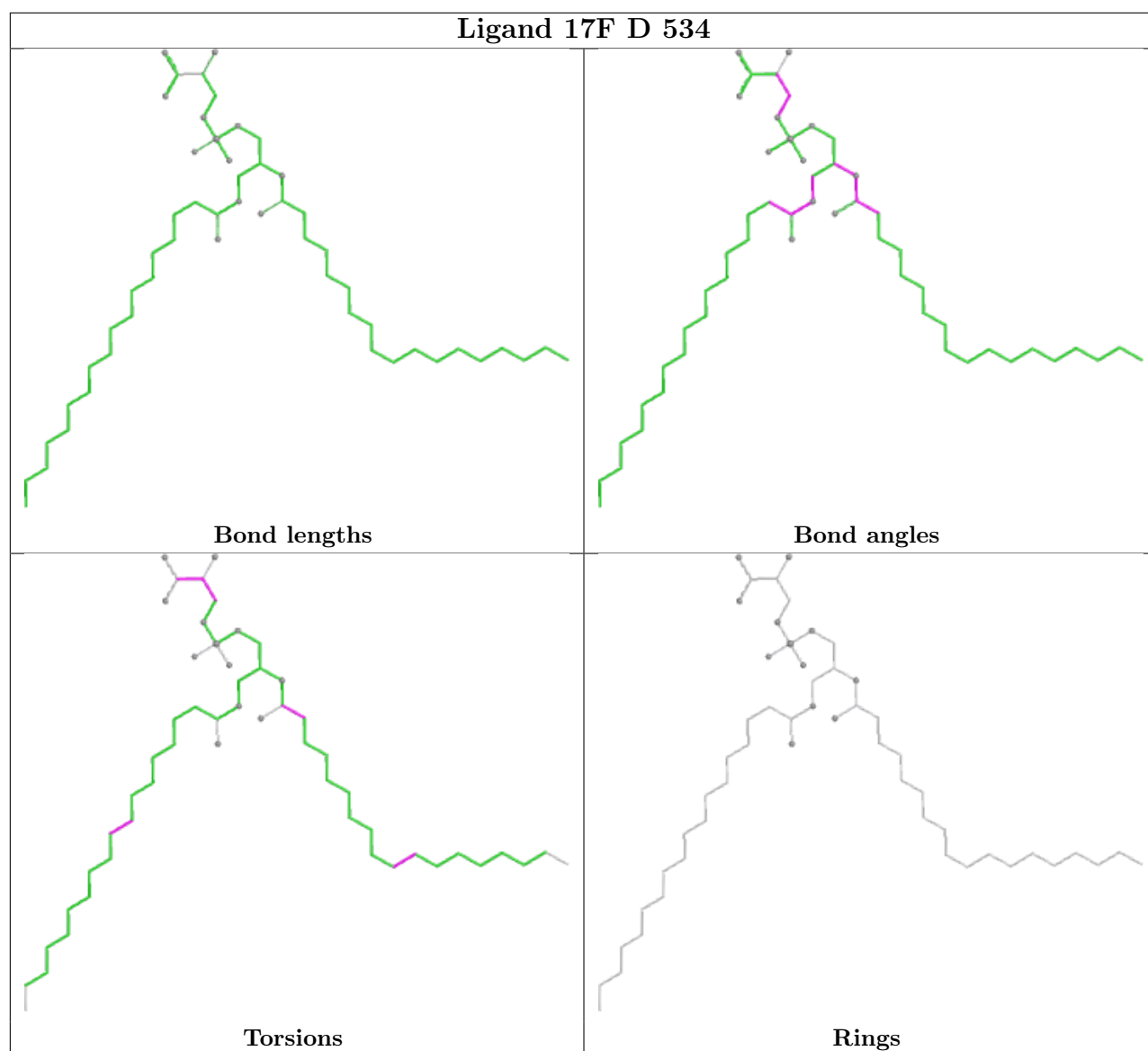


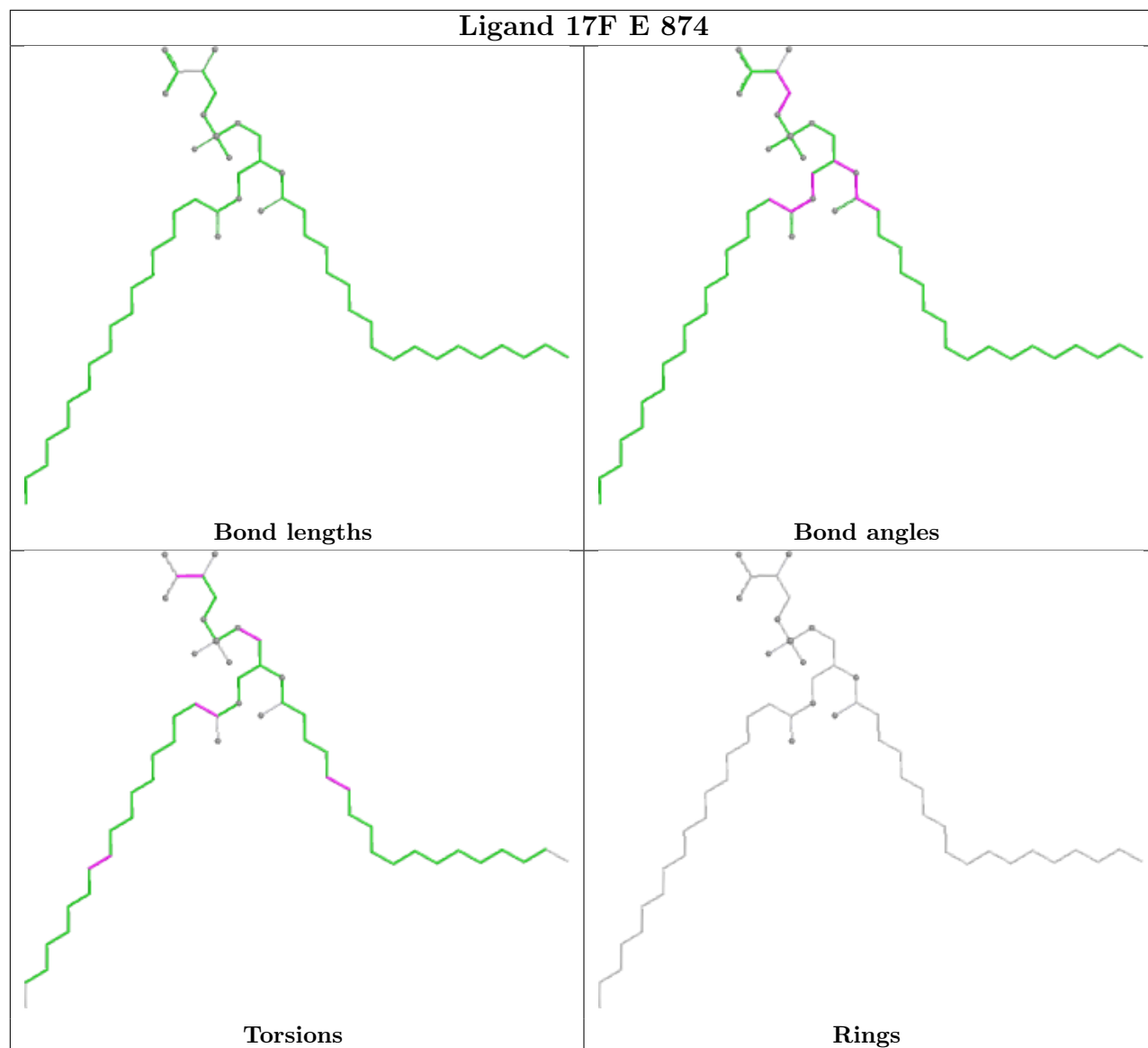
Ligand 7Q9 E 877

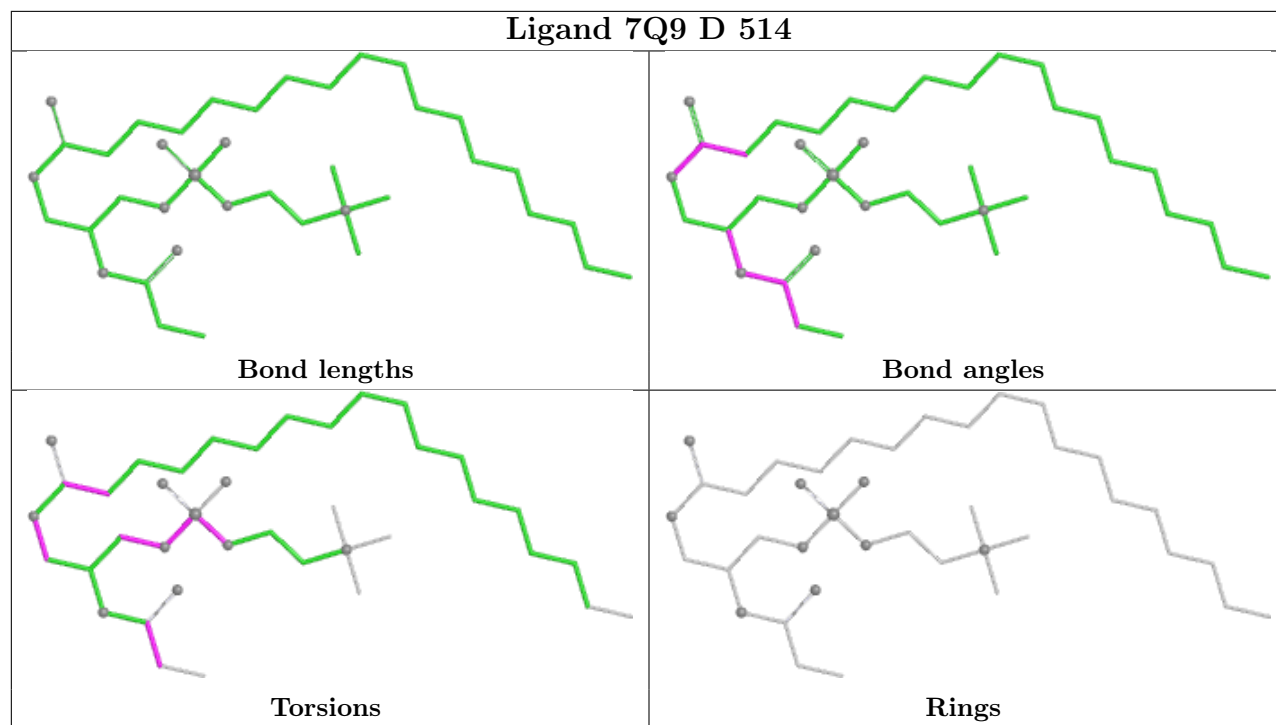
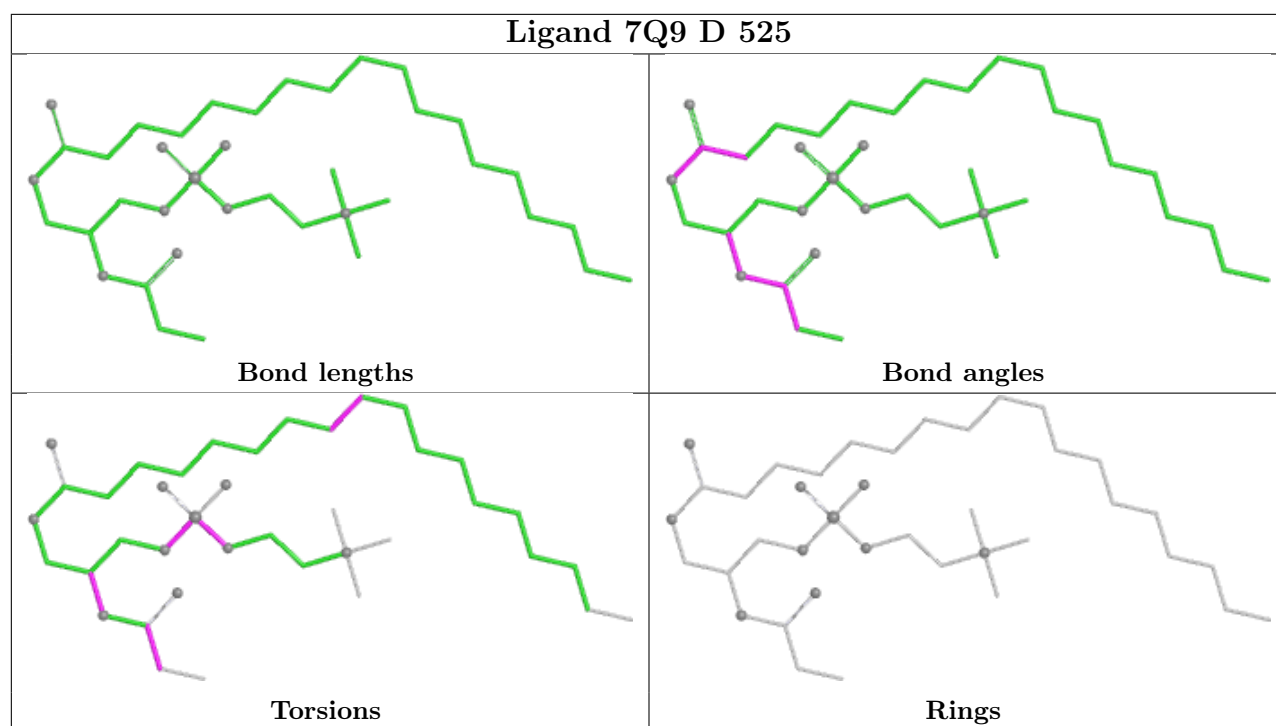


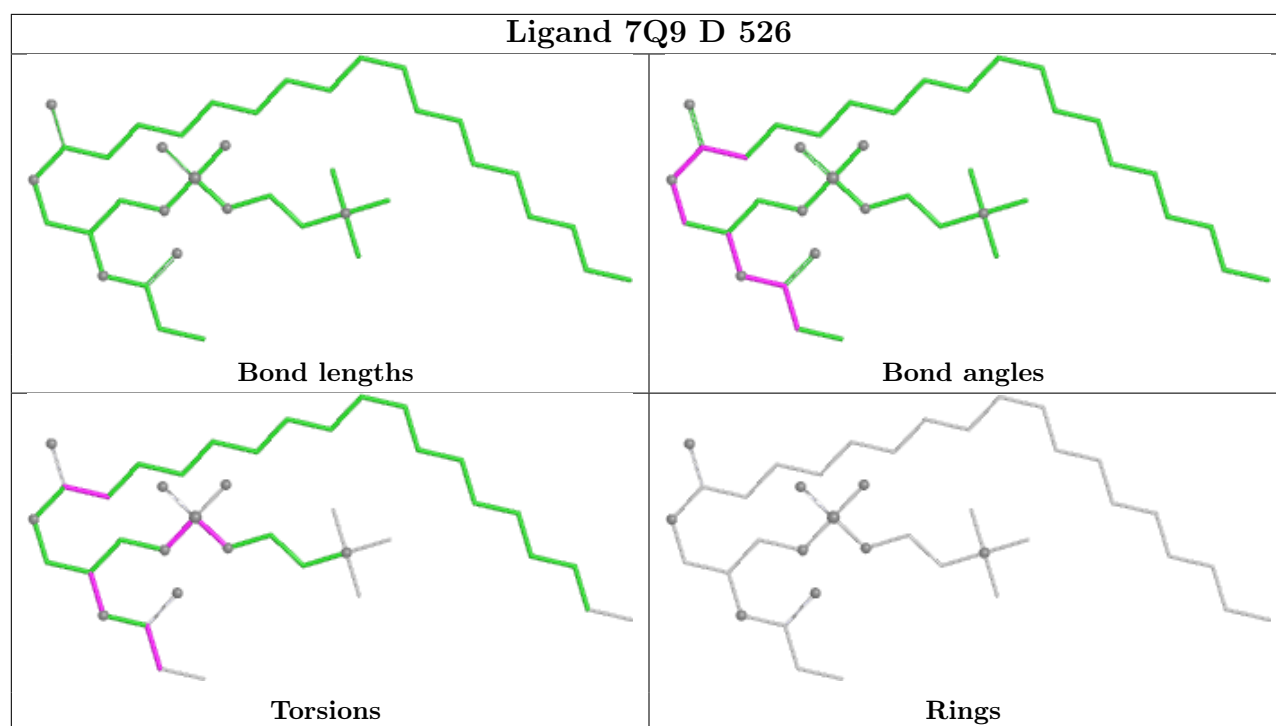
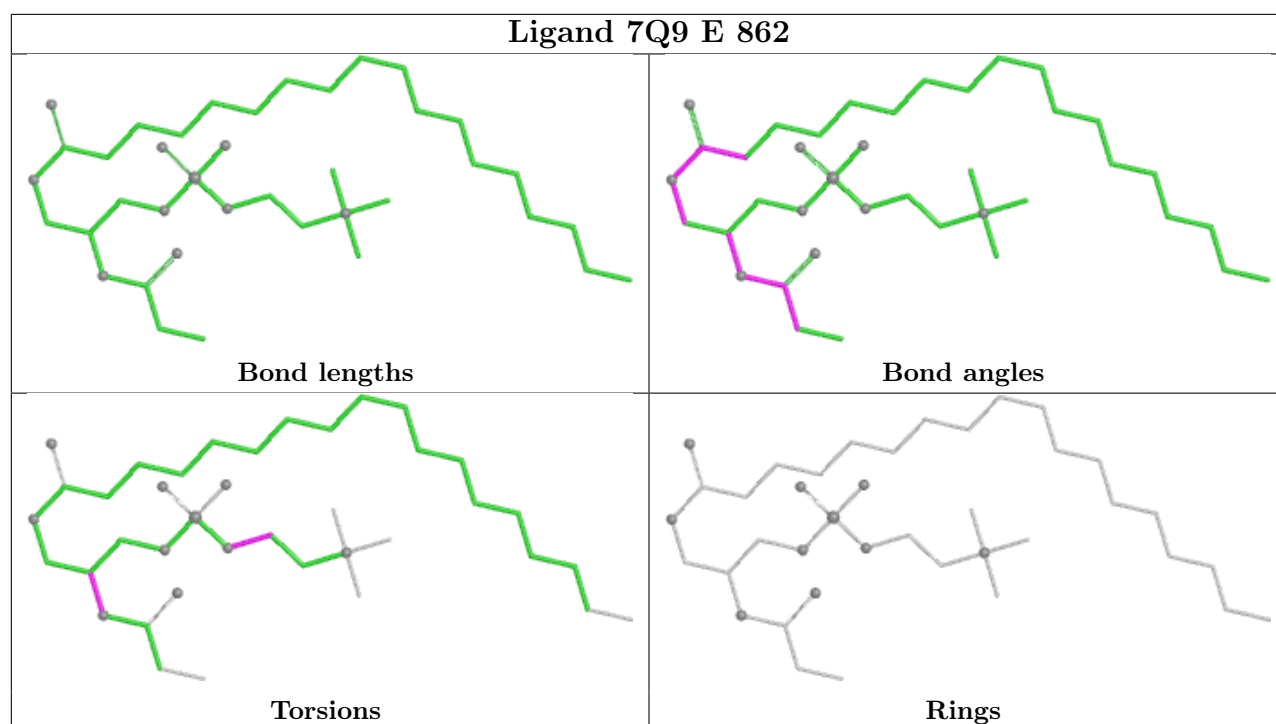
Ligand 7Q9 D 542

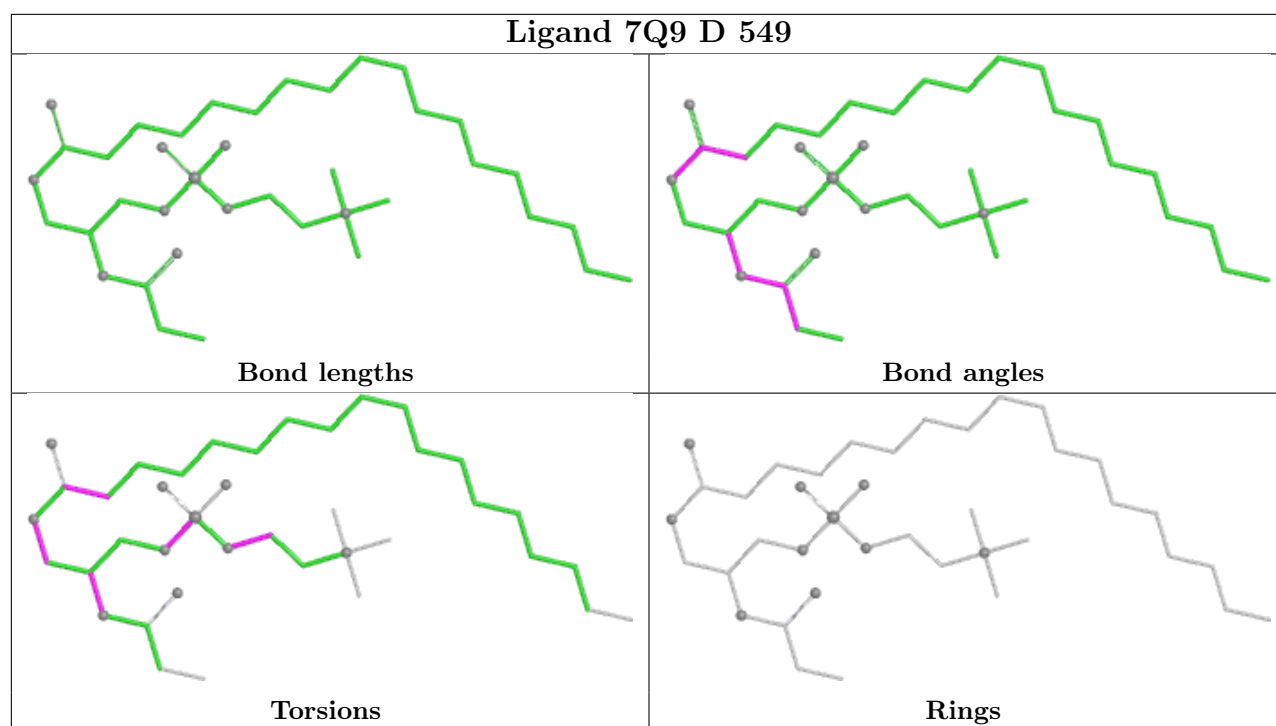


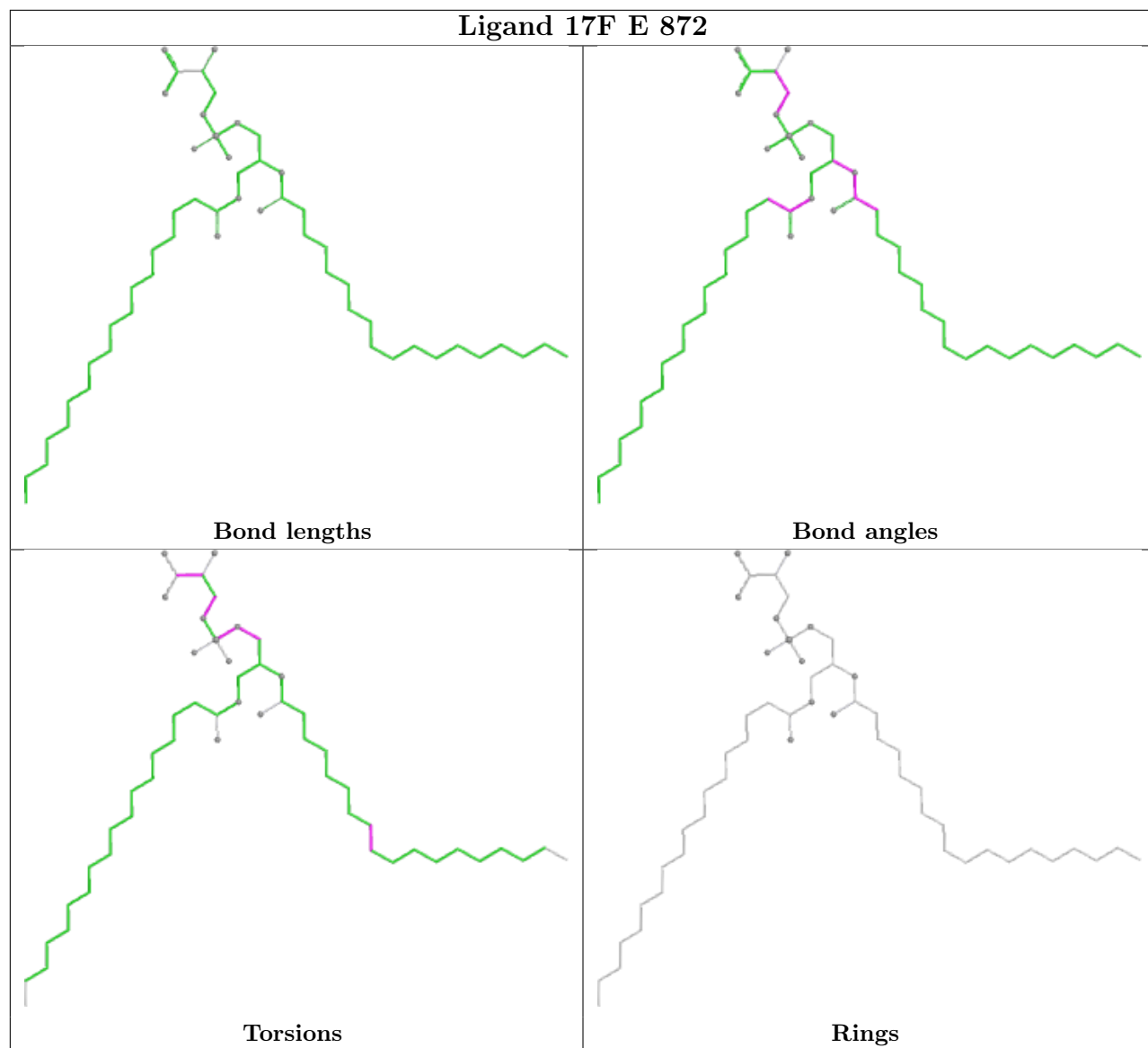




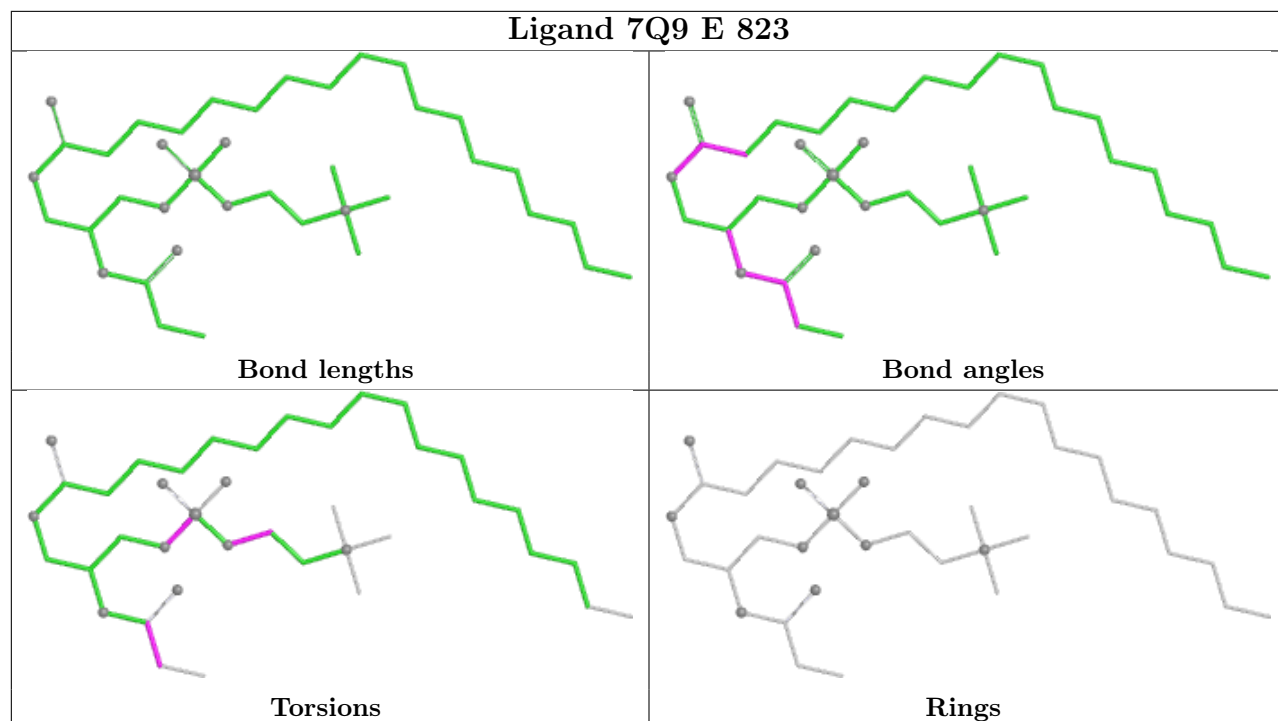




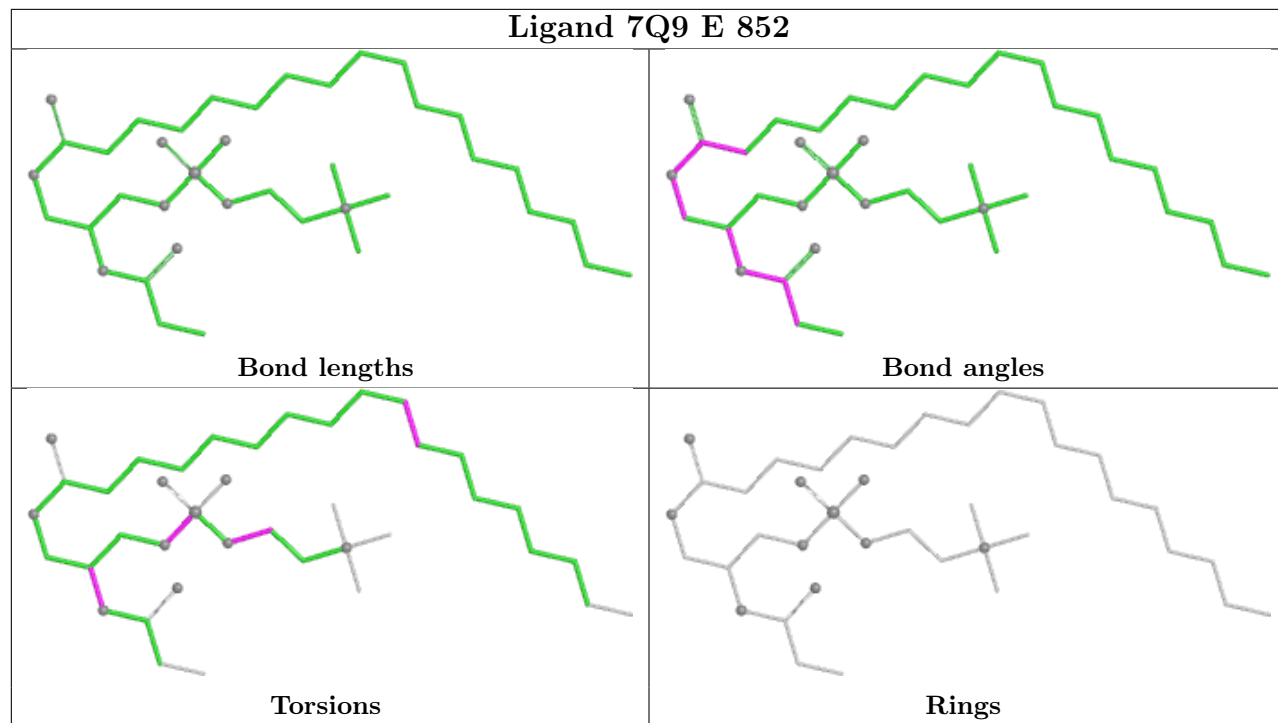


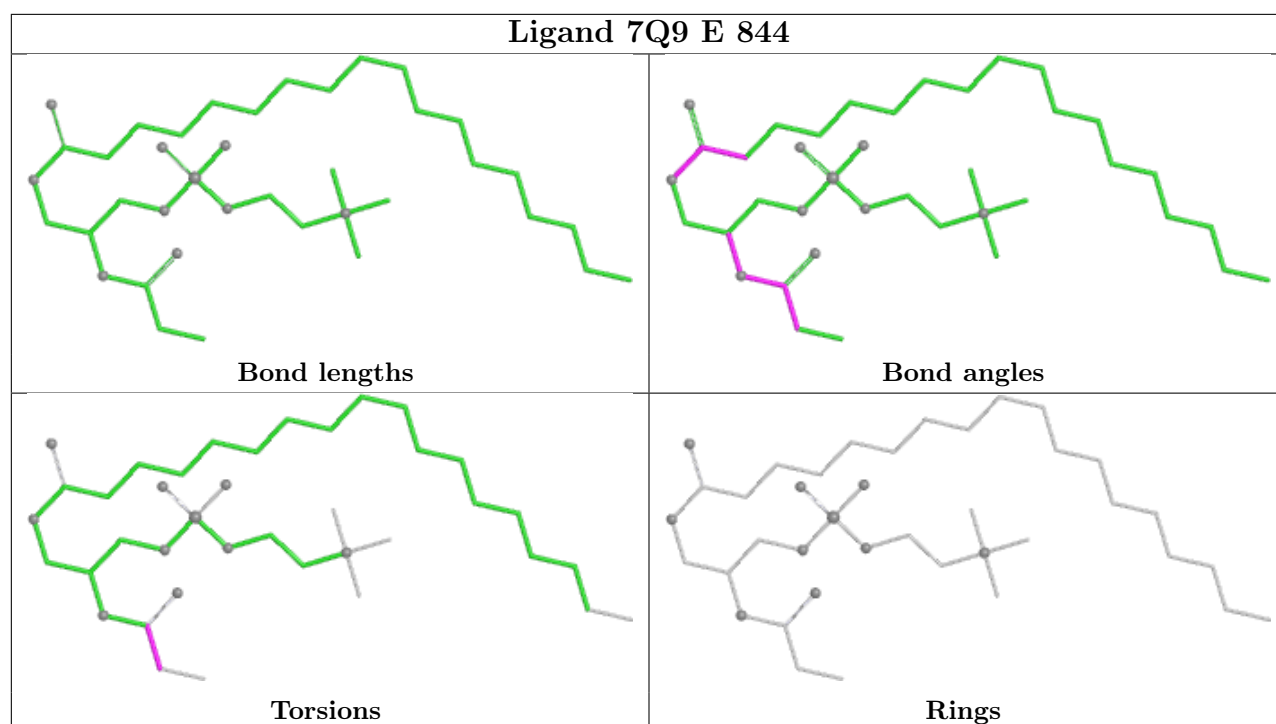


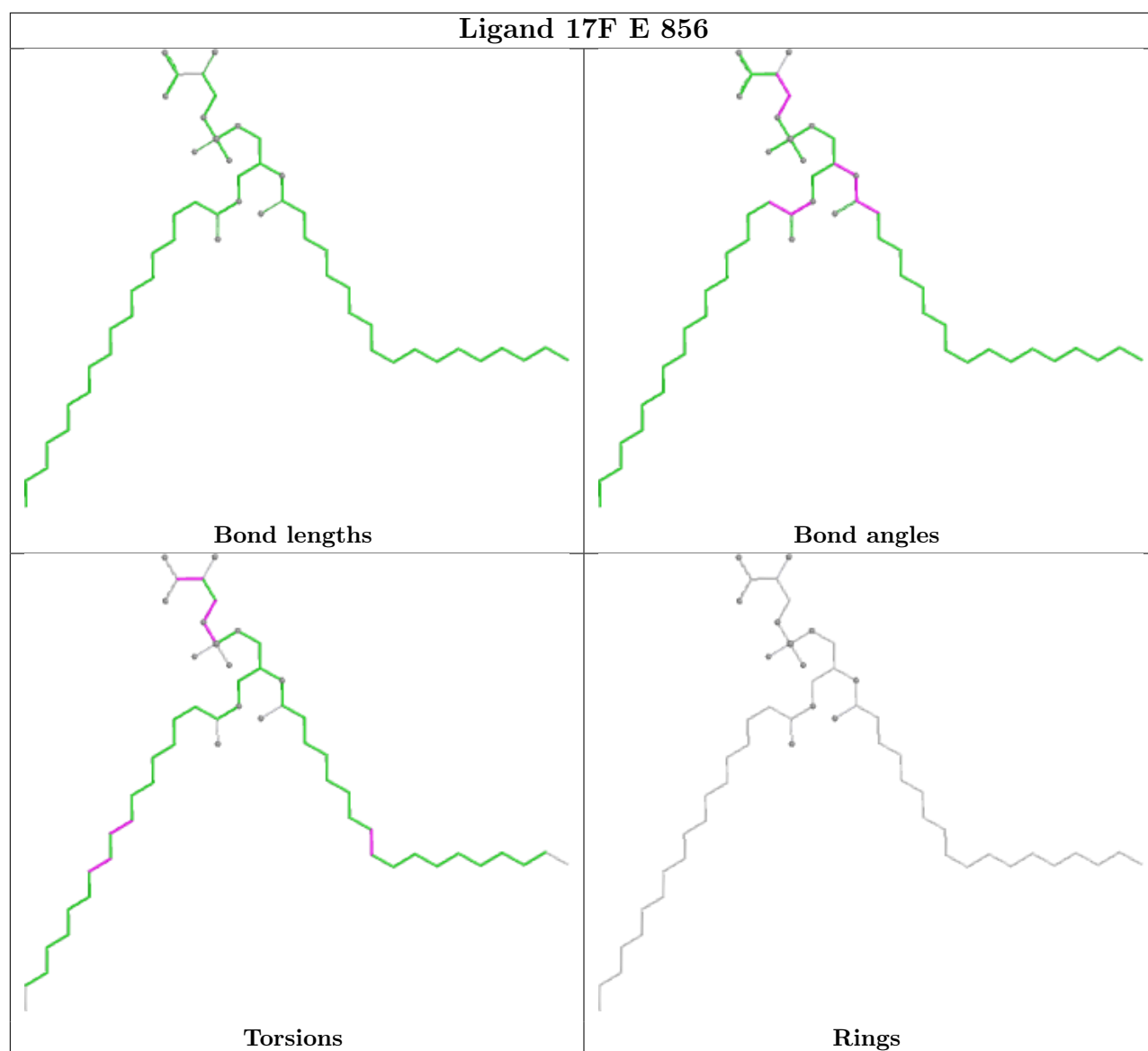
Ligand 7Q9 E 823

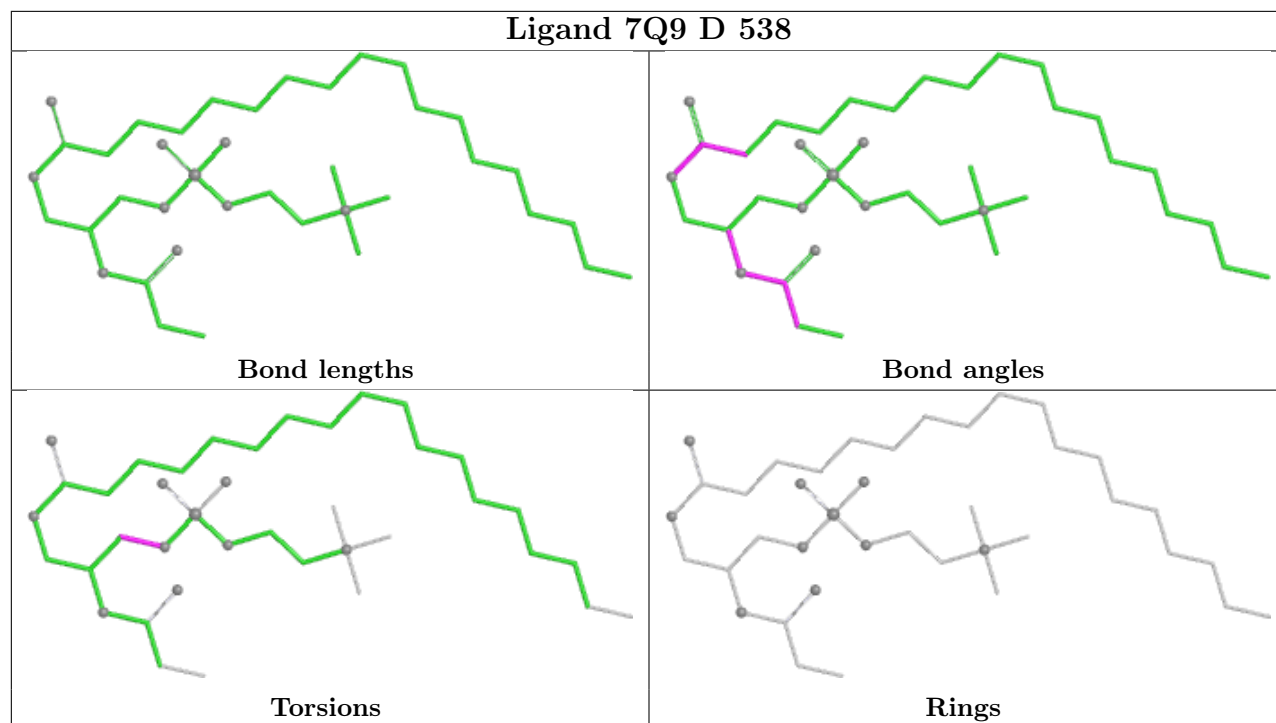


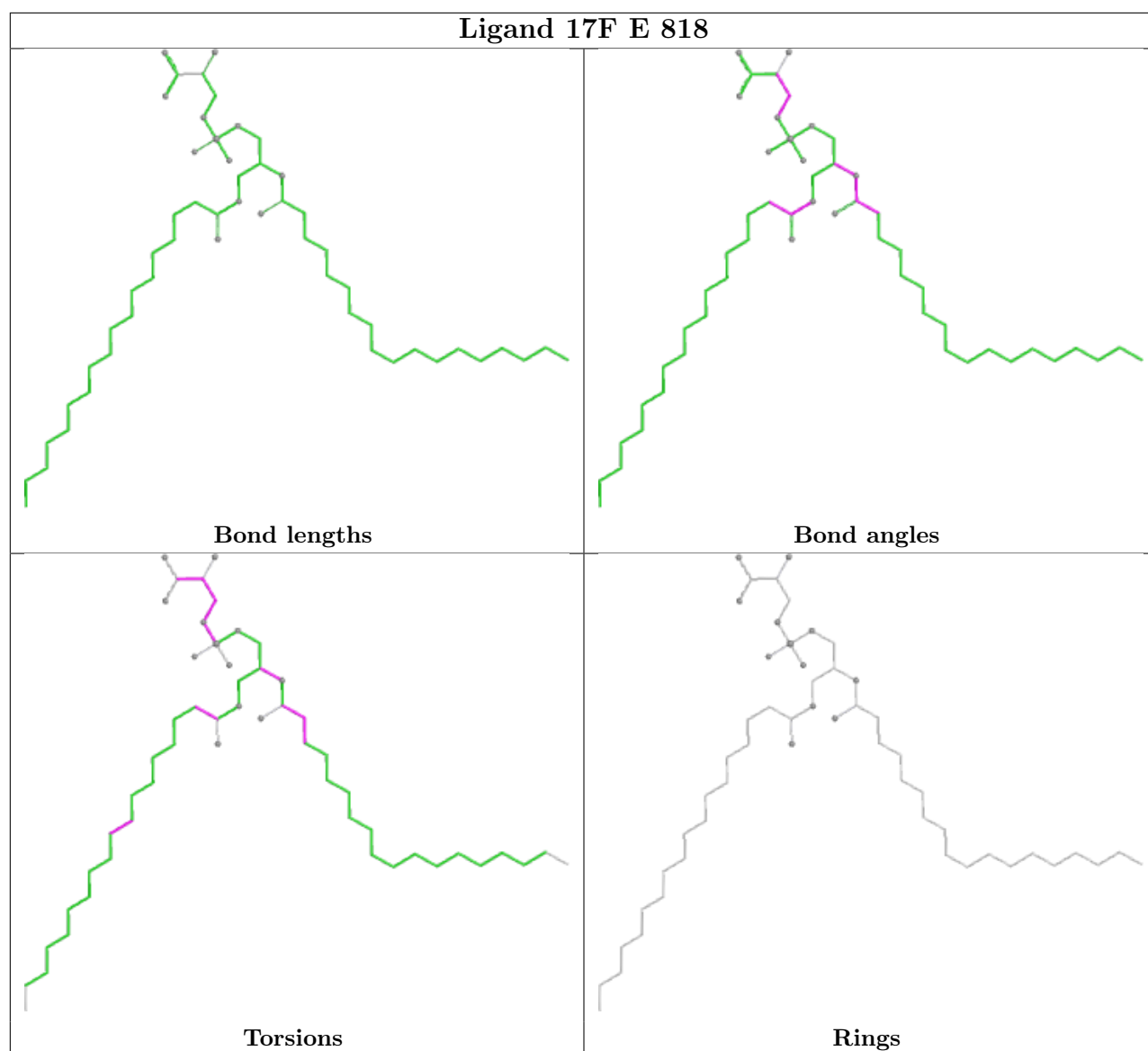
Ligand 7Q9 E 852

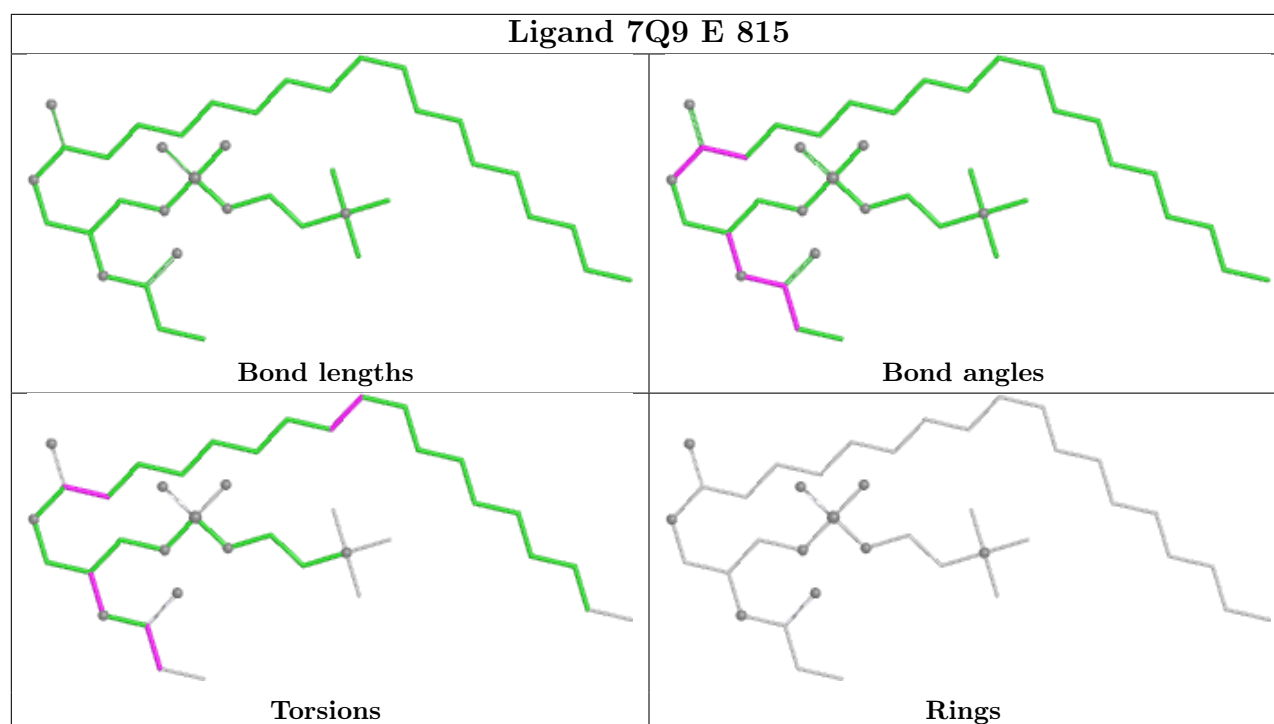


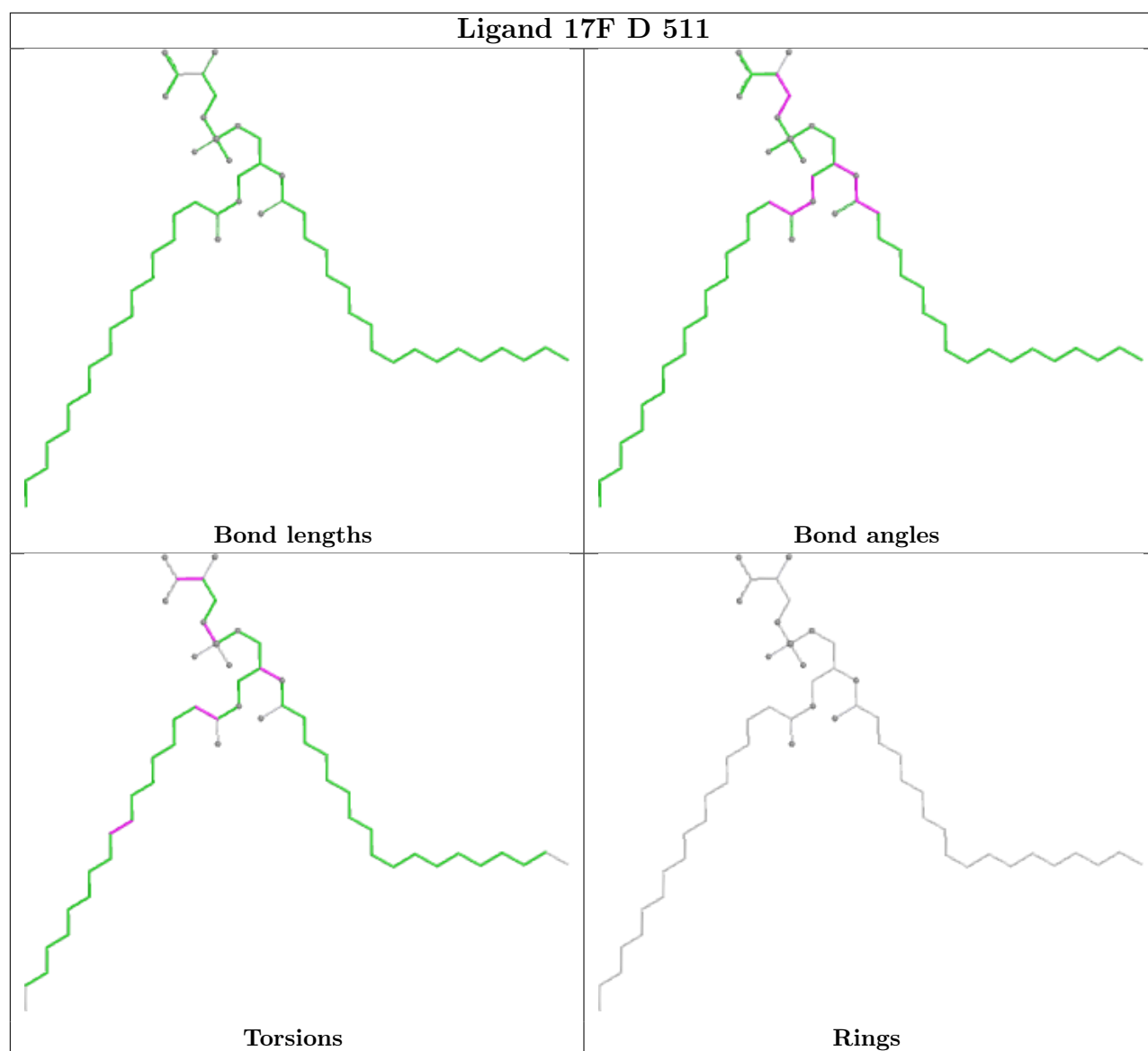




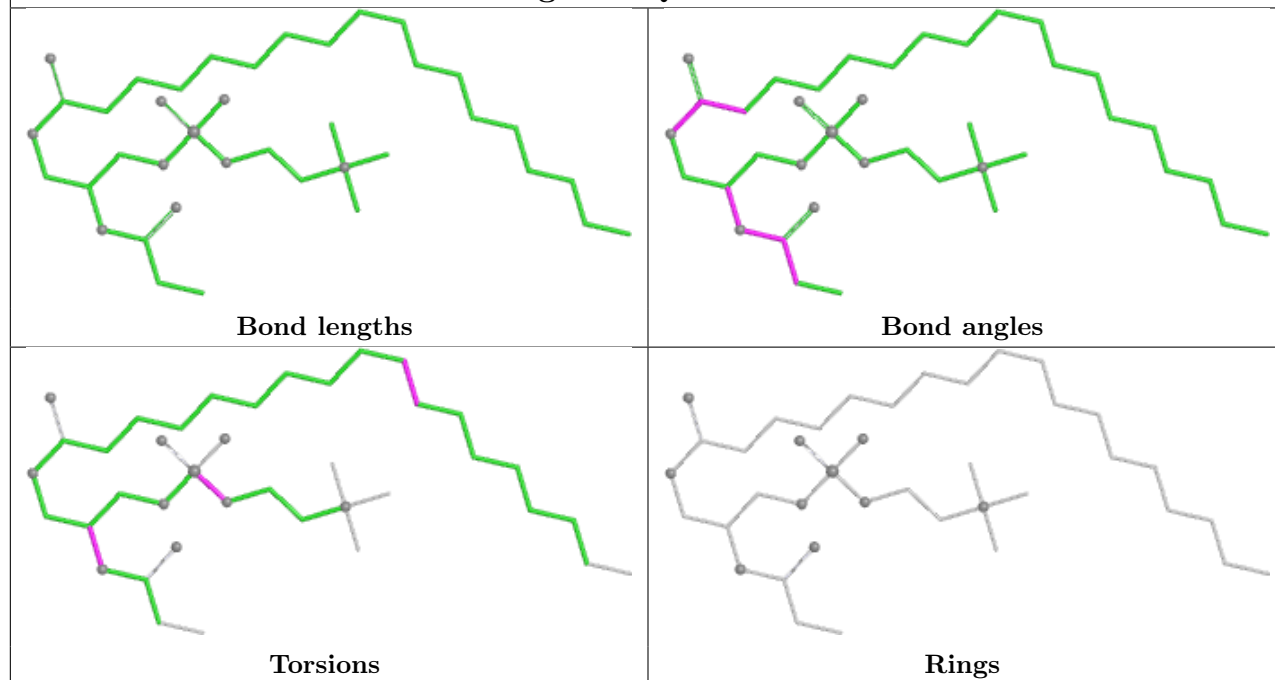




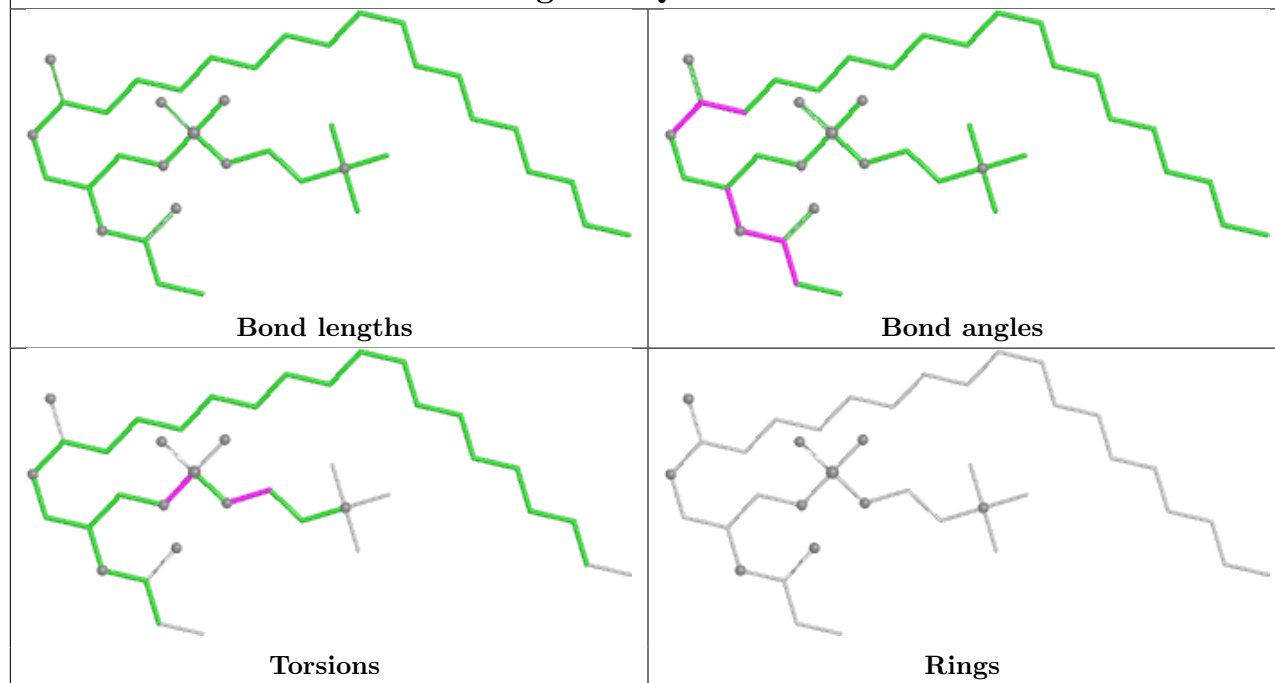


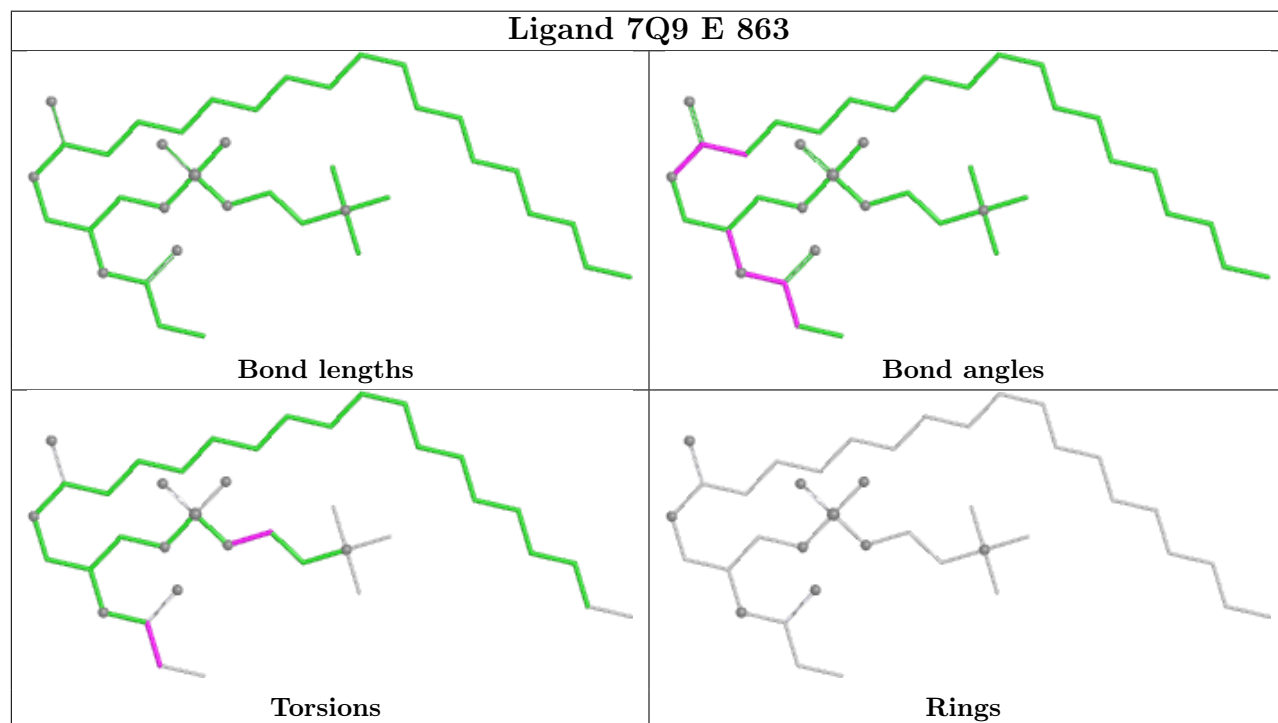
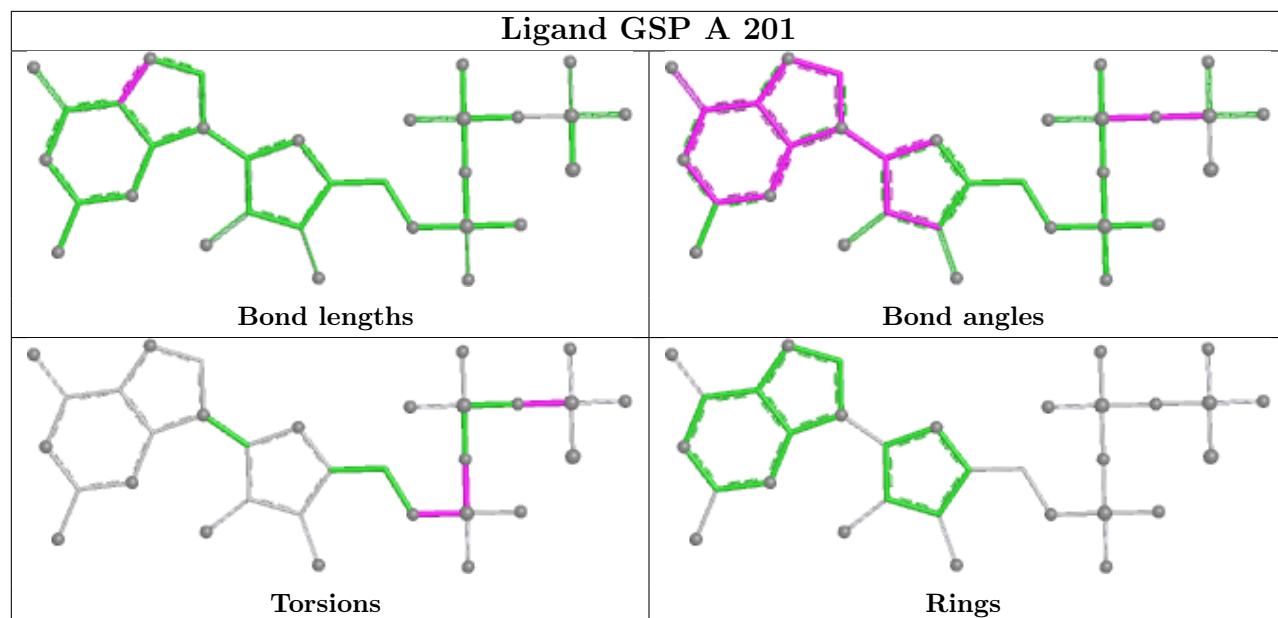


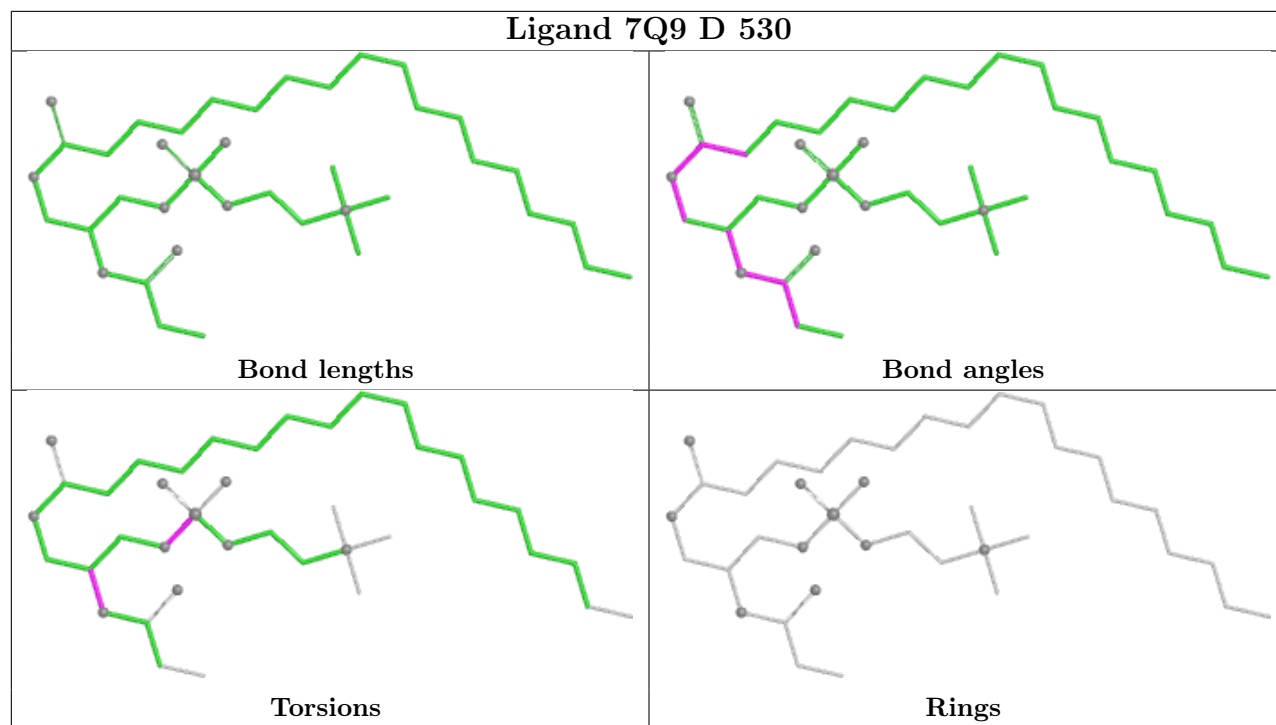
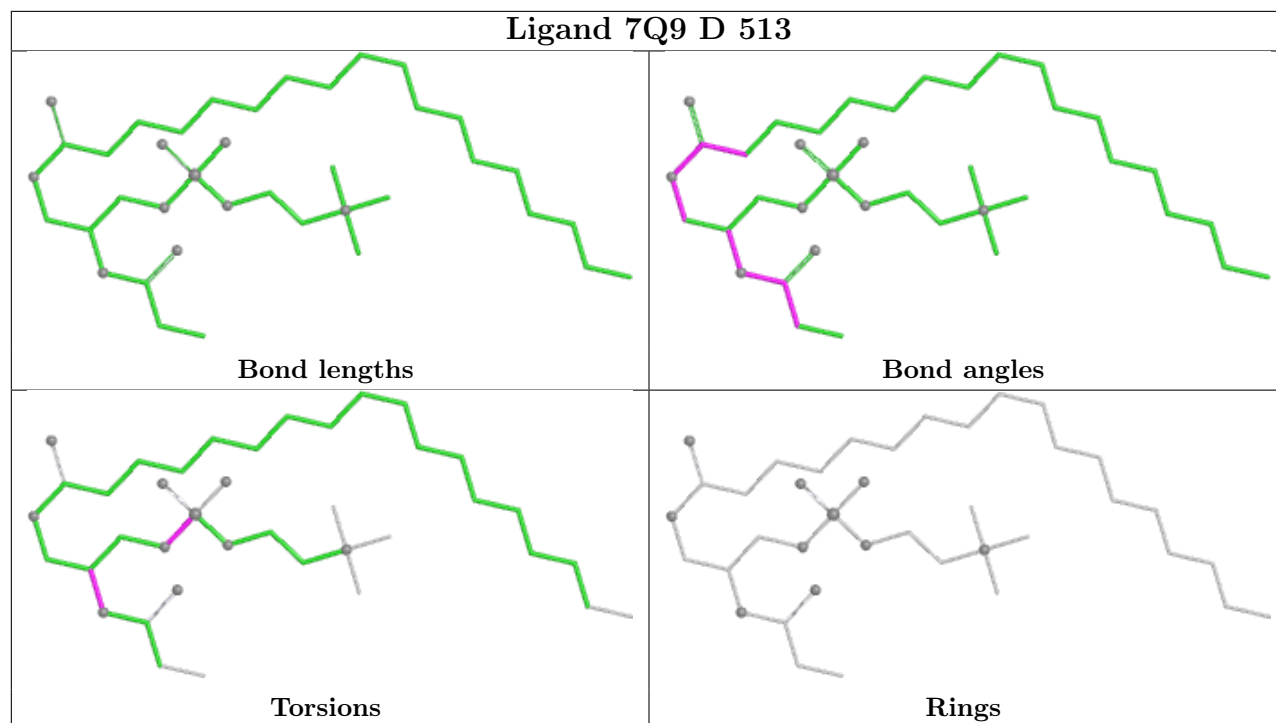
Ligand 7Q9 E 832

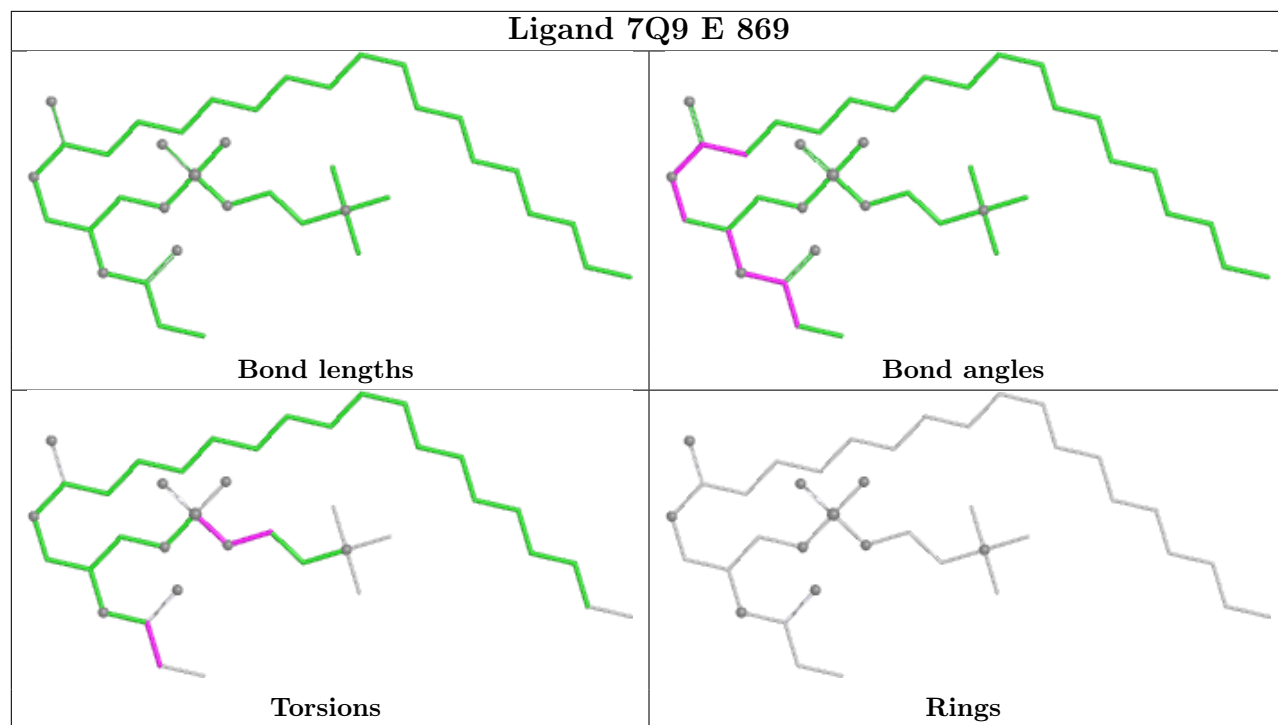
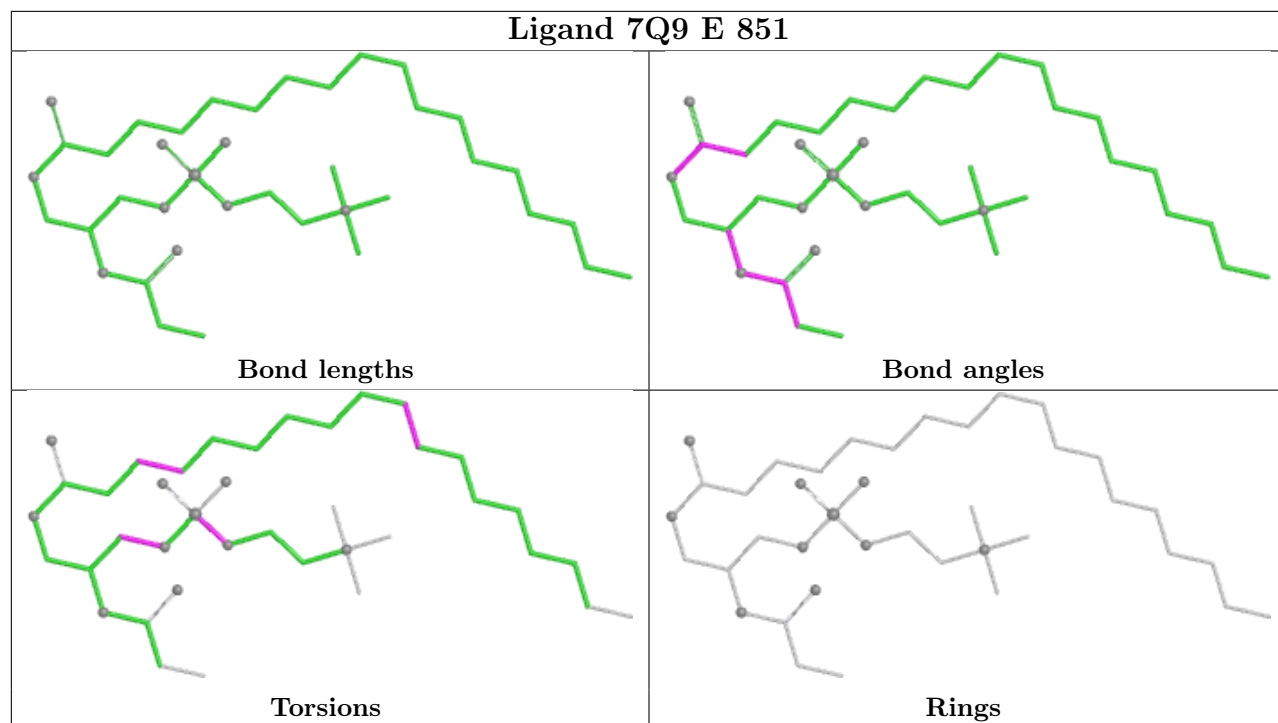


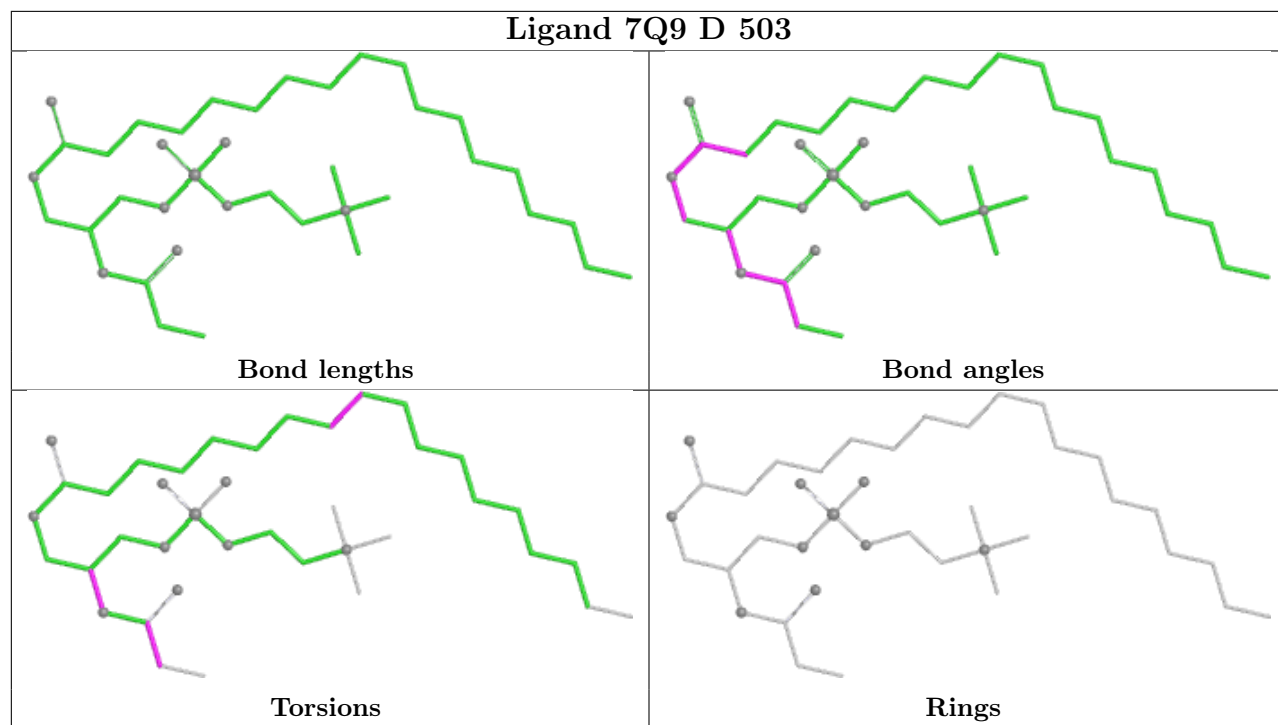
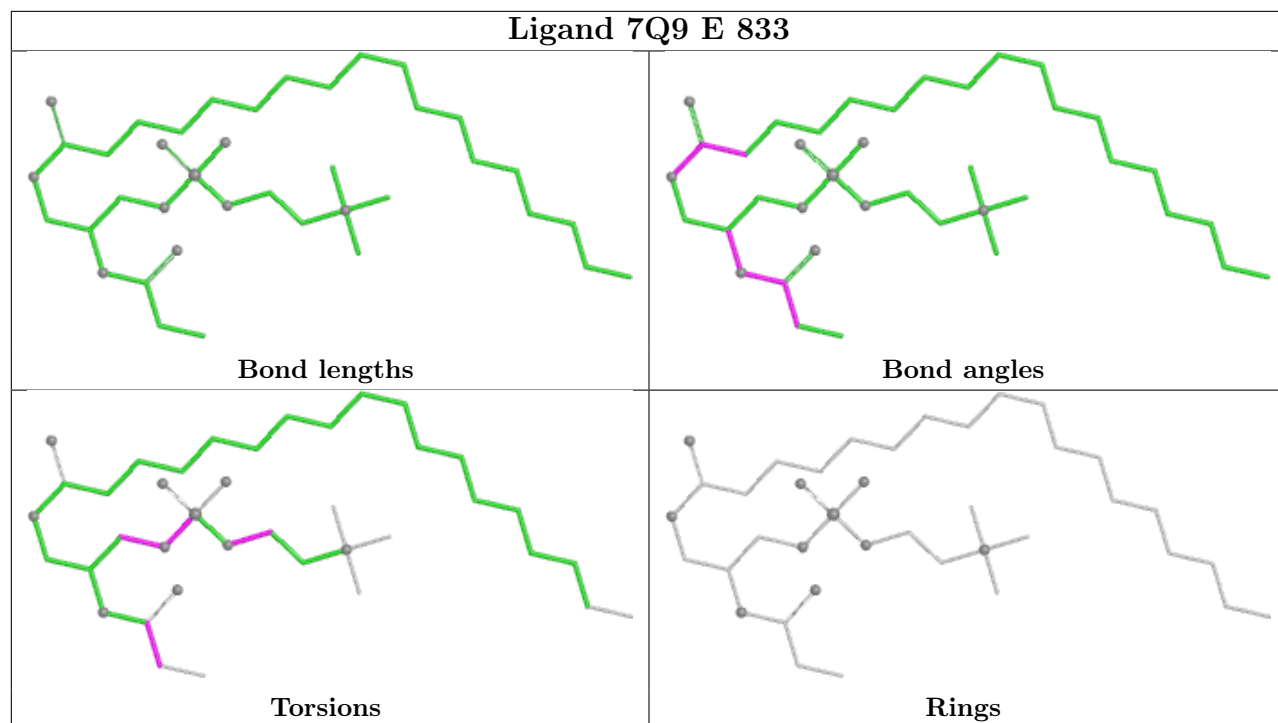
Ligand 7Q9 D 502



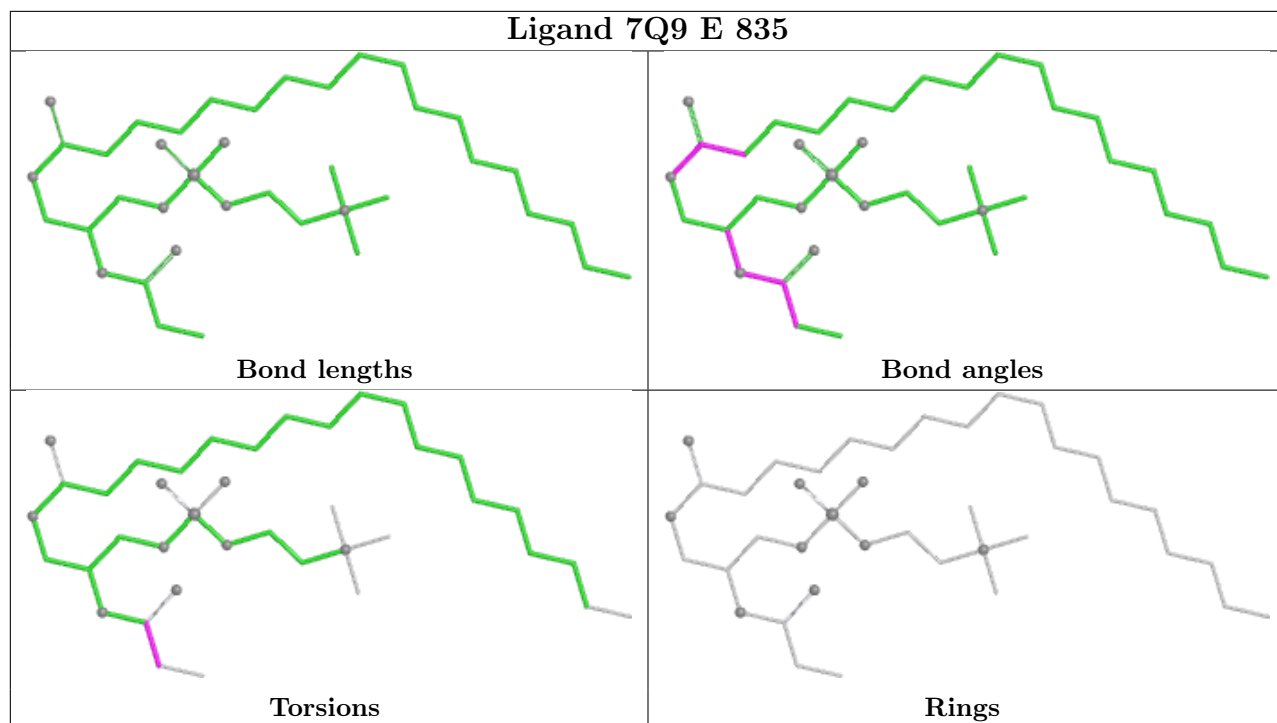




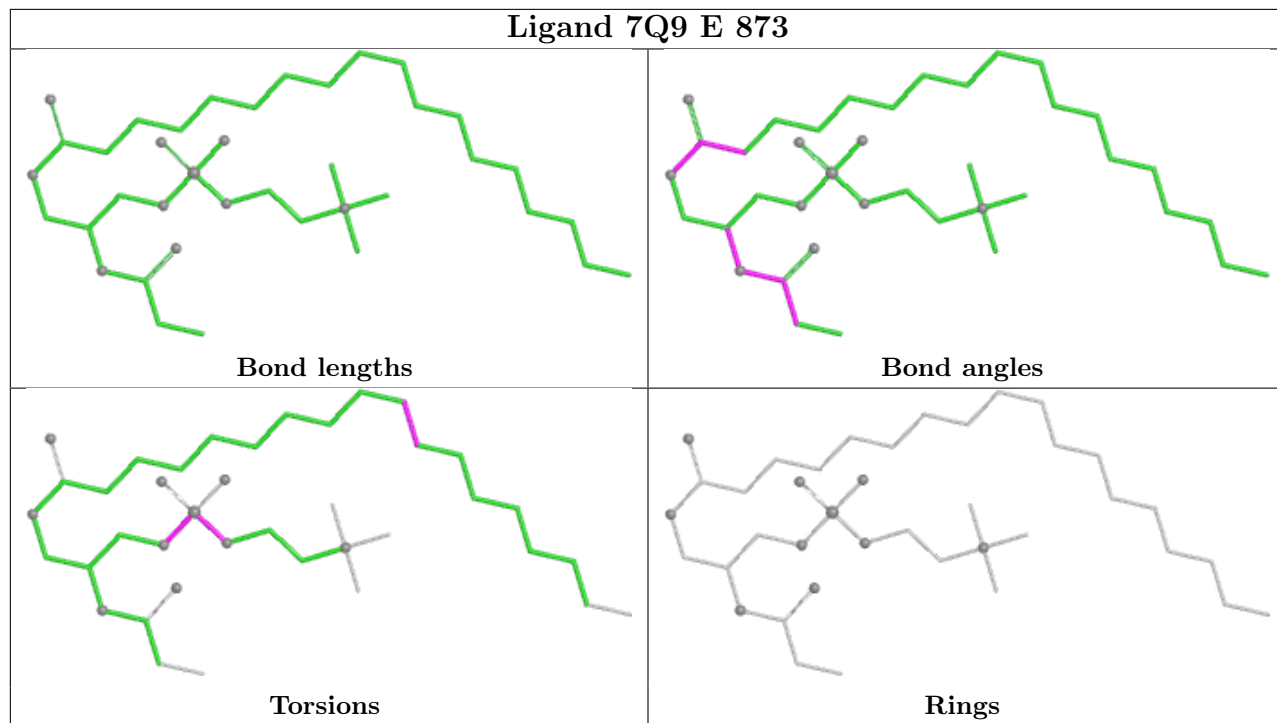


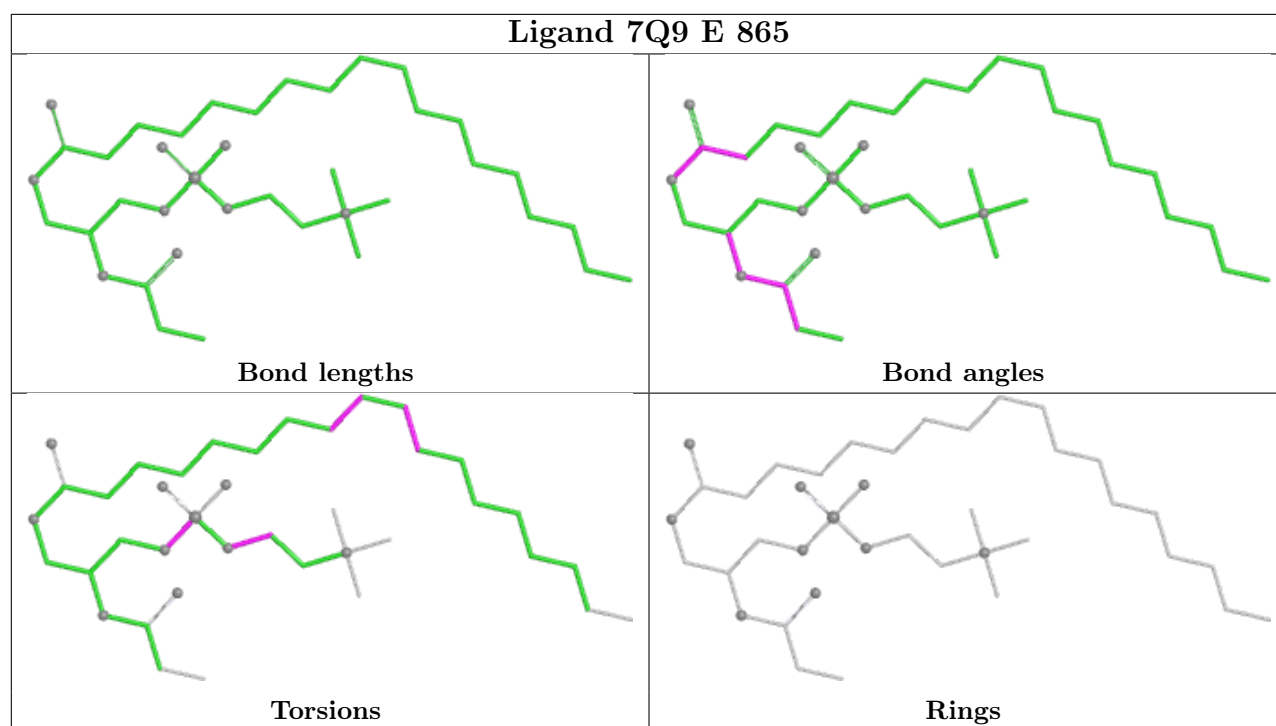


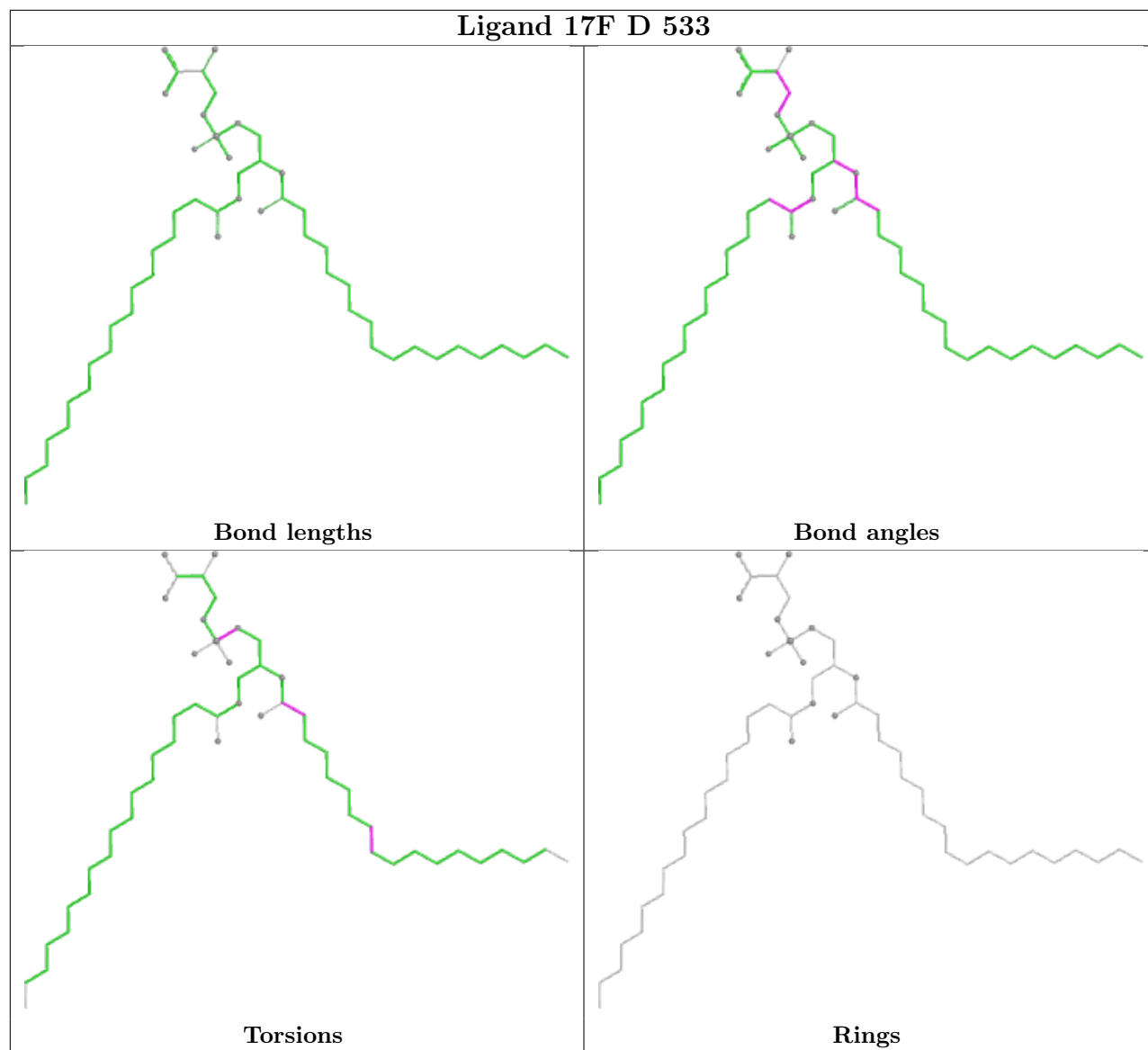
Ligand 7Q9 E 835

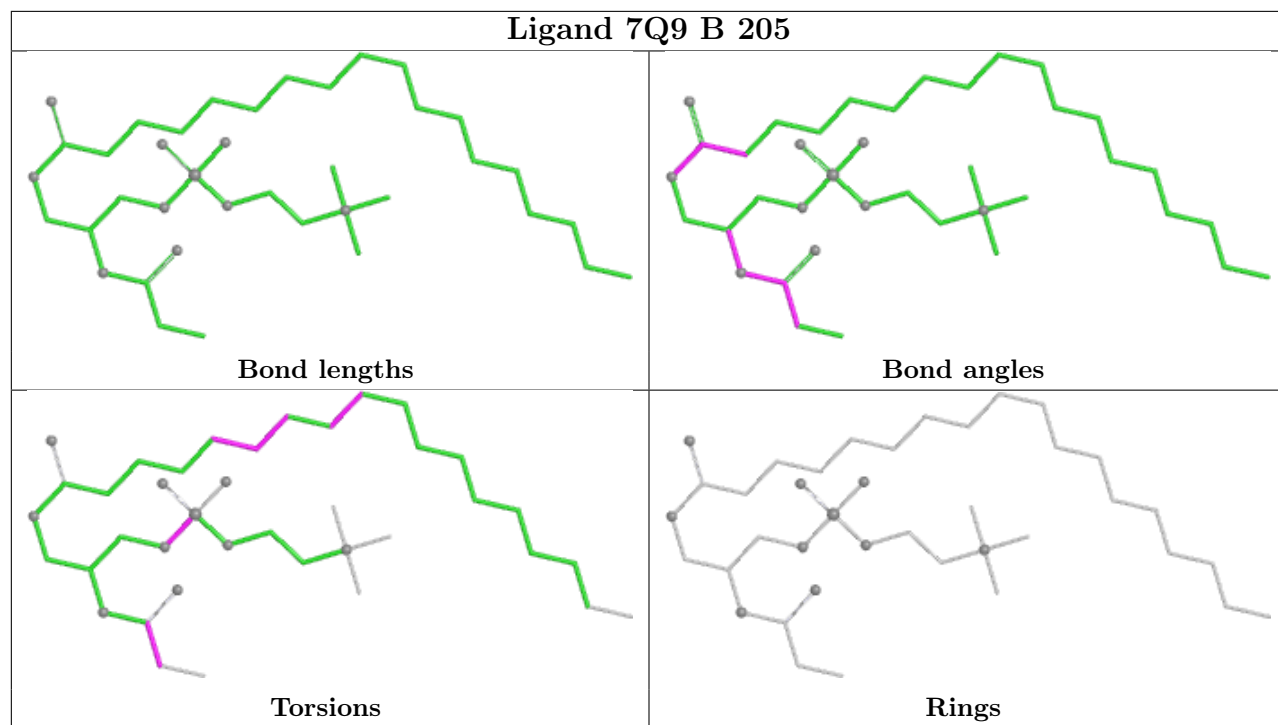
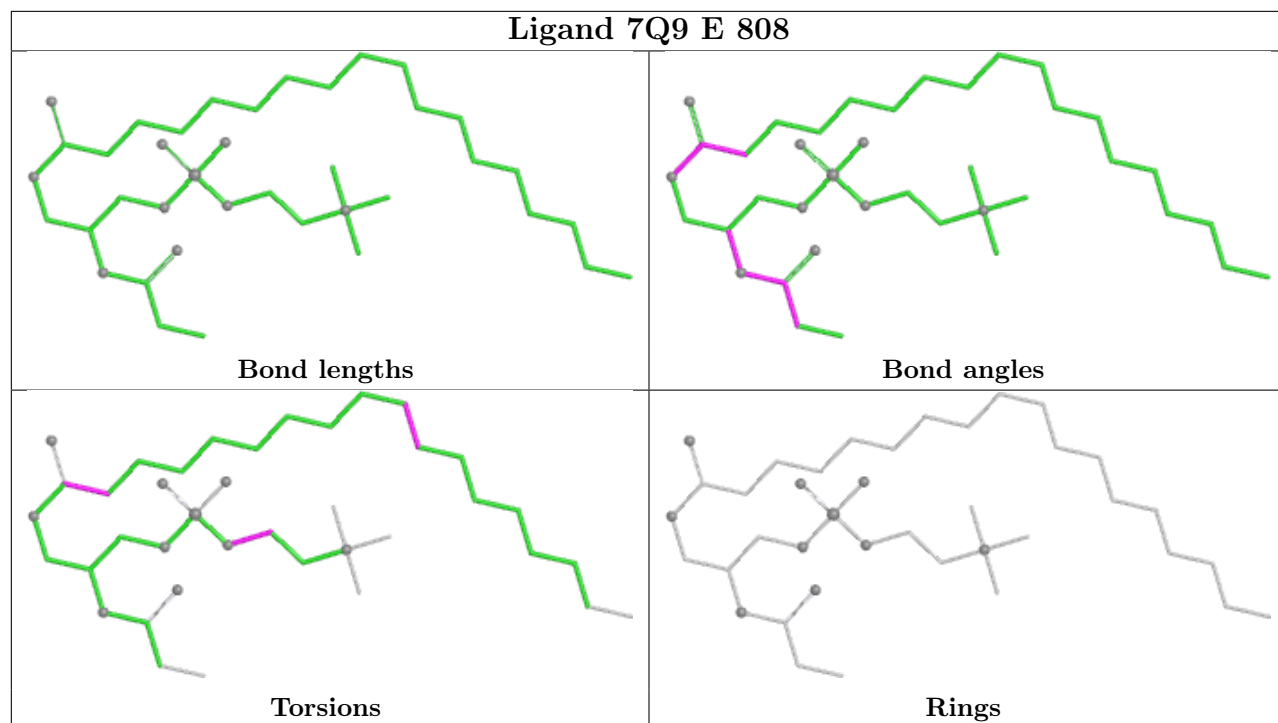


Ligand 7Q9 E 873

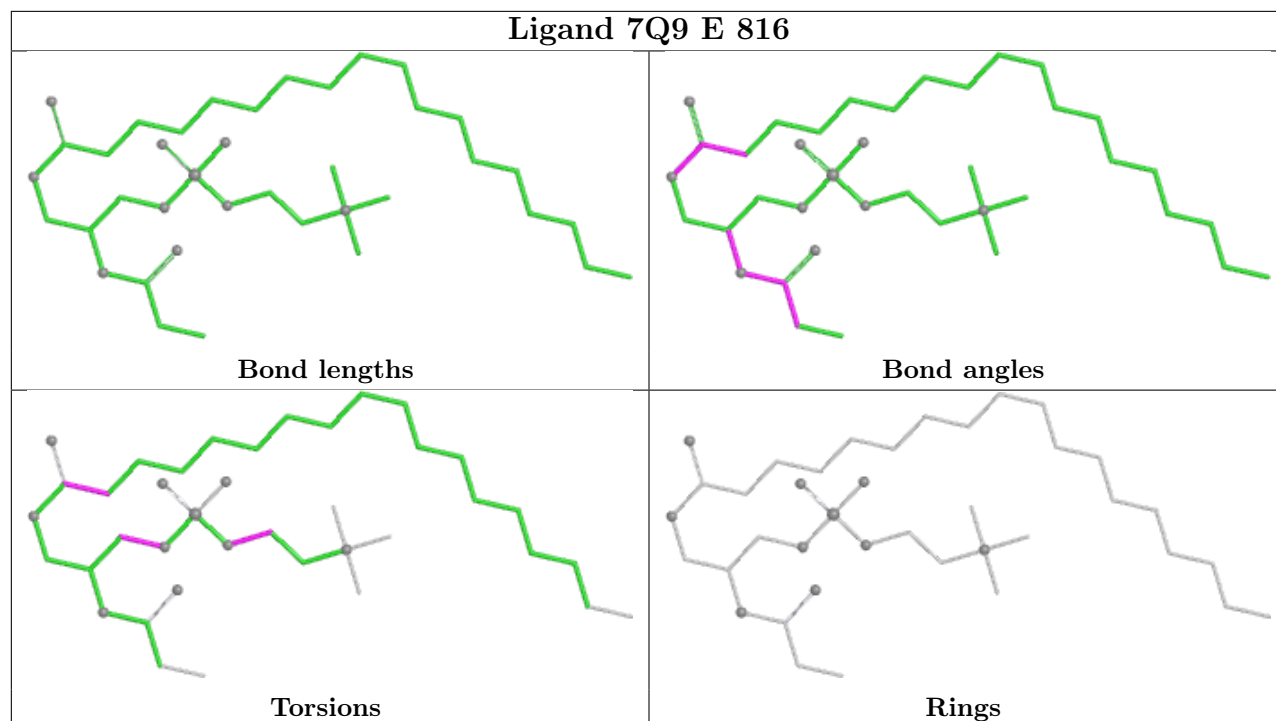




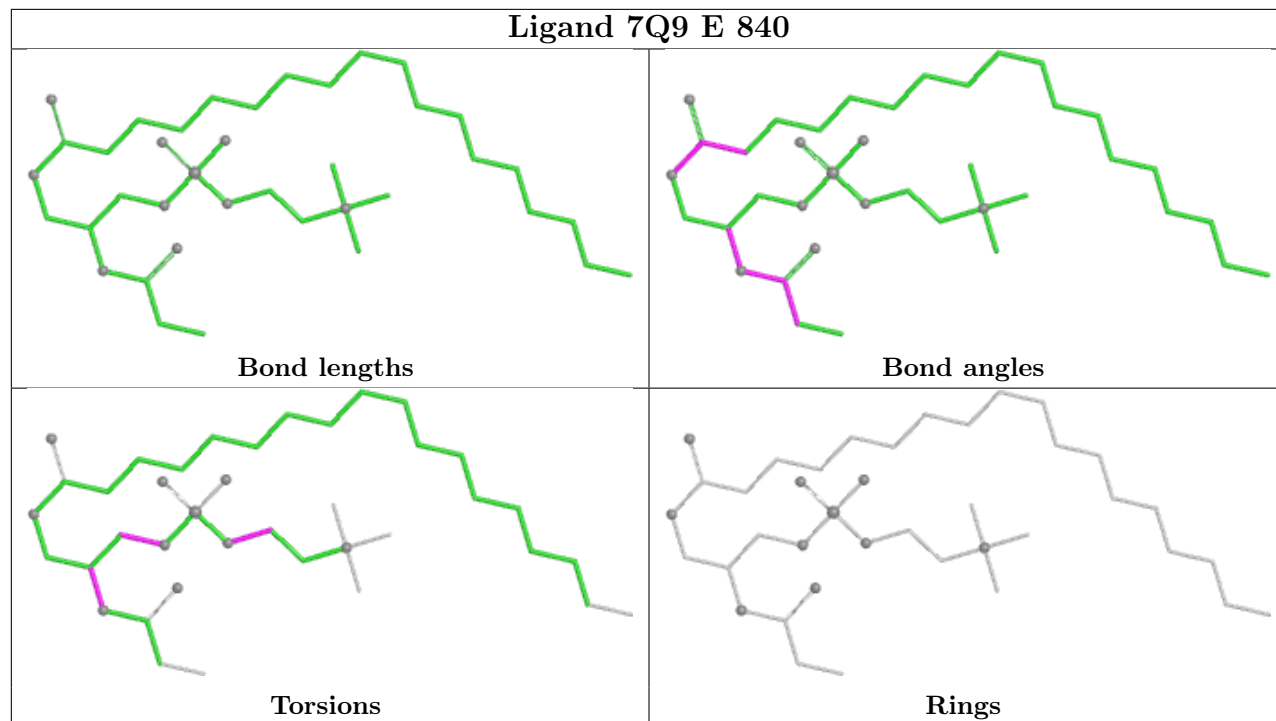


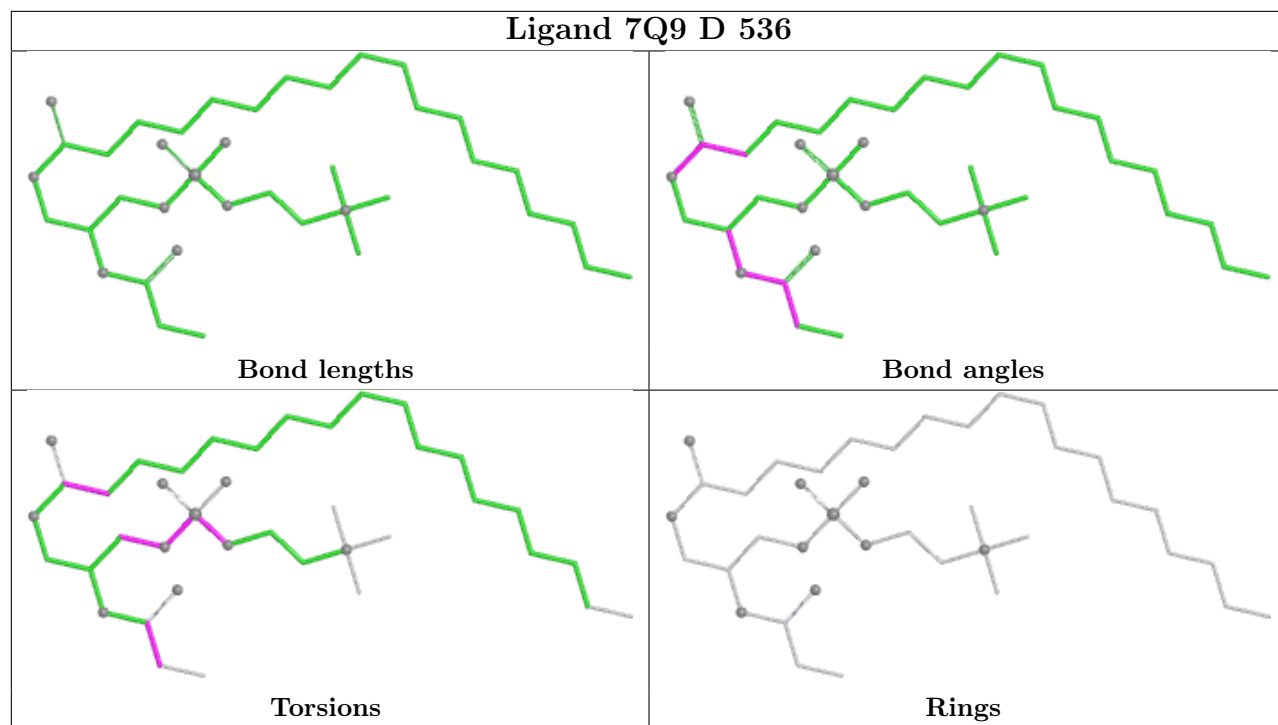
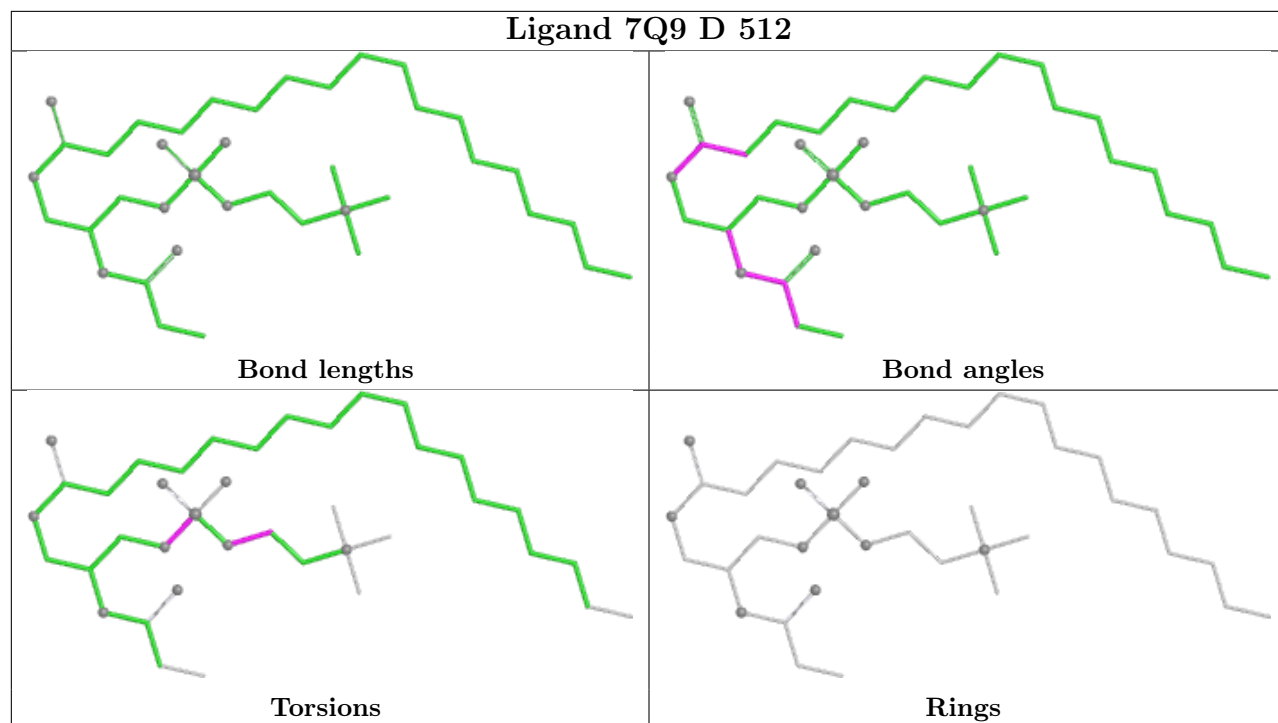


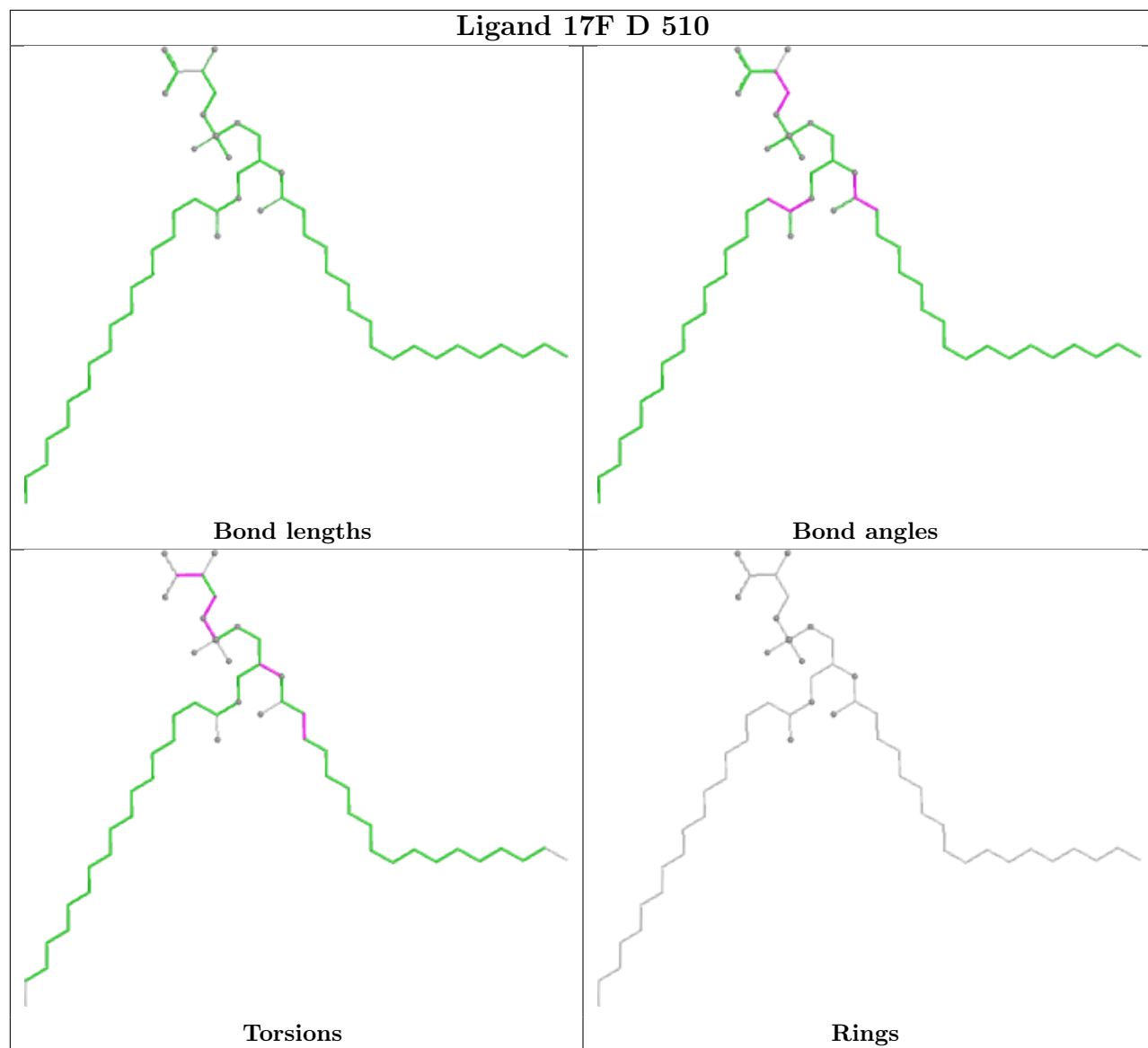
Ligand 7Q9 E 816



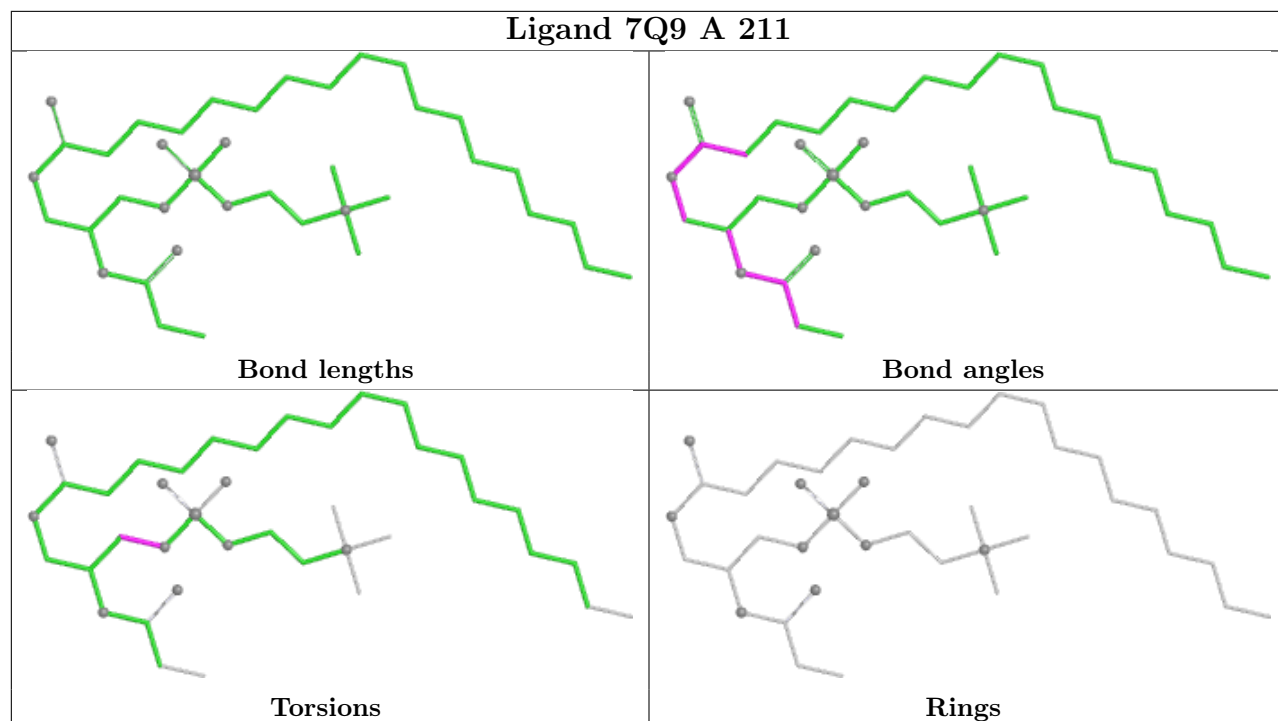
Ligand 7Q9 E 840



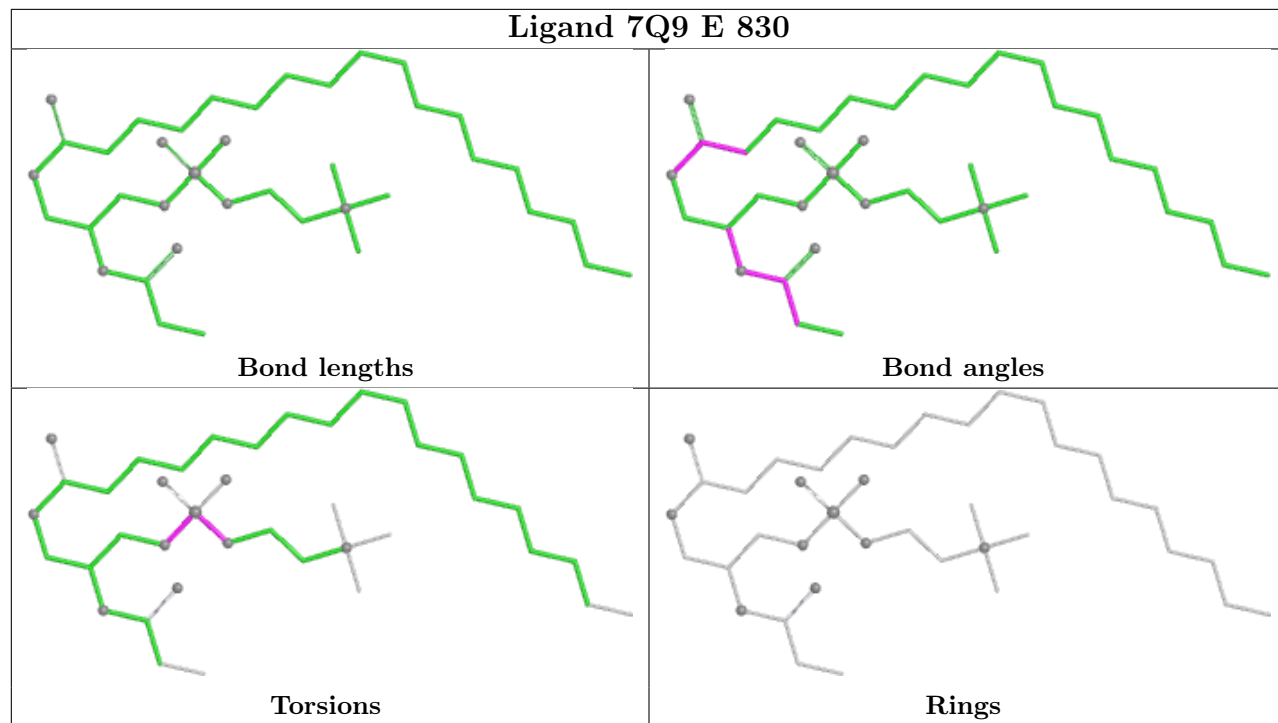


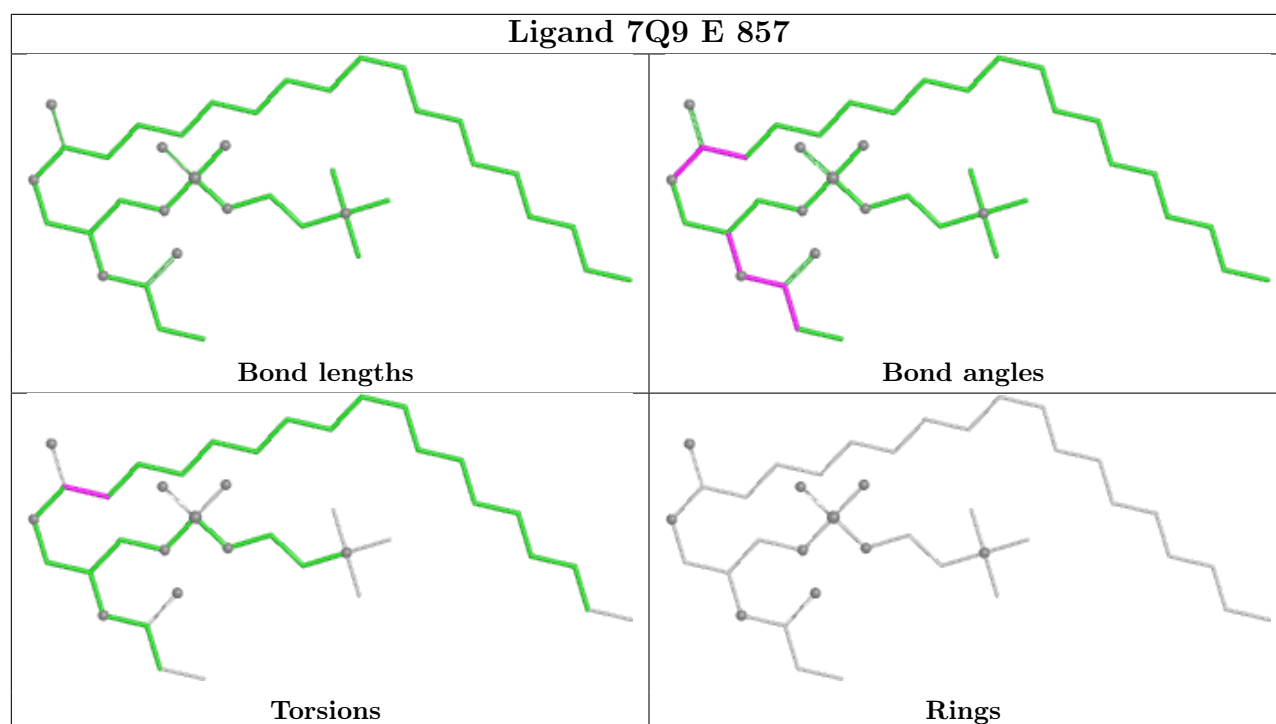


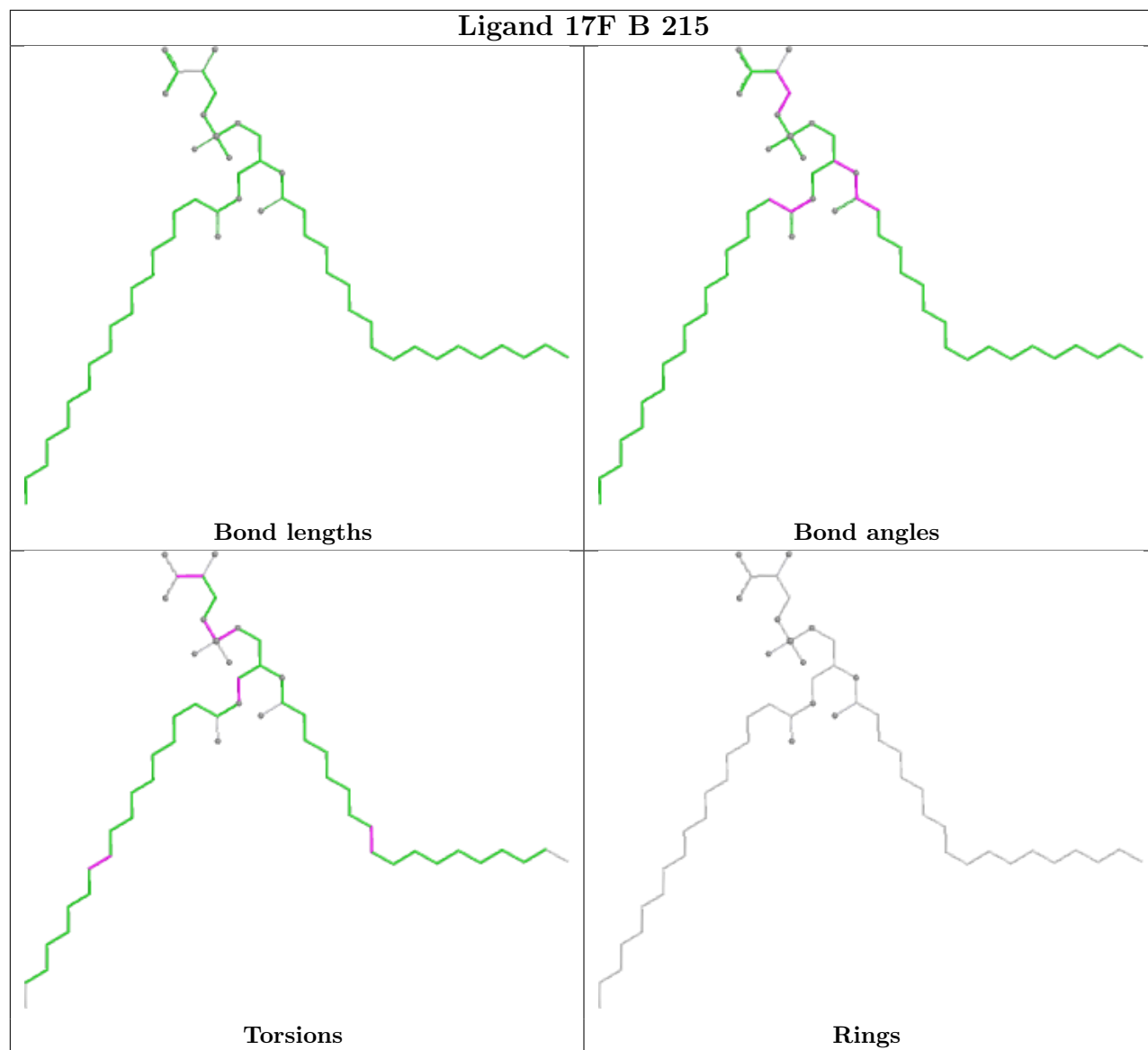
Ligand 7Q9 A 211

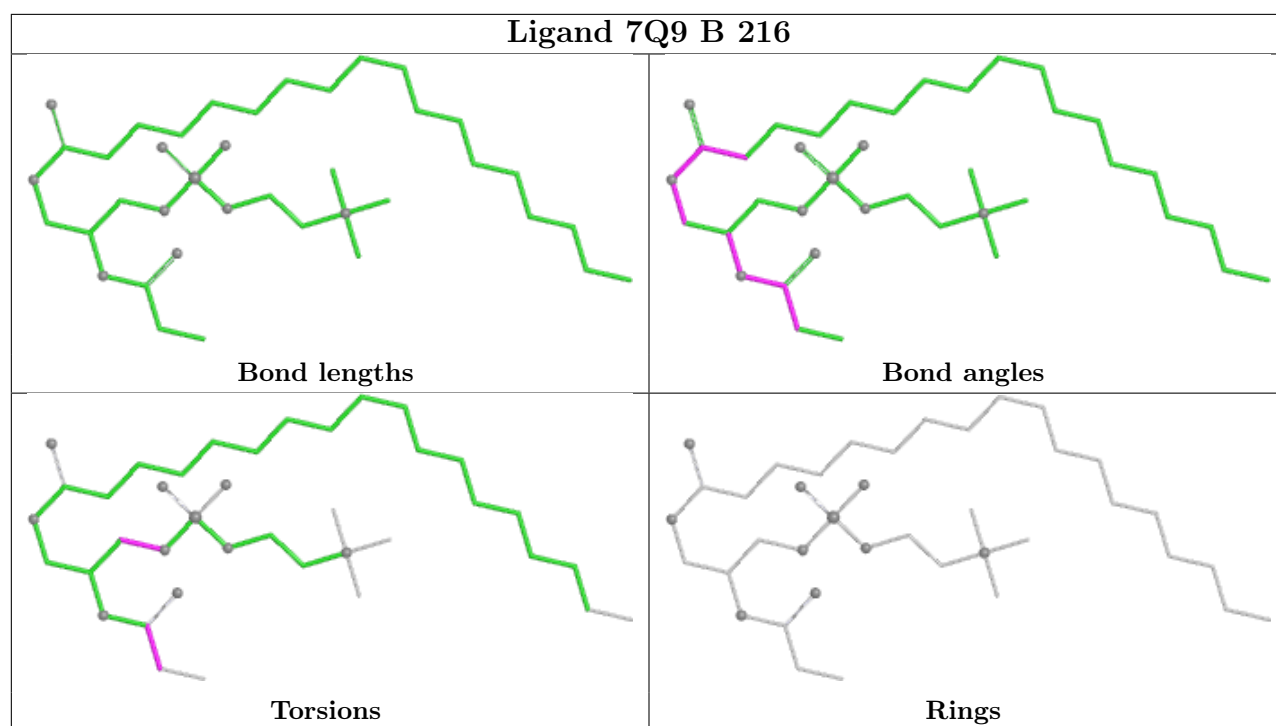
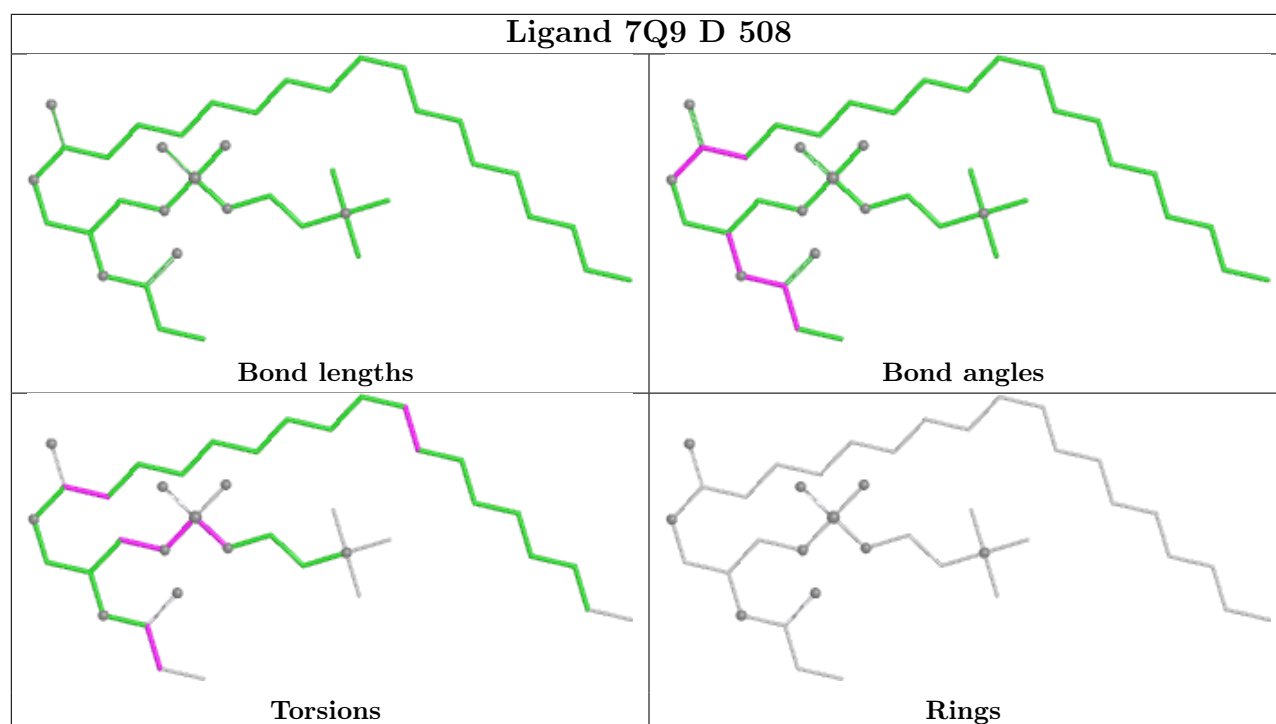


Ligand 7Q9 E 830

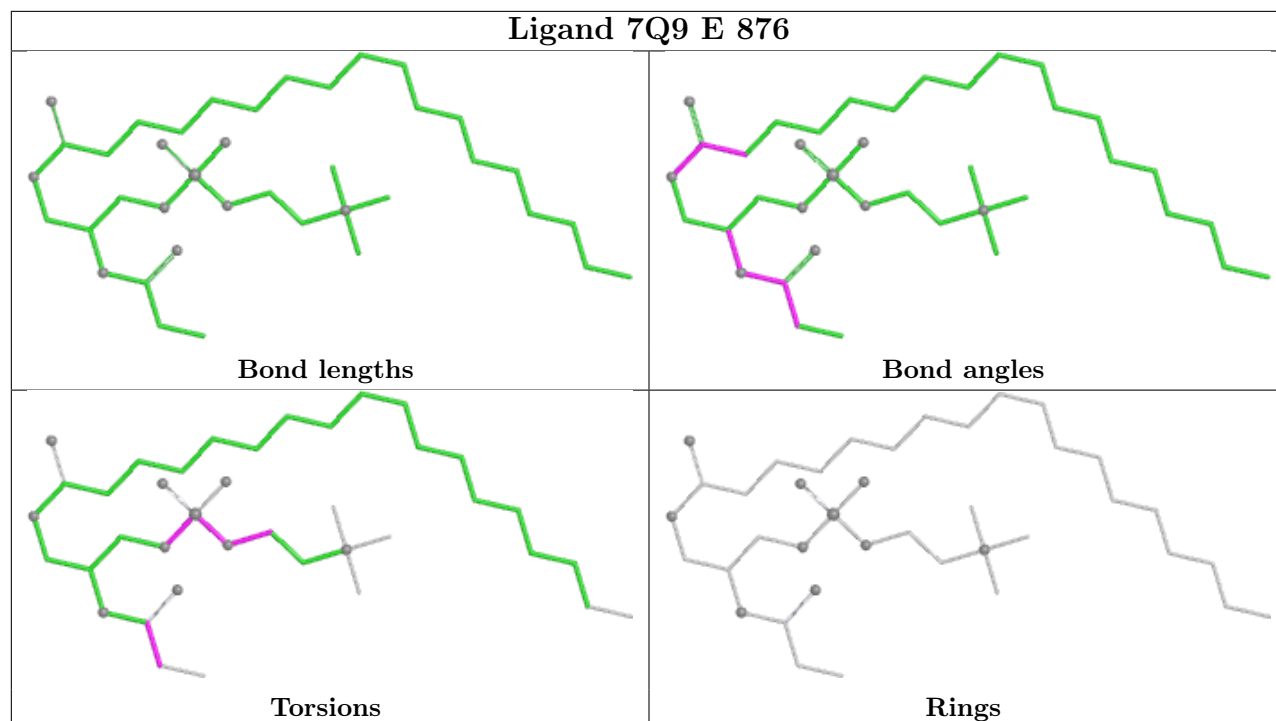




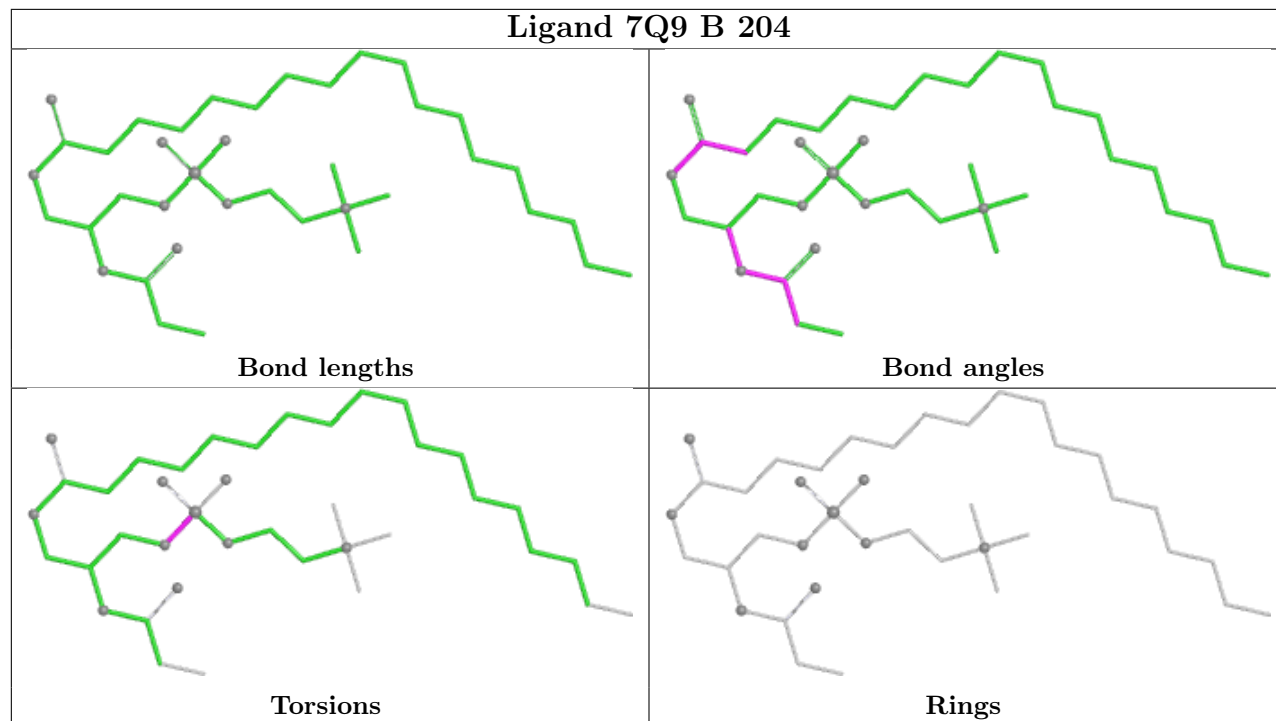


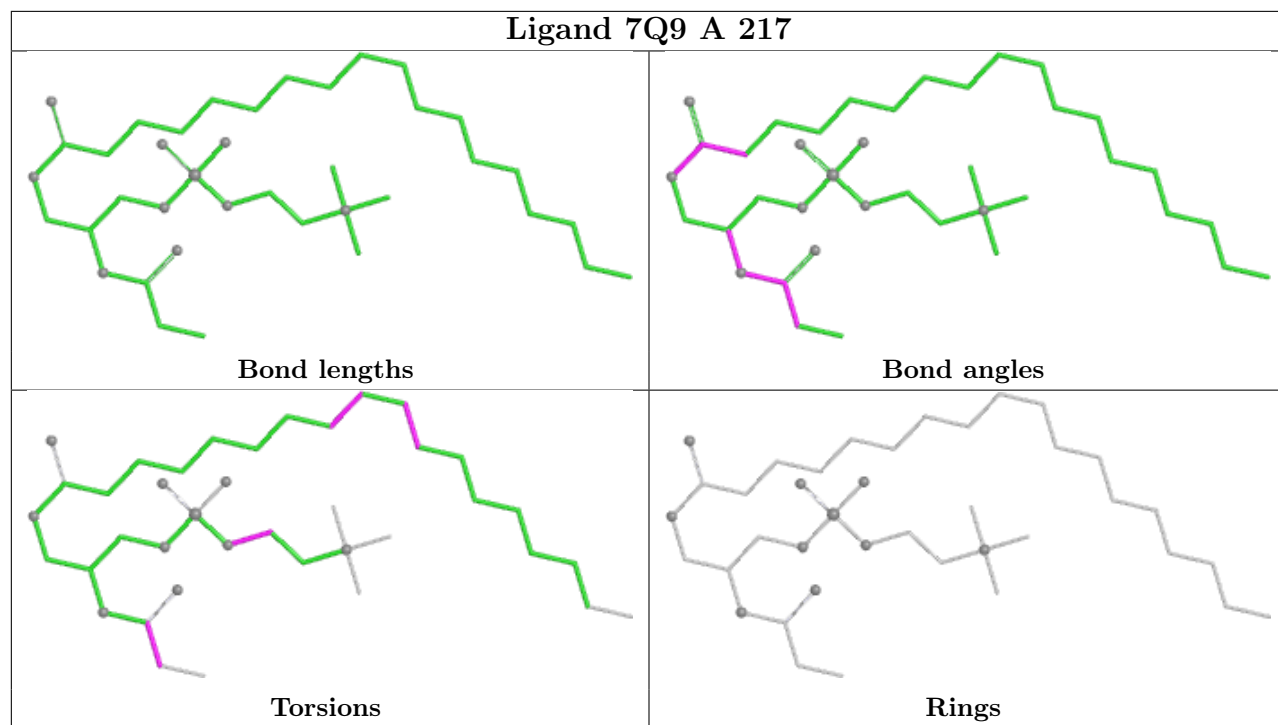
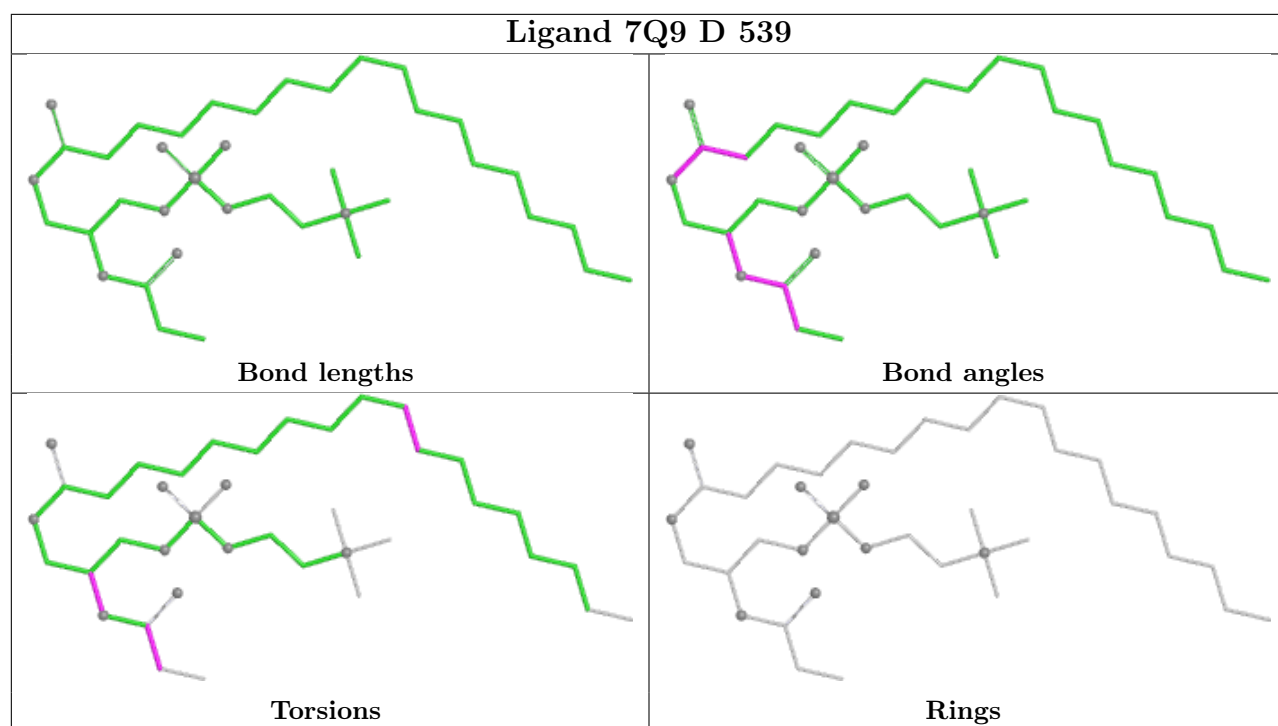


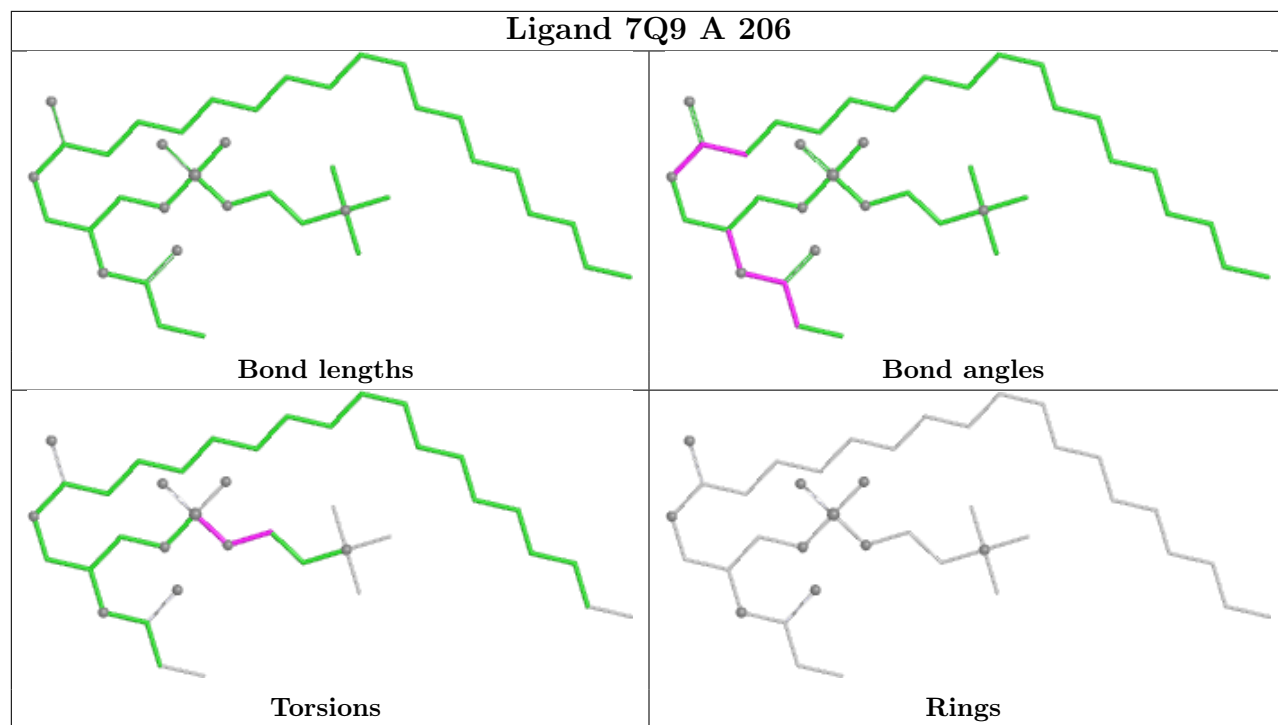
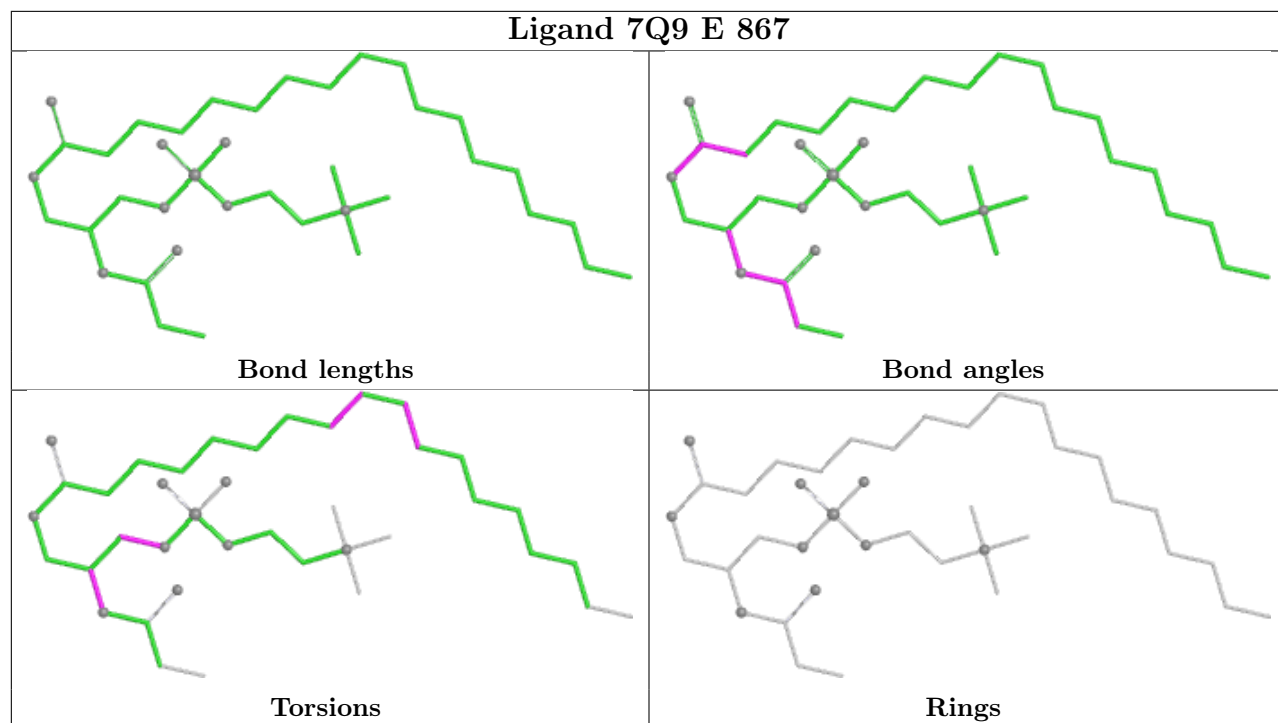
Ligand 7Q9 E 876

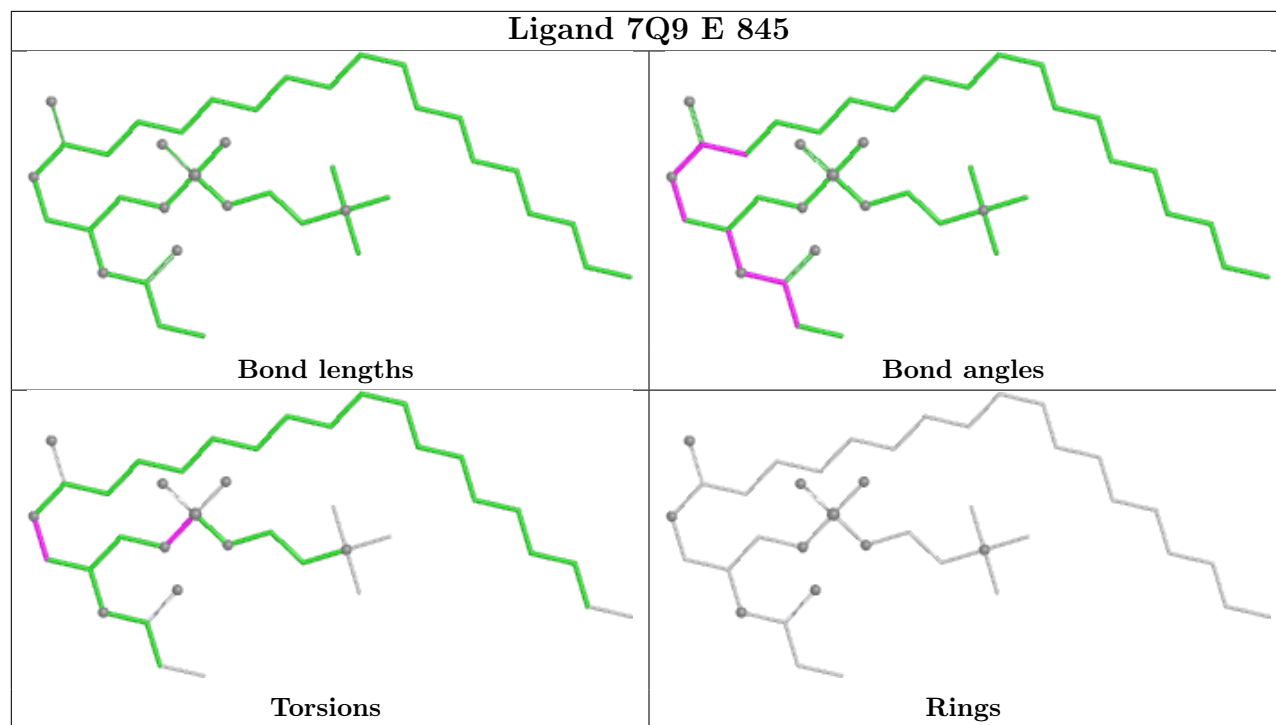
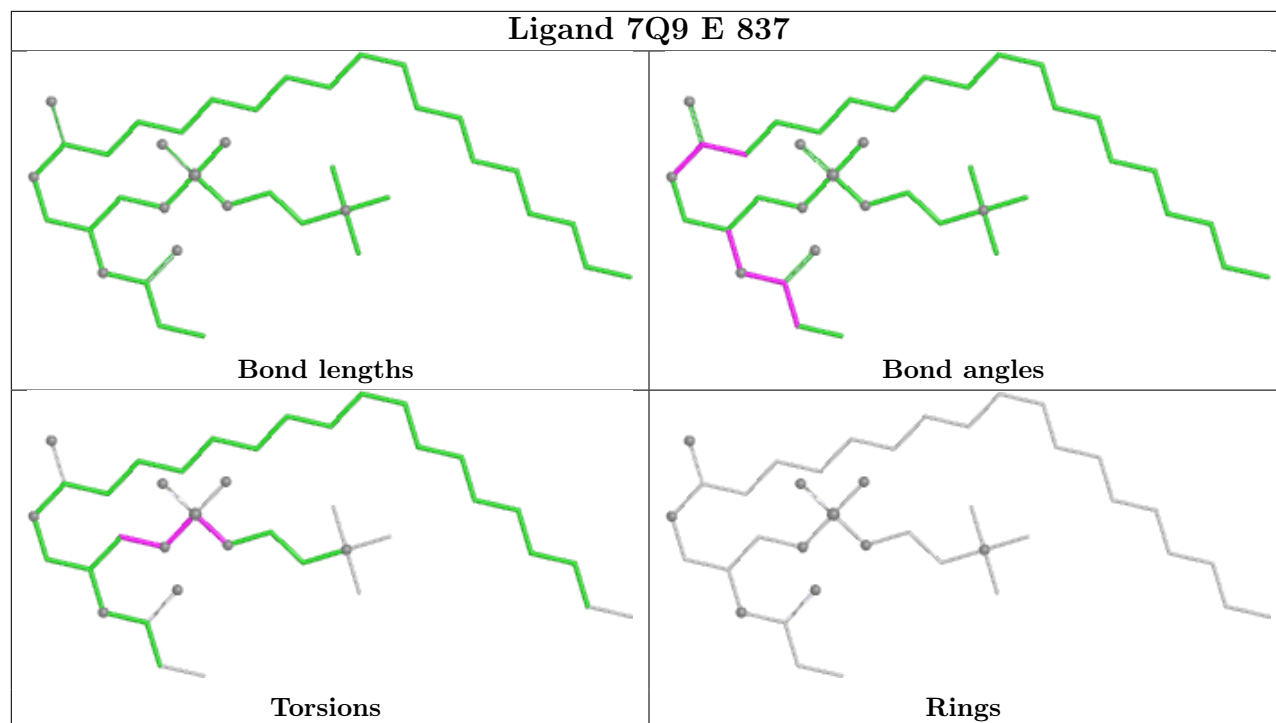


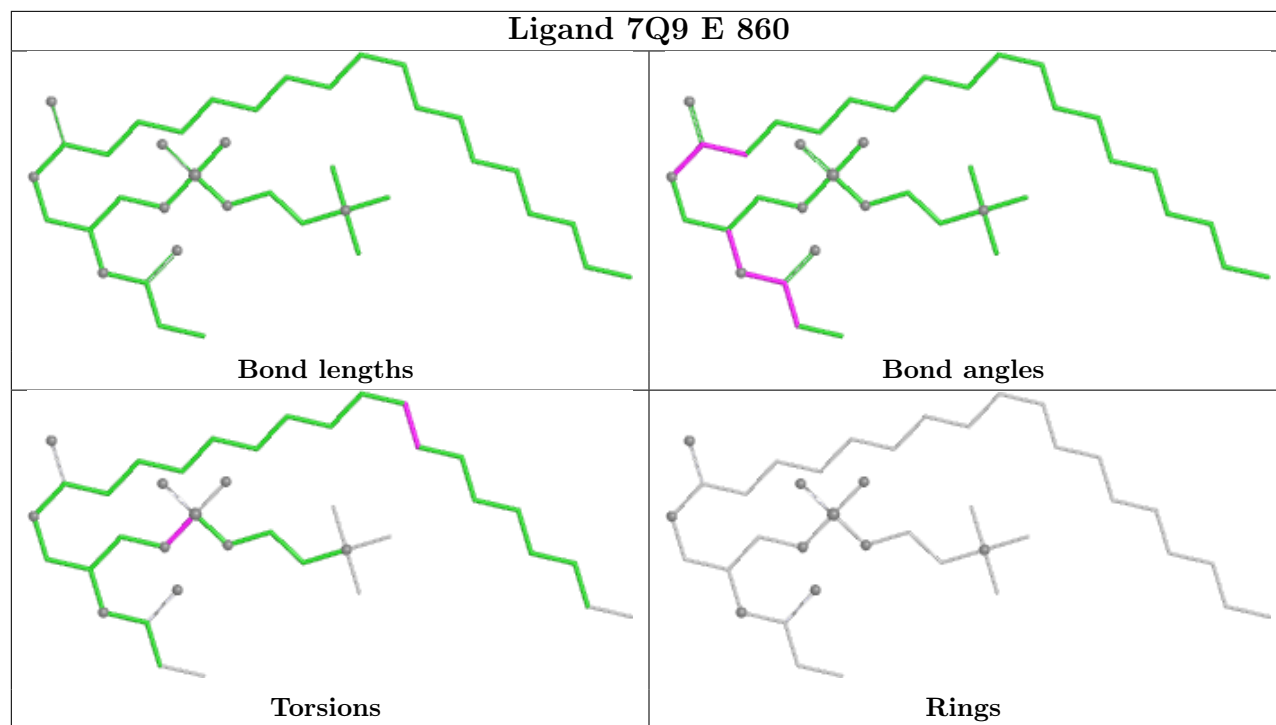
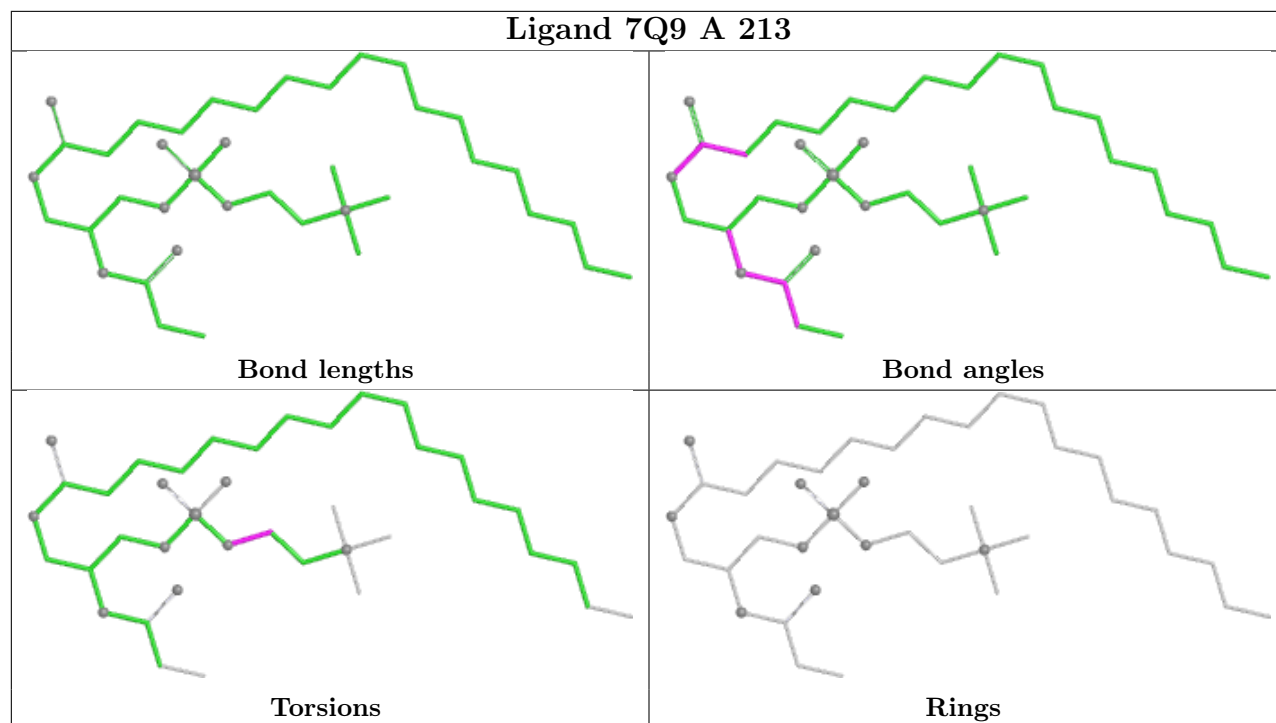
Ligand 7Q9 B 204

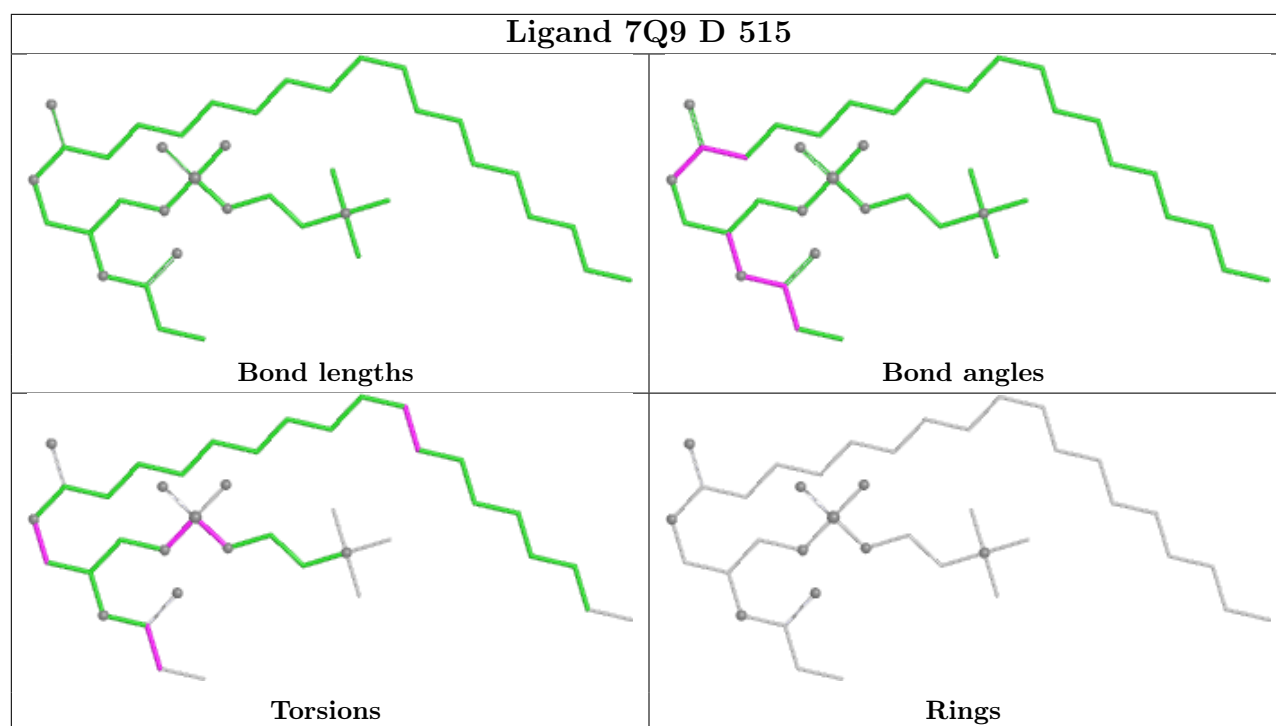


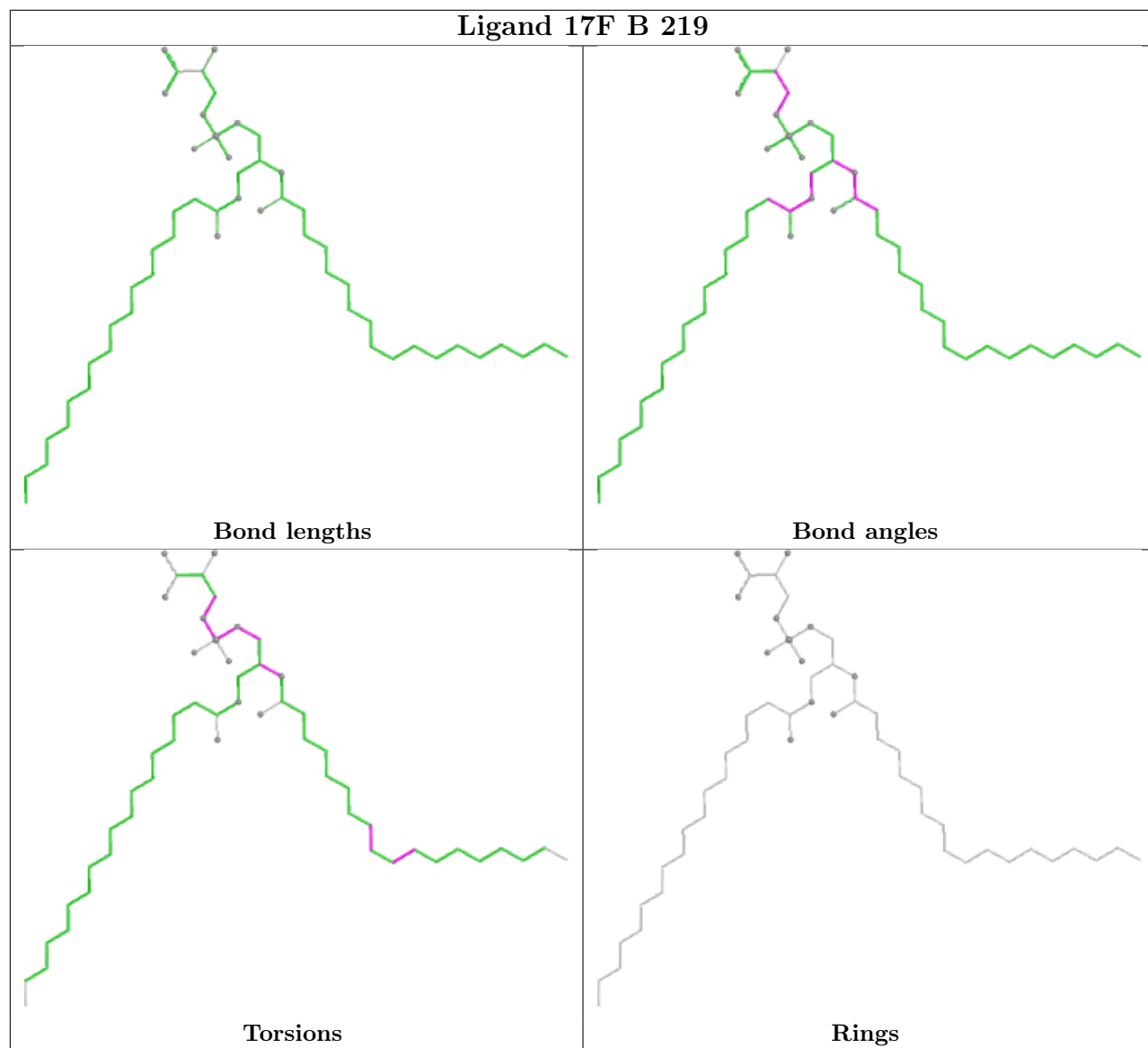


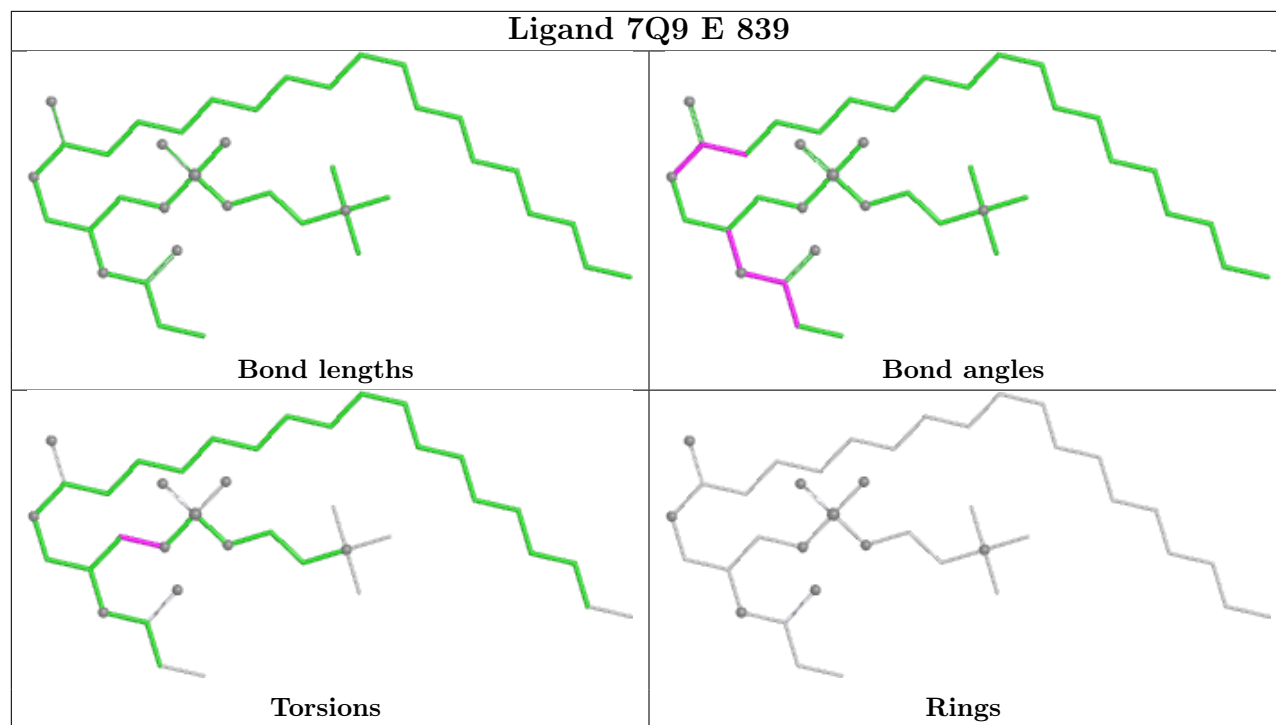
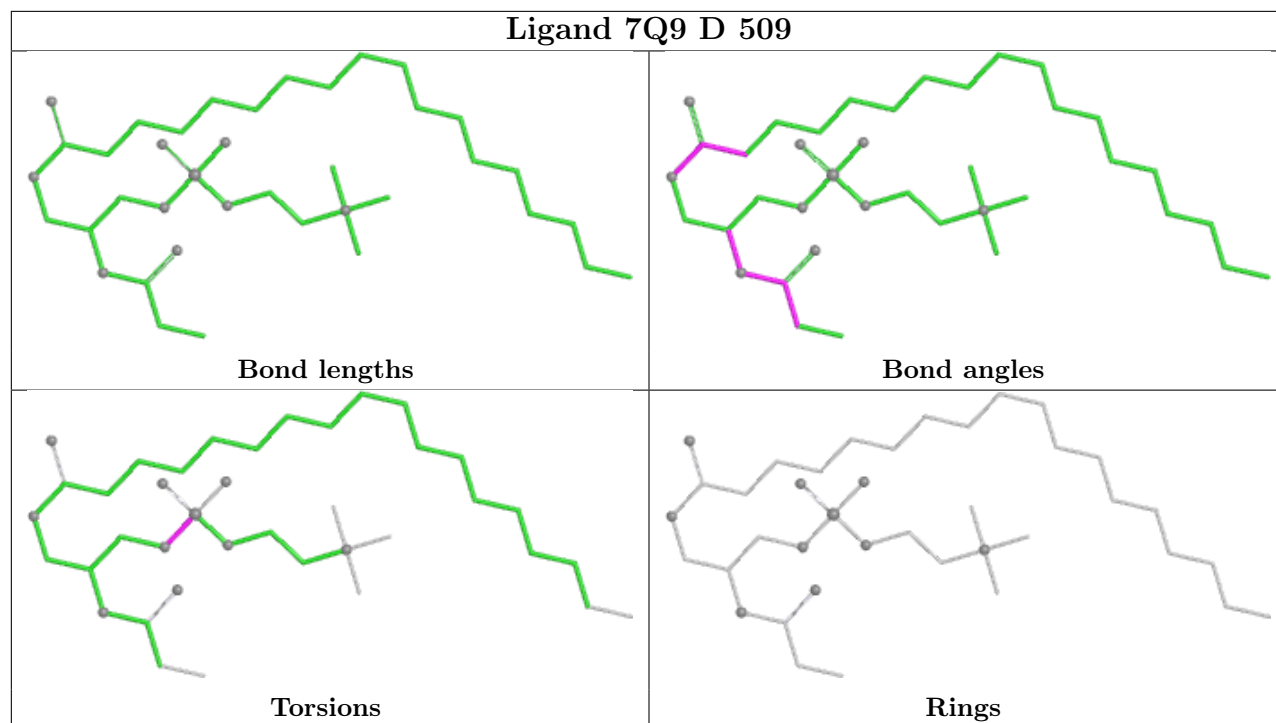


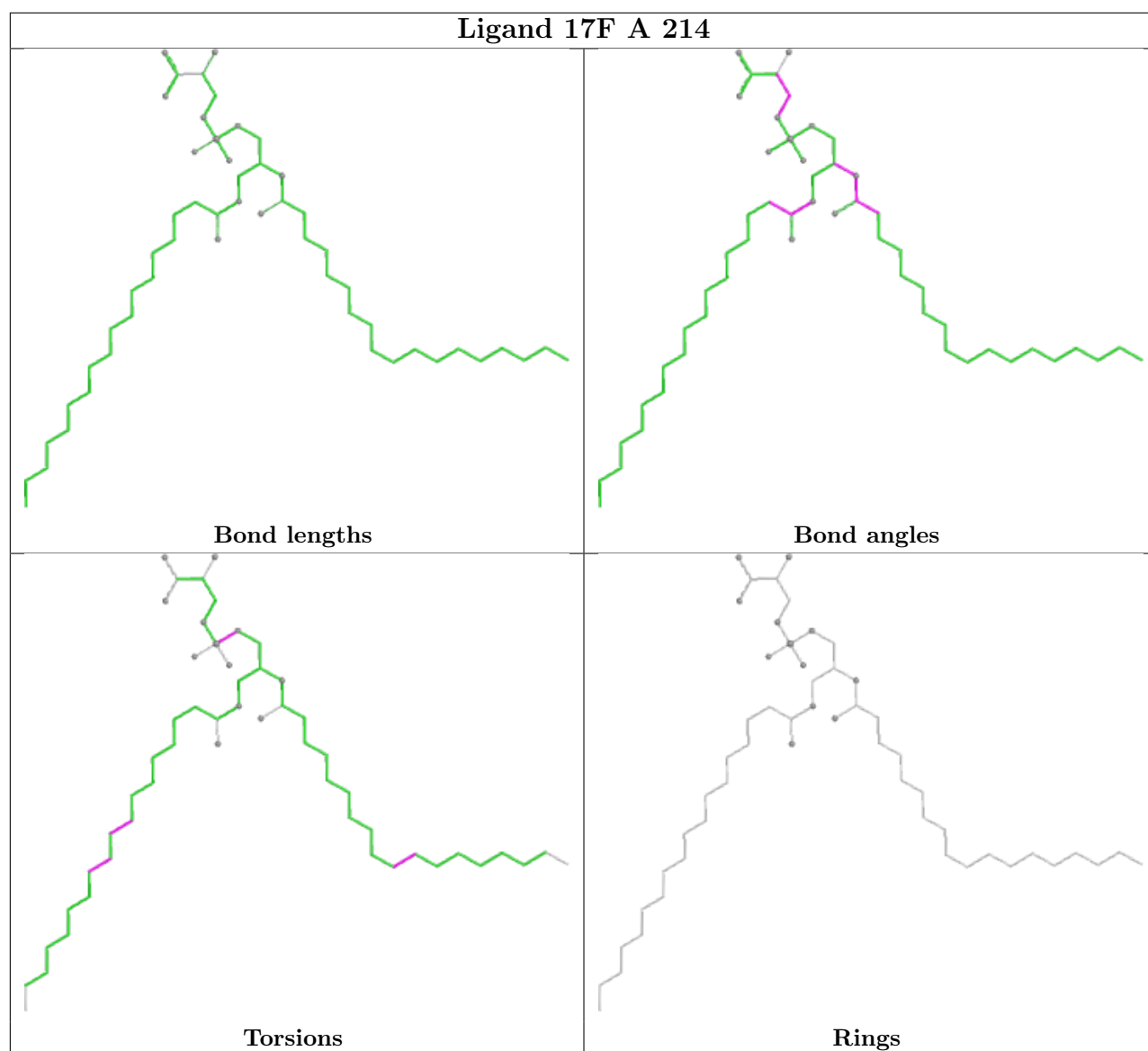


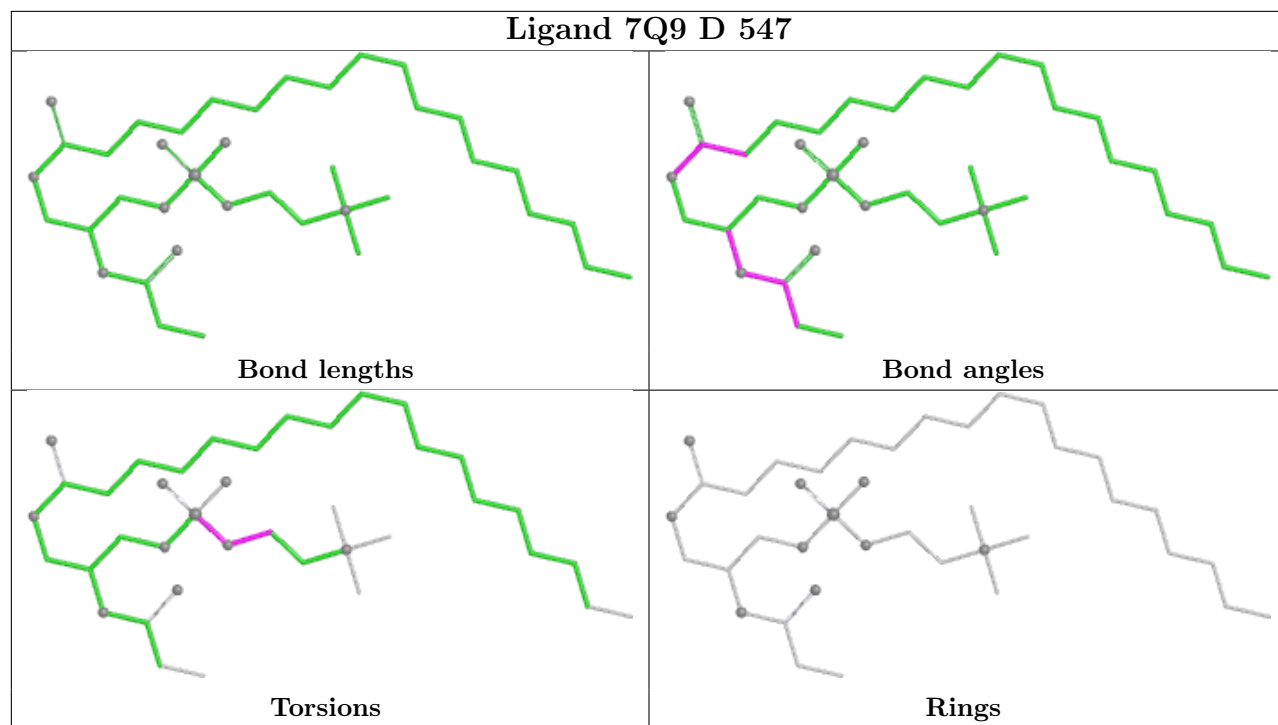
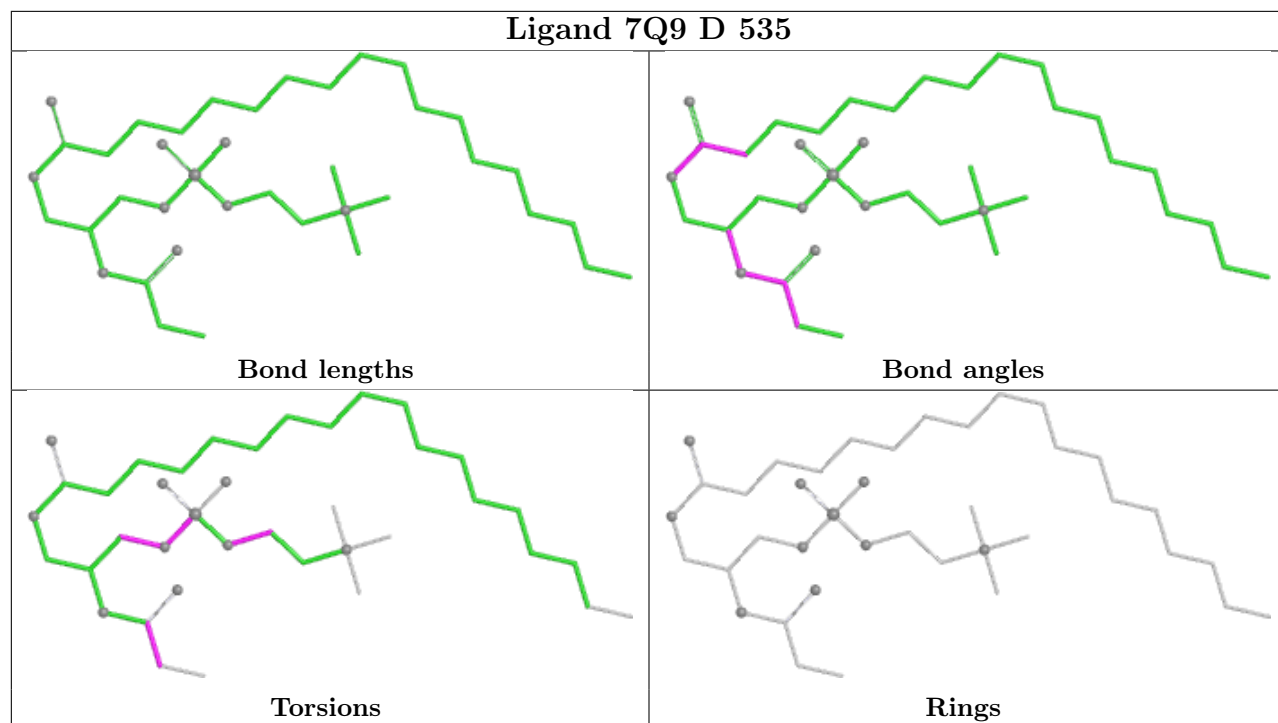


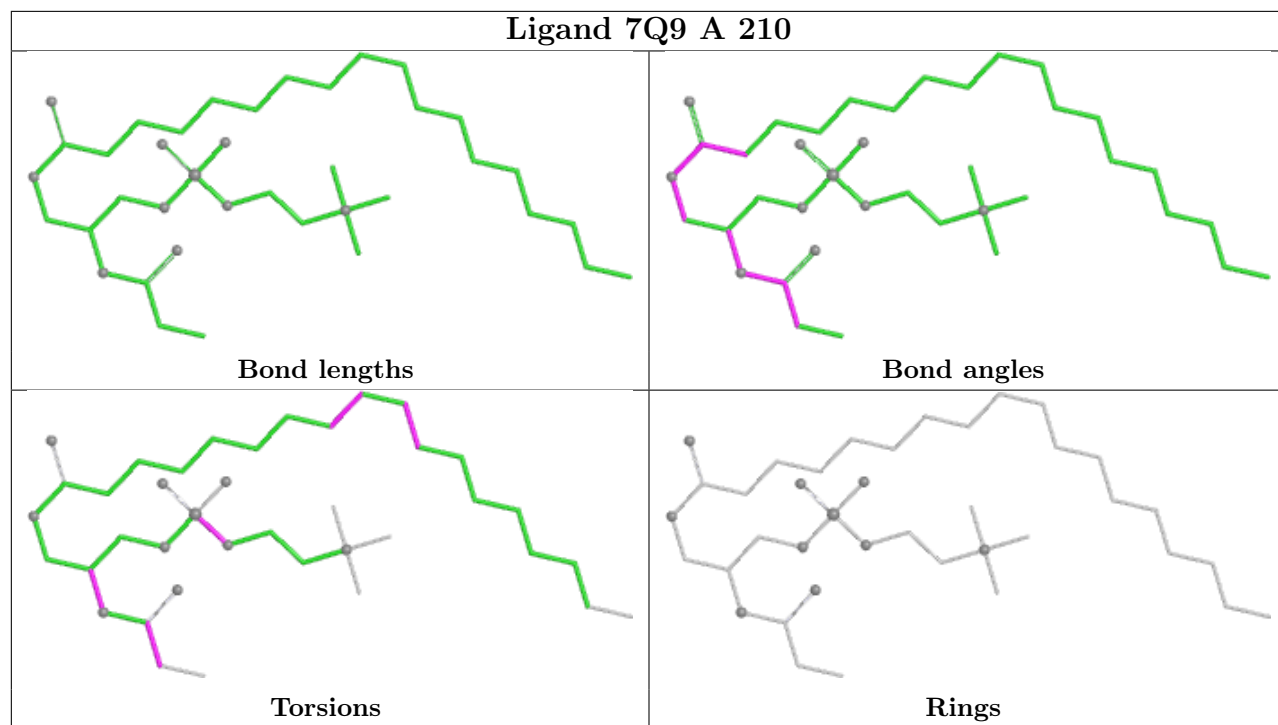
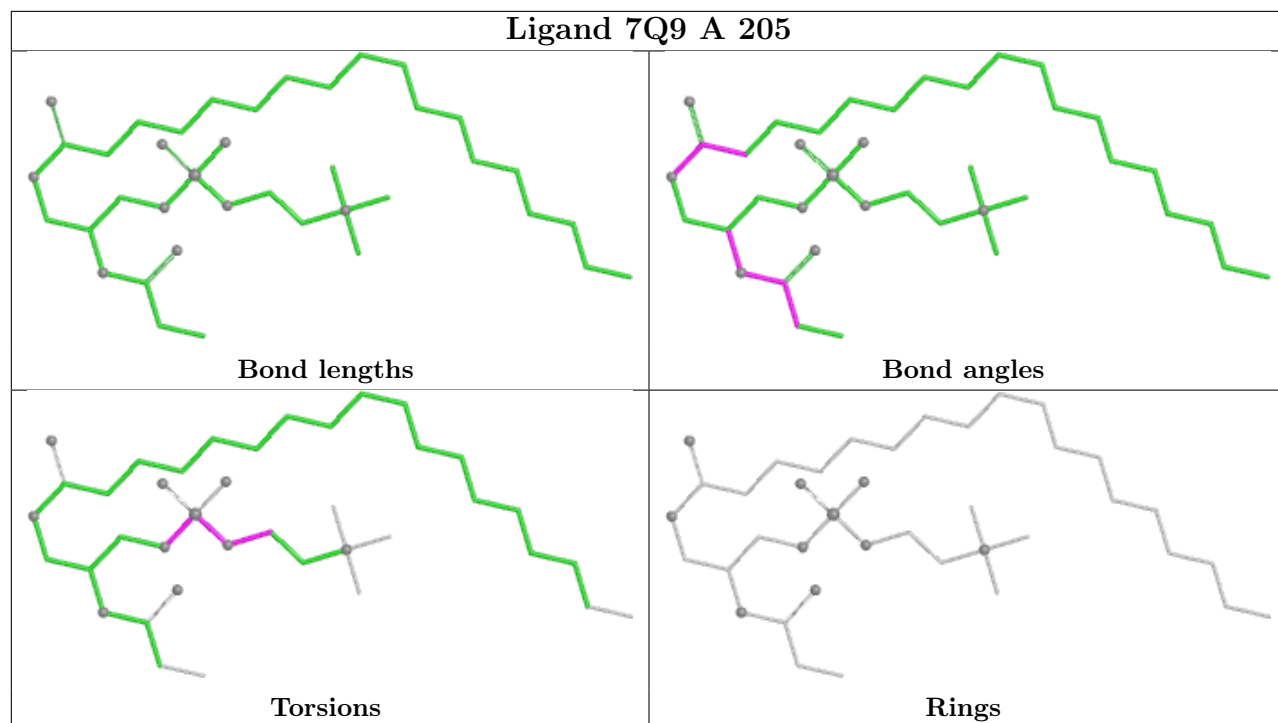


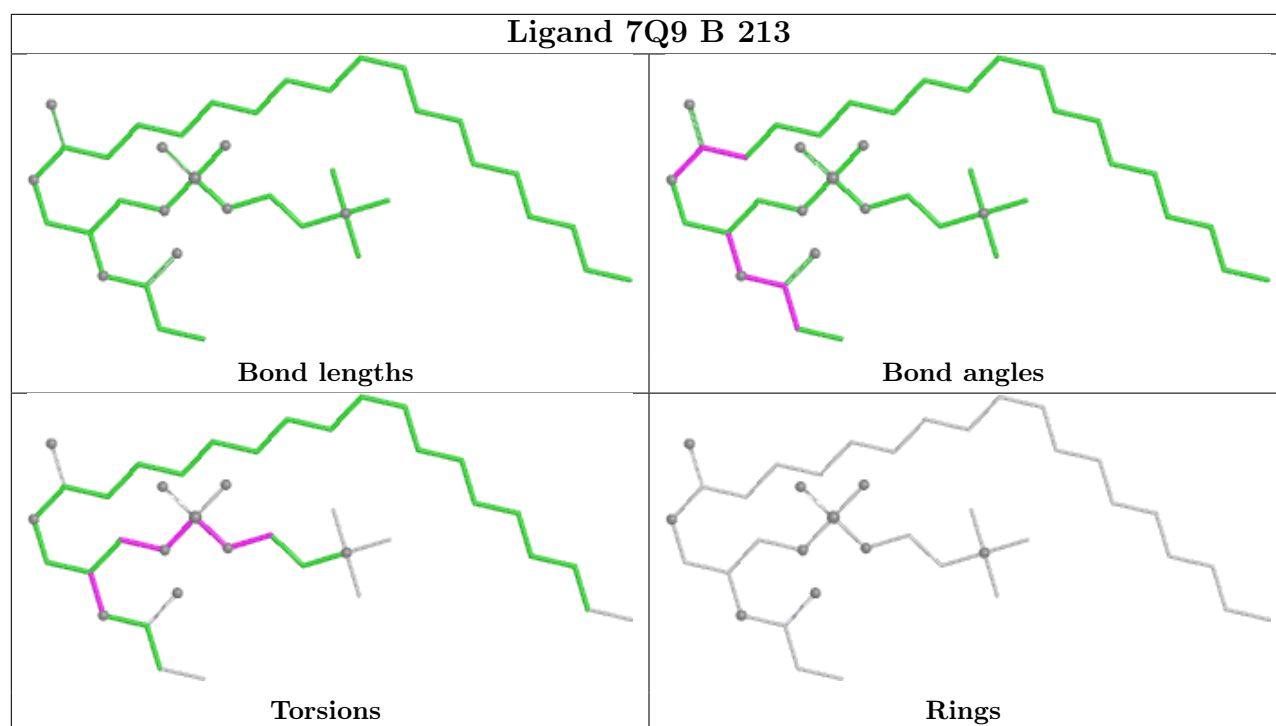


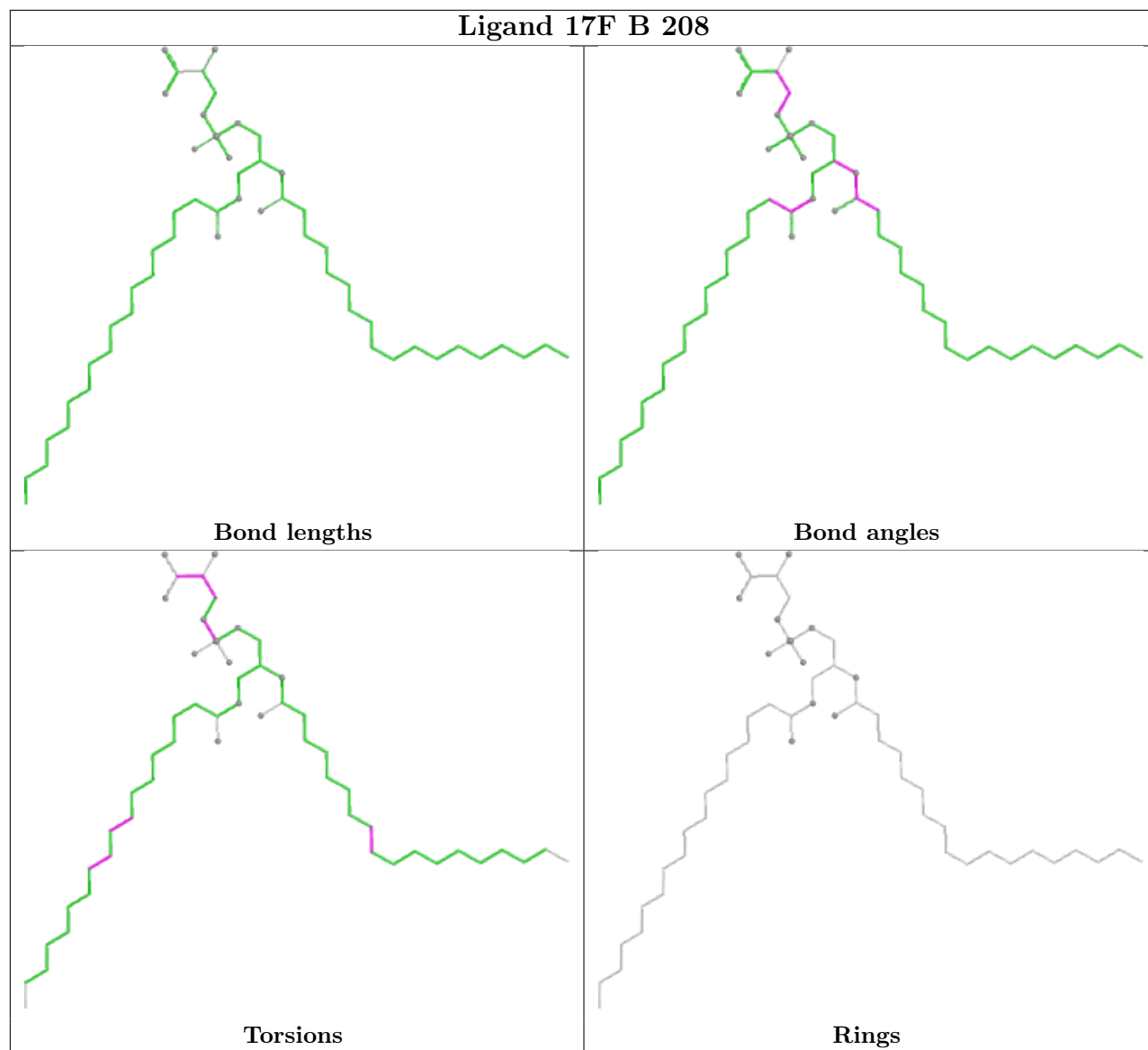


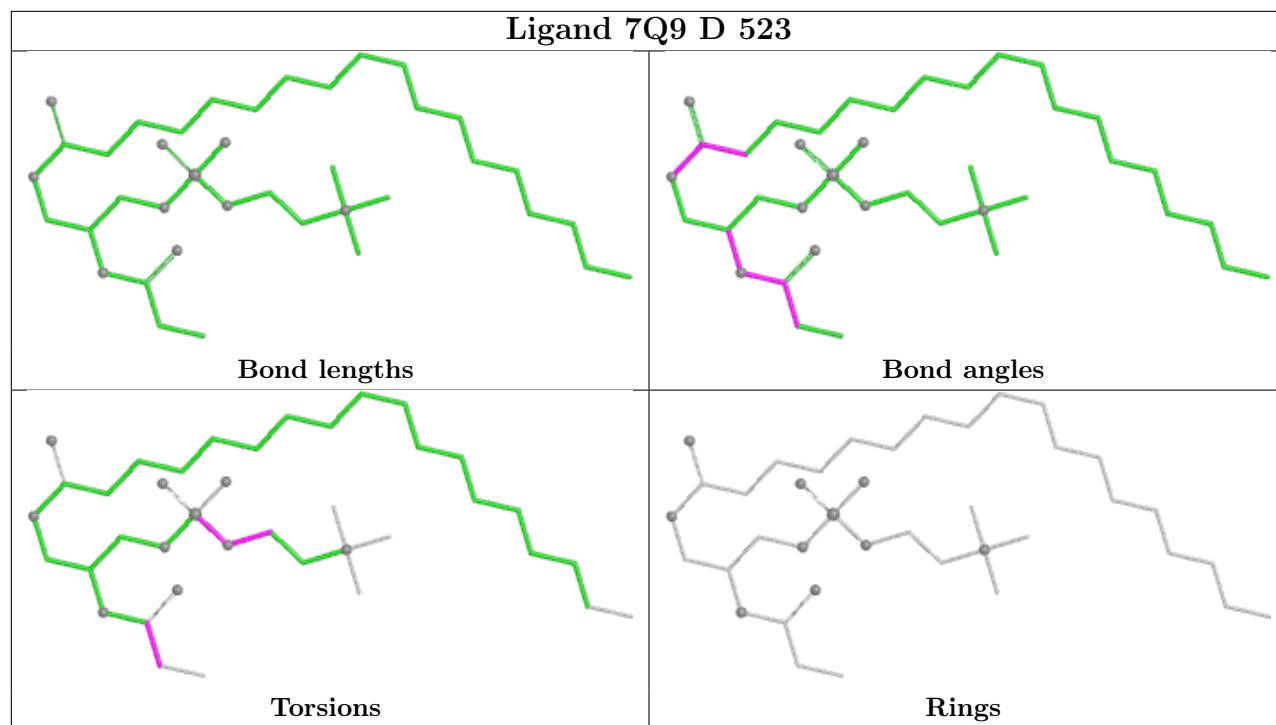
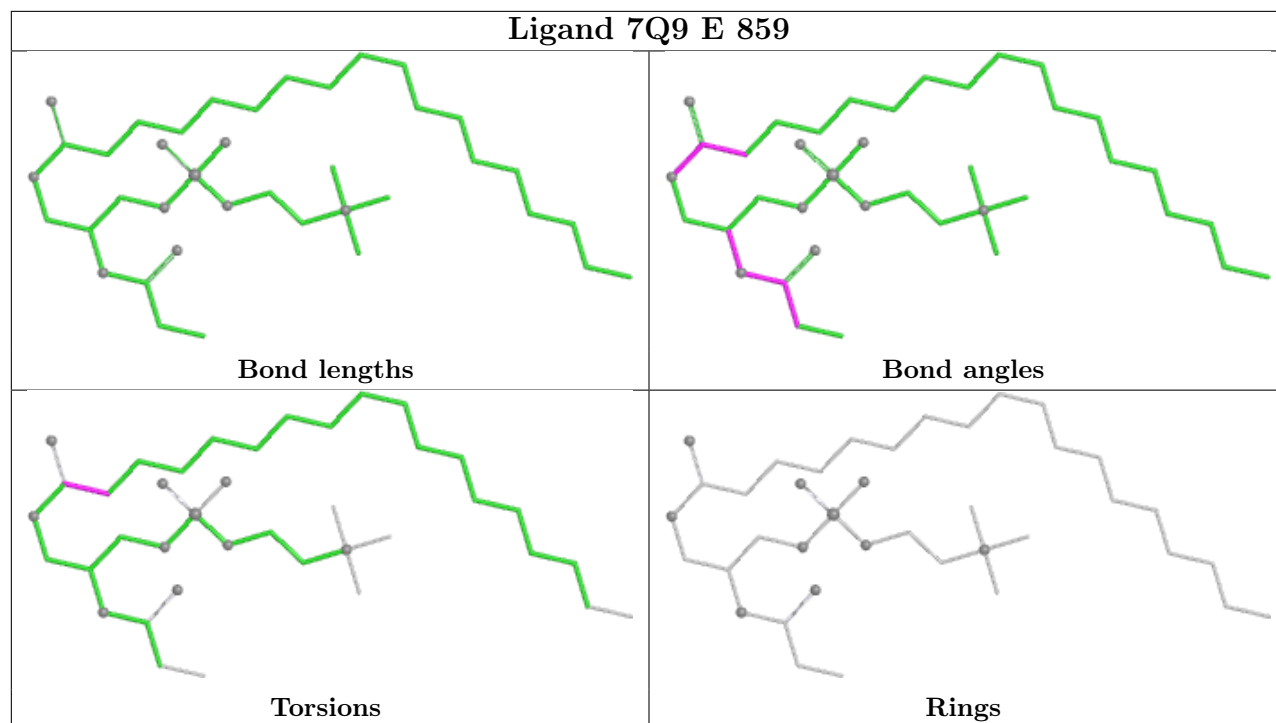




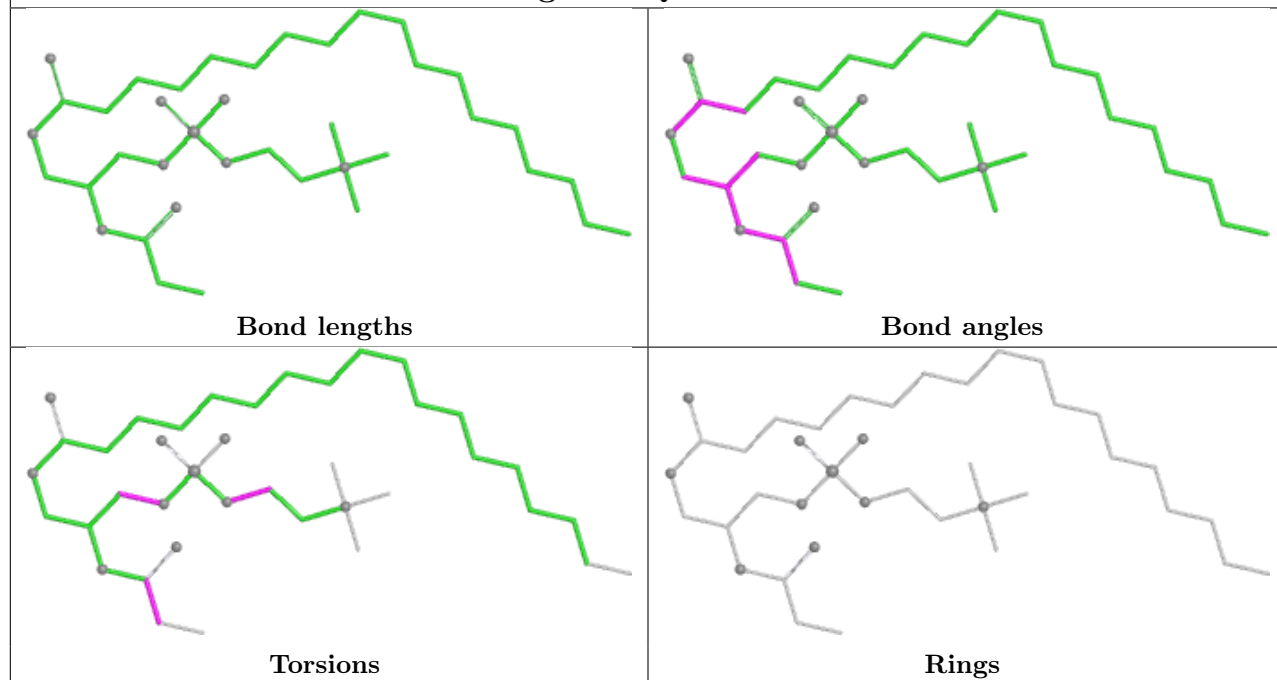




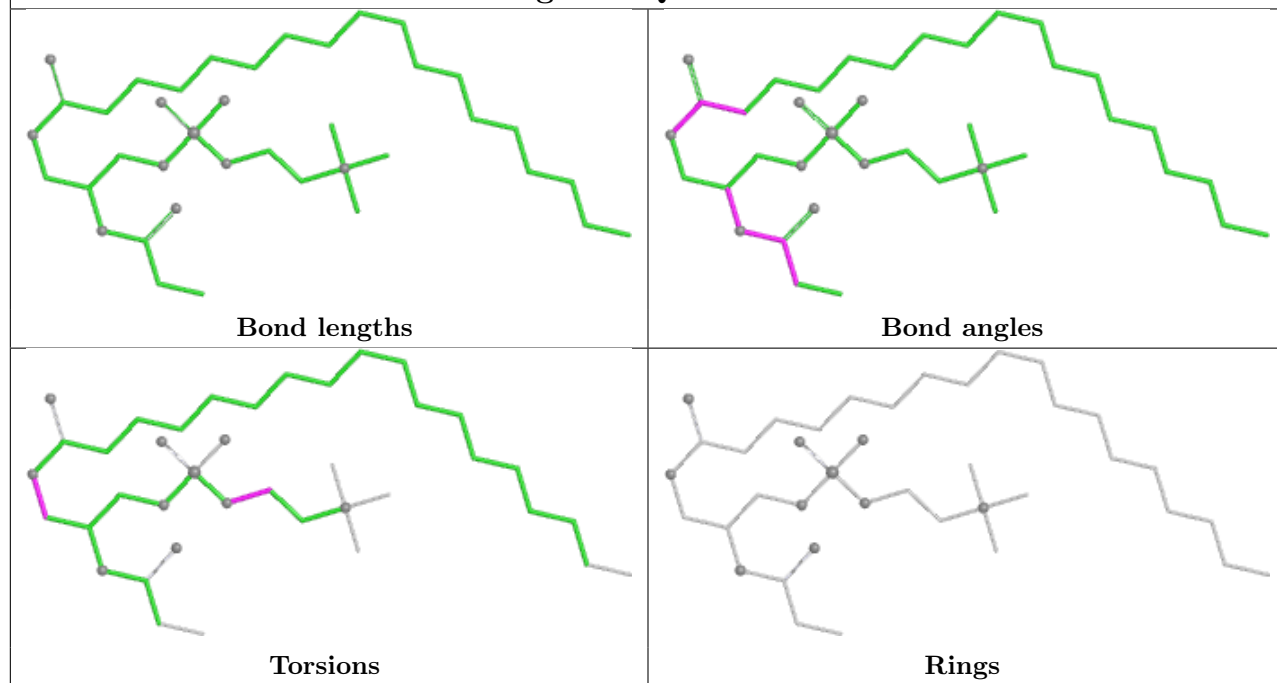


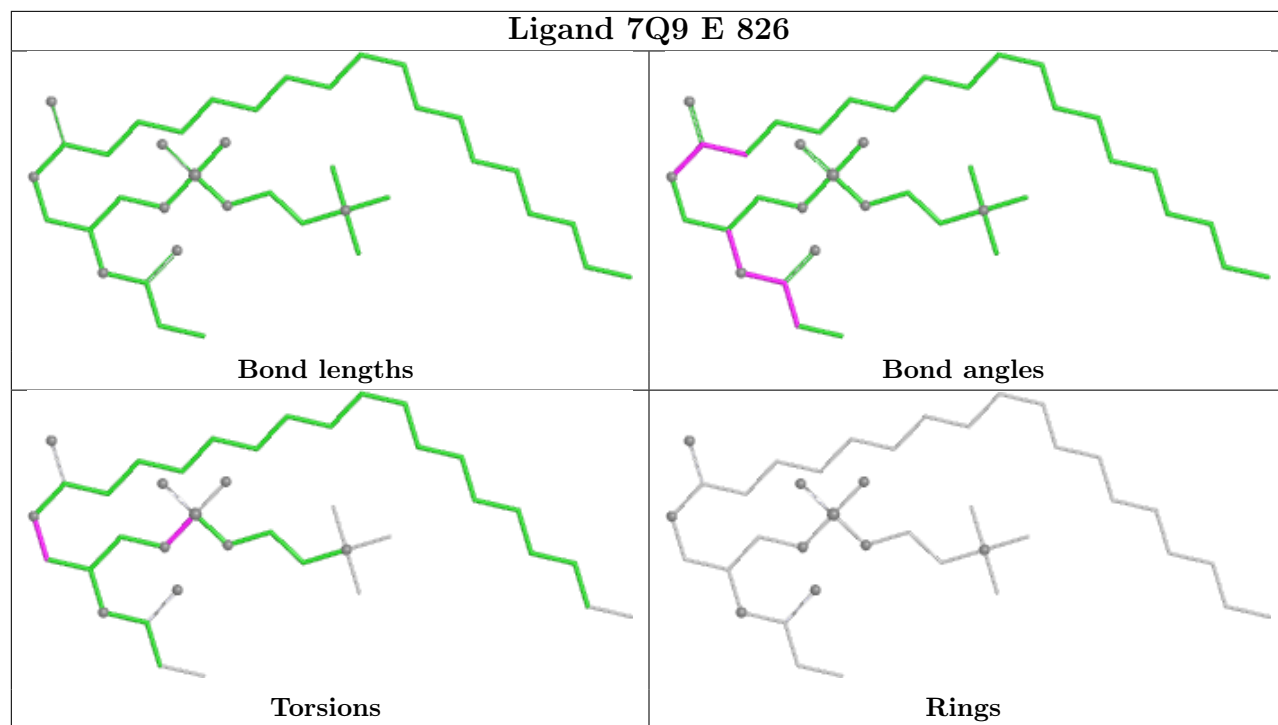
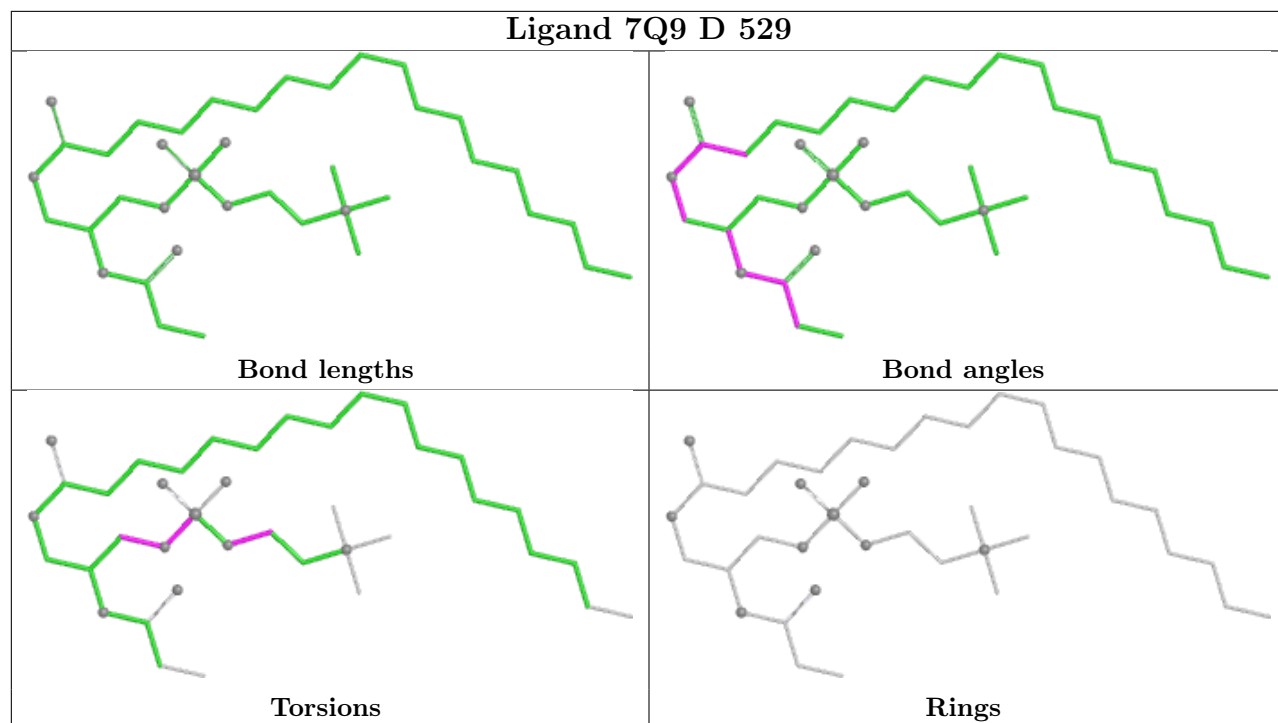


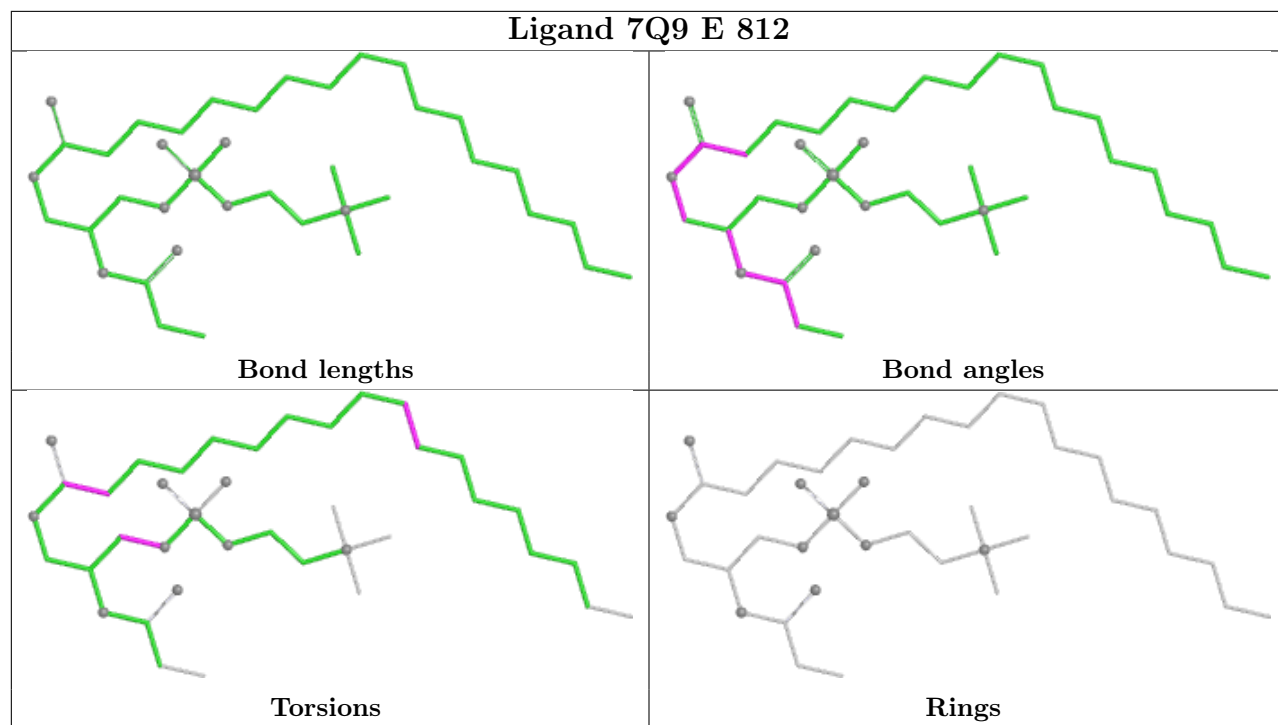
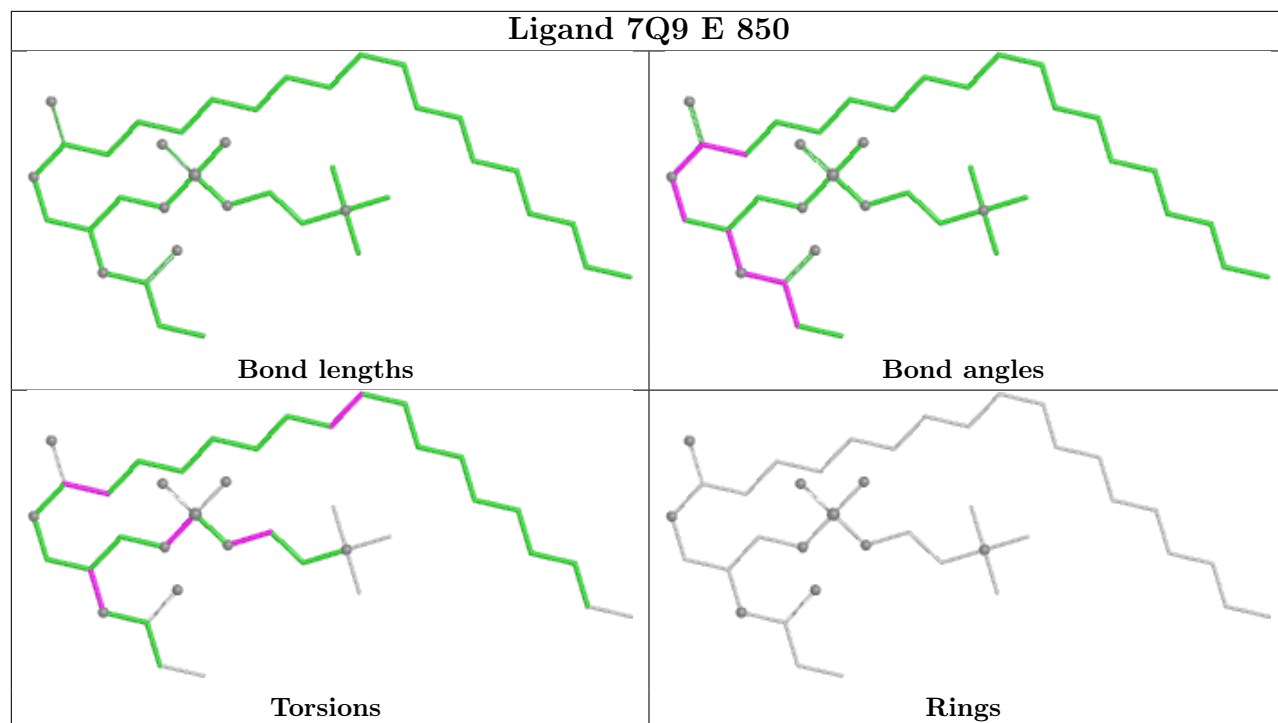
Ligand 7Q9 E 829



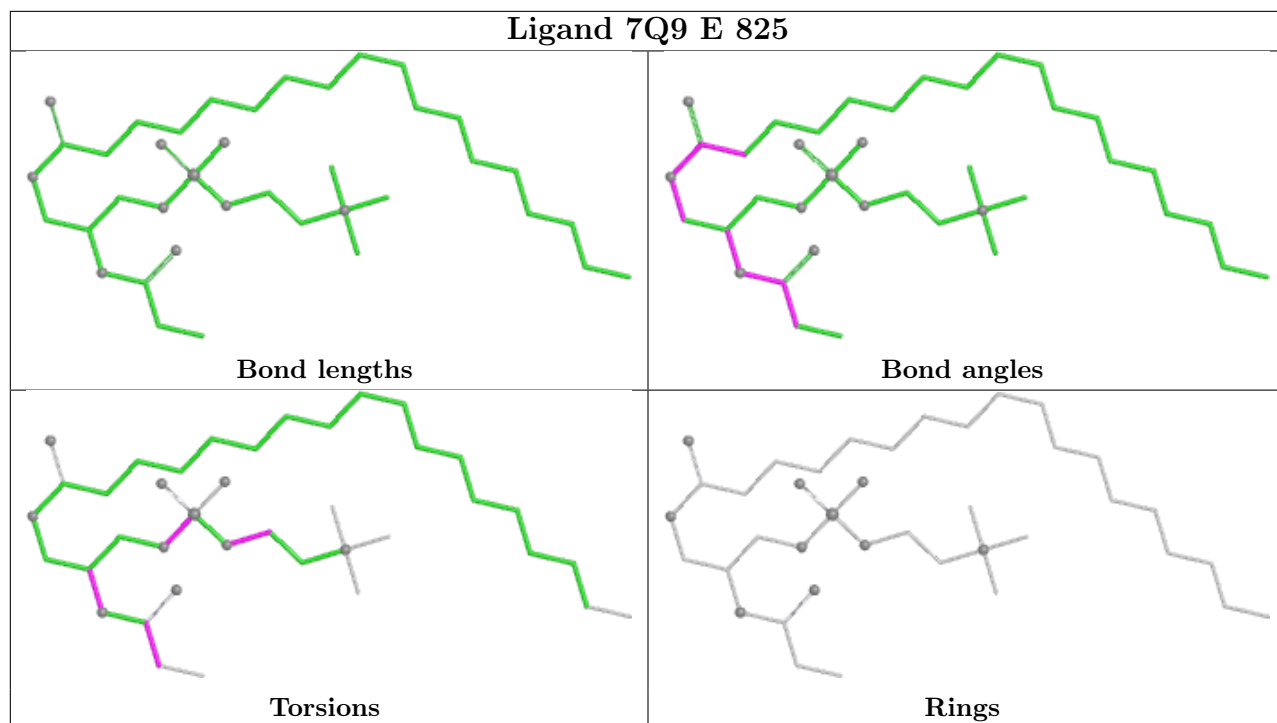
Ligand 7Q9 D 506



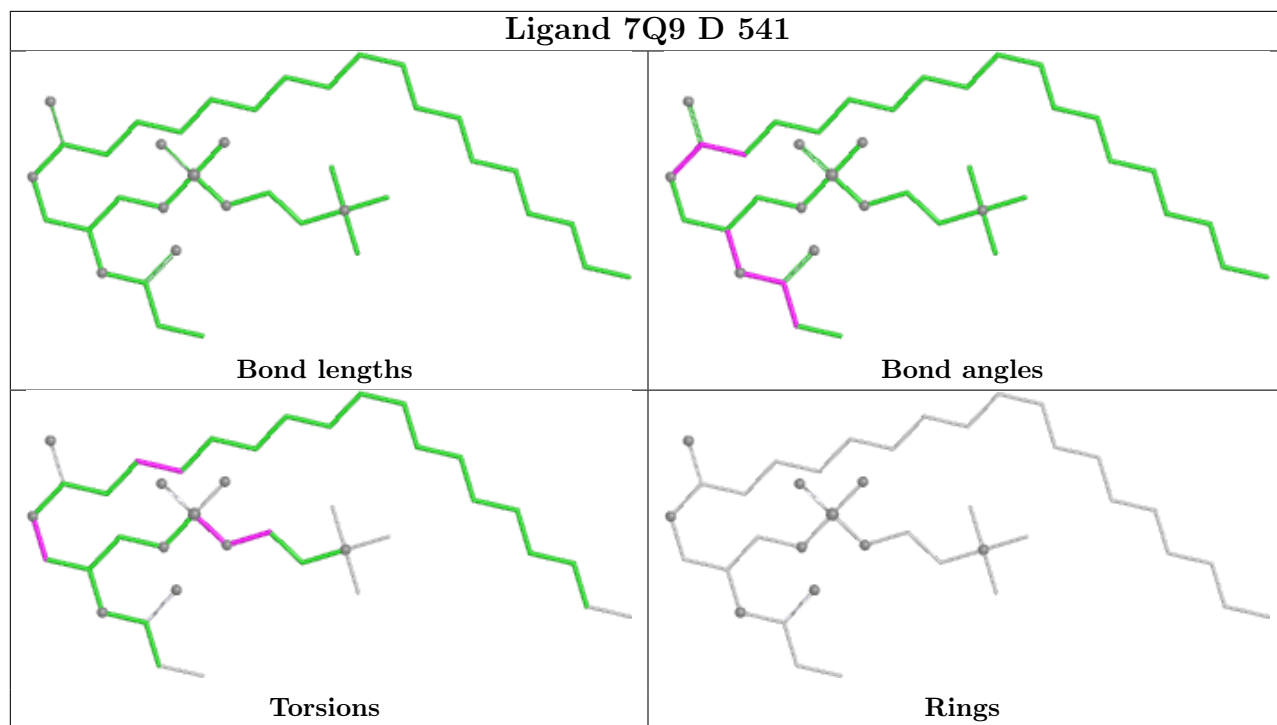


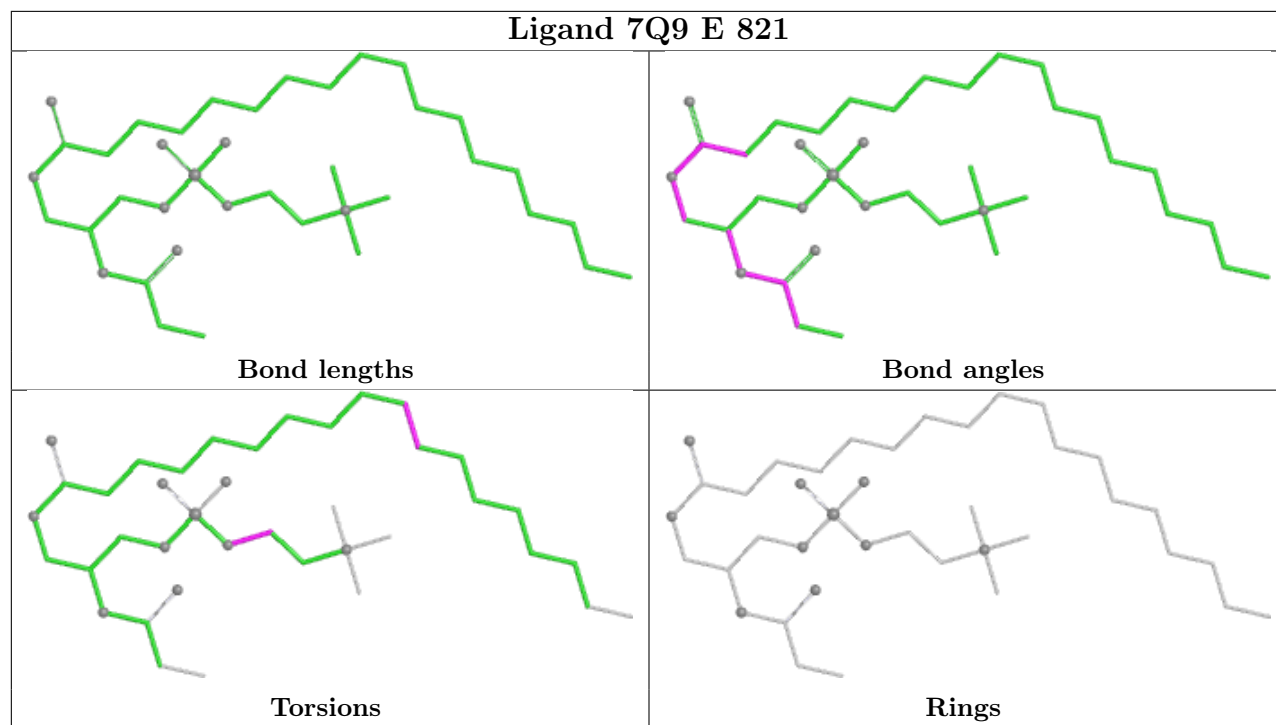
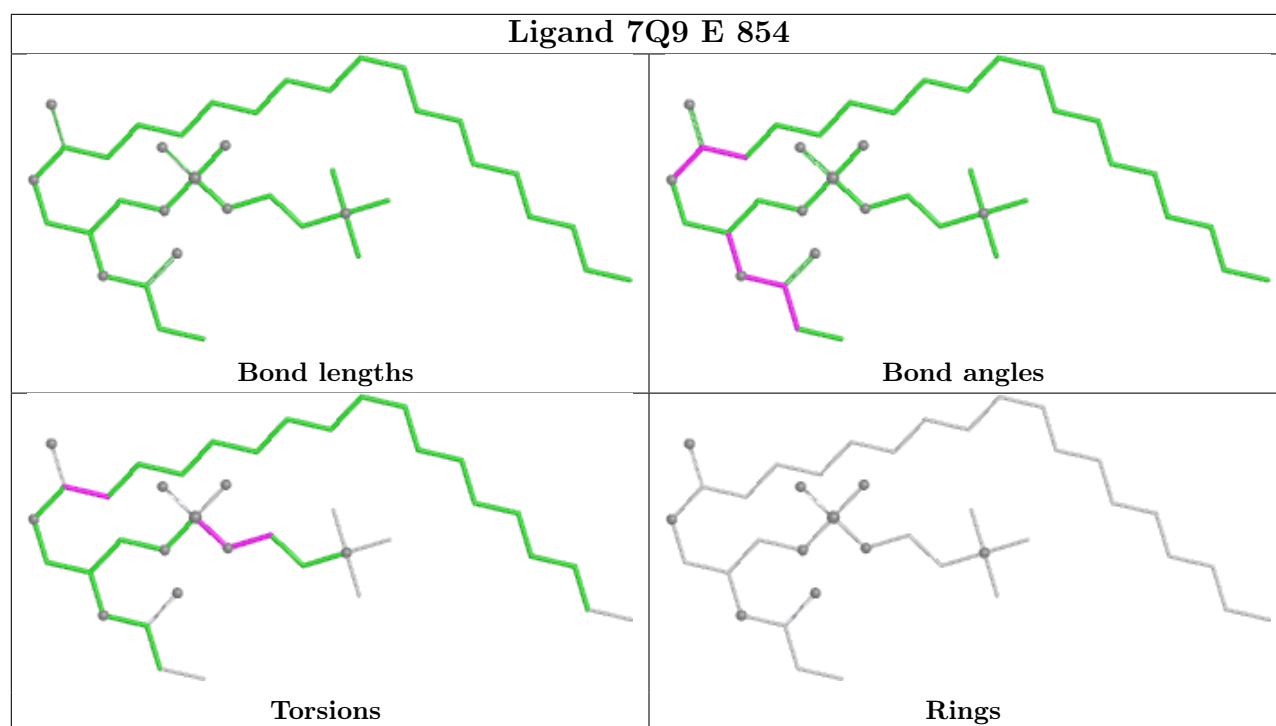


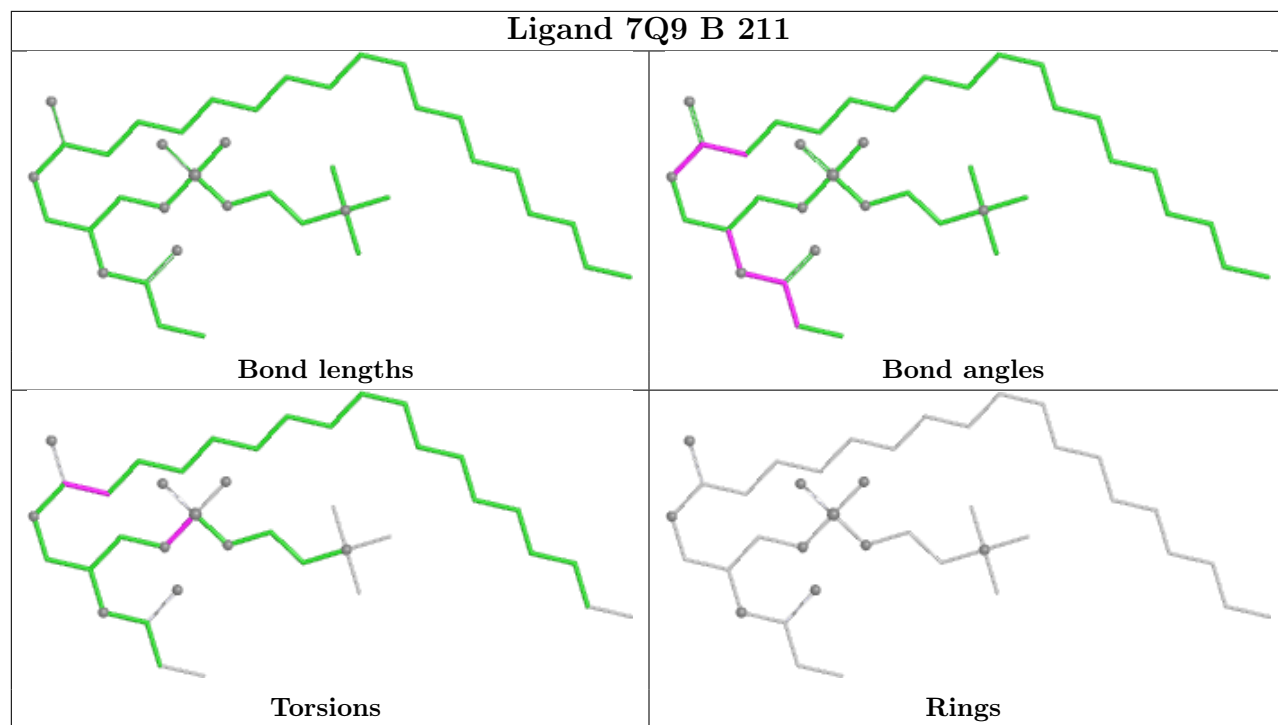
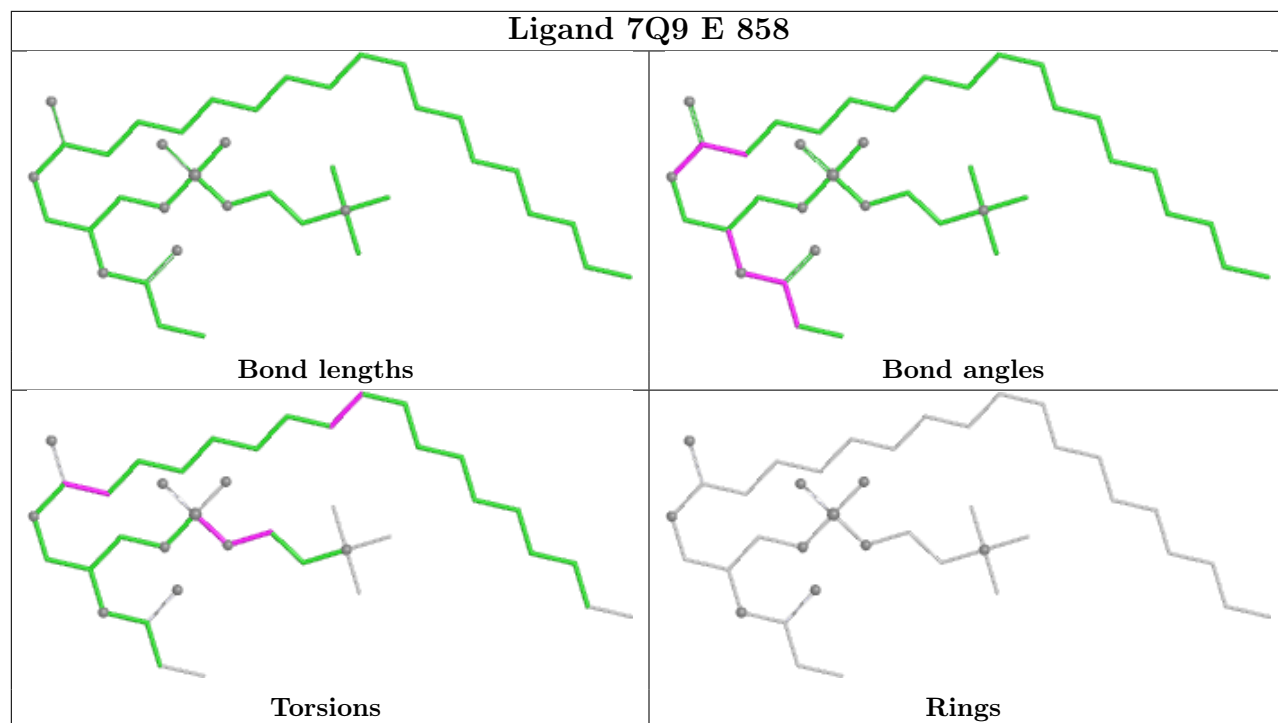
Ligand 7Q9 E 825



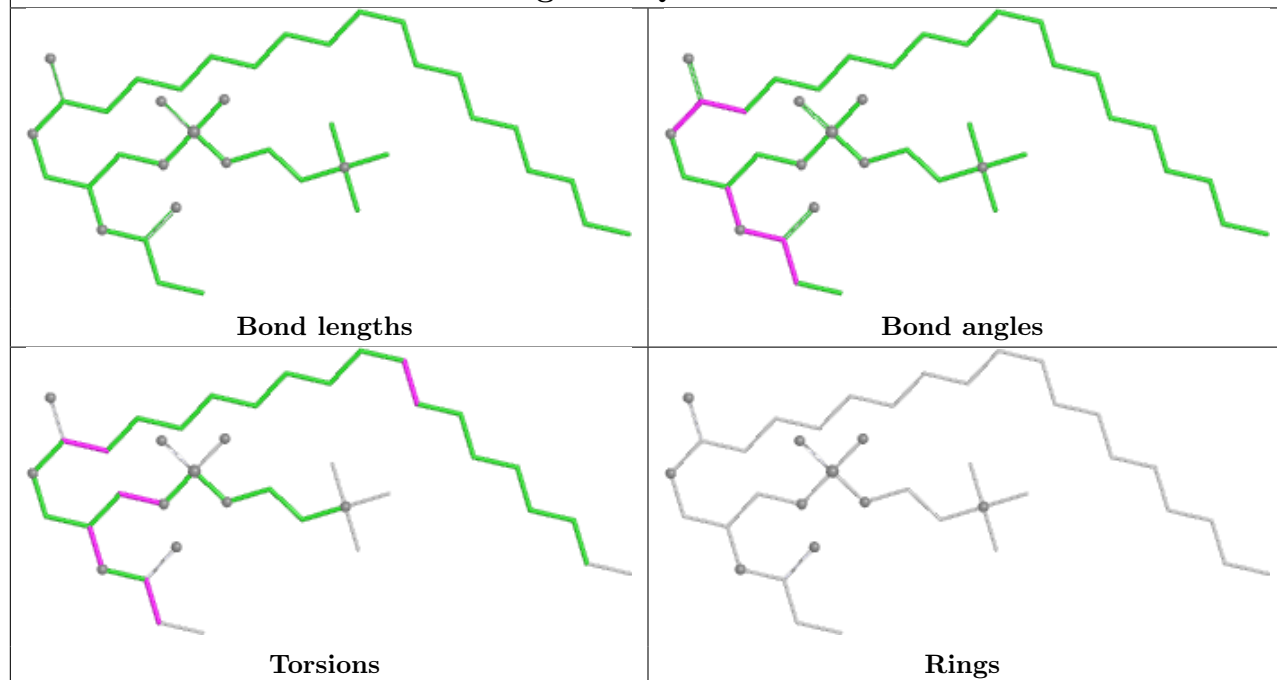
Ligand 7Q9 D 541



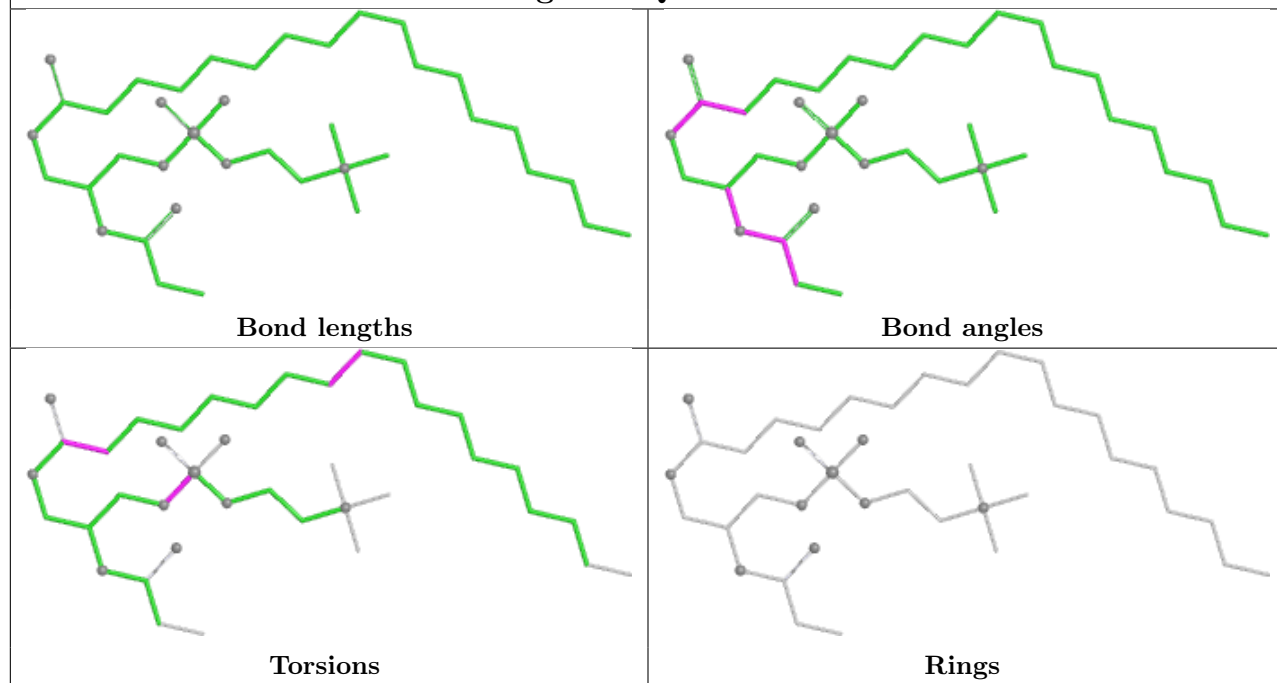




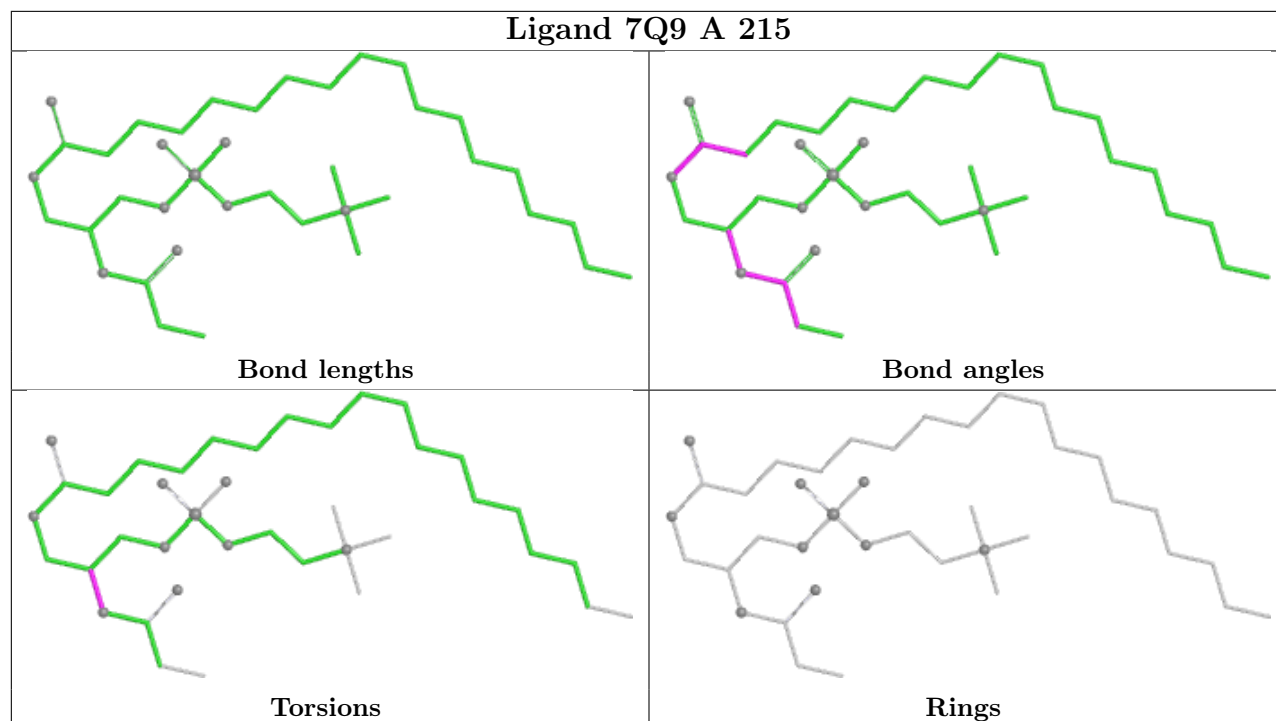
Ligand 7Q9 A 212



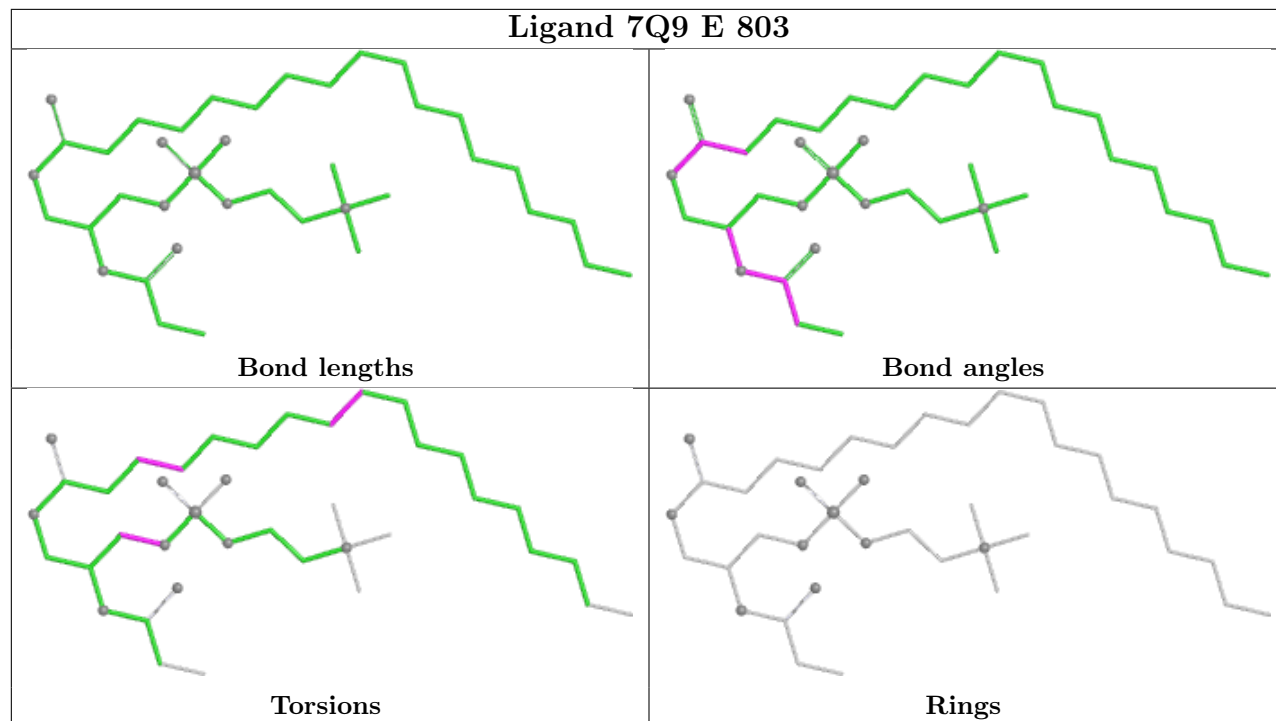
Ligand 7Q9 D 531



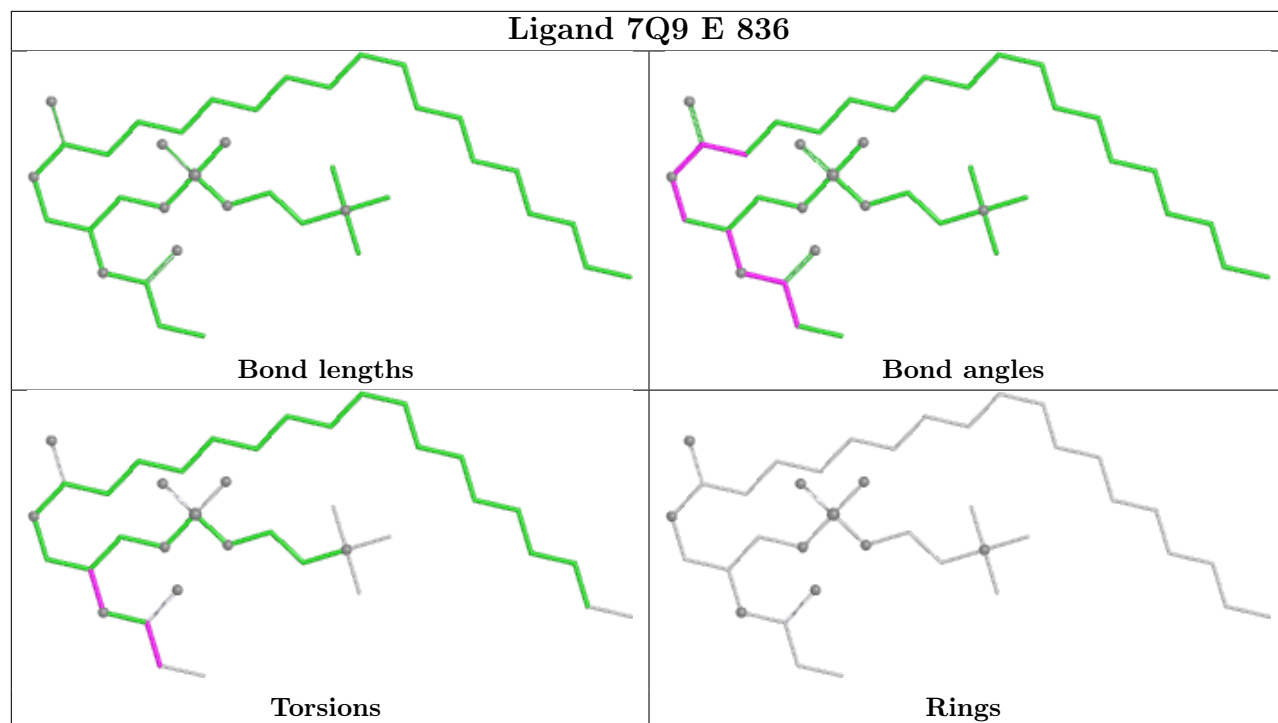
Ligand 7Q9 A 215



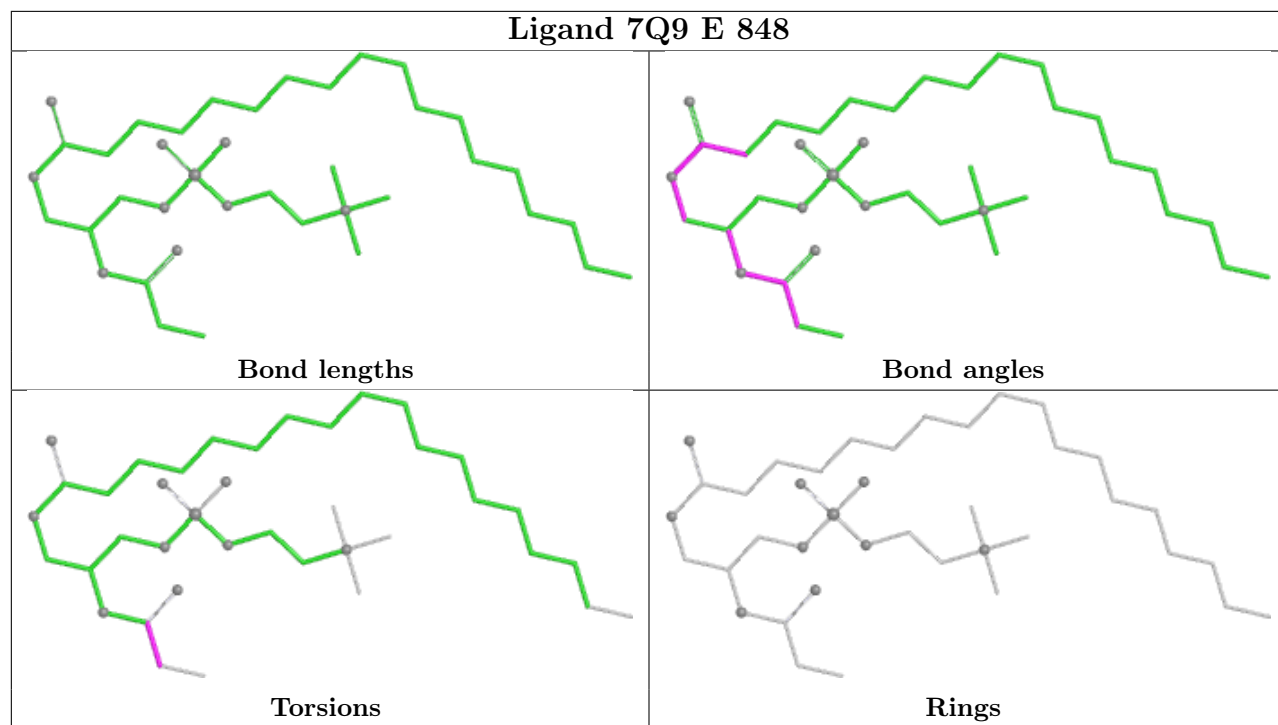
Ligand 7Q9 E 803



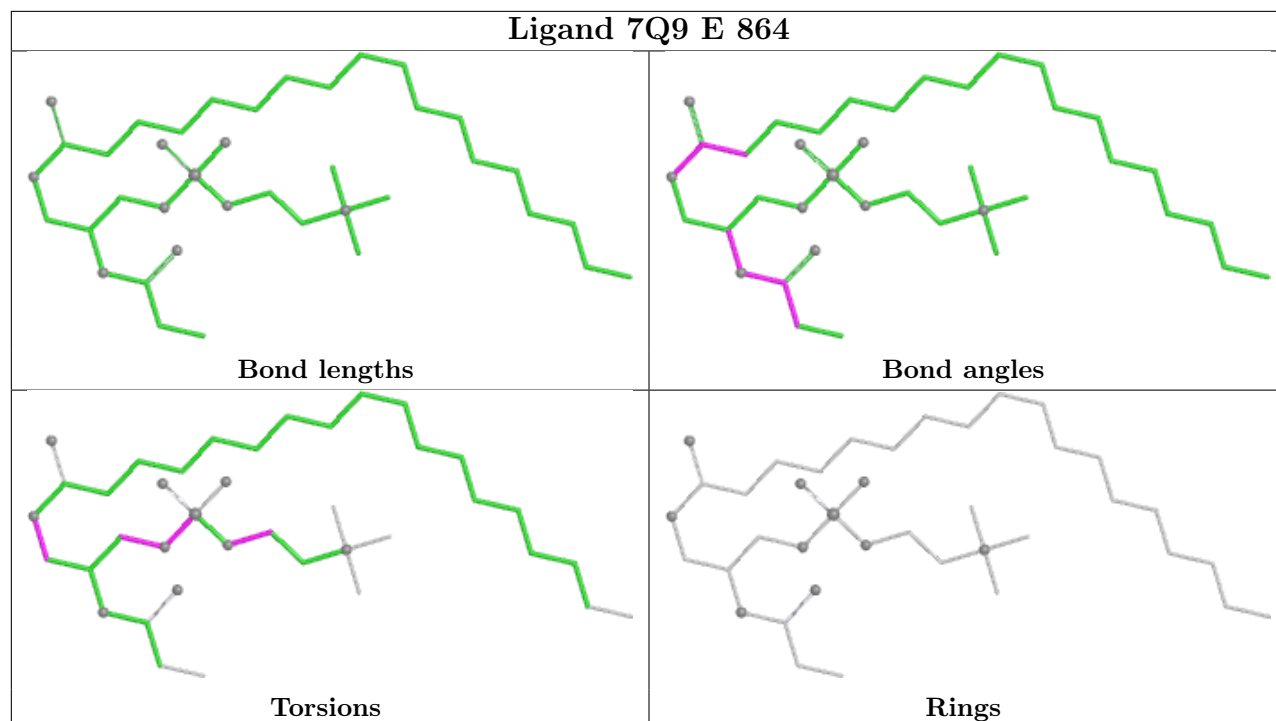
Ligand 7Q9 E 836



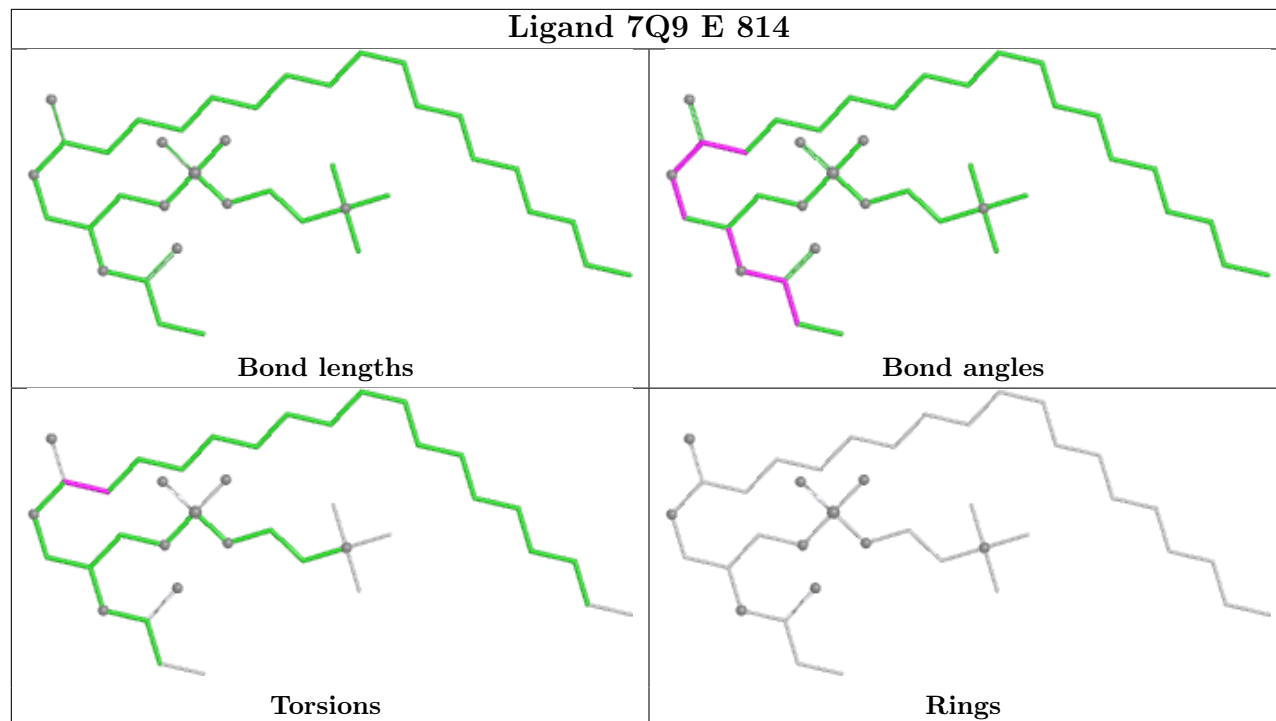
Ligand 7Q9 E 848



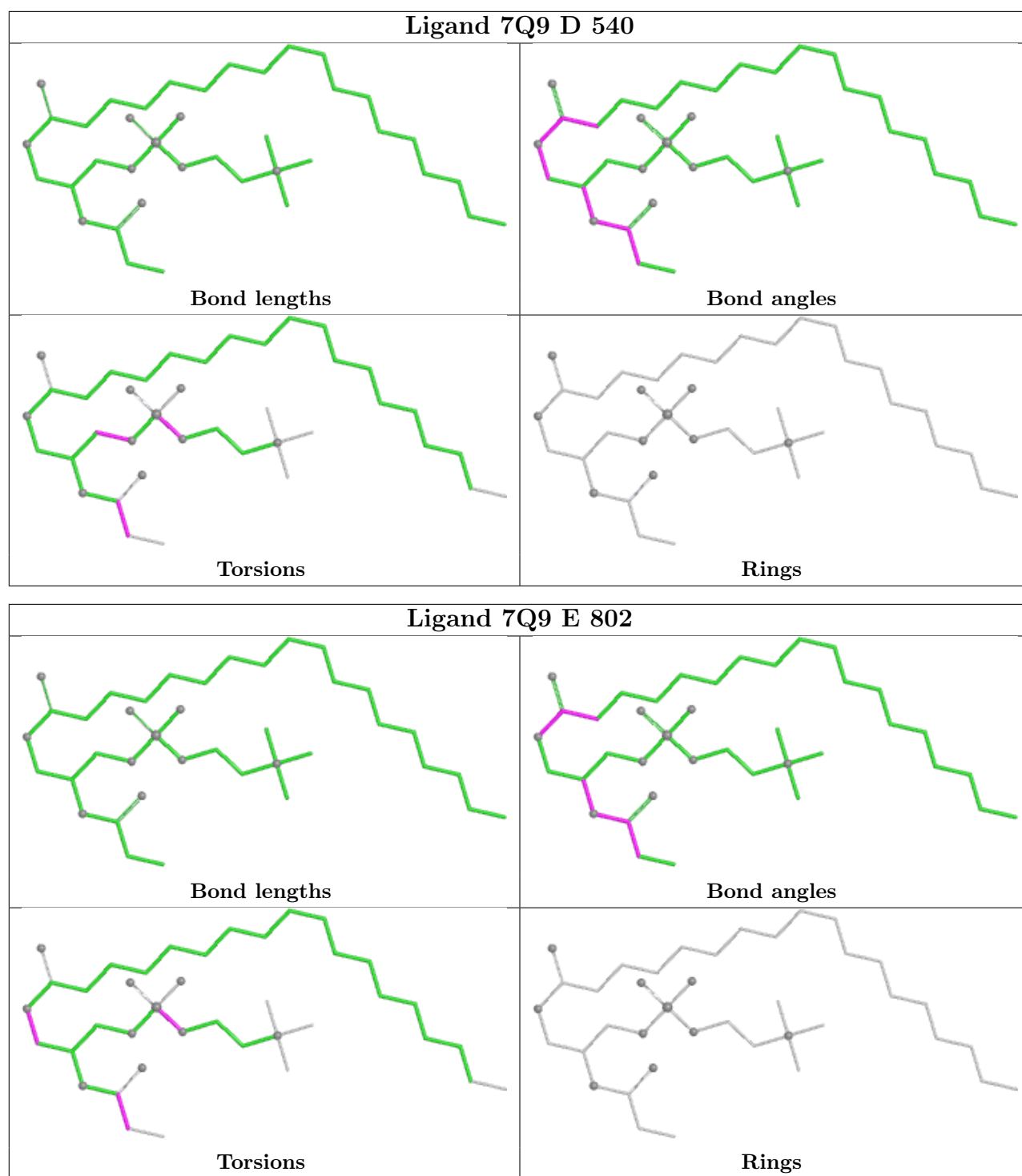
Ligand 7Q9 E 864



Ligand 7Q9 E 814







6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 1% for the well-defined parts and 1% 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

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	154
Number of shifts mapped to atoms	61
Number of unparsed shifts	0
Number of shifts with mapping errors	93
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 93) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	LEU	HD11	0.763	.	2
1	A	6	LEU	HD12	0.763	.	2
1	A	6	LEU	HD13	0.763	.	2
1	A	8	VAL	HG21	0.7528	.	2
1	A	8	VAL	HG22	0.7528	.	2
1	A	8	VAL	HG23	0.7528	.	2
1	A	14	VAL	HG21	0.9725	.	2
1	A	14	VAL	HG22	0.9725	.	2
1	A	14	VAL	HG23	0.9725	.	2
1	A	19	LEU	HD11	0.4104	.	2
1	A	19	LEU	HD12	0.4104	.	2
1	A	19	LEU	HD13	0.4104	.	2
1	A	19	LEU	HD21	0.5804	.	2
1	A	19	LEU	HD22	0.5804	.	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	19	LEU	HD23	0.5804	.	2
1	A	21	ILE	HD11	0.4182	.	1
1	A	21	ILE	HD12	0.4182	.	1
1	A	21	ILE	HD13	0.4182	.	1
1	A	23	LEU	HD11	-0.477	.	2
1	A	23	LEU	HD12	-0.477	.	2
1	A	23	LEU	HD13	-0.477	.	2
1	A	24	ILE	HD11	0.2691	.	1
1	A	24	ILE	HD12	0.2691	.	1
1	A	24	ILE	HD13	0.2691	.	1
1	A	36	ILE	HD11	0.5397	.	1
1	A	36	ILE	HD12	0.5397	.	1
1	A	36	ILE	HD13	0.5397	.	1
1	A	44	VAL	HG11	0.5353	.	2
1	A	44	VAL	HG12	0.5353	.	2
1	A	44	VAL	HG13	0.5353	.	2
1	A	45	VAL	HG11	0.4379	.	2
1	A	45	VAL	HG12	0.4379	.	2
1	A	45	VAL	HG13	0.4379	.	2
1	A	46	ILE	HD11	0.2525	.	1
1	A	46	ILE	HD12	0.2525	.	1
1	A	46	ILE	HD13	0.2525	.	1
1	A	55	ILE	HD11	0.3369	.	1
1	A	55	ILE	HD12	0.3369	.	1
1	A	55	ILE	HD13	0.3369	.	1
1	A	56	LEU	HD11	0.5372	.	2
1	A	56	LEU	HD12	0.5372	.	2
1	A	56	LEU	HD13	0.5372	.	2
1	A	79	LEU	HD11	-0.1312	.	2
1	A	79	LEU	HD12	-0.1312	.	2
1	A	79	LEU	HD13	-0.1312	.	2
1	A	79	LEU	HD21	-0.015	.	2
1	A	79	LEU	HD22	-0.015	.	2
1	A	79	LEU	HD23	-0.015	.	2
1	A	81	VAL	HG21	0.4663	.	2
1	A	81	VAL	HG22	0.4663	.	2
1	A	81	VAL	HG23	0.4663	.	2
1	A	84	ILE	HD11	0.5865	.	1
1	A	84	ILE	HD12	0.5865	.	1
1	A	84	ILE	HD13	0.5865	.	1
1	A	93	ILE	HD11	0.6063	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	ILE	HD12	0.6063	.	1
1	A	93	ILE	HD13	0.6063	.	1
1	A	100	ILE	HD11	0.0964	.	1
1	A	100	ILE	HD12	0.0964	.	1
1	A	100	ILE	HD13	0.0964	.	1
1	A	103	VAL	HG11	0.8243	.	2
1	A	103	VAL	HG12	0.8243	.	2
1	A	103	VAL	HG13	0.8243	.	2
1	A	112	VAL	HG11	0.5953	.	2
1	A	112	VAL	HG12	0.5953	.	2
1	A	112	VAL	HG13	0.5953	.	2
1	A	113	LEU	HD11	0.8748	.	2
1	A	113	LEU	HD12	0.8748	.	2
1	A	113	LEU	HD13	0.8748	.	2
1	A	120	LEU	HD11	0.6958	.	2
1	A	120	LEU	HD12	0.6958	.	2
1	A	120	LEU	HD13	0.6958	.	2
1	A	125	VAL	HG11	-0.3248	.	2
1	A	125	VAL	HG12	-0.3248	.	2
1	A	125	VAL	HG13	-0.3248	.	2
1	A	133	LEU	HD11	0.2014	.	2
1	A	133	LEU	HD12	0.2014	.	2
1	A	133	LEU	HD13	0.2014	.	2
1	A	139	ILE	HD11	0.7118	.	1
1	A	139	ILE	HD12	0.7118	.	1
1	A	139	ILE	HD13	0.7118	.	1
1	A	142	ILE	HD11	0.5035	.	1
1	A	142	ILE	HD12	0.5035	.	1
1	A	142	ILE	HD13	0.5035	.	1
1	A	159	LEU	HD11	0.51	.	2
1	A	159	LEU	HD12	0.51	.	2
1	A	159	LEU	HD13	0.51	.	2
1	A	160	VAL	HG11	-0.2062	.	2
1	A	160	VAL	HG12	-0.2062	.	2
1	A	160	VAL	HG13	-0.2062	.	2
1	A	163	ILE	HD11	0.5261	.	1
1	A	163	ILE	HD12	0.5261	.	1
1	A	163	ILE	HD13	0.5261	.	1

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 1%, i.e. 144 atoms were assigned a chemical shift out of a possible 9928. 0 out of 125 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	20/3532 (1%)	10/1429 (1%)	0/1416 (0%)	10/687 (1%)
Sidechain	124/5777 (2%)	93/3712 (3%)	31/1806 (2%)	0/259 (0%)
Aromatic	0/619 (0%)	0/306 (0%)	0/291 (0%)	0/22 (0%)
Overall	144/9928 (1%)	103/5447 (2%)	31/3513 (1%)	10/968 (1%)

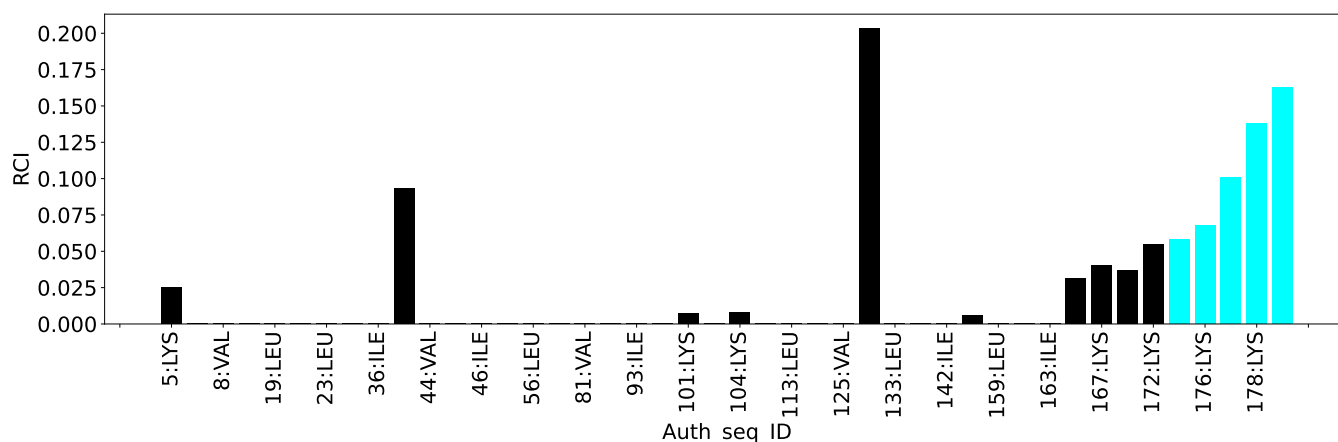
7.1.4 Statistically unusual chemical shifts [i](#)

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	45
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	14
Inter-chain	31
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	5
Number of restraints per residue	0.0
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.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	None	None
0.2-0.5 (Medium)	0.1	0.48
>0.5 (Large)	21.9	37.39

8.2.2 Average number of dihedral-angle violations per model [i](#)

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

9 Distance violation analysis ⓘ

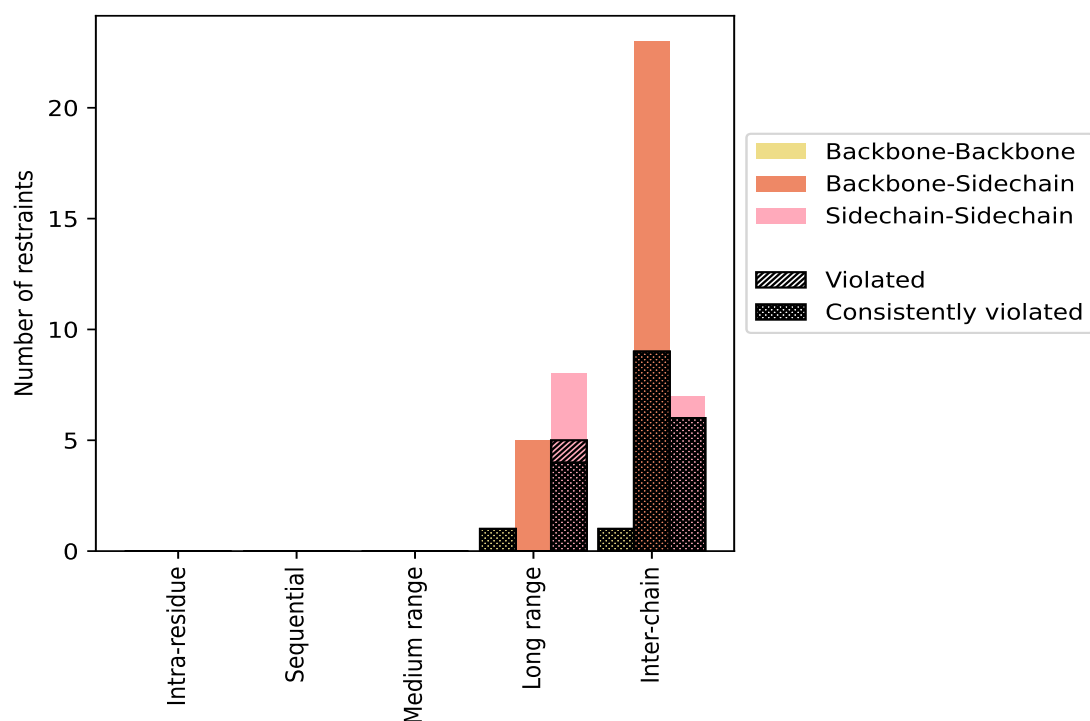
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \geq 5$)	14	31.1	6	42.9	13.3	5	35.7	11.1
Backbone-Backbone	1	2.2	1	100.0	2.2	1	100.0	2.2
Backbone-Sidechain	5	11.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	8	17.8	5	62.5	11.1	4	50.0	8.9
Inter-chain	31	68.9	16	51.6	35.6	16	51.6	35.6
Backbone-Backbone	1	2.2	1	100.0	2.2	1	100.0	2.2
Backbone-Sidechain	23	51.1	9	39.1	20.0	9	39.1	20.0
Sidechain-Sidechain	7	15.6	6	85.7	13.3	6	85.7	13.3
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	45	100.0	22	48.9	48.9	21	46.7	46.7
Backbone-Backbone	2	4.4	2	100.0	4.4	2	100.0	4.4
Backbone-Sidechain	28	62.2	9	32.1	20.0	9	32.1	20.0
Sidechain-Sidechain	15	33.3	11	73.3	24.4	10	66.7	22.2

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 disulfied bonds are counted in their appropriate category on the x-axis

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

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	2	20	22	10.63	20.24	3.97	11.02
2	0	0	0	2	20	22	9.96	15.2	3.83	10.72
3	0	0	0	1	21	22	11.21	24.53	4.62	10.5
4	0	0	0	1	21	22	11.32	37.39	6.42	10.28
5	0	0	0	0	21	21	9.62	14.55	2.5	9.56
6	0	0	0	2	20	22	11.37	28.35	5.17	11.18
7	0	0	0	2	20	22	11.05	26.13	4.59	9.85
8	0	0	0	1	21	22	11.67	35.94	6.41	10.46
9	0	0	0	1	21	22	11.09	30.01	5.21	10.26
10	0	0	0	2	20	22	11.4	27.95	4.73	10.96

Continued on next page...

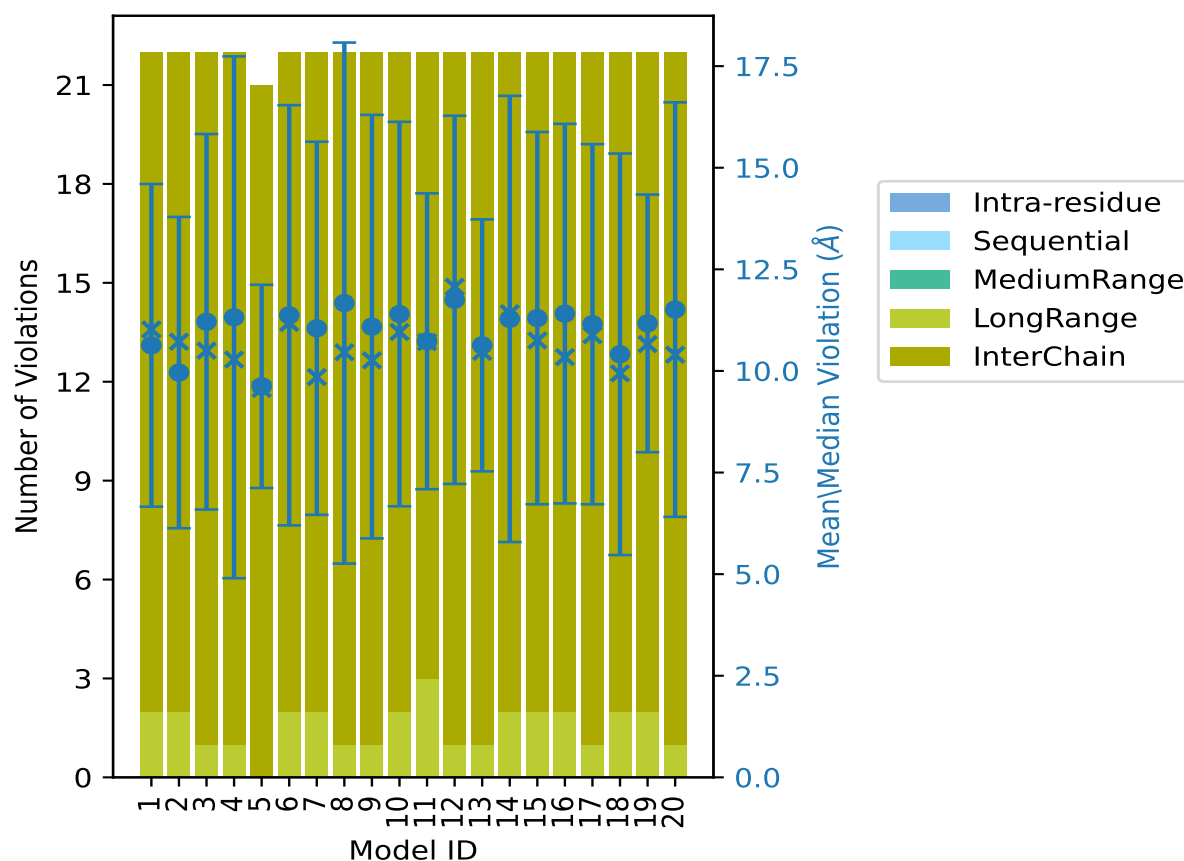
Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	3	19	22	10.73	18.46	3.64	10.71
12	0	0	0	1	21	22	11.75	24.93	4.53	12.07
13	0	0	0	1	21	22	10.63	15.03	3.1	10.47
14	0	0	0	2	20	22	11.28	29.44	5.49	11.42
15	0	0	0	2	20	22	11.3	26.6	4.58	10.75
16	0	0	0	2	20	22	11.41	28.13	4.67	10.34
17	0	0	0	1	21	22	11.15	24.67	4.43	10.88
18	0	0	0	2	20	22	10.41	26.99	4.94	9.94
19	0	0	0	2	20	22	11.17	16.37	3.17	10.66
20	0	0	0	1	21	22	11.51	29.97	5.1	10.4

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble ⓘ

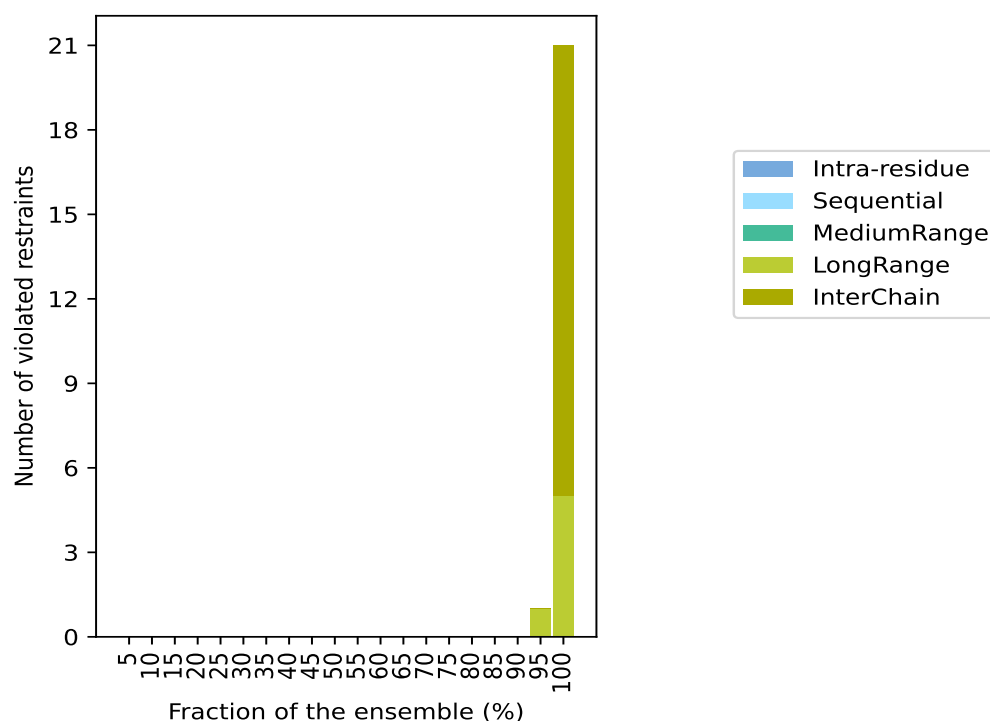
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 23(IR:0, SQ:0, MR:0, LR:8, IC:15) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	1	0	1	19	95.0
0	0	0	5	16	21	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

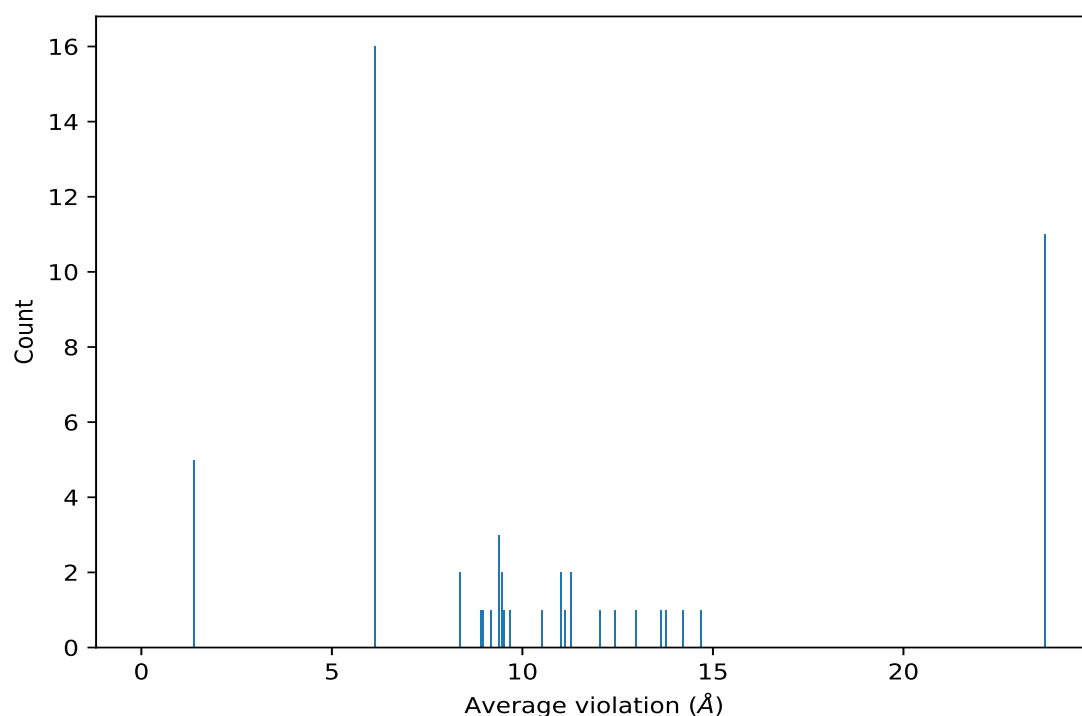
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,21)	1:184:A:LYS:HZ3	5:209:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:O	5:203:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:CE	5:209:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:CE	5:220:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:HZ2	5:209:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:HZ1	5:209:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:N	6:208:B:17F:N1	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:HZ3	5:220:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:N	5:216:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:H	6:208:B:17F:N1	20	23.74	8.95	26.36
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	20	14.66	0.68	15.04
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	20	14.21	0.73	14.3
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	20	13.75	1.57	14.19
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	20	13.64	1.42	13.94
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	20	12.99	1.43	13.18

Continued on next page...

Continued from previous page...

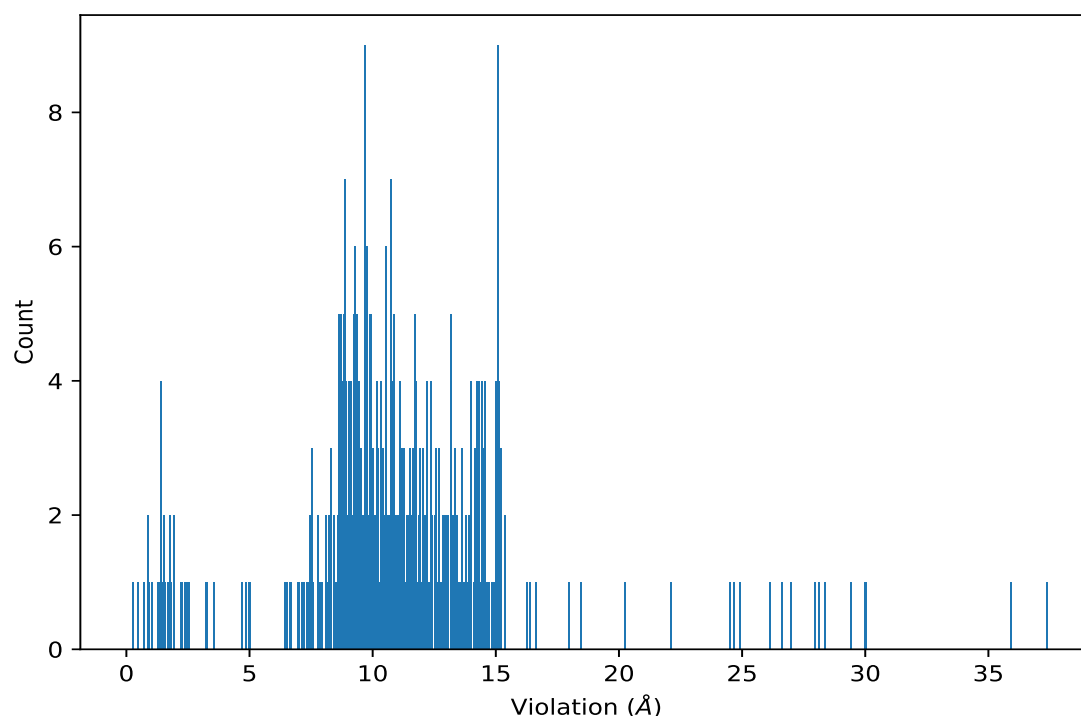
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	20	12.44	0.74	12.51
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	20	12.01	0.88	11.98
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	20	11.27	1.09	11.15
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD2	20	11.27	1.09	11.15
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	20	11.12	0.86	10.84

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table provides the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	4	37.39
(1,21)	1:184:A:LYS:HZ1	5:209:B:7Q9:N	8	35.94
(1,21)	1:184:A:LYS:N	6:208:B:17F:N1	9	30.01
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	20	29.97
(1,21)	1:184:A:LYS:H	6:208:B:17F:N1	14	29.44
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	6	28.35
(1,21)	1:184:A:LYS:HZ1	5:209:B:7Q9:N	16	28.13
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	10	27.95
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	18	26.99
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	15	26.6

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found