



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 04:37 AM JST

PDB ID : 7EQD
EMDB ID : EMD-31258
Title : STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF RHODOSPIRILLUM RUBRUM
Authors : Tani, K.; Kanno, R.; Ji, X.-C.; Yu, L.-J.; Hall, M.; Kimura, Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on : 2021-05-01
Resolution : 2.76 Å (reported)
Based on initial model : 5Y5S

This is a wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

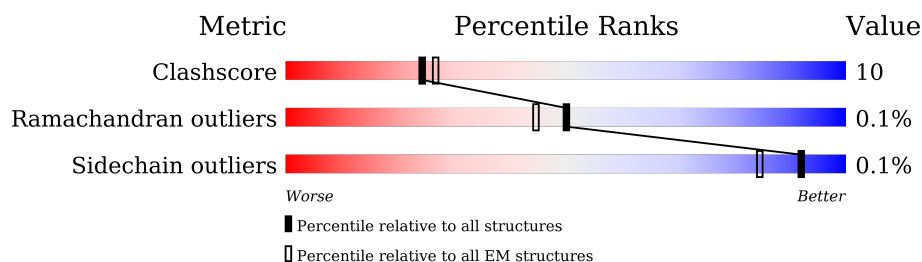
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.76 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	275	
2	M	305	
3	H	256	
4	1	62	
4	3	62	
4	5	62	
4	7	62	
4	9	62	

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Mol	Chain	Length	Quality of chain
4	A	62	
4	D	62	
4	F	62	
4	I	62	
4	K	62	
4	O	62	
4	Q	62	
4	S	62	
4	U	62	
4	W	62	
4	Y	62	
5	0	55	
5	2	55	
5	4	55	
5	6	55	
5	8	55	
5	B	55	
5	E	55	
5	G	55	
5	J	55	
5	N	55	
5	P	55	
5	R	55	
5	T	55	
5	V	55	

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Mol	Chain	Length	Quality of chain
5	X	55	<div><div></div><div>29%</div><div></div><div>64%</div><div></div><div>18%</div><div></div><div>18%</div></div>
5	Z	55	<div><div></div><div>18%</div><div></div><div>71%</div><div></div><div>9%</div><div></div><div>20%</div></div>

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 23122 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	275	Total	C	N	O	S	0	0
			2169	1458	345	356	10		

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	304	Total	C	N	O	S	0	0
			2408	1608	396	395	9		

- Molecule 3 is a protein called Photoreaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	256	Total	C	N	O	S	0	0
			1951	1248	339	361	3		

- Molecule 4 is a protein called Light-harvesting protein B-870 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
4	D	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
4	F	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
4	I	47	Total	C	N	O	S	0	0
			391	266	62	62	1		
4	K	47	Total	C	N	O	S	0	0
			391	266	62	62	1		
4	O	47	Total	C	N	O	S	0	0
			387	264	61	61	1		
4	Q	47	Total	C	N	O	S	0	0
			391	266	62	62	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	47	Total	C	N	O	S	0	0
			382	258	61	62	1		
4	U	47	Total	C	N	O	S	0	0
			391	266	62	62	1		
4	W	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
4	Y	47	Total	C	N	O	S	0	0
			391	266	62	62	1		
4	1	47	Total	C	N	O	S	0	0
			393	266	64	62	1		
4	3	47	Total	C	N	O	S	0	0
			393	266	64	62	1		
4	5	47	Total	C	N	O	S	0	0
			393	266	64	62	1		
4	7	47	Total	C	N	O	S	0	0
			382	258	61	62	1		
4	9	47	Total	C	N	O	S	0	0
			391	266	62	62	1		

- Molecule 5 is a protein called Light-harvesting protein B-870 beta chain.

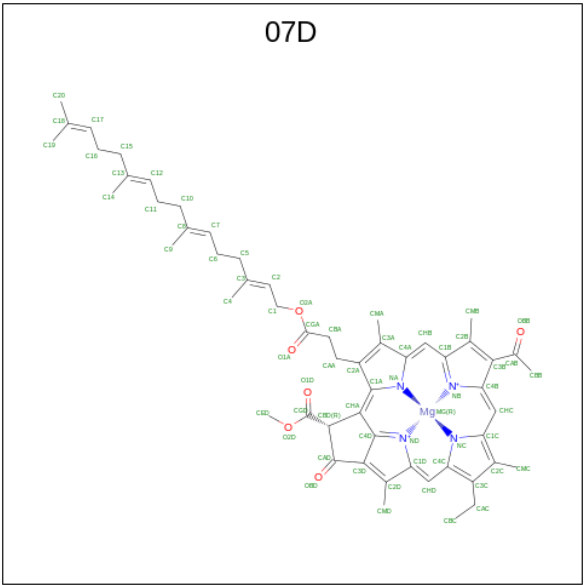
Mol	Chain	Residues	Atoms				AltConf	Trace
5	B	45	Total	C	N	O	0	0
			367	250	58	59		
5	E	44	Total	C	N	O	0	0
			351	240	57	54		
5	G	45	Total	C	N	O	0	0
			367	250	58	59		
5	J	45	Total	C	N	O	0	0
			367	250	58	59		
5	N	45	Total	C	N	O	0	0
			367	250	58	59		
5	P	44	Total	C	N	O	0	0
			359	244	57	58		
5	R	45	Total	C	N	O	0	0
			363	248	58	57		
5	T	45	Total	C	N	O	0	0
			350	239	57	54		
5	V	45	Total	C	N	O	0	0
			354	242	58	54		
5	X	45	Total	C	N	O	0	0
			362	246	58	58		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	Z	44	Total	C	N	O	0	0
			355	242	57	56		
5	2	44	Total	C	N	O	0	0
			351	239	56	56		
5	4	45	Total	C	N	O	0	0
			350	239	57	54		
5	6	45	Total	C	N	O	0	0
			346	237	57	52		
5	8	44	Total	C	N	O	0	0
			349	239	57	53		
5	0	45	Total	C	N	O	0	0
			367	250	58	59		

- Molecule 6 is Trans-Geranyl BACTERIOCHLOROPHYLL A (three-letter code: 07D) (formula: $C_{55}H_{64}MgN_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
6	L	1	Total	C	Mg	N	O
			66	55	1	4	6
6	L	1	Total	C	Mg	N	O
			66	55	1	4	6
6	M	1	Total	C	Mg	N	O
			66	55	1	4	6
6	M	1	Total	C	Mg	N	O
			66	55	1	4	6
6	A	1	Total	C	Mg	N	O
			66	55	1	4	6

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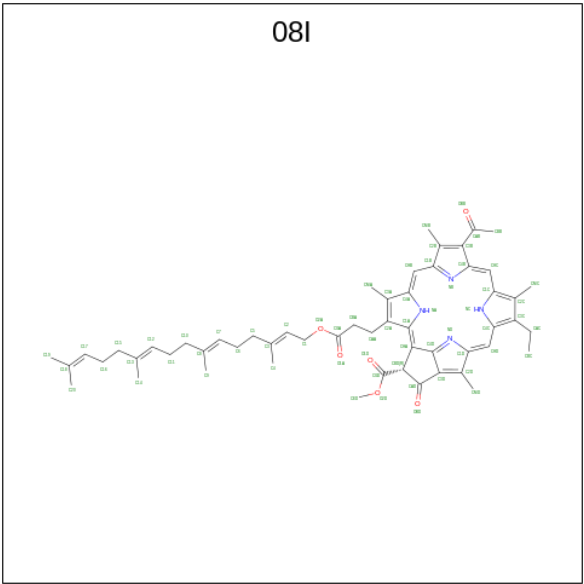
Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
6	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
6	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 7 is Trans-Geranyl BACTERIOPHEOPHYTIN A (three-letter code: 08I) (formula: C₅₅H₆₆N₄O₆).



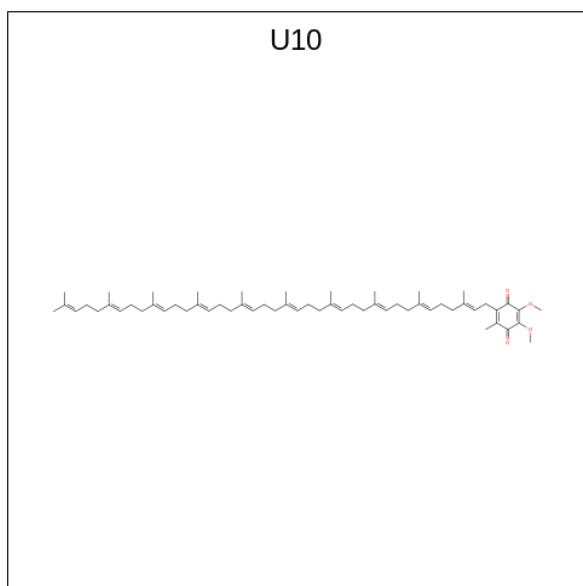
Mol	Chain	Residues	Atoms				AltConf
7	L	1	Total	C	N	O	0
			65	55	4	6	

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Mol	Chain	Residues	Atoms				AltConf
7	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms				AltConf
8	L	1	Total	C	O		0
			28	24	4		
8	M	1	Total	C	O		0
			18	14	4		

- Molecule 9 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).

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Mol	Chain	Residues	Atoms			AltConf
10	L	1	Total	C	O	0
			32	21	11	
10	M	1	Total	C	O	0
			35	24	11	
10	M	1	Total	C	O	0
			29	18	11	
10	H	1	Total	C	O	0
			35	24	11	
10	B	1	Total	C	O	0
			35	24	11	
10	E	1	Total	C	O	0
			35	24	11	
10	G	1	Total	C	O	0
			35	24	11	
10	J	1	Total	C	O	0
			35	24	11	
10	N	1	Total	C	O	0
			35	24	11	
10	P	1	Total	C	O	0
			35	24	11	
10	R	1	Total	C	O	0
			35	24	11	
10	T	1	Total	C	O	0
			35	24	11	
10	V	1	Total	C	O	0
			35	24	11	
10	X	1	Total	C	O	0
			35	24	11	
10	Z	1	Total	C	O	0
			35	24	11	
10	2	1	Total	C	O	0
			35	24	11	
10	4	1	Total	C	O	0
			35	24	11	
10	5	1	Total	C	O	0
			31	20	11	
10	5	1	Total	C	O	0
			35	24	11	
10	6	1	Total	C	O	0
			35	24	11	
10	8	1	Total	C	O	0
			35	24	11	

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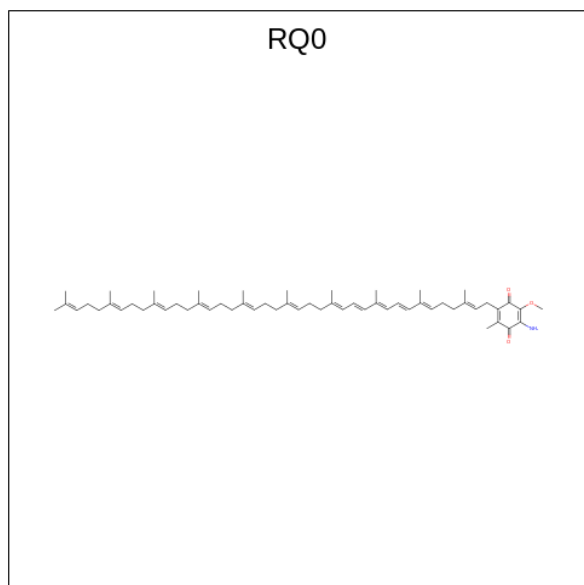
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Mol	Chain	Residues	Atoms			AltConf
10	0	1	Total	C	O	0
			35	24	11	

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

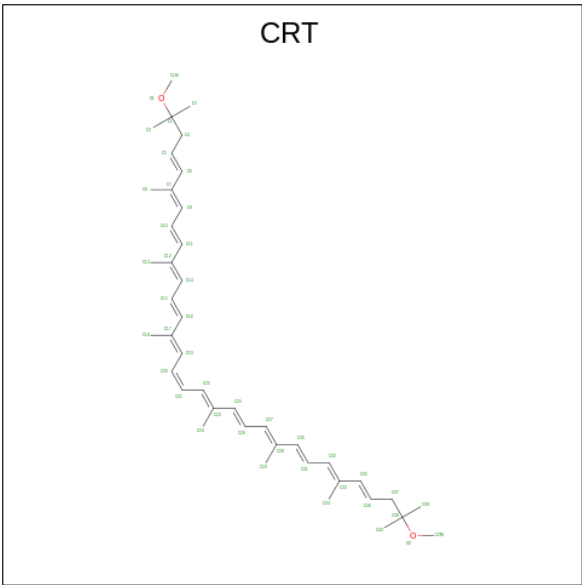
Mol	Chain	Residues	Atoms		AltConf
11	M	1	Total	Fe	0
			1	1	

- Molecule 12 is 2-azanyl-5-[(2 {E},6 {E},8 {E},10 {E},12 {E},14 {E},18 {E},22 {E},26 {E},30 {E},34 {E})-3,7,11,15,19,23,27,31,35,39-decamethyltetraconta-2,6,8,10,12,14,18,22,26,30,34,38-dodecaenyl]-3-methoxy-6-methyl-cyclohexa-2,5-diene-1,4-dione (three-letter code: RQ0) (formula: C₅₈H₈₅NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
12	M	1	Total	C	N	O	0
			62	58	1	3	

- Molecule 13 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: C₄₂H₆₀O₂).



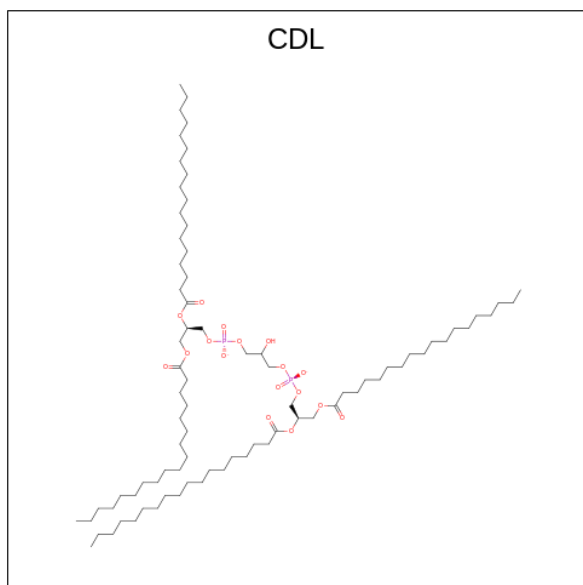
Mol	Chain	Residues	Atoms			AltConf
13	M	1	Total	C	O	0
			44	42	2	
13	A	1	Total	C	O	0
			44	42	2	
13	E	1	Total	C	O	0
			44	42	2	
13	G	1	Total	C	O	0
			44	42	2	
13	J	1	Total	C	O	0
			44	42	2	
13	N	1	Total	C	O	0
			44	42	2	
13	P	1	Total	C	O	0
			44	42	2	
13	R	1	Total	C	O	0
			44	42	2	
13	T	1	Total	C	O	0
			44	42	2	
13	V	1	Total	C	O	0
			44	42	2	
13	X	1	Total	C	O	0
			44	42	2	
13	Z	1	Total	C	O	0
			44	42	2	
13	2	1	Total	C	O	0
			44	42	2	
13	4	1	Total	C	O	0
			44	42	2	

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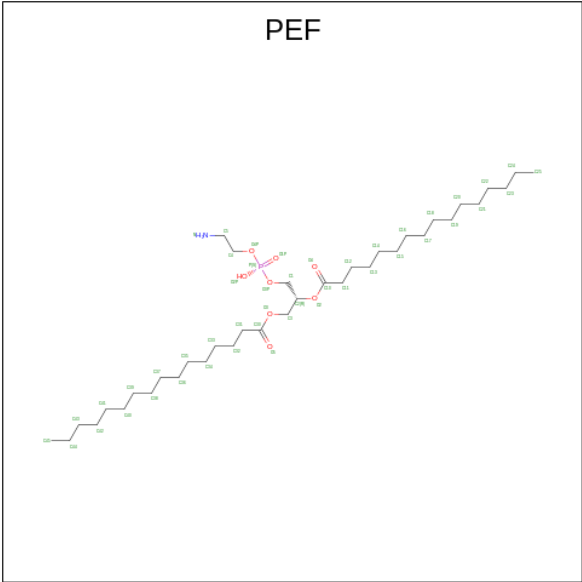
Mol	Chain	Residues	Atoms			AltConf
13	6	1	Total	C	O	0
			44	42	2	
13	8	1	Total	C	O	0
			44	42	2	
13	0	1	Total	C	O	0
			44	42	2	

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
14	M	1	Total	C	O	P	0
			68	49	17	2	
14	M	1	Total	C	O	P	0
			68	49	17	2	
14	H	1	Total	C	O	P	0
			64	45	17	2	
14	H	1	Total	C	O	P	0
			59	40	17	2	
14	H	1	Total	C	O	P	0
			33	15	16	2	

- Molecule 15 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).

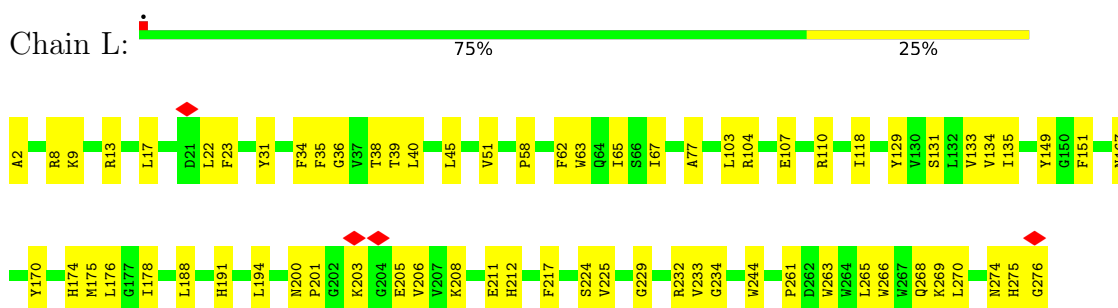


Mol	Chain	Residues	Atoms					AltConf
15	H	1	Total	C	N	O	P	0
			13	5	1	6	1	
15	K	1	Total	C	N	O	P	0
			31	21	1	8	1	
15	K	1	Total	C	N	O	P	0
			42	32	1	8	1	

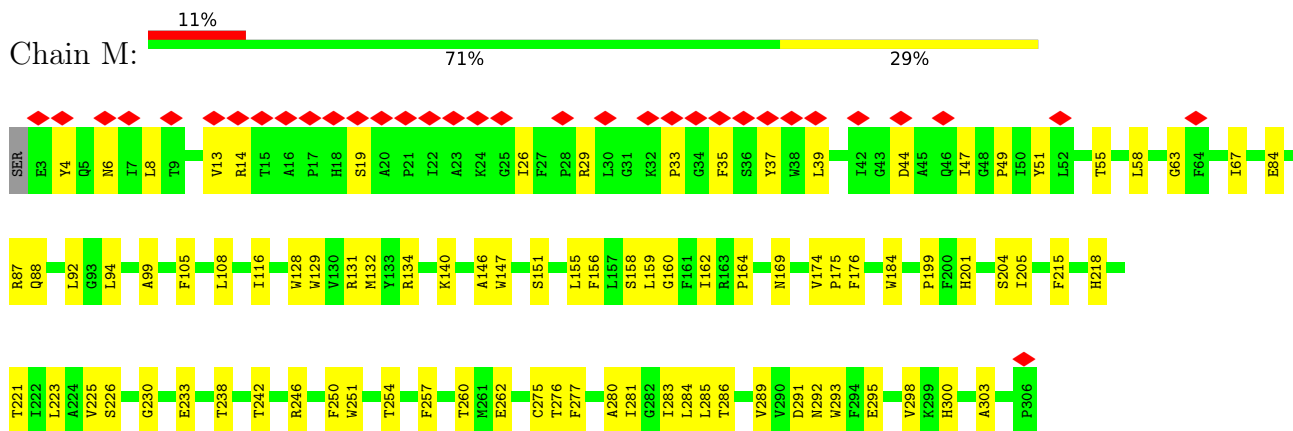
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

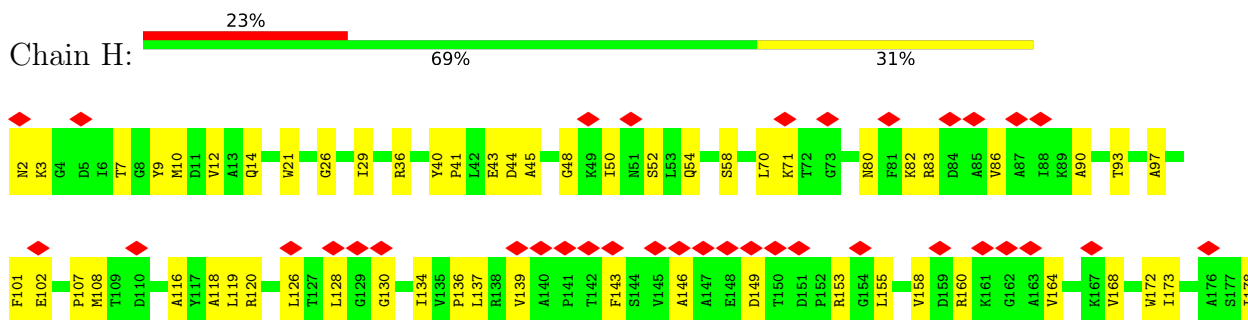
- Molecule 1: Reaction center protein L chain

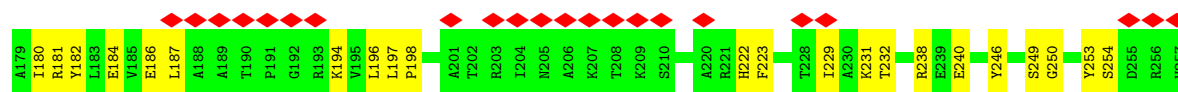


- Molecule 2: Reaction center protein M chain

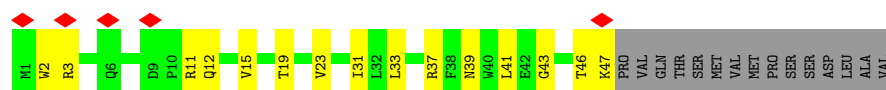


- Molecule 3: Photoreaction center protein H

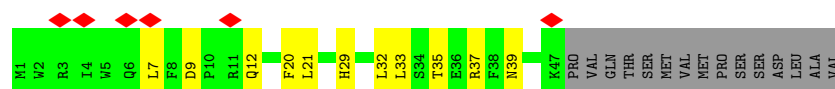




- Molecule 4: Light-harvesting protein B-870 alpha chain



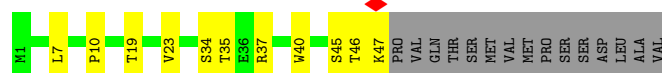
- Molecule 4: Light-harvesting protein B-870 alpha chain



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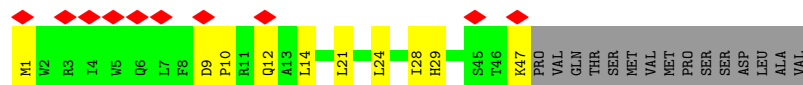
- Molecule 4: Light-harvesting protein B-870 alpha chain



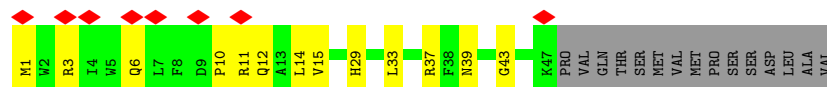
- Molecule 4: Light-harvesting protein B-870 alpha chain



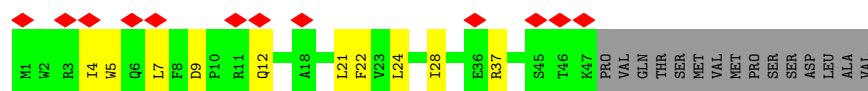
- Molecule 4: Light-harvesting protein B-870 alpha chain



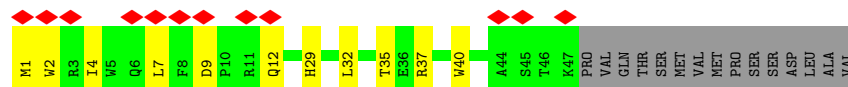
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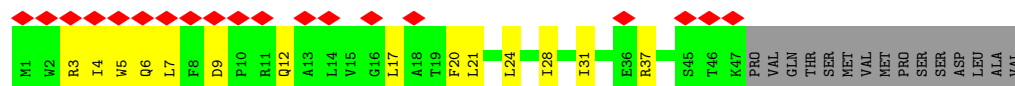
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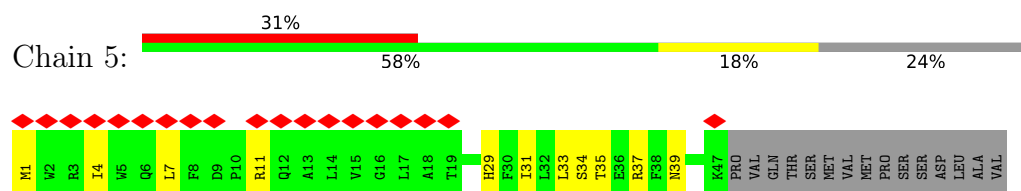
- Molecule 4: Light-harvesting protein B-870 alpha chain



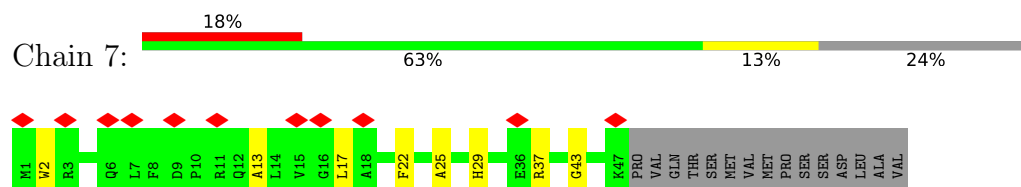
- Molecule 4: Light-harvesting protein B-870 alpha chain



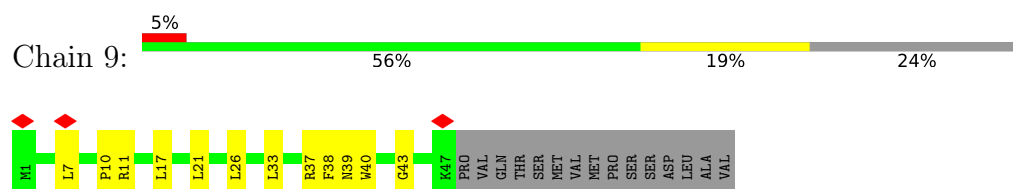
- Molecule 4: Light-harvesting protein B-870 alpha chain



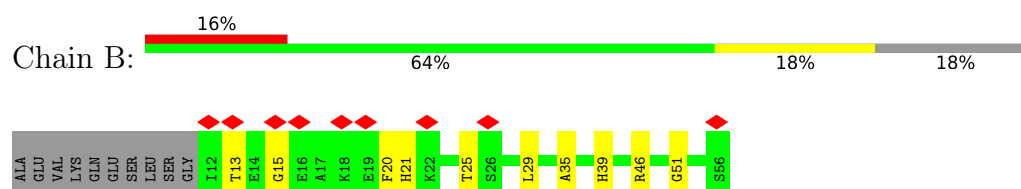
- Molecule 4: Light-harvesting protein B-870 alpha chain



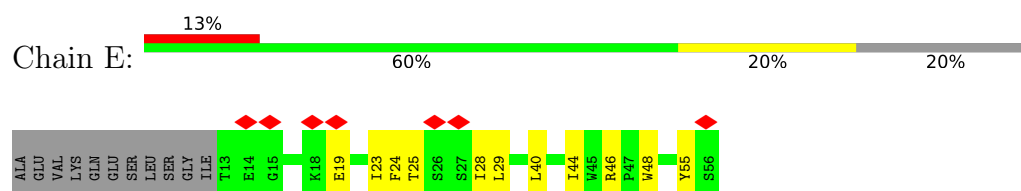
- Molecule 4: Light-harvesting protein B-870 alpha chain



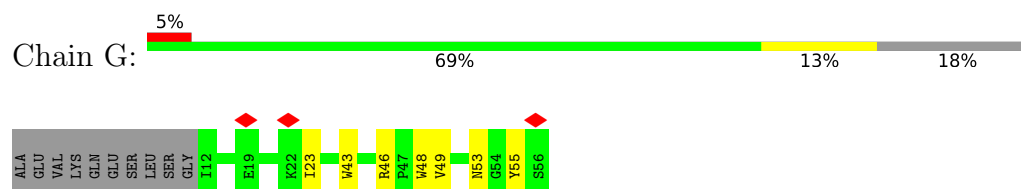
- Molecule 5: Light-harvesting protein B-870 beta chain



- Molecule 5: Light-harvesting protein B-870 beta chain

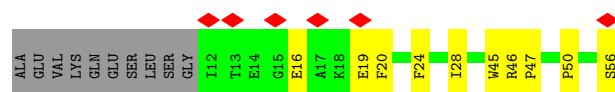


- Molecule 5: Light-harvesting protein B-870 beta chain

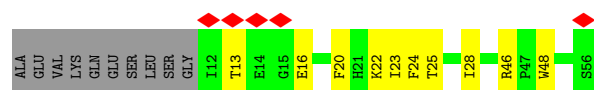


- Molecule 5: Light-harvesting protein B-870 beta chain

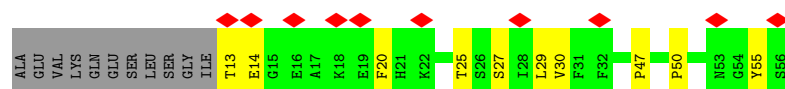




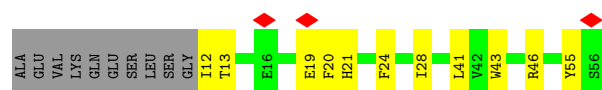
- Molecule 5: Light-harvesting protein B-870 beta chain



- Molecule 5: Light-harvesting protein B-870 beta chain



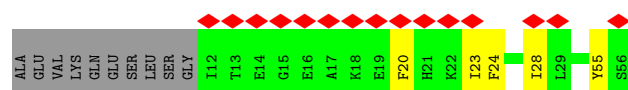
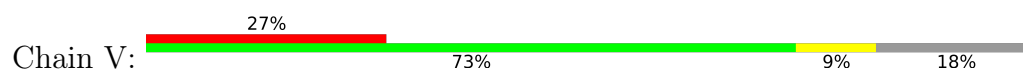
- Molecule 5: Light-harvesting protein B-870 beta chain



- Molecule 5: Light-harvesting protein B-870 beta chain



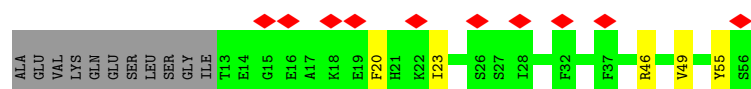
- Molecule 5: Light-harvesting protein B-870 beta chain



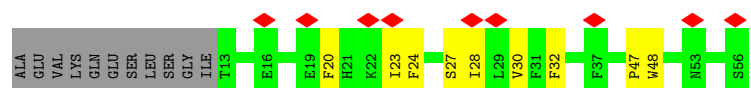
- Molecule 5: Light-harvesting protein B-870 beta chain



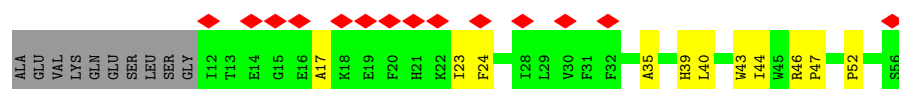
- Molecule 5: Light-harvesting protein B-870 beta chain



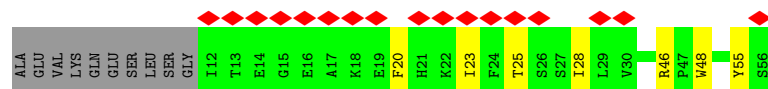
- Molecule 5: Light-harvesting protein B-870 beta chain



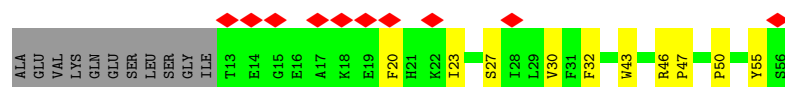
- Molecule 5: Light-harvesting protein B-870 beta chain



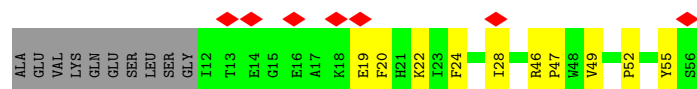
- Molecule 5: Light-harvesting protein B-870 beta chain



- Molecule 5: Light-harvesting protein B-870 beta chain



- Molecule 5: Light-harvesting protein B-870 beta chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145033	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.238	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.033	Depositor
Map size (\AA)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82000005, 0.82000005, 0.82000005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 07D, PGV, CDL, 08I, FME, FE, LMT, PEF, U10, RQ0, CRT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	0.30	0/2253	0.48	0/3082
2	M	0.30	0/2499	0.47	0/3408
3	H	0.28	0/1993	0.54	0/2714
4	1	0.25	0/395	0.46	0/539
4	3	0.27	0/395	0.48	0/539
4	5	0.26	0/395	0.51	0/539
4	7	0.26	0/382	0.45	0/520
4	9	0.27	0/393	0.45	0/536
4	A	0.26	0/399	0.45	0/543
4	D	0.28	0/399	0.47	0/543
4	F	0.27	0/399	0.48	0/543
4	I	0.29	0/393	0.43	0/536
4	K	0.30	0/393	0.53	1/536 (0.2%)
4	O	0.30	0/389	0.60	1/531 (0.2%)
4	Q	0.28	0/393	0.47	0/536
4	S	0.26	0/382	0.43	0/520
4	U	0.26	0/393	0.44	0/536
4	W	0.27	0/399	0.48	0/543
4	Y	0.26	0/393	0.49	0/536
5	0	0.28	0/383	0.38	0/522
5	2	0.27	0/367	0.42	0/502
5	4	0.28	0/366	0.50	0/501
5	6	0.27	0/362	0.38	0/496
5	8	0.27	0/365	0.45	0/498
5	B	0.27	0/383	0.41	0/522
5	E	0.28	0/367	0.43	0/501
5	G	0.28	0/383	0.39	0/522
5	J	0.29	0/383	0.39	0/522
5	N	0.28	0/383	0.39	0/522
5	P	0.30	0/375	0.43	0/511
5	R	0.29	0/379	0.40	0/517
5	T	0.27	0/366	0.39	0/501

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	V	0.28	0/370	0.36	0/505
5	X	0.27	0/378	0.37	0/515
5	Z	0.27	0/371	0.43	0/506
All	All	0.28	0/19018	0.46	2/25943 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	10	PRO	CA-N-CD	-8.07	100.20	111.50
4	K	10	PRO	CA-N-CD	-5.71	103.50	111.50

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	L	2169	0	2129	57	0
2	M	2408	0	2336	68	0
3	H	1951	0	1973	66	0
4	1	393	0	396	10	0
4	3	393	0	396	11	0
4	5	393	0	396	10	0
4	7	382	0	388	7	0
4	9	391	0	396	14	0
4	A	397	0	407	13	0
4	D	397	0	407	10	0
4	F	397	0	407	9	0
4	I	391	0	396	11	0
4	K	391	0	396	12	0
4	O	387	0	390	5	0
4	Q	391	0	396	14	0
4	S	382	0	388	6	0
4	U	391	0	396	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	W	397	0	407	11	0
4	Y	391	0	396	10	0
5	0	367	0	355	8	0
5	2	351	0	329	11	0
5	4	350	0	322	9	0
5	6	346	0	318	8	0
5	8	349	0	331	11	0
5	B	367	0	355	7	0
5	E	351	0	336	9	0
5	G	367	0	355	9	0
5	J	367	0	355	11	0
5	N	367	0	355	11	0
5	P	359	0	344	8	0
5	R	363	0	351	9	0
5	T	350	0	322	7	0
5	V	354	0	333	5	0
5	X	362	0	341	10	0
5	Z	355	0	340	6	0
6	0	66	0	0	0	0
6	1	66	0	0	0	0
6	2	66	0	0	3	0
6	3	66	0	0	0	0
6	4	66	0	0	0	0
6	5	66	0	0	0	0
6	6	66	0	0	0	0
6	7	66	0	0	1	0
6	8	66	0	0	2	0
6	9	66	0	0	0	0
6	A	66	0	0	0	0
6	B	66	0	0	0	0
6	D	66	0	0	0	0
6	E	66	0	0	1	0
6	F	66	0	0	0	0
6	G	66	0	0	1	0
6	I	66	0	0	0	0
6	J	66	0	0	0	0
6	K	66	0	0	0	0
6	L	132	0	0	0	0
6	M	132	0	0	0	0
6	N	66	0	0	1	0
6	O	66	0	0	0	0
6	P	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	132	0	0	0	0
6	S	66	0	0	0	0
6	T	66	0	0	0	0
6	U	66	0	0	0	0
6	V	66	0	0	0	0
6	W	66	0	0	0	0
6	X	66	0	0	0	0
6	Y	66	0	0	1	0
6	Z	66	0	0	0	0
7	L	65	0	0	0	0
7	M	65	0	0	0	0
8	L	28	0	31	4	0
8	M	18	0	15	1	0
9	H	36	0	42	6	0
9	L	43	0	59	4	0
10	0	35	0	46	1	0
10	2	35	0	46	1	0
10	4	35	0	46	0	0
10	5	66	0	81	4	0
10	6	35	0	46	2	0
10	8	35	0	46	1	0
10	B	35	0	46	2	0
10	E	35	0	46	2	0
10	G	35	0	46	3	0
10	H	35	0	46	6	0
10	J	35	0	46	2	0
10	L	60	0	66	0	0
10	M	64	0	77	5	0
10	N	35	0	46	0	0
10	P	35	0	46	1	0
10	R	35	0	46	2	0
10	T	35	0	46	1	0
10	V	35	0	46	0	0
10	X	35	0	46	1	0
10	Z	35	0	46	2	0
11	M	1	0	0	0	0
12	M	62	0	0	0	0
13	0	44	0	60	5	0
13	2	44	0	60	9	0
13	4	44	0	60	8	0
13	6	44	0	60	7	0
13	8	44	0	60	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	44	0	60	3	0
13	E	44	0	60	7	0
13	G	44	0	60	6	0
13	J	44	0	60	8	0
13	M	44	0	60	6	0
13	N	44	0	60	9	0
13	P	44	0	60	4	0
13	R	44	0	60	6	0
13	T	44	0	60	4	0
13	V	44	0	60	6	0
13	X	44	0	60	8	0
13	Z	44	0	60	7	0
14	H	156	0	155	8	0
14	M	136	0	160	7	0
15	H	13	0	11	3	0
15	K	73	0	95	5	0
All	All	23122	0	20832	460	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 460 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)
3:H:172:TRP:HB2	3:H:182:TYR:HB2	1.59	0.84
5:Z:23:ILE:HD11	13:Z:101:CRT:H6	1.57	0.84
5:2:23:ILE:HD11	13:2:101:CRT:H6	1.64	0.78
4:9:37:ARG:NH1	5:0:47:PRO:O	2.16	0.77
4:I:37:ARG:NH1	5:J:47:PRO:O	2.18	0.76

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	L	273/275 (99%)	258 (94%)	15 (6%)	0	100	100
2	M	302/305 (99%)	292 (97%)	10 (3%)	0	100	100
3	H	254/256 (99%)	233 (92%)	21 (8%)	0	100	100
4	1	45/62 (73%)	44 (98%)	0	1 (2%)	5	9
4	3	45/62 (73%)	45 (100%)	0	0	100	100
4	5	45/62 (73%)	42 (93%)	3 (7%)	0	100	100
4	7	45/62 (73%)	44 (98%)	0	1 (2%)	5	9
4	9	45/62 (73%)	45 (100%)	0	0	100	100
4	A	45/62 (73%)	45 (100%)	0	0	100	100
4	D	45/62 (73%)	45 (100%)	0	0	100	100
4	F	45/62 (73%)	45 (100%)	0	0	100	100
4	I	45/62 (73%)	45 (100%)	0	0	100	100
4	K	45/62 (73%)	45 (100%)	0	0	100	100
4	O	45/62 (73%)	45 (100%)	0	0	100	100
4	Q	45/62 (73%)	44 (98%)	1 (2%)	0	100	100
4	S	45/62 (73%)	45 (100%)	0	0	100	100
4	U	45/62 (73%)	42 (93%)	3 (7%)	0	100	100
4	W	45/62 (73%)	43 (96%)	2 (4%)	0	100	100
4	Y	45/62 (73%)	41 (91%)	4 (9%)	0	100	100
5	0	43/55 (78%)	43 (100%)	0	0	100	100
5	2	42/55 (76%)	40 (95%)	2 (5%)	0	100	100
5	4	43/55 (78%)	42 (98%)	1 (2%)	0	100	100
5	6	43/55 (78%)	43 (100%)	0	0	100	100
5	8	42/55 (76%)	41 (98%)	1 (2%)	0	100	100
5	B	43/55 (78%)	41 (95%)	2 (5%)	0	100	100
5	E	42/55 (76%)	41 (98%)	1 (2%)	0	100	100
5	G	43/55 (78%)	43 (100%)	0	0	100	100
5	J	43/55 (78%)	42 (98%)	1 (2%)	0	100	100
5	N	43/55 (78%)	41 (95%)	2 (5%)	0	100	100
5	P	42/55 (76%)	42 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	43/55 (78%)	43 (100%)	0	0	100	100
5	T	43/55 (78%)	43 (100%)	0	0	100	100
5	V	43/55 (78%)	42 (98%)	1 (2%)	0	100	100
5	X	43/55 (78%)	42 (98%)	1 (2%)	0	100	100
5	Z	42/55 (76%)	40 (95%)	2 (5%)	0	100	100
All	All	2232/2708 (82%)	2157 (97%)	73 (3%)	2 (0%)	50	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	7	2	TRP
4	1	2	TRP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	219/219 (100%)	219 (100%)	0	100	100
2	M	235/239 (98%)	235 (100%)	0	100	100
3	H	199/203 (98%)	199 (100%)	0	100	100
4	1	39/54 (72%)	39 (100%)	0	100	100
4	3	39/54 (72%)	39 (100%)	0	100	100
4	5	39/54 (72%)	39 (100%)	0	100	100
4	7	38/54 (70%)	38 (100%)	0	100	100
4	9	39/54 (72%)	39 (100%)	0	100	100
4	A	40/54 (74%)	40 (100%)	0	100	100
4	D	40/54 (74%)	40 (100%)	0	100	100
4	F	40/54 (74%)	40 (100%)	0	100	100
4	I	39/54 (72%)	39 (100%)	0	100	100
4	K	39/54 (72%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	38/54 (70%)	38 (100%)	0	100	100
4	Q	39/54 (72%)	39 (100%)	0	100	100
4	S	38/54 (70%)	38 (100%)	0	100	100
4	U	39/54 (72%)	39 (100%)	0	100	100
4	W	40/54 (74%)	40 (100%)	0	100	100
4	Y	39/54 (72%)	39 (100%)	0	100	100
5	0	37/45 (82%)	37 (100%)	0	100	100
5	2	34/45 (76%)	34 (100%)	0	100	100
5	4	32/45 (71%)	31 (97%)	1 (3%)	35	56
5	6	31/45 (69%)	31 (100%)	0	100	100
5	8	33/45 (73%)	33 (100%)	0	100	100
5	B	37/45 (82%)	37 (100%)	0	100	100
5	E	34/45 (76%)	34 (100%)	0	100	100
5	G	37/45 (82%)	37 (100%)	0	100	100
5	J	37/45 (82%)	37 (100%)	0	100	100
5	N	37/45 (82%)	37 (100%)	0	100	100
5	P	36/45 (80%)	36 (100%)	0	100	100
5	R	36/45 (80%)	36 (100%)	0	100	100
5	T	32/45 (71%)	32 (100%)	0	100	100
5	V	33/45 (73%)	33 (100%)	0	100	100
5	X	35/45 (78%)	35 (100%)	0	100	100
5	Z	35/45 (78%)	35 (100%)	0	100	100
All	All	1834/2245 (82%)	1833 (100%)	1 (0%)	92	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	4	52	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	12	GLN

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Mol	Chain	Res	Type
4	U	12	GLN
5	8	53	ASN
4	Y	12	GLN
4	7	12	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
4	FME	7	1	4	8,9,10	0.93	0	7,9,11	0.88	0
4	FME	U	1	4	8,9,10	0.92	0	7,9,11	1.03	1 (14%)
4	FME	W	1	4	8,9,10	0.91	0	7,9,11	1.56	2 (28%)
4	FME	1	1	4	8,9,10	0.91	0	7,9,11	0.98	0
4	FME	S	1	4	8,9,10	0.91	0	7,9,11	0.86	0
4	FME	5	1	4	8,9,10	0.95	0	7,9,11	0.85	0
4	FME	K	1	4	8,9,10	0.92	0	7,9,11	0.83	0
4	FME	F	1	4	8,9,10	0.87	0	7,9,11	0.90	0
4	FME	A	1	4	8,9,10	0.95	0	7,9,11	0.97	0
4	FME	3	1	4	8,9,10	0.92	0	7,9,11	0.97	0
4	FME	9	1	4	8,9,10	0.94	0	7,9,11	0.89	0
4	FME	Y	1	4	8,9,10	0.92	0	7,9,11	0.81	0
4	FME	D	1	4	8,9,10	0.91	0	7,9,11	0.98	0
4	FME	Q	1	4	8,9,10	0.84	0	7,9,11	1.63	2 (28%)
4	FME	I	1	4	8,9,10	0.93	0	7,9,11	0.92	0
4	FME	O	1	4	8,9,10	0.88	0	7,9,11	1.26	2 (28%)

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
4	FME	7	1	4	-	4/7/9/11	-
4	FME	U	1	4	-	5/7/9/11	-
4	FME	W	1	4	-	3/7/9/11	-
4	FME	1	1	4	-	0/7/9/11	-
4	FME	S	1	4	-	2/7/9/11	-
4	FME	5	1	4	-	0/7/9/11	-
4	FME	K	1	4	-	5/7/9/11	-
4	FME	F	1	4	-	3/7/9/11	-
4	FME	A	1	4	-	2/7/9/11	-
4	FME	3	1	4	-	4/7/9/11	-
4	FME	9	1	4	-	4/7/9/11	-
4	FME	Y	1	4	-	4/7/9/11	-
4	FME	D	1	4	-	4/7/9/11	-
4	FME	Q	1	4	-	3/7/9/11	-
4	FME	I	1	4	-	6/7/9/11	-
4	FME	O	1	4	-	2/7/9/11	-

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	1	FME	C-CA-N	3.03	115.20	109.73
4	W	1	FME	CA-N-CN	2.75	127.05	122.82
4	W	1	FME	C-CA-N	2.66	114.53	109.73
4	Q	1	FME	CA-N-CN	2.53	126.72	122.82
4	U	1	FME	C-CA-N	2.22	113.74	109.73

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	FME	O-C-CA-CB
4	D	1	FME	N-CA-CB-CG
4	I	1	FME	CB-CA-N-CN
4	I	1	FME	N-CA-CB-CG
4	I	1	FME	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	1	1	FME	2	0
4	5	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 1 is monoatomic - leaving 91 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	U10	L	303	-	28,28,63	0.90	2 (7%)	34,37,79	0.65	0
15	PEF	K	103	-	41,41,46	1.01	2 (4%)	44,46,51	1.11	4 (9%)
10	LMT	8	103	-	36,36,36	0.42	0	47,47,47	0.79	1 (2%)
6	07D	2	102	-	69,74,74	1.73	9 (13%)	74,115,115	2.69	19 (25%)
6	07D	G	102	-	69,74,74	1.72	7 (10%)	74,115,115	2.67	17 (22%)
10	LMT	V	103	-	36,36,36	0.48	0	47,47,47	0.96	4 (8%)
6	07D	6	102	-	69,74,74	1.74	8 (11%)	74,115,115	2.80	19 (25%)
6	07D	V	102	-	69,74,74	1.71	8 (11%)	74,115,115	2.71	19 (25%)
10	LMT	X	103	-	36,36,36	0.44	0	47,47,47	0.78	1 (2%)
6	07D	Q	101	-	69,74,74	1.72	9 (13%)	74,115,115	2.80	20 (27%)
6	07D	9	101	-	69,74,74	1.75	8 (11%)	74,115,115	2.75	21 (28%)
10	LMT	G	103	-	36,36,36	0.44	0	47,47,47	0.76	0
6	07D	7	101	-	69,74,74	1.72	8 (11%)	74,115,115	2.74	18 (24%)
6	07D	O	101	-	69,74,74	1.76	10 (14%)	74,115,115	2.68	18 (24%)
13	CRT	P	101	-	41,43,43	0.70	0	50,54,54	1.71	11 (22%)
6	07D	5	202	-	69,74,74	1.75	9 (13%)	74,115,115	2.86	25 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CDL	H	301	-	63,63,99	1.14	4 (6%)	69,75,111	1.21	4 (5%)
10	LMT	N	103	-	36,36,36	0.43	0	47,47,47	0.97	3 (6%)
13	CRT	G	101	-	41,43,43	0.72	0	50,54,54	1.77	10 (20%)
10	LMT	H	306	-	36,36,36	0.44	0	47,47,47	0.88	1 (2%)
13	CRT	Z	101	-	41,43,43	0.71	0	50,54,54	1.67	13 (26%)
6	07D	4	102	-	69,74,74	1.78	10 (14%)	74,115,115	2.70	21 (28%)
10	LMT	R	102	-	36,36,36	0.38	0	47,47,47	0.91	2 (4%)
6	07D	M	404	-	69,74,74	1.74	10 (14%)	74,115,115	2.79	20 (27%)
10	LMT	L	306	-	33,33,36	0.42	0	44,44,47	0.65	1 (2%)
6	07D	L	301	-	69,74,74	1.74	9 (13%)	74,115,115	2.74	17 (22%)
6	07D	F	101	-	69,74,74	1.77	8 (11%)	74,115,115	2.72	19 (25%)
10	LMT	2	103	-	36,36,36	0.47	0	47,47,47	0.84	1 (2%)
10	LMT	5	203	-	36,36,36	0.41	0	47,47,47	0.74	0
14	CDL	M	408	-	67,67,99	1.10	4 (5%)	73,79,111	1.23	8 (10%)
10	LMT	T	103	-	36,36,36	0.42	0	47,47,47	0.87	2 (4%)
10	LMT	4	103	-	36,36,36	0.47	0	47,47,47	0.79	0
6	07D	U	101	-	69,74,74	1.76	8 (11%)	74,115,115	2.68	21 (28%)
7	08I	L	302	-	50,70,70	1.49	3 (6%)	45,101,101	2.21	13 (28%)
13	CRT	4	101	-	41,43,43	0.72	0	50,54,54	1.64	9 (18%)
13	CRT	N	101	-	41,43,43	0.70	0	50,54,54	1.58	8 (16%)
13	CRT	X	101	-	41,43,43	0.69	0	50,54,54	1.74	9 (18%)
10	LMT	E	103	-	36,36,36	0.41	0	47,47,47	0.79	0
6	07D	M	403	-	69,74,74	1.76	9 (13%)	74,115,115	2.67	15 (20%)
6	07D	Y	101	-	69,74,74	1.77	9 (13%)	74,115,115	2.73	21 (28%)
6	07D	Q	102	-	69,74,74	1.72	7 (10%)	74,115,115	2.70	17 (22%)
10	LMT	J	103	-	36,36,36	0.45	0	47,47,47	0.83	1 (2%)
13	CRT	J	101	-	41,43,43	0.69	0	50,54,54	1.61	9 (18%)
10	LMT	L	305	-	29,29,36	0.41	0	40,40,47	0.76	1 (2%)
13	CRT	2	101	-	41,43,43	0.73	0	50,54,54	1.64	10 (20%)
13	CRT	M	407	-	41,43,43	0.75	0	50,54,54	3.81	16 (32%)
6	07D	8	102	-	69,74,74	1.72	8 (11%)	74,115,115	2.89	21 (28%)
6	07D	S	101	-	69,74,74	1.76	9 (13%)	74,115,115	2.69	19 (25%)
13	CRT	E	101	-	41,43,43	0.70	0	50,54,54	1.68	14 (28%)
7	08I	M	405	-	50,70,70	1.52	3 (6%)	45,101,101	1.94	8 (17%)
6	07D	L	307	-	69,74,74	1.74	8 (11%)	74,115,115	2.90	22 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	07D	K	101	-	69,74,74	1.72	8 (11%)	74,115,115	2.72	20 (27%)
10	LMT	0	103	-	36,36,36	0.38	0	47,47,47	0.70	1 (2%)
12	RQ0	M	406	-	62,62,62	2.87	28 (45%)	69,78,78	2.37	27 (39%)
10	LMT	M	410	-	36,36,36	0.42	0	47,47,47	0.90	1 (2%)
9	PGV	H	302	-	35,35,50	1.09	2 (5%)	38,41,56	1.29	4 (10%)
6	07D	Z	102	-	69,74,74	1.71	8 (11%)	74,115,115	2.68	15 (20%)
10	LMT	5	201	-	32,32,36	0.50	0	43,43,47	0.92	2 (4%)
13	CRT	0	101	-	41,43,43	0.70	0	50,54,54	1.62	13 (26%)
15	PEF	H	305	-	12,12,46	0.45	0	13,15,51	0.47	0
13	CRT	A	102	-	41,43,43	0.71	0	50,54,54	1.71	14 (28%)
6	07D	E	102	-	69,74,74	1.71	7 (10%)	74,115,115	2.67	18 (24%)
10	LMT	6	103	-	36,36,36	0.45	0	47,47,47	0.83	0
6	07D	0	102	-	69,74,74	1.71	7 (10%)	74,115,115	2.70	17 (22%)
10	LMT	P	103	-	36,36,36	0.43	0	47,47,47	0.68	1 (2%)
13	CRT	V	101	-	41,43,43	0.75	0	50,54,54	1.80	13 (26%)
6	07D	X	102	-	69,74,74	1.73	8 (11%)	74,115,115	2.72	18 (24%)
6	07D	T	102	-	69,74,74	1.73	9 (13%)	74,115,115	2.81	18 (24%)
10	LMT	Z	103	-	36,36,36	0.45	0	47,47,47	0.76	0
6	07D	P	102	-	69,74,74	1.73	8 (11%)	74,115,115	2.73	18 (24%)
8	U10	M	401	-	18,18,63	1.02	2 (11%)	22,25,79	0.69	0
14	CDL	M	409	-	67,67,99	1.14	4 (5%)	73,79,111	1.10	5 (6%)
10	LMT	B	102	-	36,36,36	0.43	0	47,47,47	0.76	1 (2%)
13	CRT	8	101	-	41,43,43	0.69	0	50,54,54	1.58	9 (18%)
6	07D	3	101	-	69,74,74	1.76	9 (13%)	74,115,115	2.69	18 (24%)
9	PGV	L	304	-	42,42,50	0.98	2 (4%)	45,48,56	1.23	4 (8%)
13	CRT	T	101	-	41,43,43	0.70	0	50,54,54	1.79	11 (22%)
6	07D	W	101	-	69,74,74	1.79	10 (14%)	74,115,115	2.71	20 (27%)
13	CRT	R	101	-	41,43,43	0.71	0	50,54,54	1.52	9 (18%)
6	07D	A	101	-	69,74,74	1.76	9 (13%)	74,115,115	2.70	19 (25%)
14	CDL	H	303	-	58,58,99	1.24	4 (6%)	64,70,111	1.22	5 (7%)
13	CRT	6	101	-	41,43,43	0.71	0	50,54,54	1.57	9 (18%)
15	PEF	K	102	-	30,30,46	1.17	2 (6%)	33,35,51	1.17	2 (6%)
6	07D	D	101	-	69,74,74	1.79	9 (13%)	74,115,115	2.77	21 (28%)
6	07D	1	101	-	69,74,74	1.80	8 (11%)	74,115,115	2.70	20 (27%)
6	07D	B	101	-	69,74,74	1.74	8 (11%)	74,115,115	2.86	22 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	07D	J	102	-	69,74,74	1.70	8 (11%)	74,115,115	2.81	19 (25%)
6	07D	I	101	-	69,74,74	1.78	11 (15%)	74,115,115	2.83	20 (27%)
10	LMT	M	411	-	30,30,36	0.46	0	41,41,47	0.76	0
14	CDL	H	304	-	32,32,99	1.37	3 (9%)	35,42,111	1.52	4 (11%)
6	07D	N	102	-	69,74,74	1.73	8 (11%)	74,115,115	2.75	21 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	U10	L	303	-	-	6/21/45/87	0/1/1/1
15	PEF	K	103	-	-	14/45/45/50	-
10	LMT	8	103	-	-	3/21/61/61	0/2/2/2
6	07D	2	102	-	-	12/41/137/137	-
6	07D	G	102	-	-	10/41/137/137	-
10	LMT	V	103	-	-	3/21/61/61	0/2/2/2
6	07D	6	102	-	-	13/41/137/137	-
6	07D	V	102	-	-	9/41/137/137	-
10	LMT	X	103	-	-	3/21/61/61	0/2/2/2
6	07D	Q	101	-	-	10/41/137/137	-
6	07D	9	101	-	-	5/41/137/137	-
10	LMT	G	103	-	-	2/21/61/61	0/2/2/2
6	07D	7	101	-	-	12/41/137/137	-
6	07D	O	101	-	-	11/41/137/137	-
13	CRT	P	101	-	-	15/51/51/51	-
6	07D	5	202	-	-	11/41/137/137	-
14	CDL	H	301	-	-	19/74/74/110	-
10	LMT	N	103	-	-	4/21/61/61	0/2/2/2
13	CRT	G	101	-	-	10/51/51/51	-
10	LMT	H	306	-	-	10/21/61/61	0/2/2/2
13	CRT	Z	101	-	-	10/51/51/51	-
6	07D	4	102	-	-	9/41/137/137	-
10	LMT	R	102	-	-	4/21/61/61	0/2/2/2
6	07D	M	404	-	-	9/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LMT	L	306	-	-	6/18/58/61	0/2/2/2
6	07D	L	301	-	-	4/41/137/137	-
6	07D	F	101	-	-	7/41/137/137	-
10	LMT	2	103	-	-	7/21/61/61	0/2/2/2
10	LMT	5	203	-	-	5/21/61/61	0/2/2/2
14	CDL	M	408	-	-	23/78/78/110	-
10	LMT	T	103	-	-	7/21/61/61	0/2/2/2
10	LMT	4	103	-	-	8/21/61/61	0/2/2/2
6	07D	U	101	-	-	7/41/137/137	-
7	08I	L	302	-	-	12/37/105/105	0/5/6/6
13	CRT	4	101	-	-	4/51/51/51	-
13	CRT	N	101	-	-	5/51/51/51	-
13	CRT	X	101	-	-	7/51/51/51	-
10	LMT	E	103	-	-	4/21/61/61	0/2/2/2
6	07D	M	403	-	-	13/41/137/137	-
6	07D	Y	101	-	-	9/41/137/137	-
6	07D	Q	102	-	-	13/41/137/137	-
10	LMT	J	103	-	-	5/21/61/61	0/2/2/2
13	CRT	J	101	-	-	2/51/51/51	-
10	LMT	L	305	-	-	0/14/54/61	0/2/2/2
13	CRT	2	101	-	-	11/51/51/51	-
13	CRT	M	407	-	-	10/51/51/51	-
6	07D	8	102	-	-	16/41/137/137	-
6	07D	S	101	-	-	7/41/137/137	-
13	CRT	E	101	-	-	11/51/51/51	-
7	08I	M	405	-	-	2/37/105/105	0/5/6/6
6	07D	L	307	-	-	12/41/137/137	-
6	07D	K	101	-	-	4/41/137/137	-
10	LMT	0	103	-	-	3/21/61/61	0/2/2/2
12	RQ0	M	406	-	-	22/61/85/85	0/1/1/1
10	LMT	M	410	-	-	8/21/61/61	0/2/2/2
9	PGV	H	302	-	-	16/40/40/55	-
6	07D	Z	102	-	-	15/41/137/137	-
10	LMT	5	201	-	-	13/17/57/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CRT	0	101	-	-	7/51/51/51	-
15	PEF	H	305	-	-	4/13/13/50	-
13	CRT	A	102	-	-	0/51/51/51	-
6	07D	E	102	-	-	13/41/137/137	-
10	LMT	6	103	-	-	4/21/61/61	0/2/2/2
6	07D	0	102	-	-	9/41/137/137	-
10	LMT	P	103	-	-	9/21/61/61	0/2/2/2
13	CRT	V	101	-	-	7/51/51/51	-
6	07D	X	102	-	-	14/41/137/137	-
6	07D	T	102	-	-	13/41/137/137	-
10	LMT	Z	103	-	-	6/21/61/61	0/2/2/2
6	07D	P	102	-	-	12/41/137/137	-
8	U10	M	401	-	-	1/9/33/87	0/1/1/1
14	CDL	M	409	-	-	23/78/78/110	-
10	LMT	B	102	-	-	8/21/61/61	0/2/2/2
13	CRT	8	101	-	-	7/51/51/51	-
6	07D	3	101	-	-	8/41/137/137	-
9	PGV	L	304	-	-	9/47/47/55	-
13	CRT	T	101	-	-	7/51/51/51	-
6	07D	W	101	-	-	6/41/137/137	-
13	CRT	R	101	-	-	7/51/51/51	-
6	07D	A	101	-	-	5/41/137/137	-
14	CDL	H	303	-	-	30/68/68/110	-
13	CRT	6	101	-	-	13/51/51/51	-
15	PEF	K	102	-	-	11/34/34/50	-
6	07D	D	101	-	-	5/41/137/137	-
6	07D	1	101	-	-	12/41/137/137	-
6	07D	B	101	-	-	12/41/137/137	-
6	07D	J	102	-	-	10/41/137/137	-
6	07D	I	101	-	-	11/41/137/137	-
10	LMT	M	411	-	-	5/15/55/61	0/2/2/2
14	CDL	H	304	-	-	20/40/40/110	-
6	07D	N	102	-	-	7/41/137/137	-

The worst 5 of 371 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	406	RQ0	C18-C14	9.55	1.59	1.34
12	M	406	RQ0	C11-C07	9.55	1.59	1.34
6	F	101	07D	C2A-C3A	8.25	1.54	1.36
6	G	102	07D	C2A-C3A	8.19	1.54	1.36
6	1	101	07D	C2A-C3A	8.14	1.54	1.36

The worst 5 of 992 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	407	CRT	C2-C1-C4	-15.77	86.64	110.86
13	M	407	CRT	C3-C1-C4	-15.66	86.81	110.86
6	W	101	07D	CMC-C2C-C1C	-10.64	112.11	128.46
6	V	102	07D	CMC-C2C-C1C	-10.48	112.36	128.46
6	I	101	07D	CMC-C2C-C1C	-10.45	112.41	128.46

There are no chirality outliers.

5 of 827 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	301	07D	C1A-C2A-CAA-CBA
6	L	301	07D	C4C-C3C-CAC-CBC
6	L	307	07D	C12-C13-C15-C16
6	L	307	07D	C14-C13-C15-C16
6	L	307	07D	C2B-C3B-CAB-CBB

There are no ring outliers.

53 monomers are involved in 185 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	303	U10	4	0
15	K	103	PEF	1	0
10	8	103	LMT	1	0
6	2	102	07D	3	0
6	G	102	07D	1	0
10	X	103	LMT	1	0
10	G	103	LMT	3	0
6	7	101	07D	1	0
13	P	101	CRT	4	0
13	G	101	CRT	6	0
10	H	306	LMT	6	0
13	Z	101	CRT	7	0
10	R	102	LMT	2	0

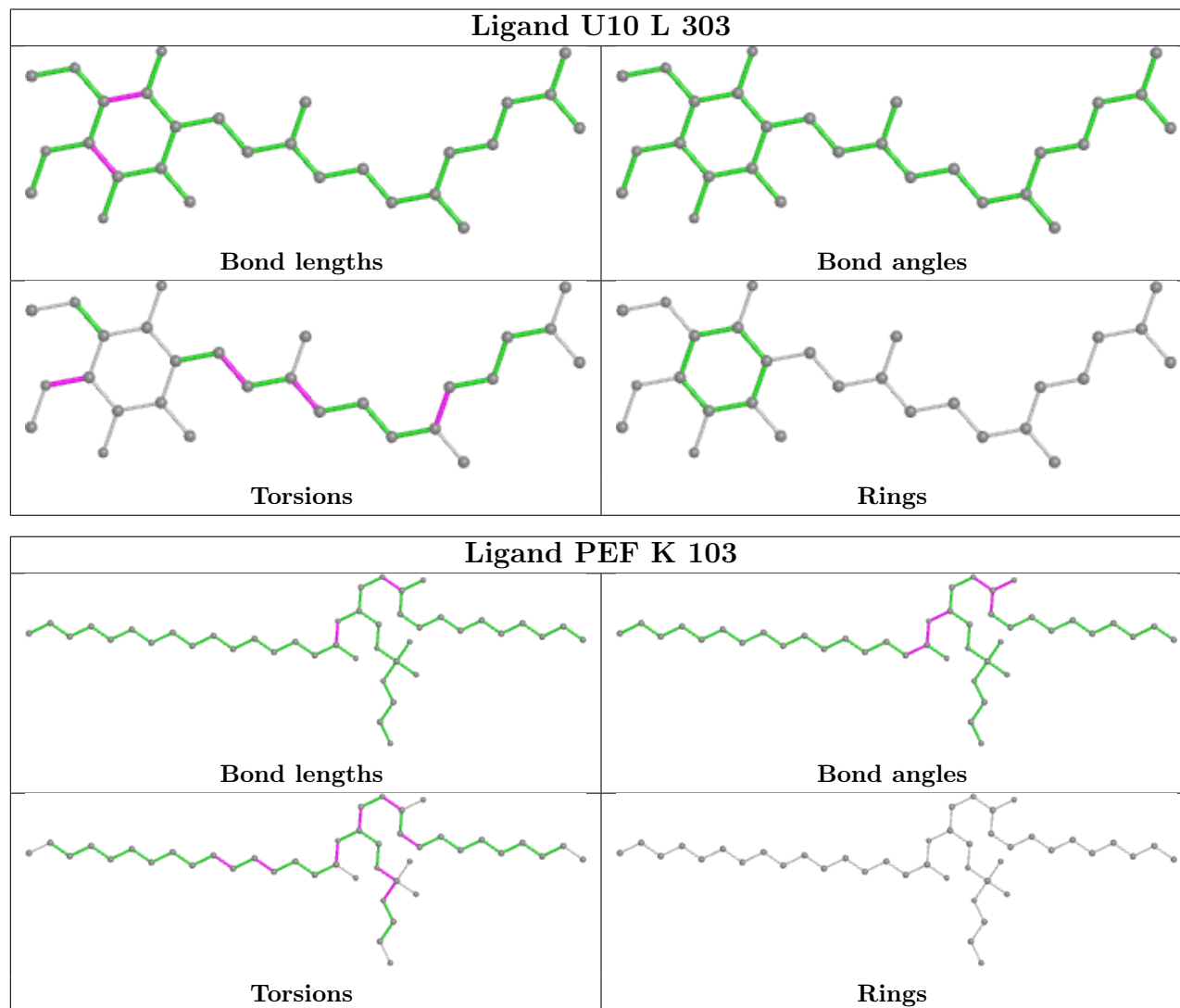
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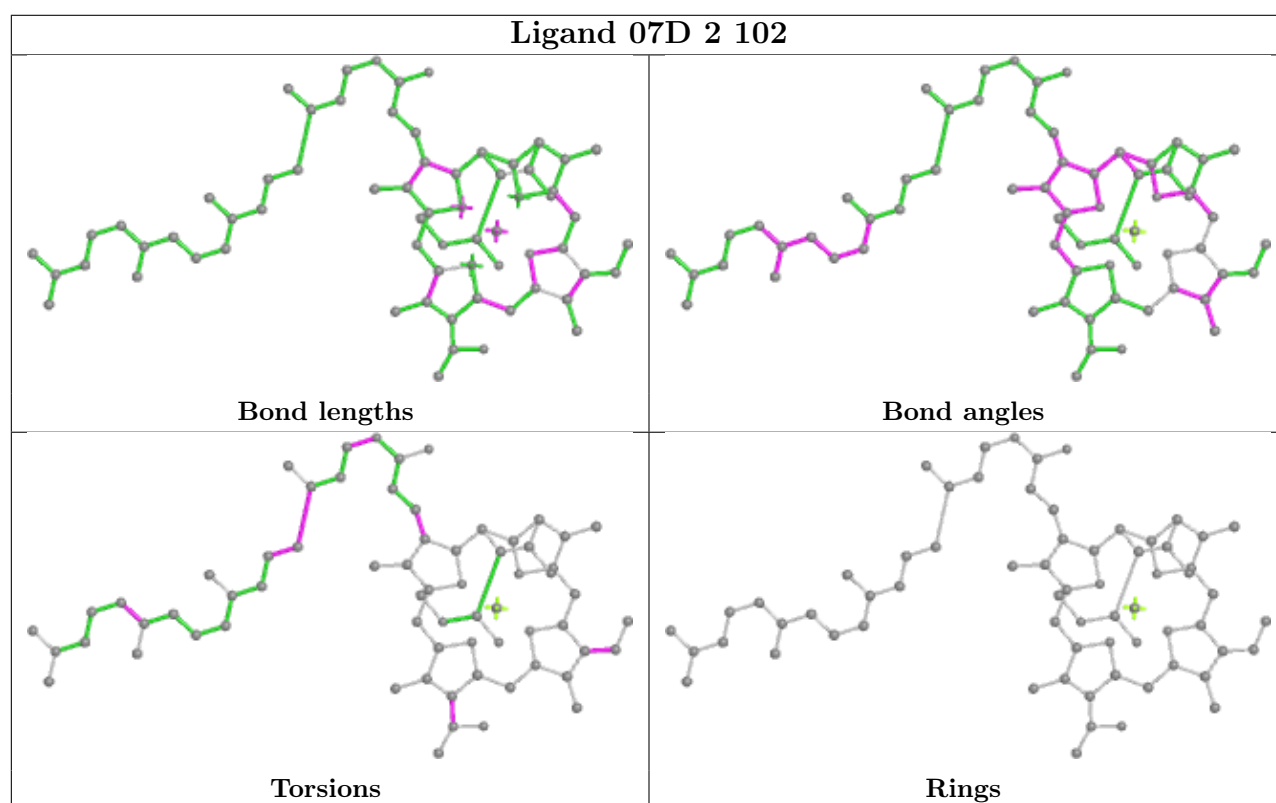
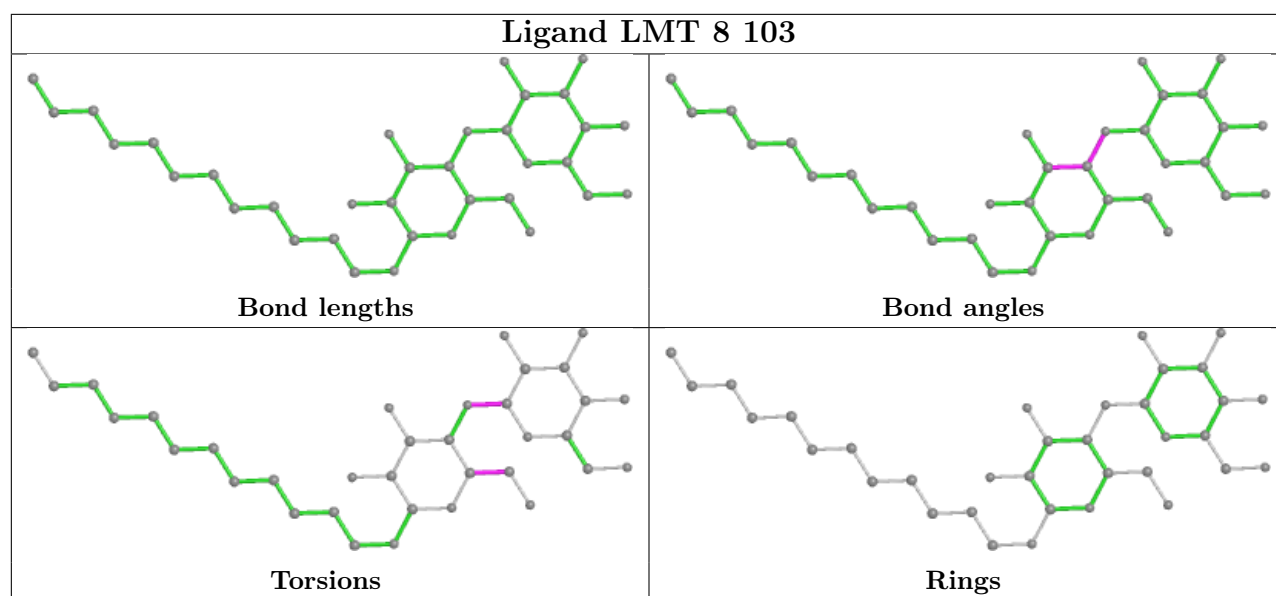
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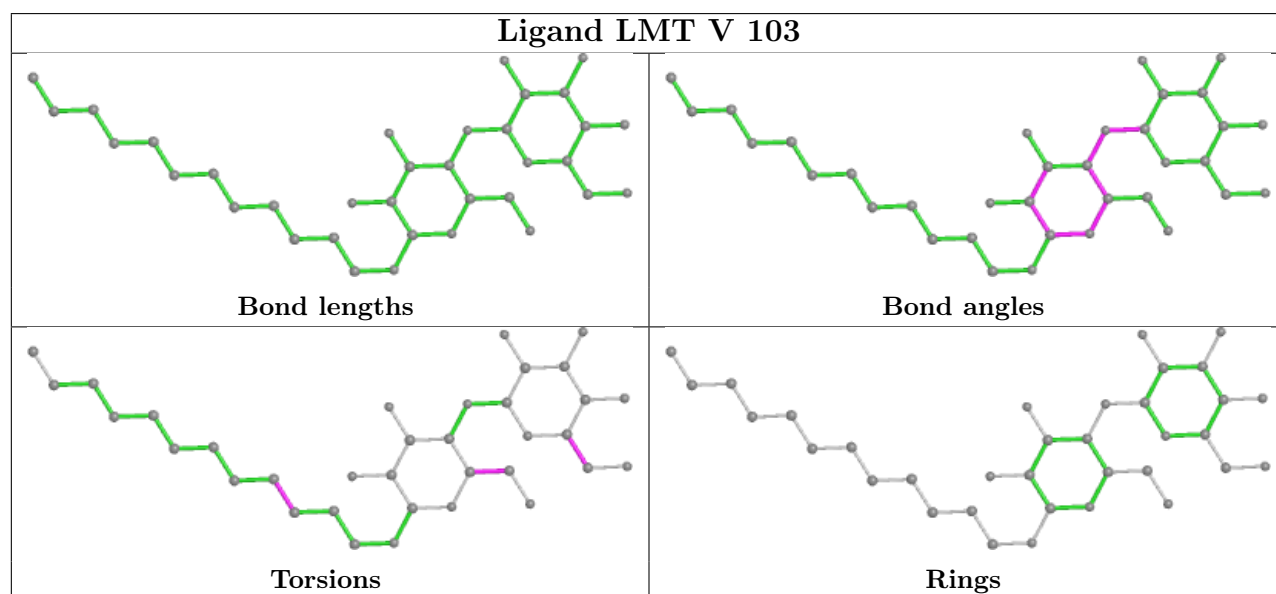
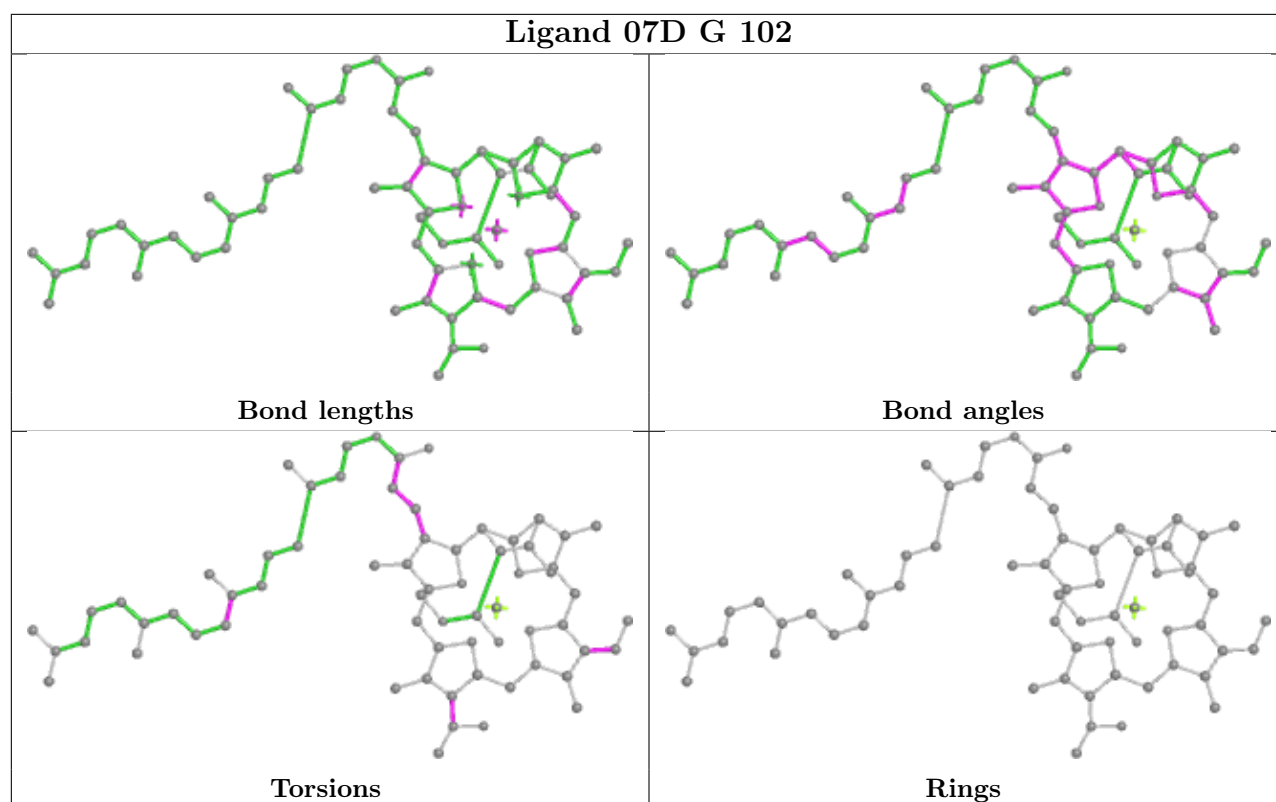
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	2	103	LMT	1	0
10	5	203	LMT	2	0
14	M	408	CDL	5	0
10	T	103	LMT	1	0
13	4	101	CRT	8	0
13	N	101	CRT	9	0
13	X	101	CRT	8	0
10	E	103	LMT	2	0
6	Y	101	07D	1	0
10	J	103	LMT	2	0
13	J	101	CRT	8	0
13	2	101	CRT	9	0
13	M	407	CRT	6	0
6	8	102	07D	2	0
13	E	101	CRT	7	0
10	0	103	LMT	1	0
10	M	410	LMT	4	0
9	H	302	PGV	6	0
10	5	201	LMT	2	0
13	0	101	CRT	5	0
15	H	305	PEF	3	0
13	A	102	CRT	3	0
6	E	102	07D	1	0
10	6	103	LMT	2	0
10	P	103	LMT	1	0
13	V	101	CRT	6	0
10	Z	103	LMT	2	0
8	M	401	U10	1	0
14	M	409	CDL	2	0
10	B	102	LMT	2	0
13	8	101	CRT	7	0
9	L	304	PGV	4	0
13	T	101	CRT	4	0
13	R	101	CRT	6	0
14	H	303	CDL	6	0
13	6	101	CRT	7	0
15	K	102	PEF	4	0
10	M	411	LMT	1	0
14	H	304	CDL	2	0
6	N	102	07D	1	0

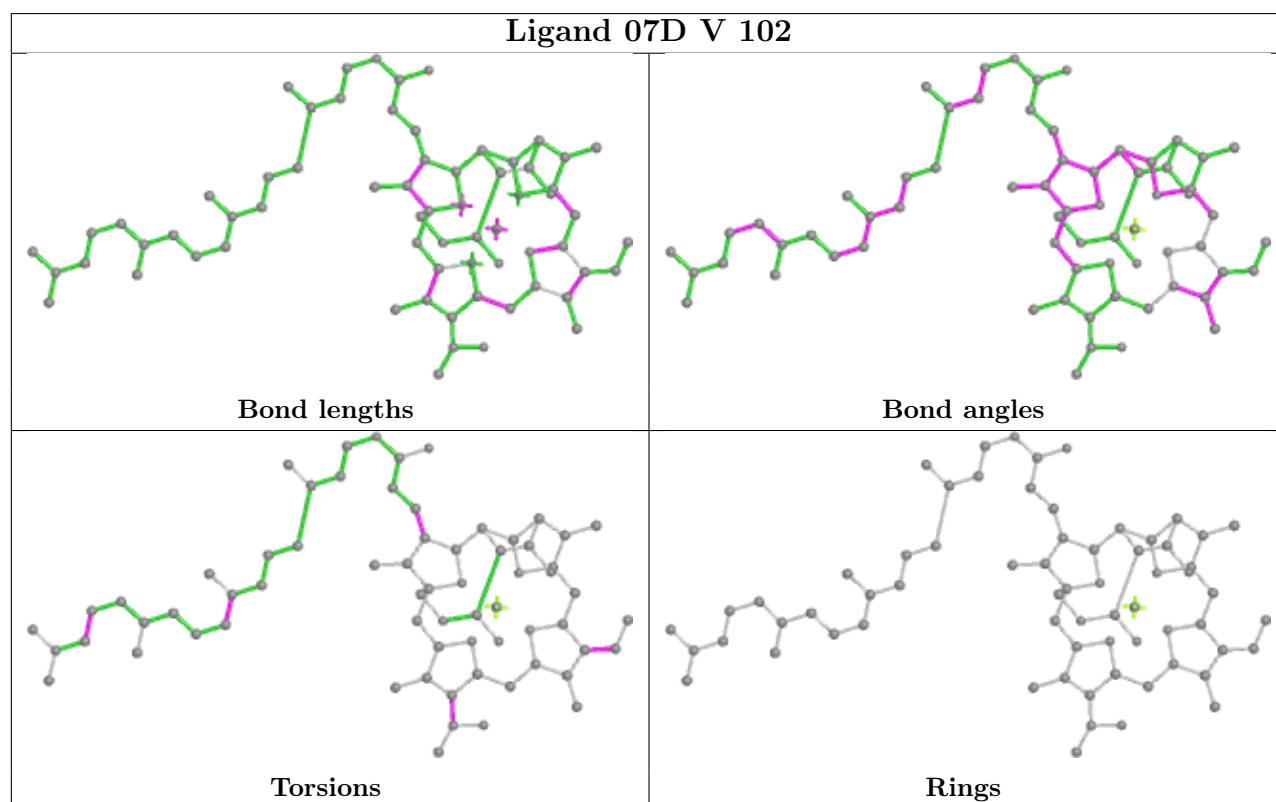
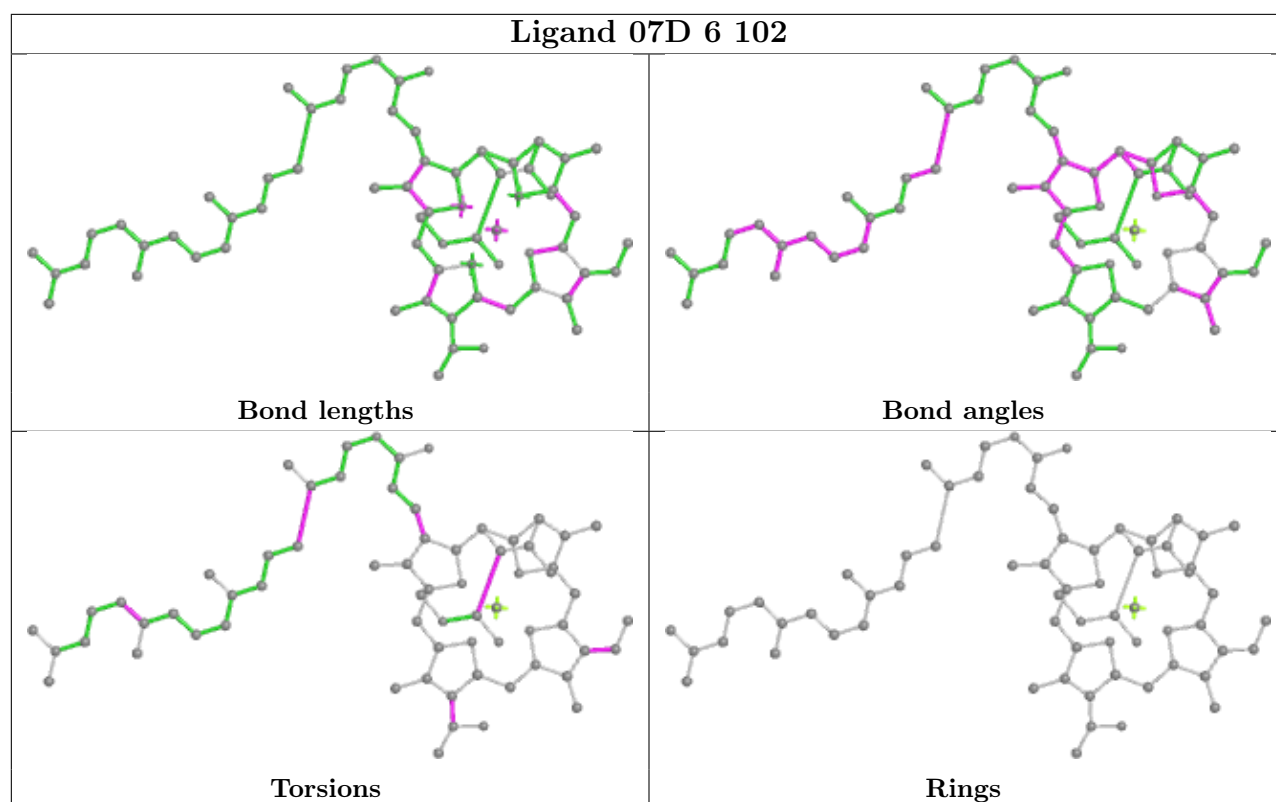
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

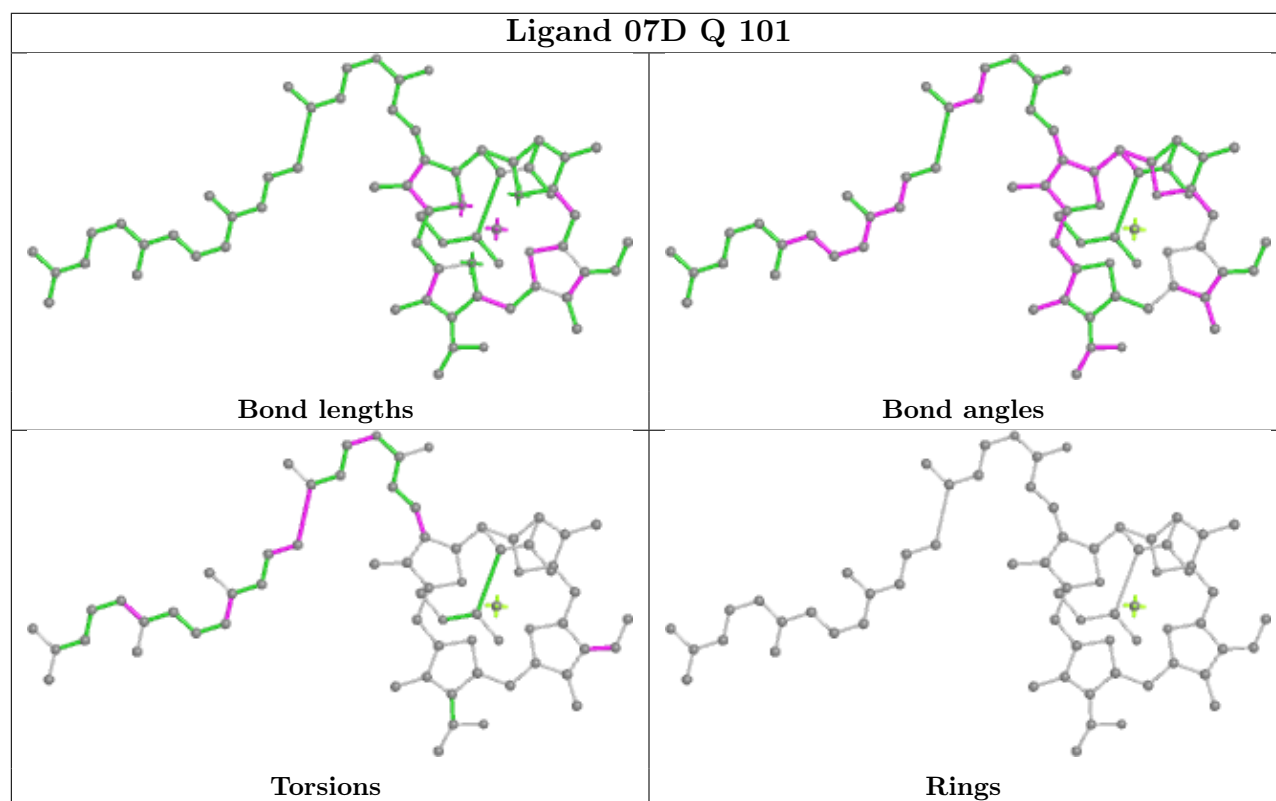
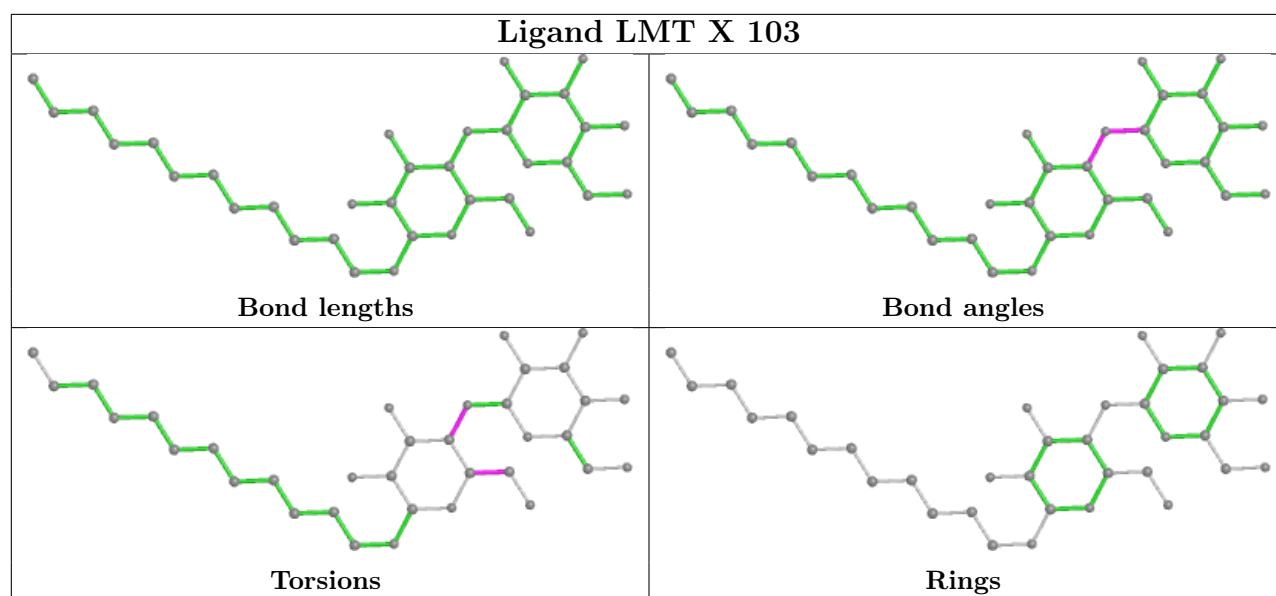
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

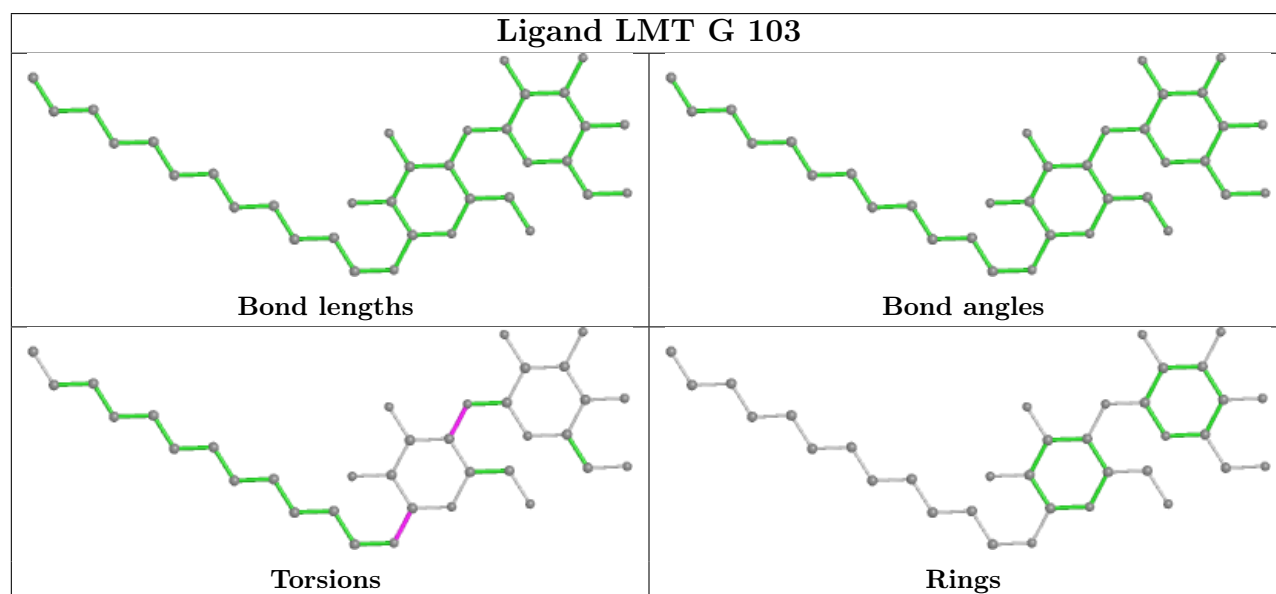
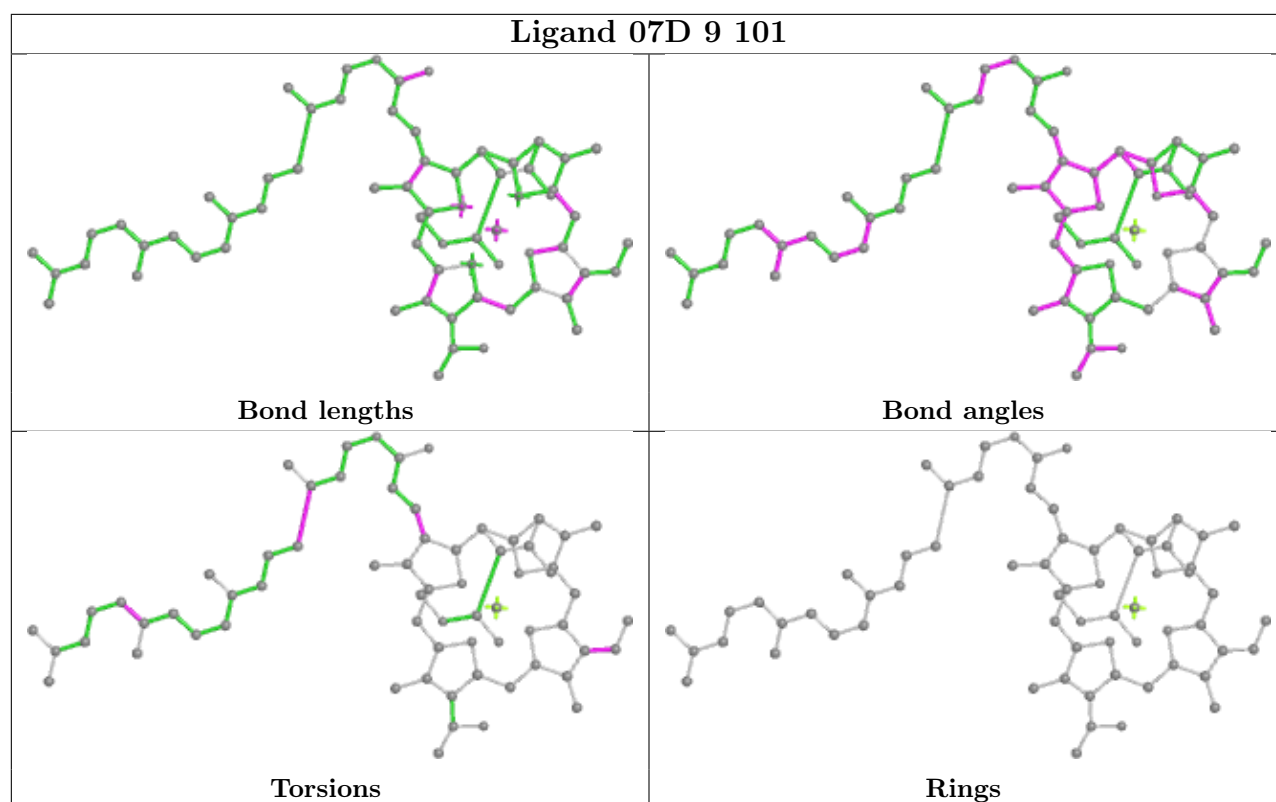


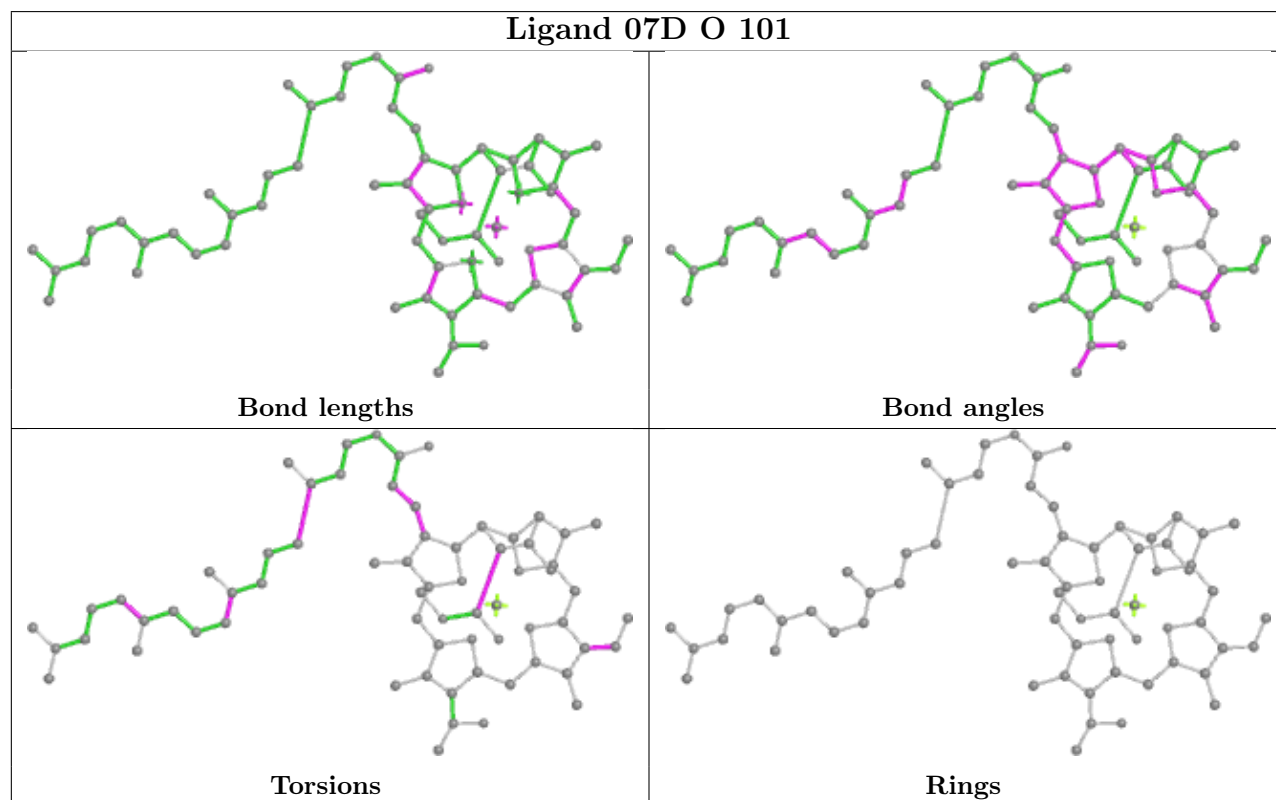
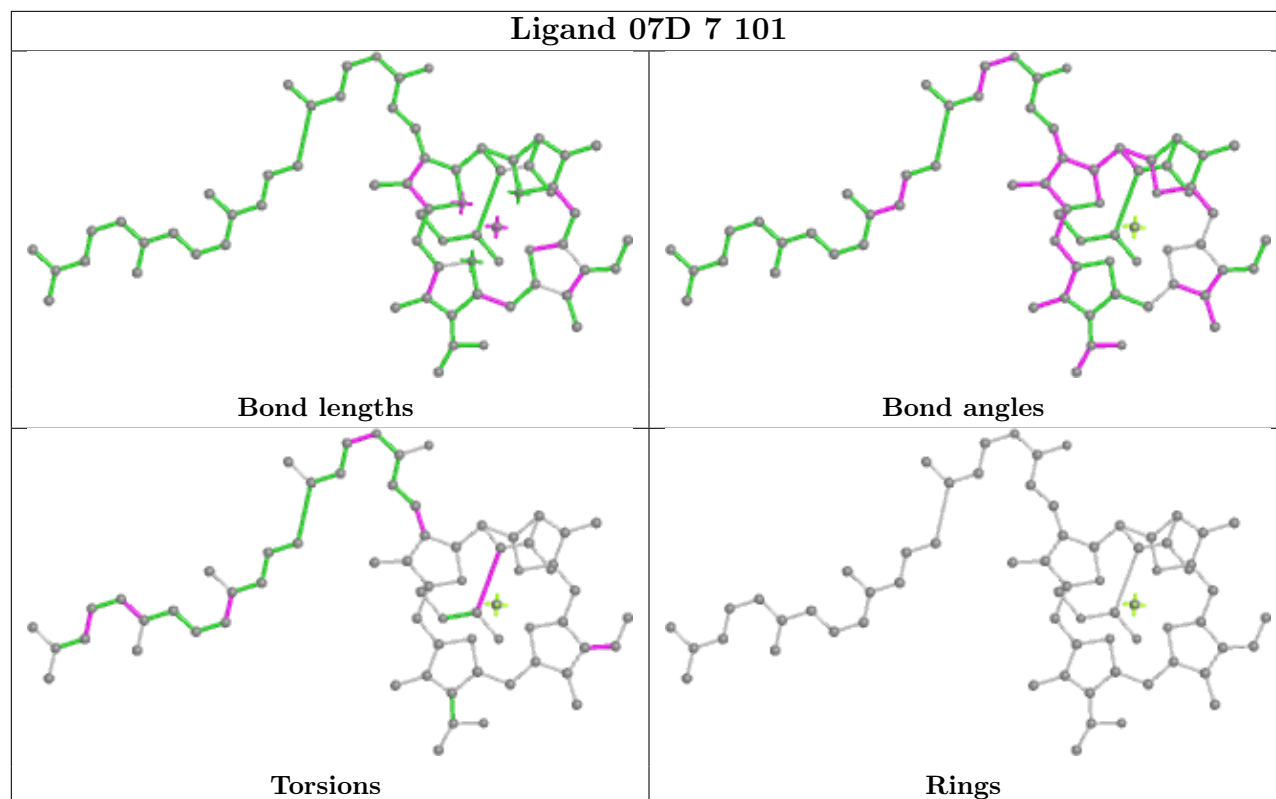


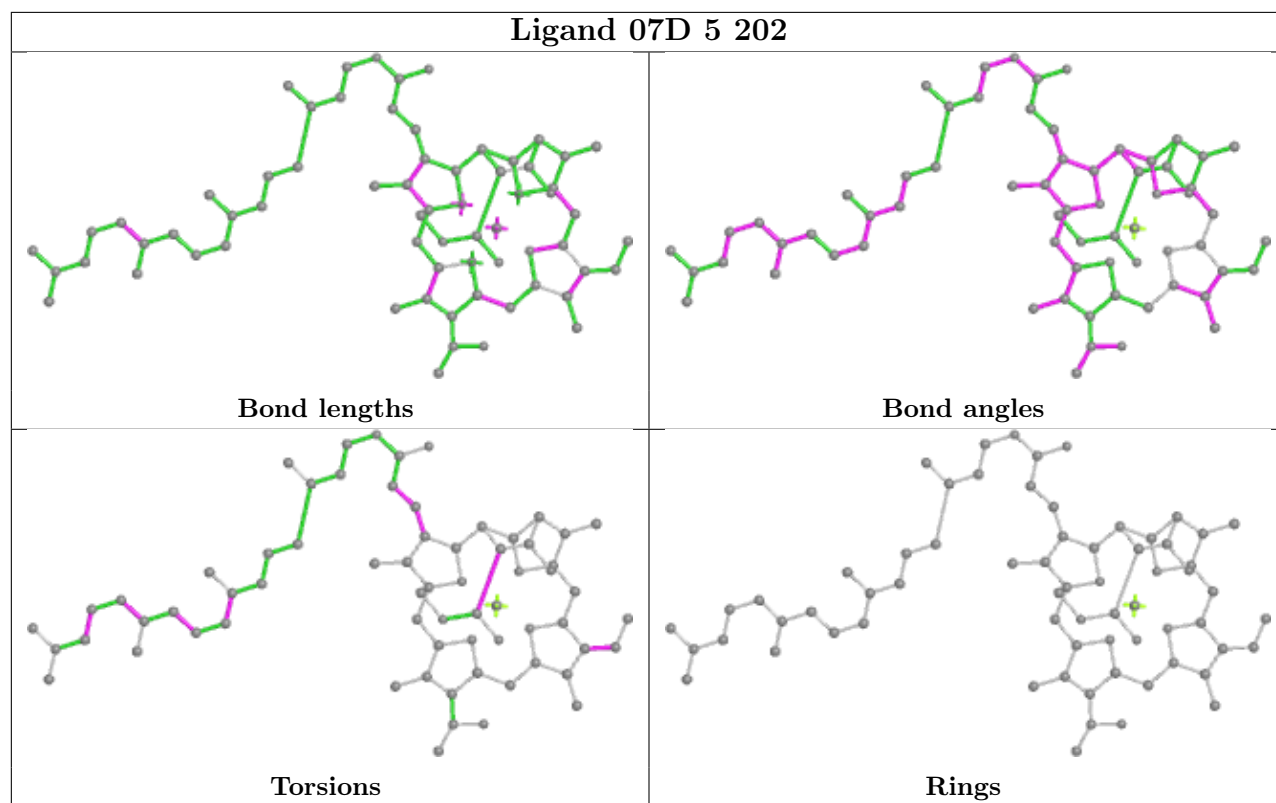
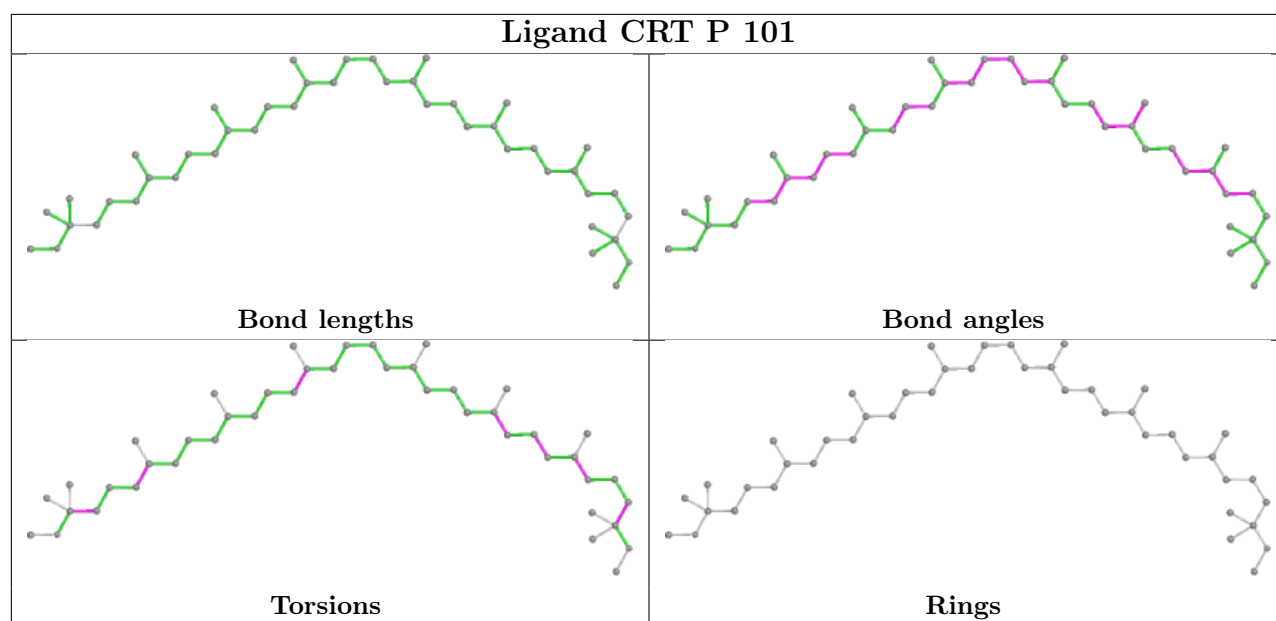


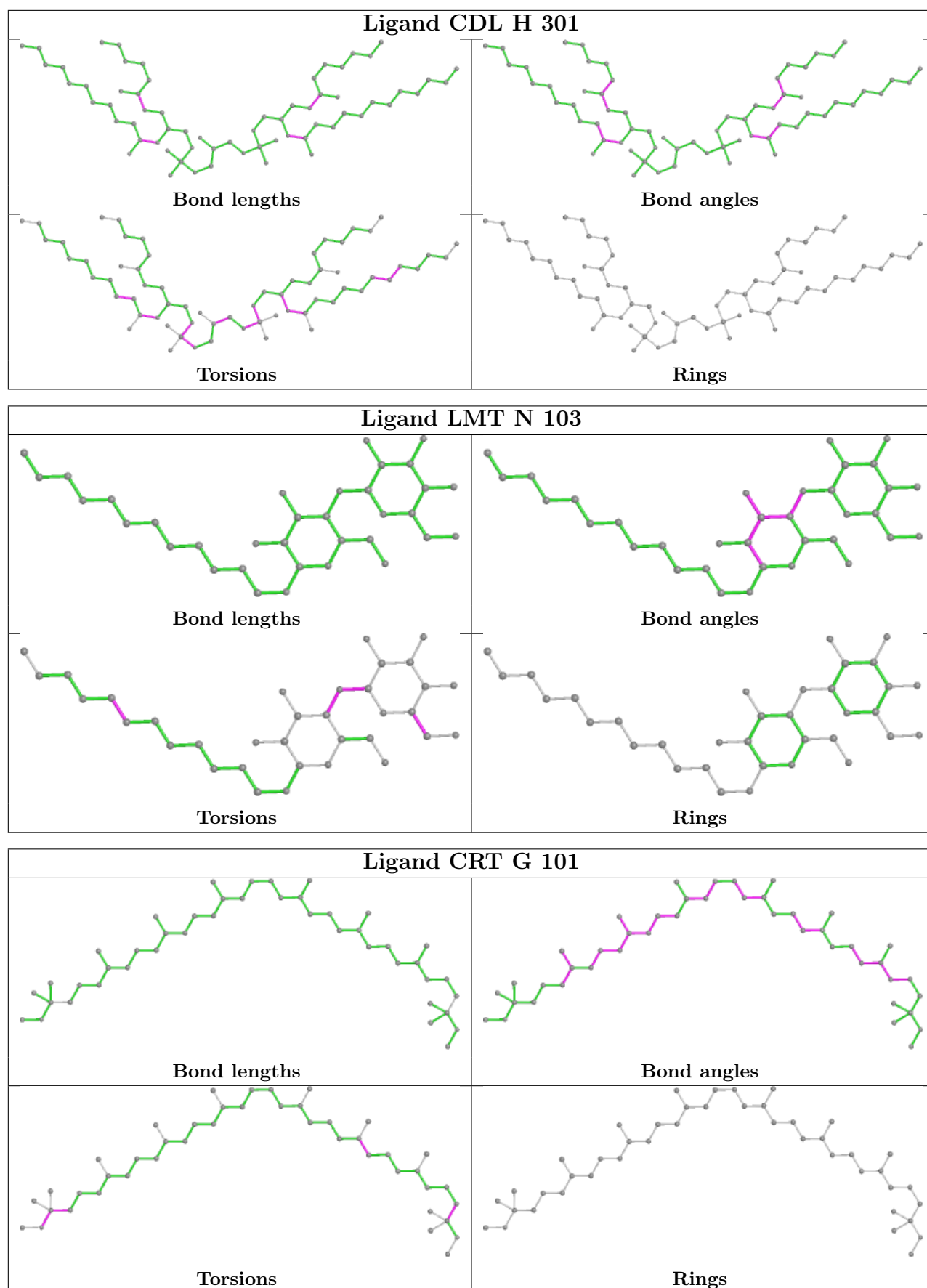


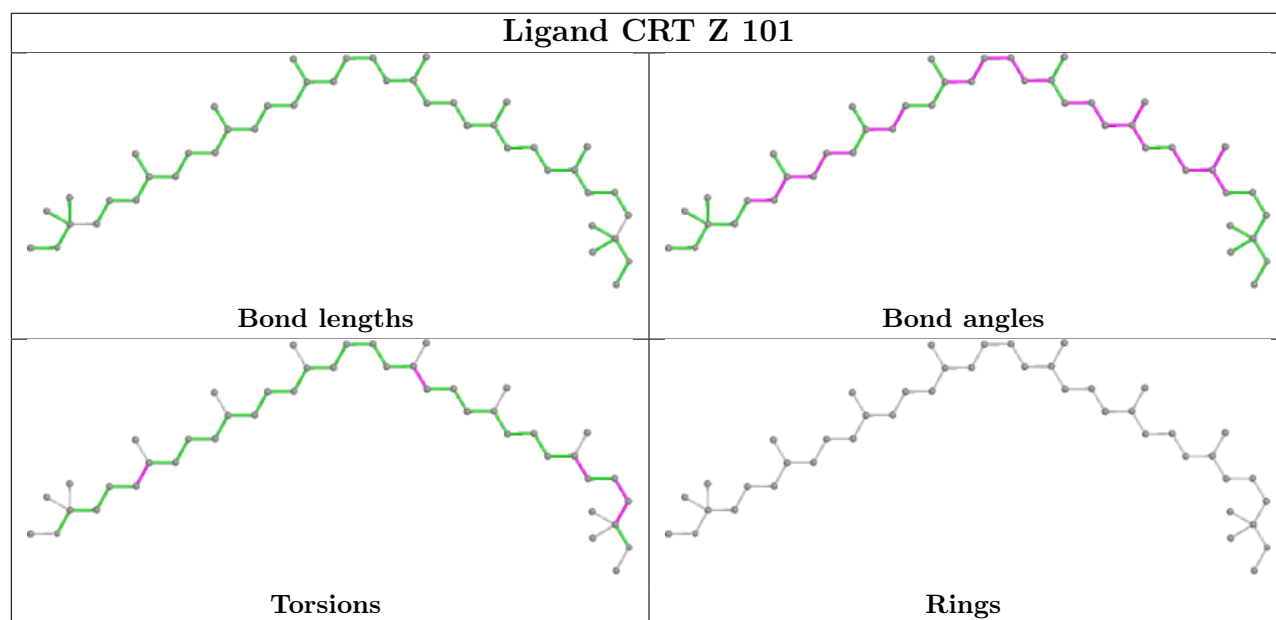
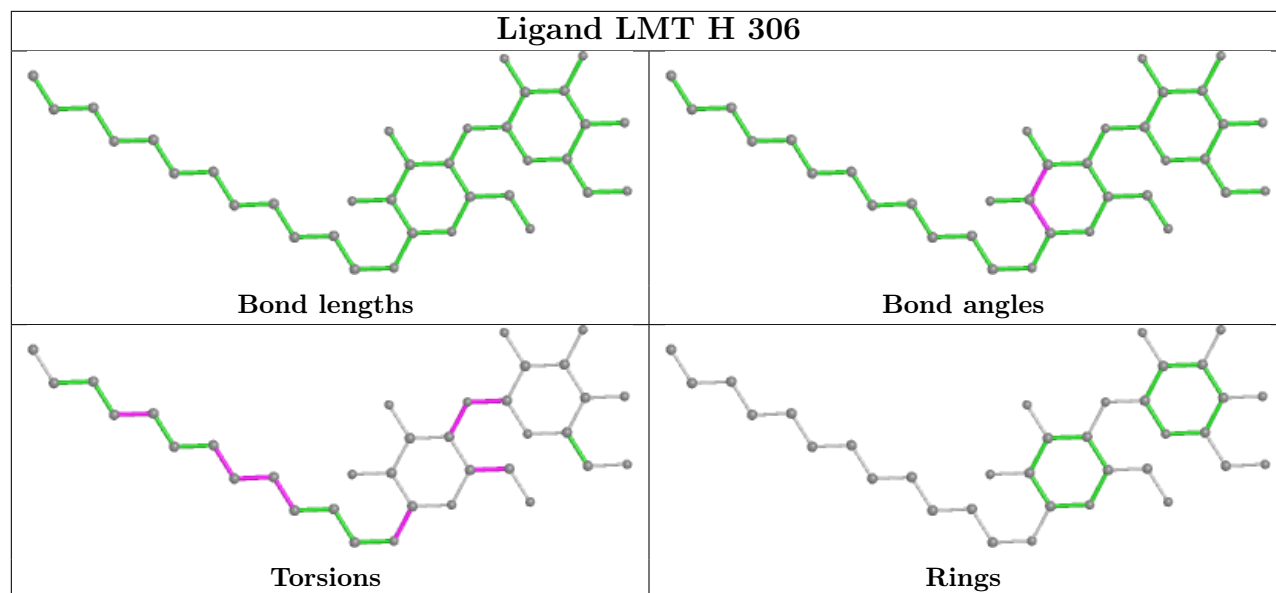


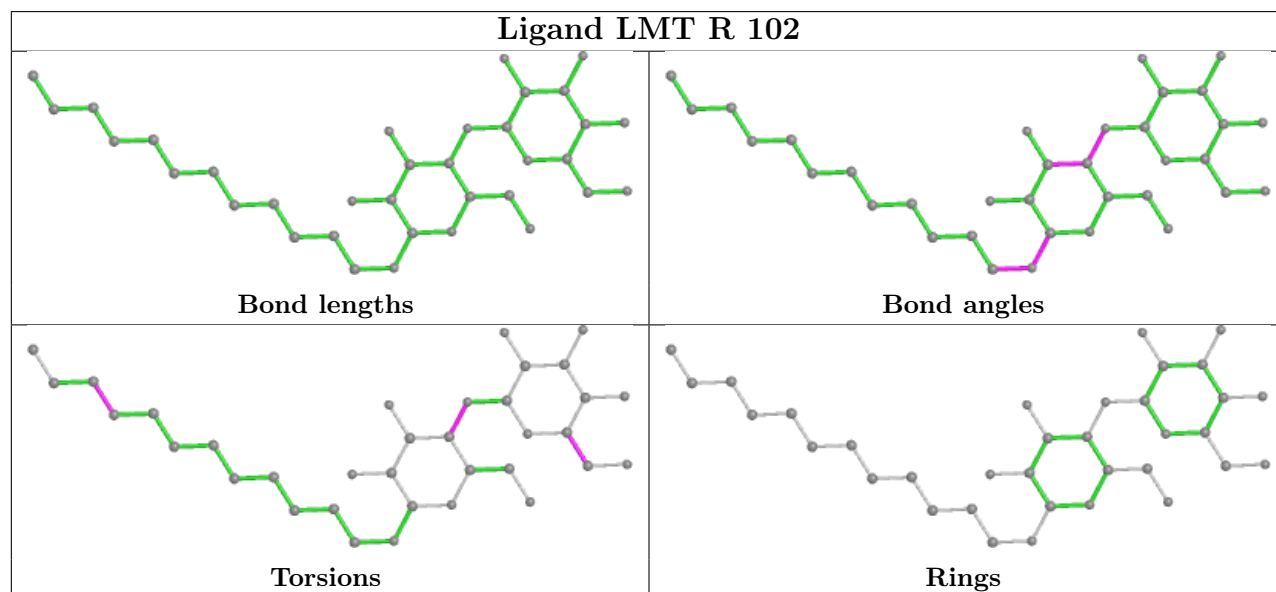
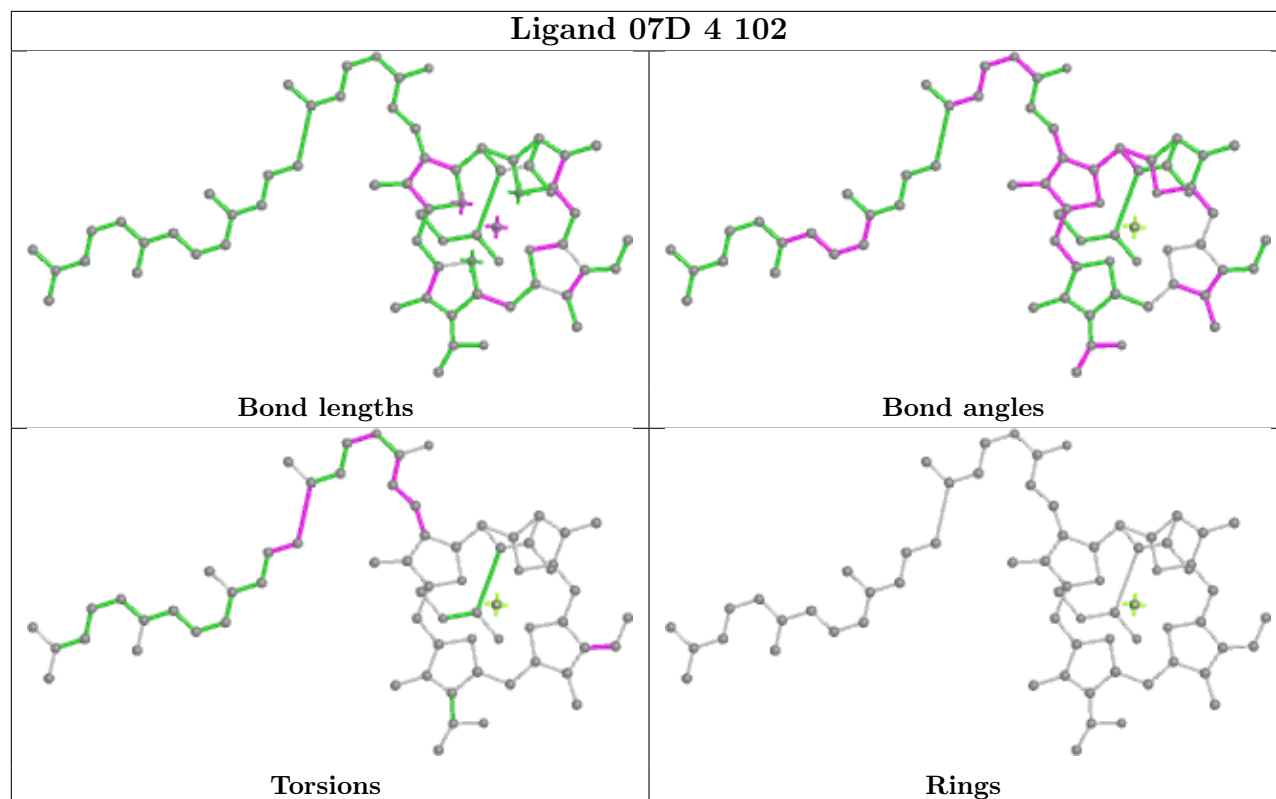


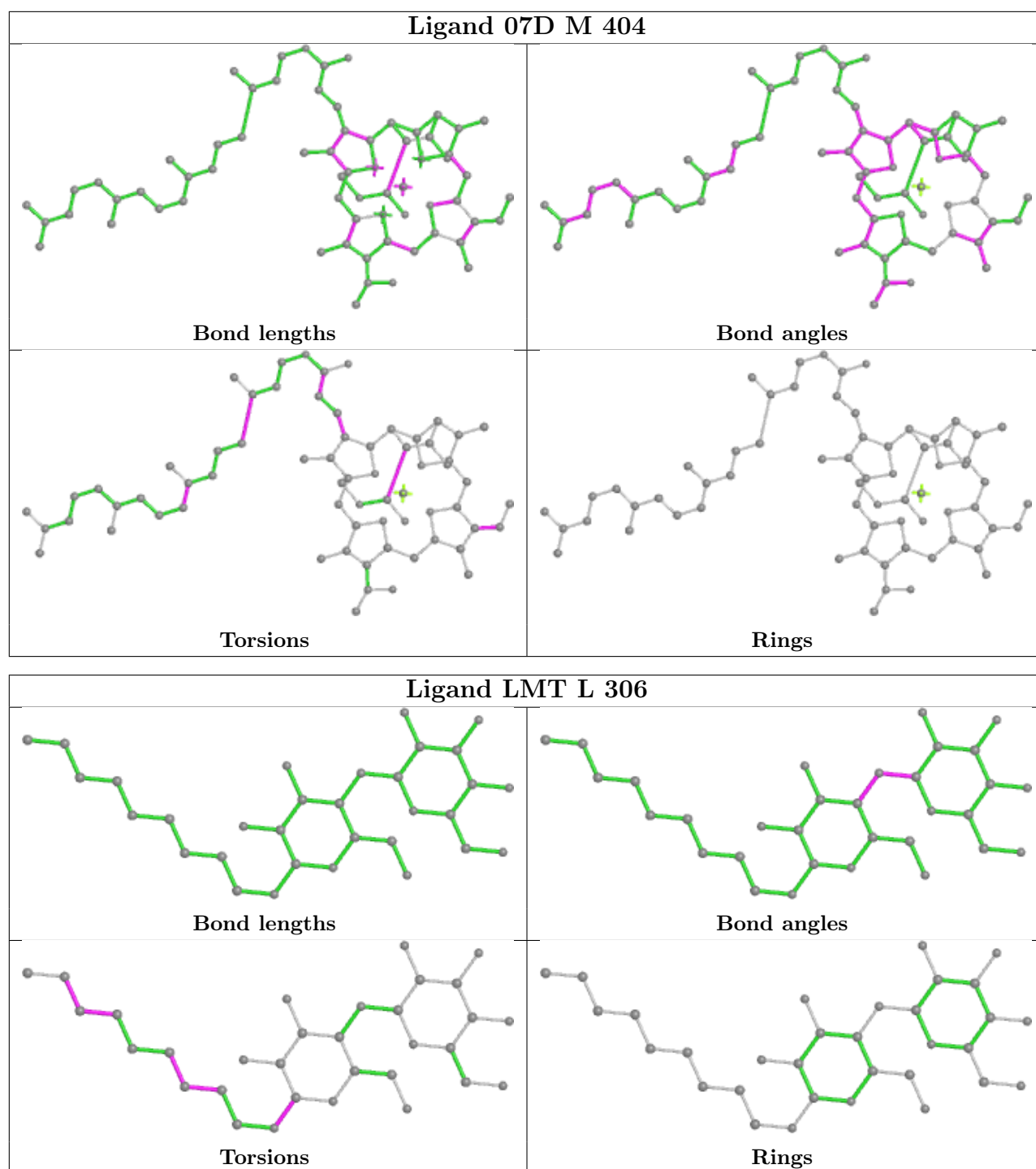


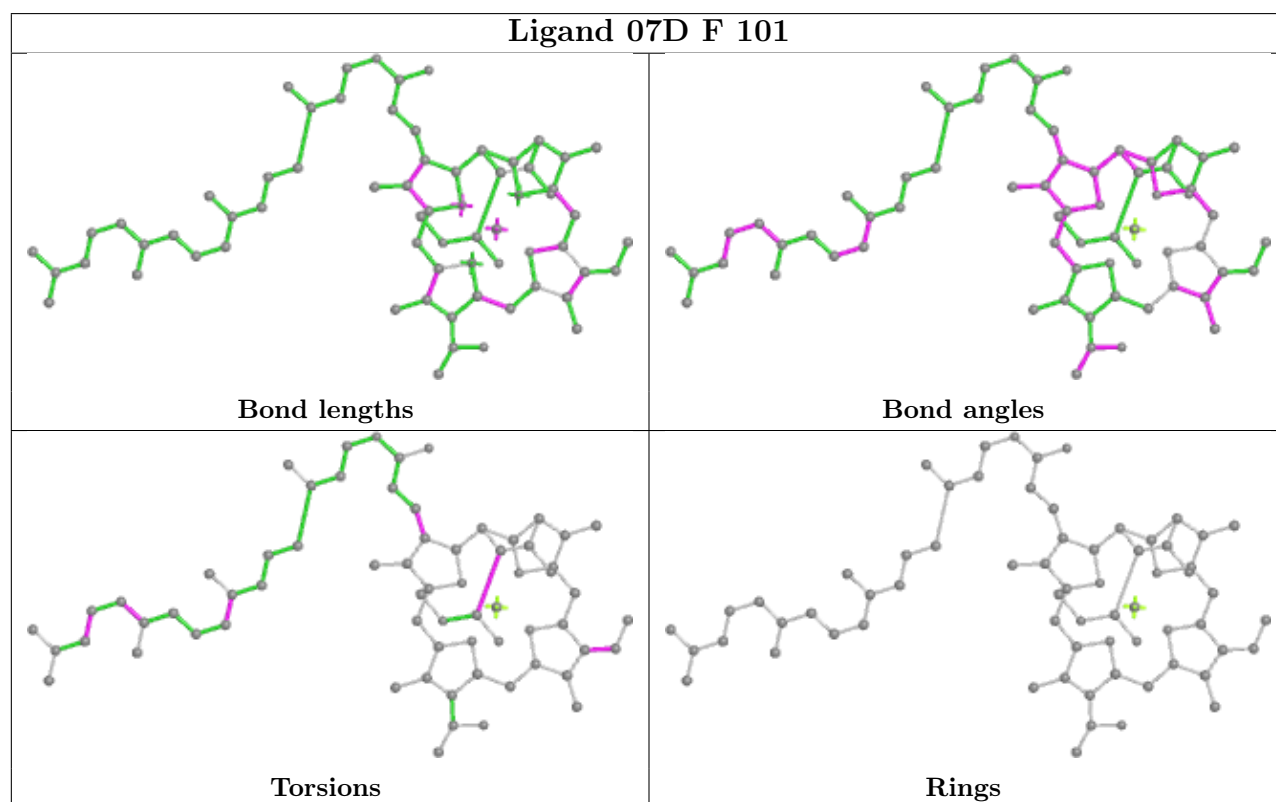
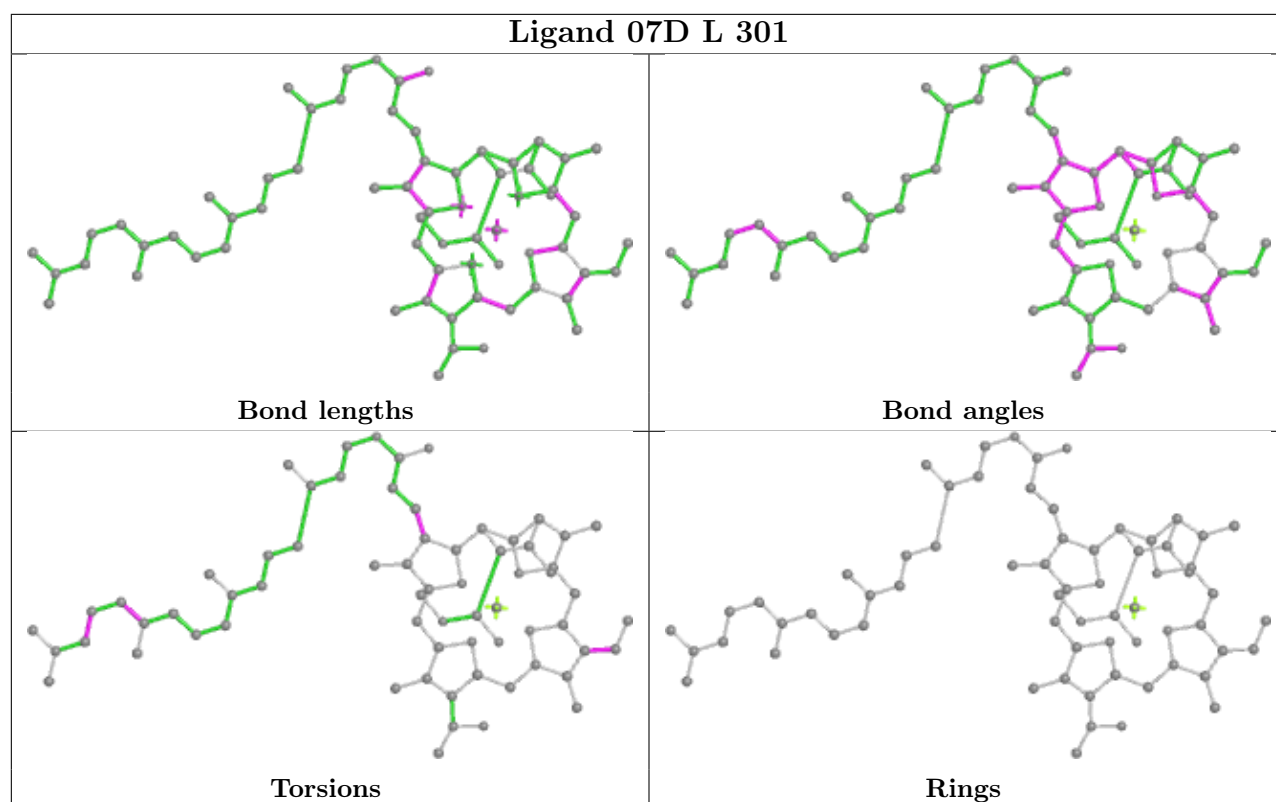


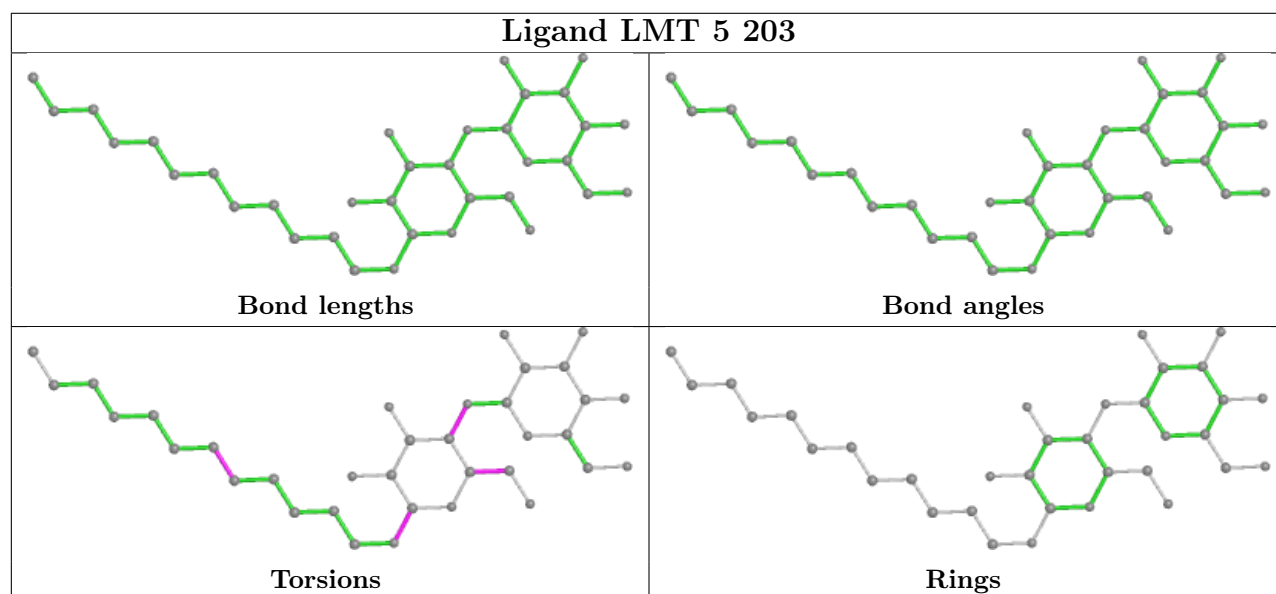
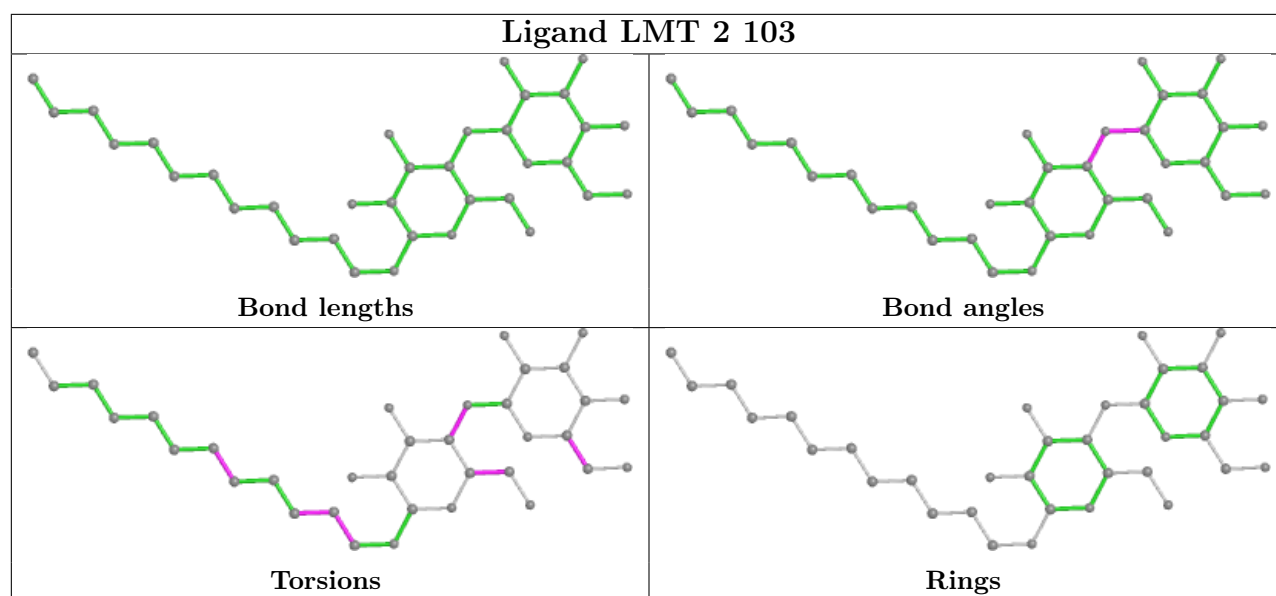


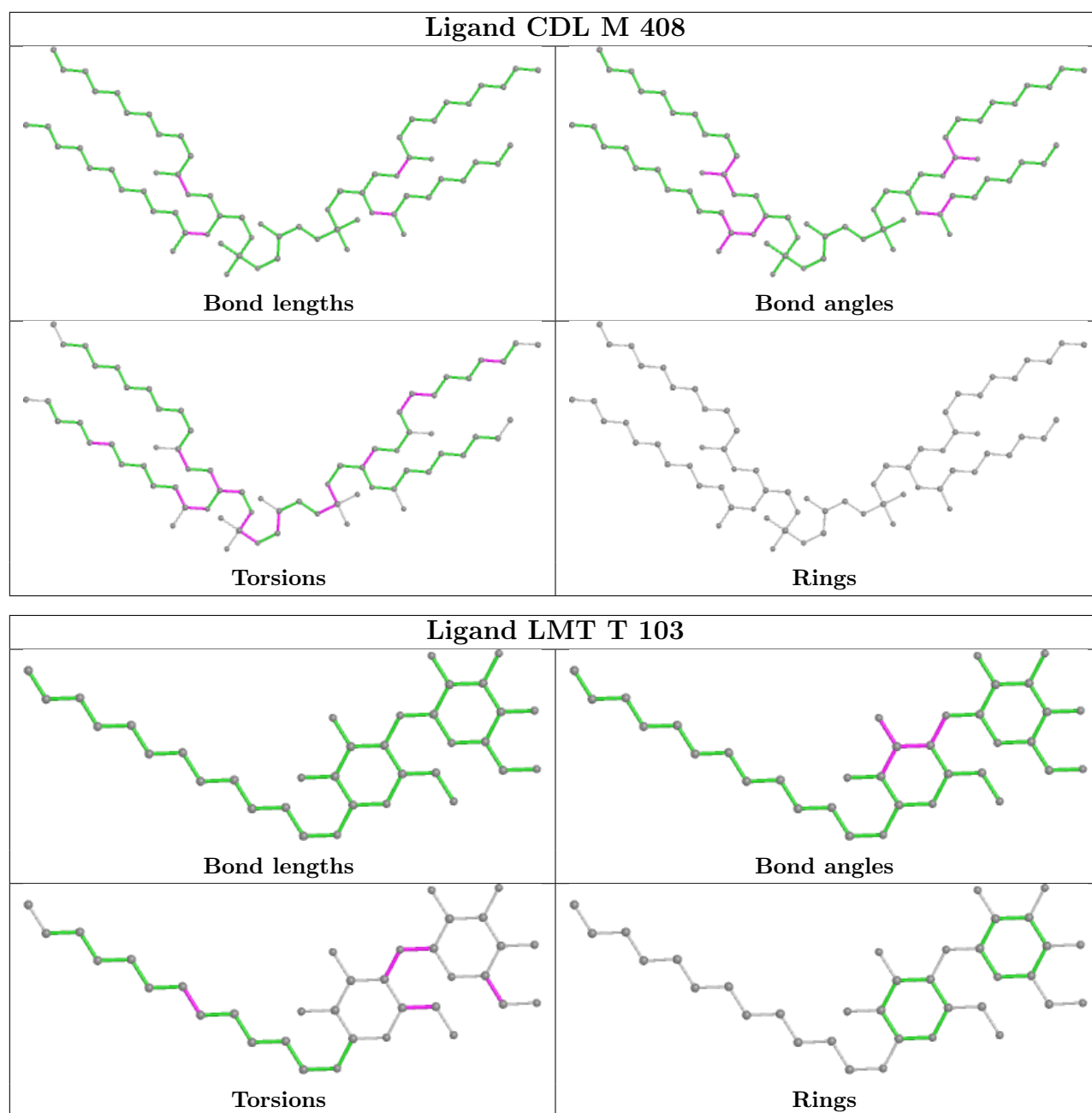


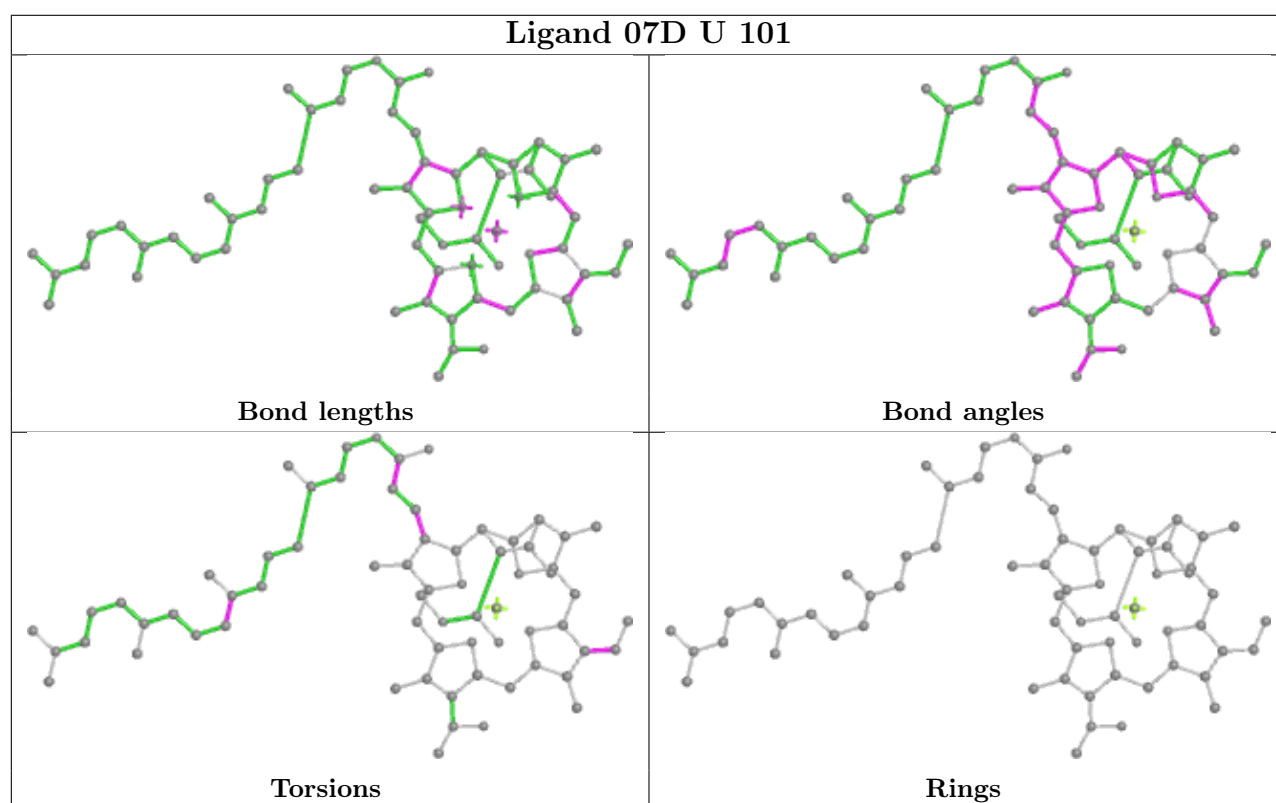
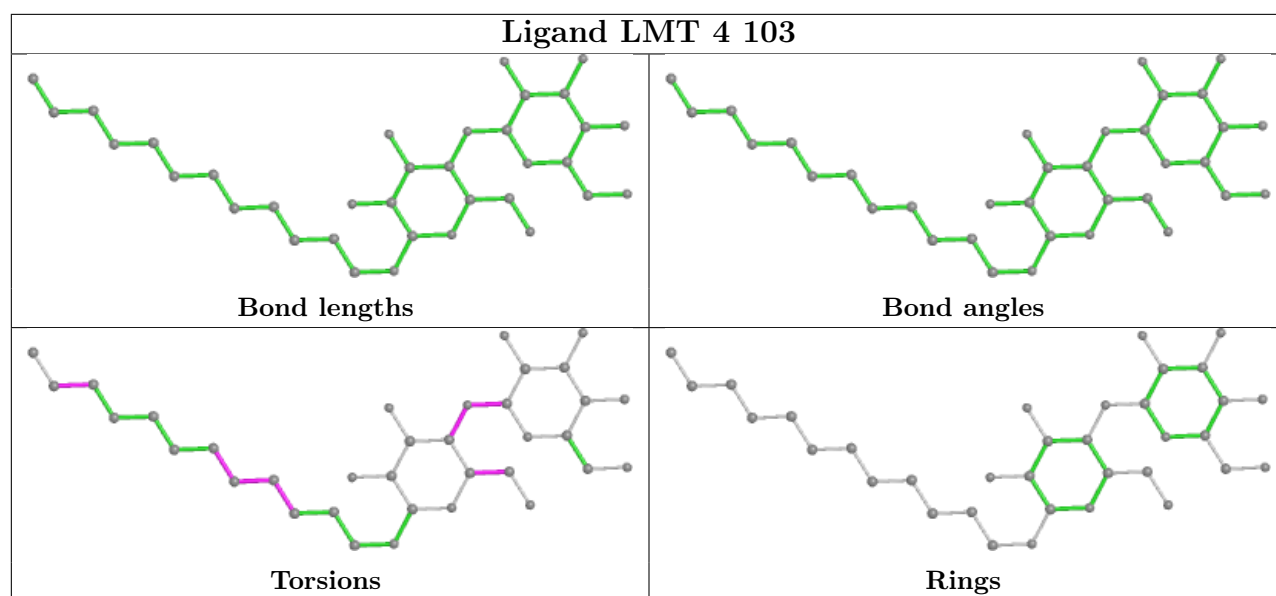


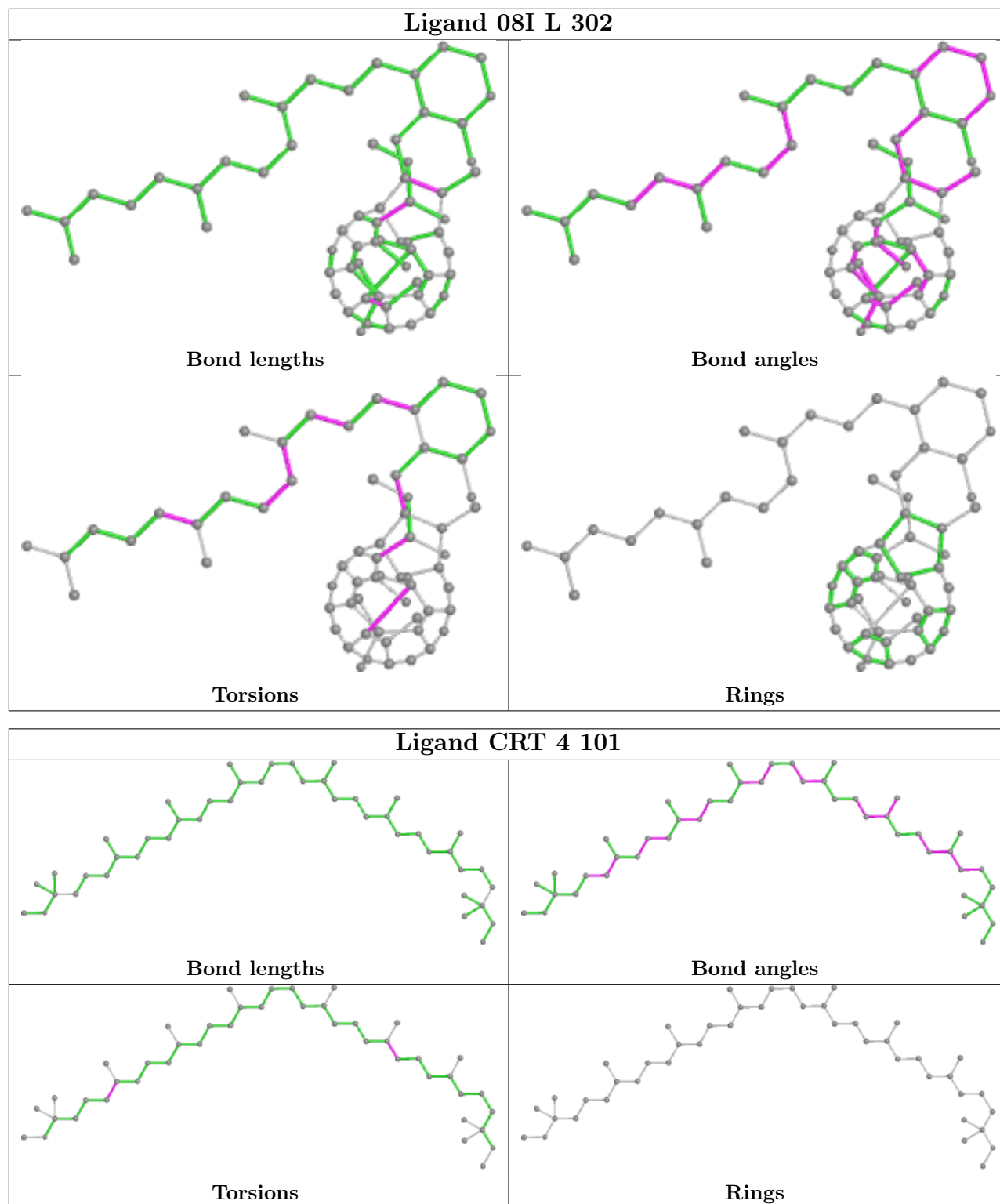


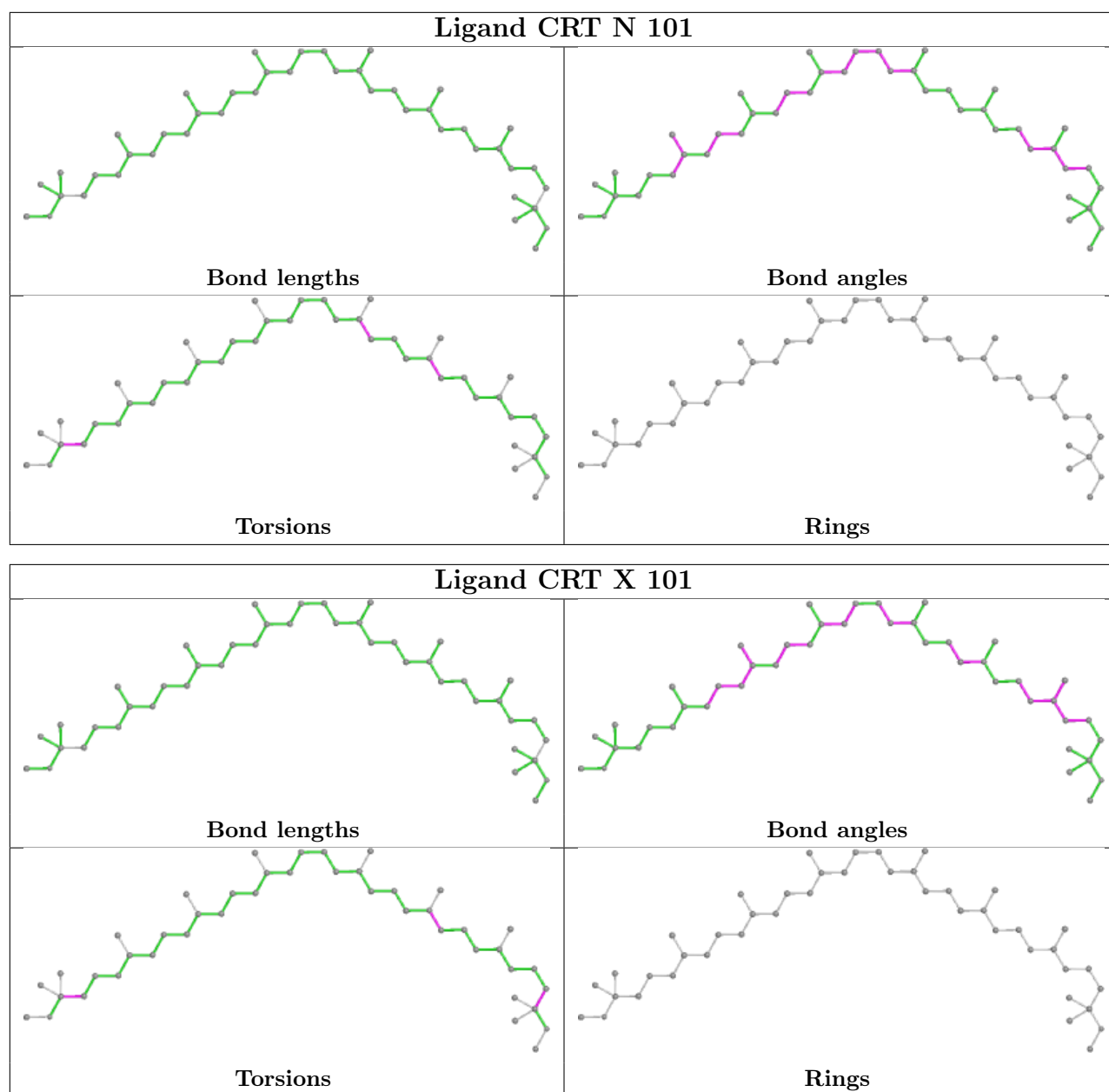


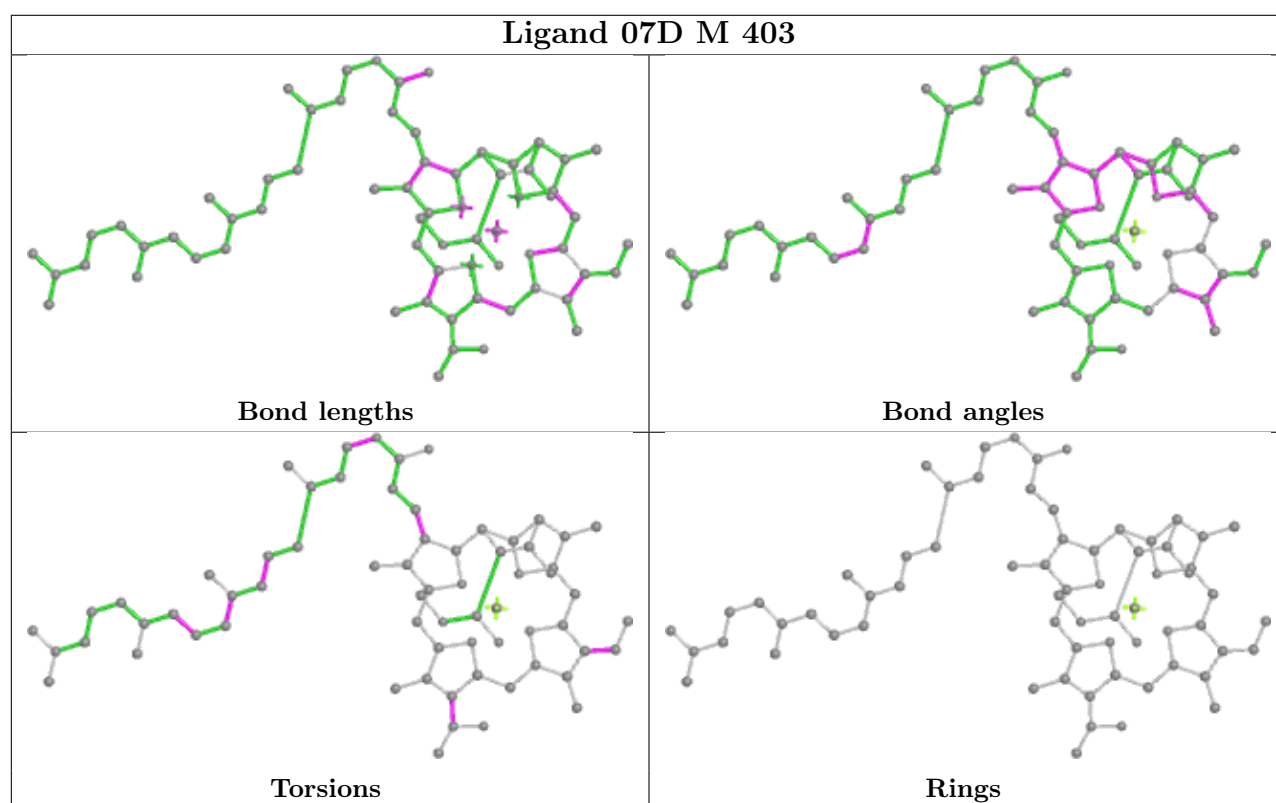
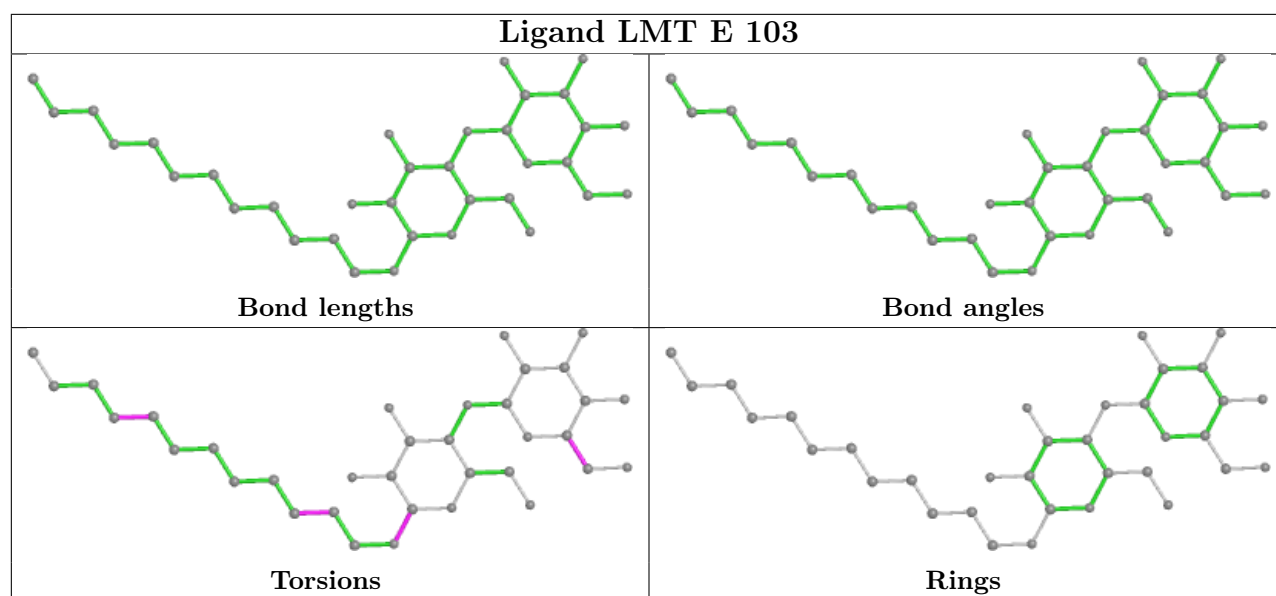


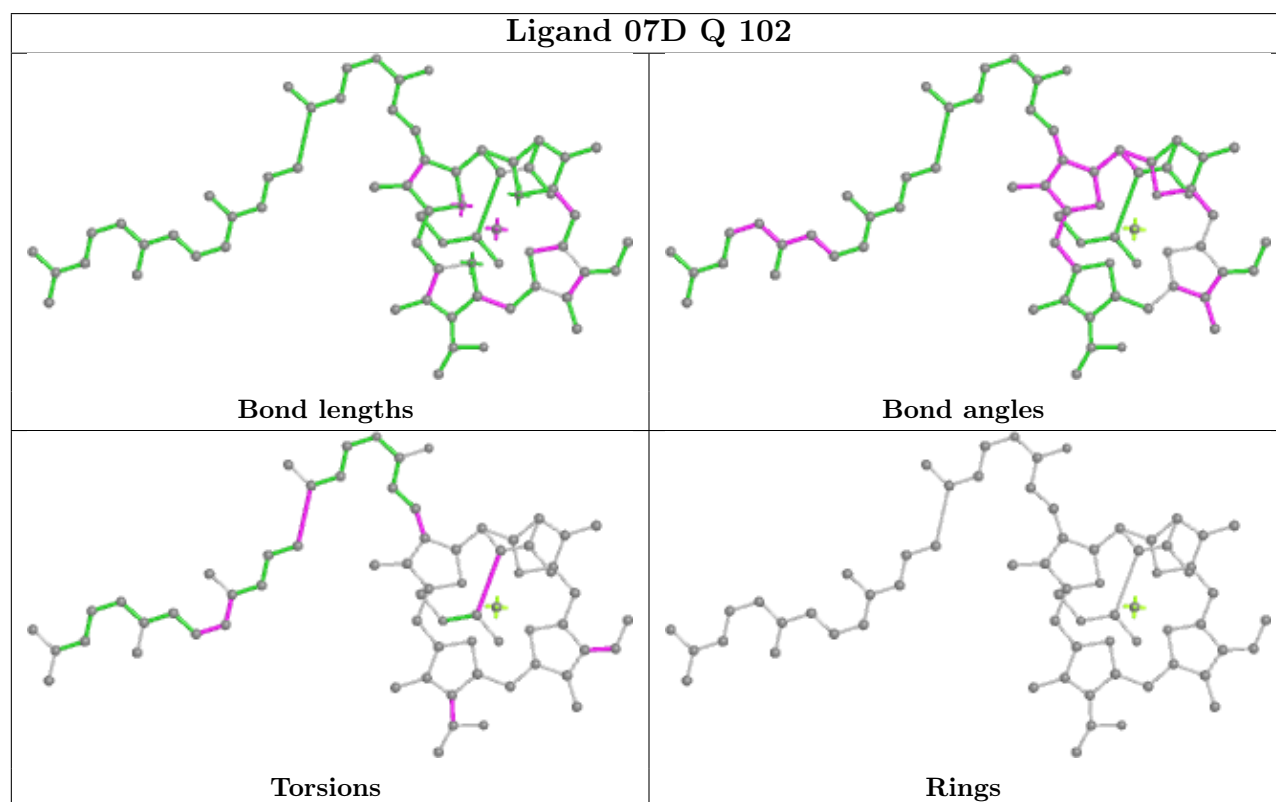
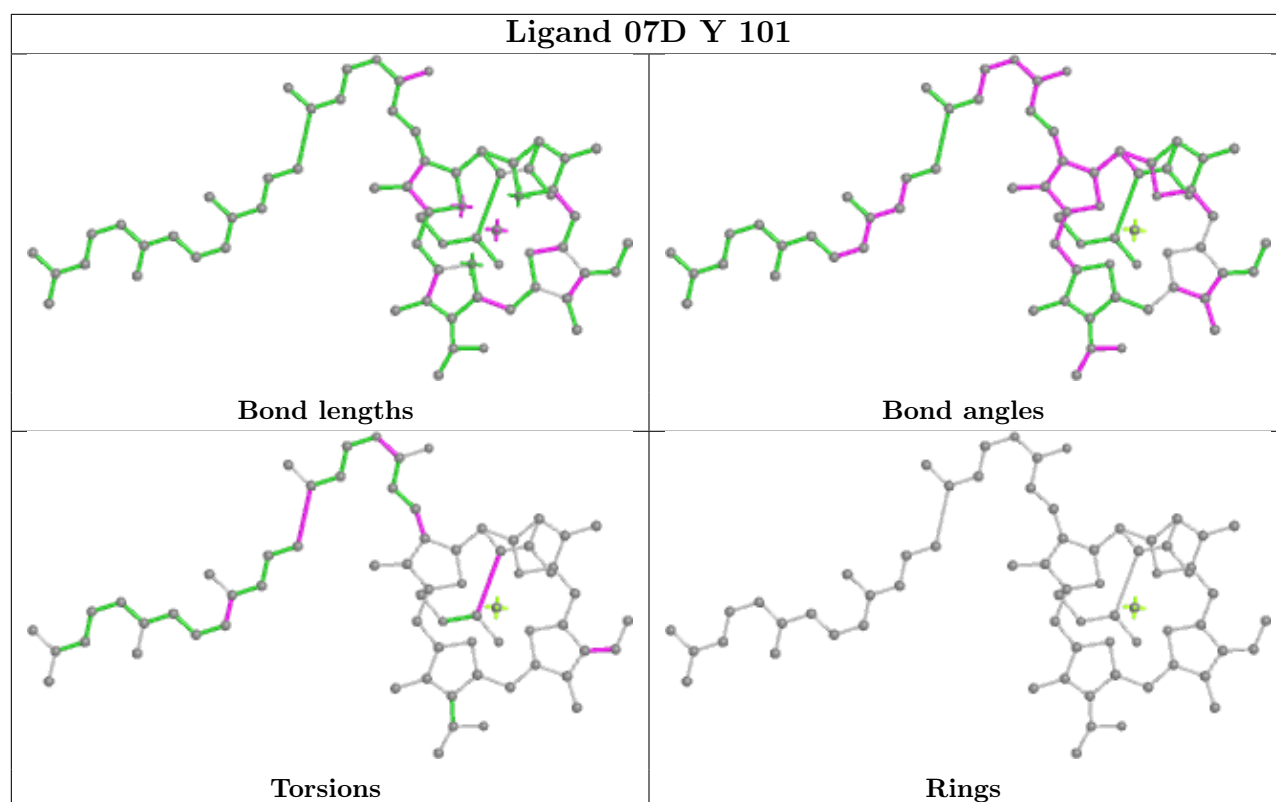


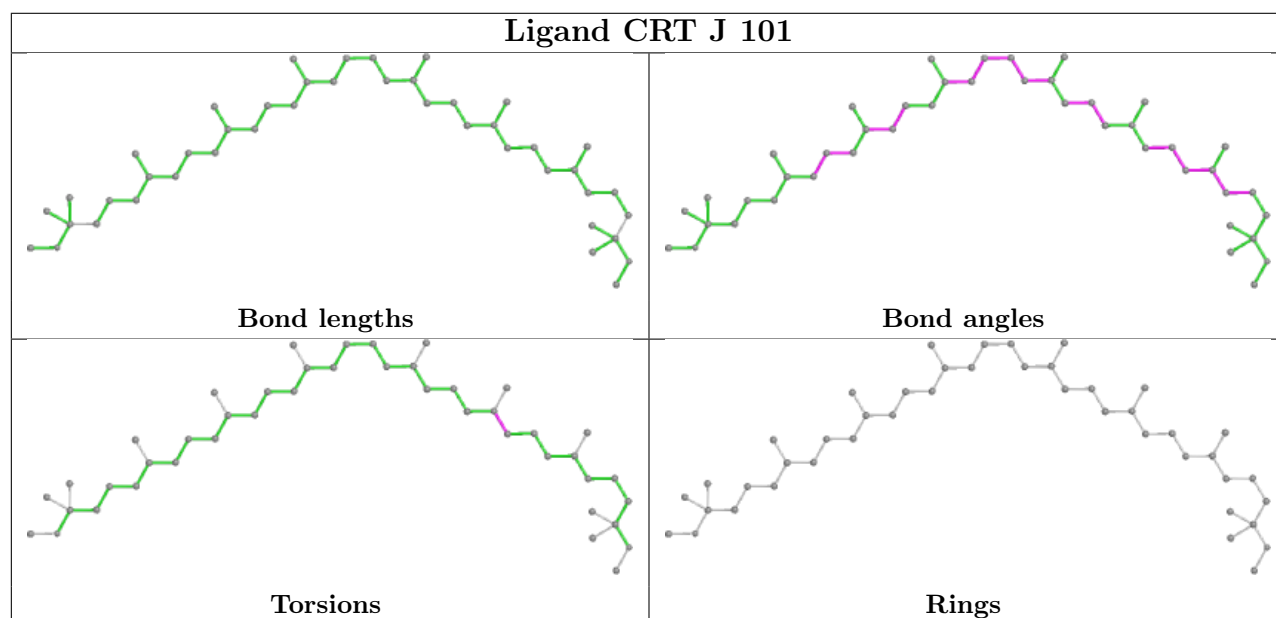
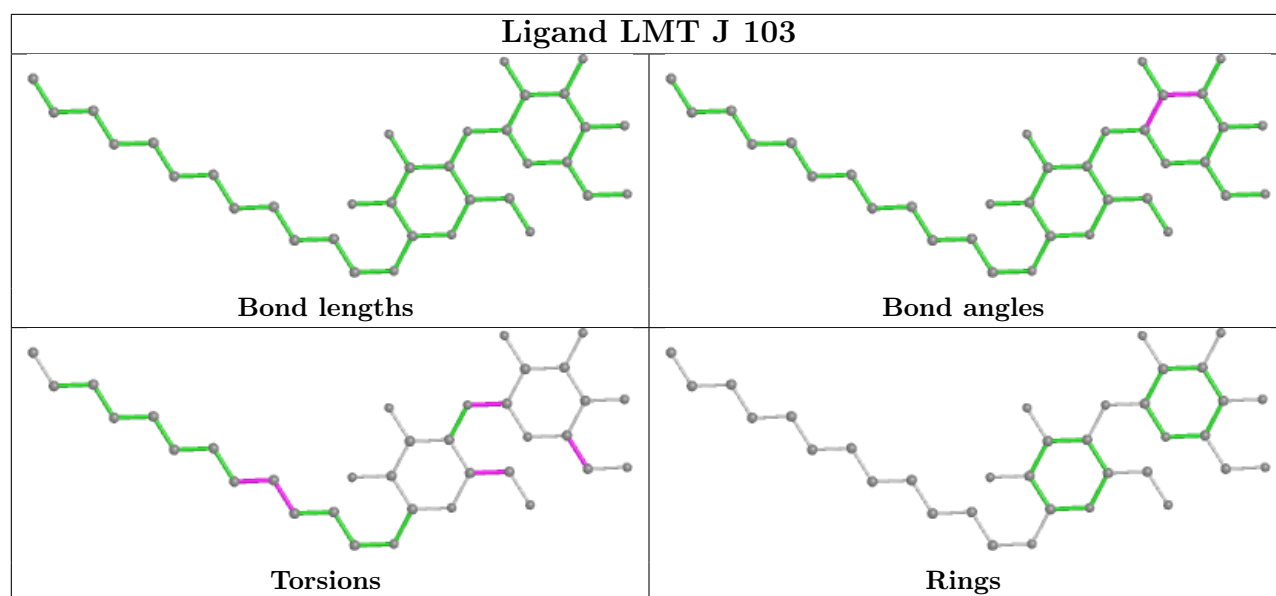


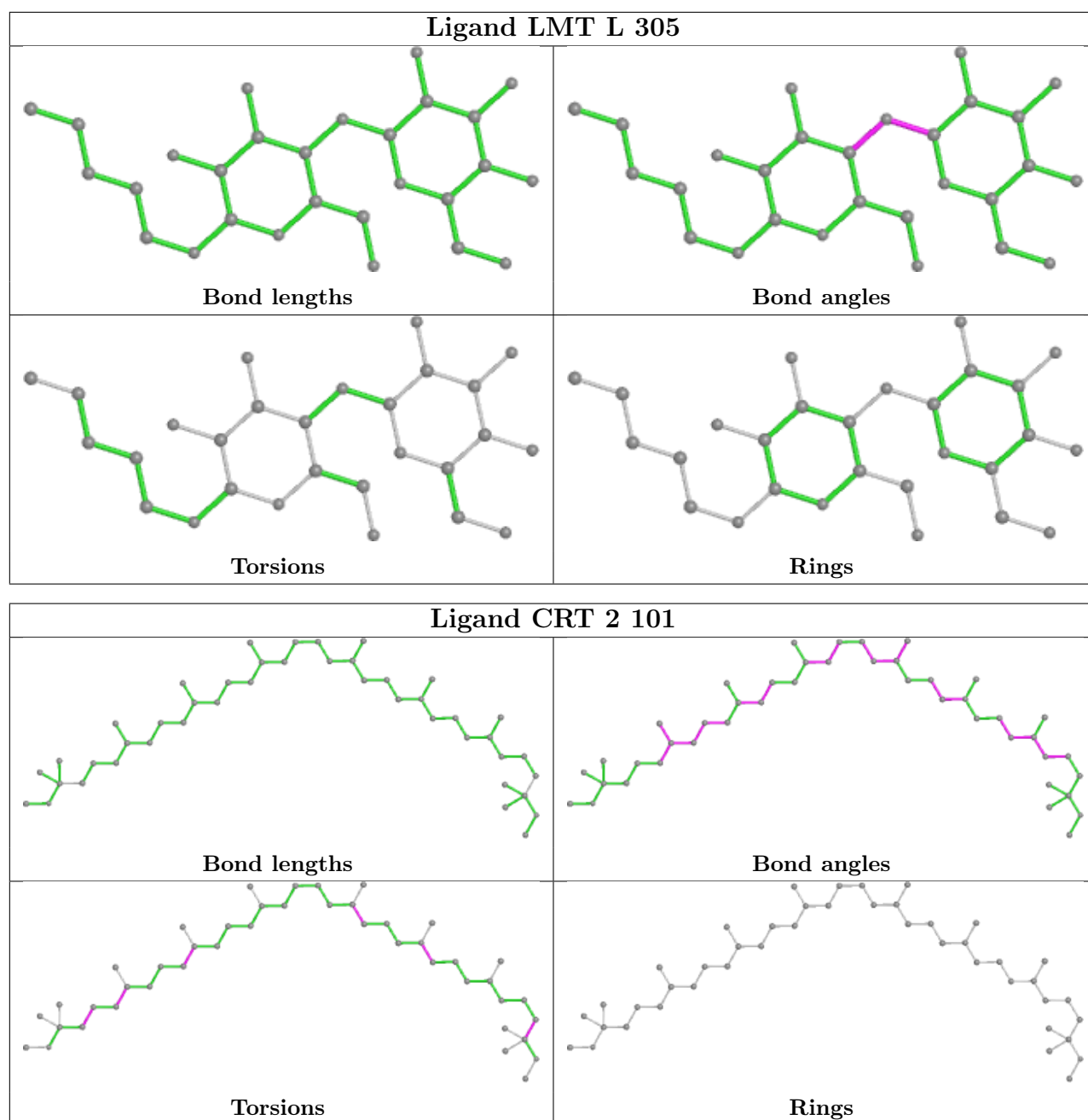


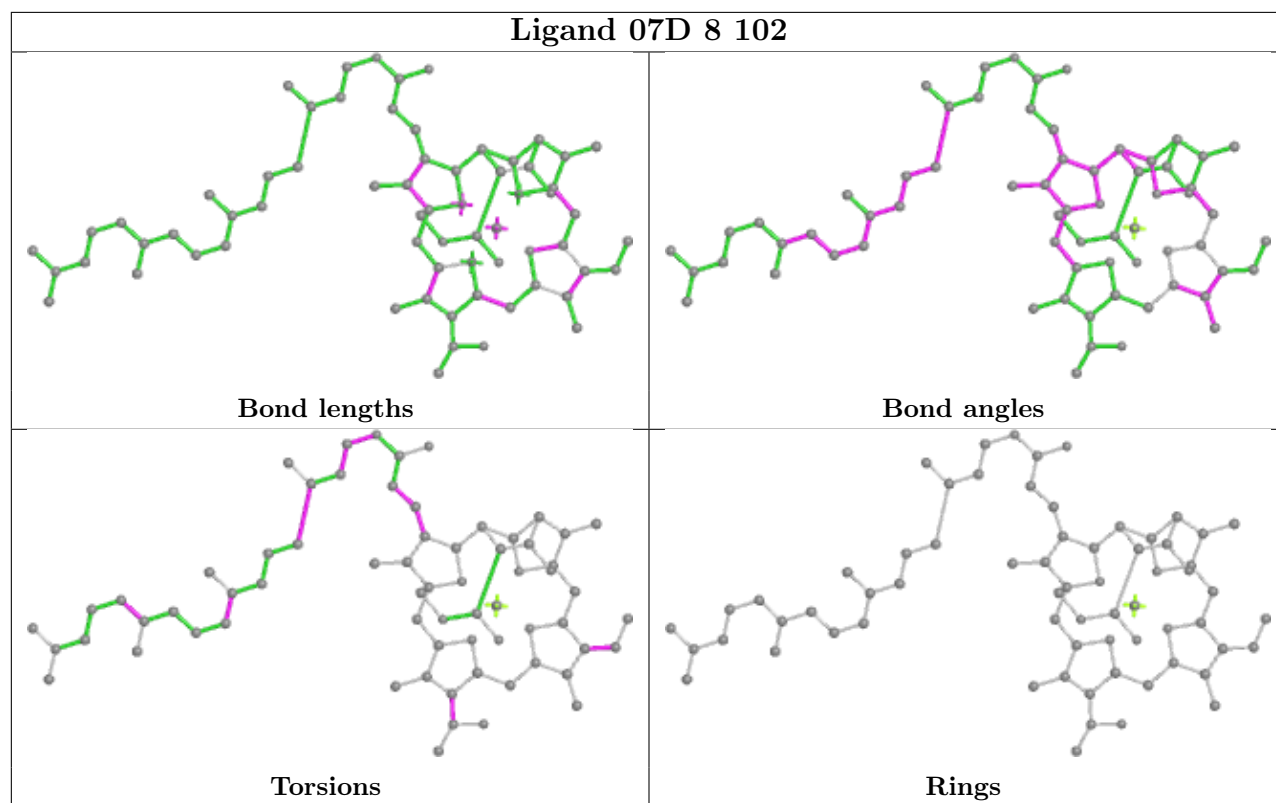
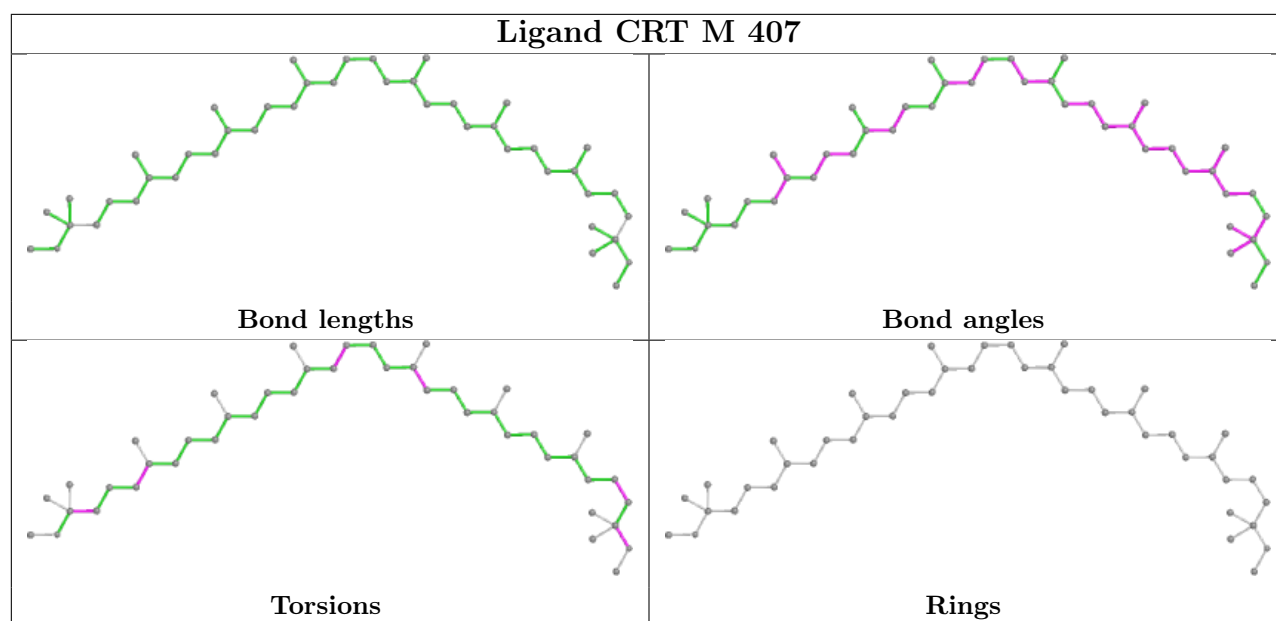


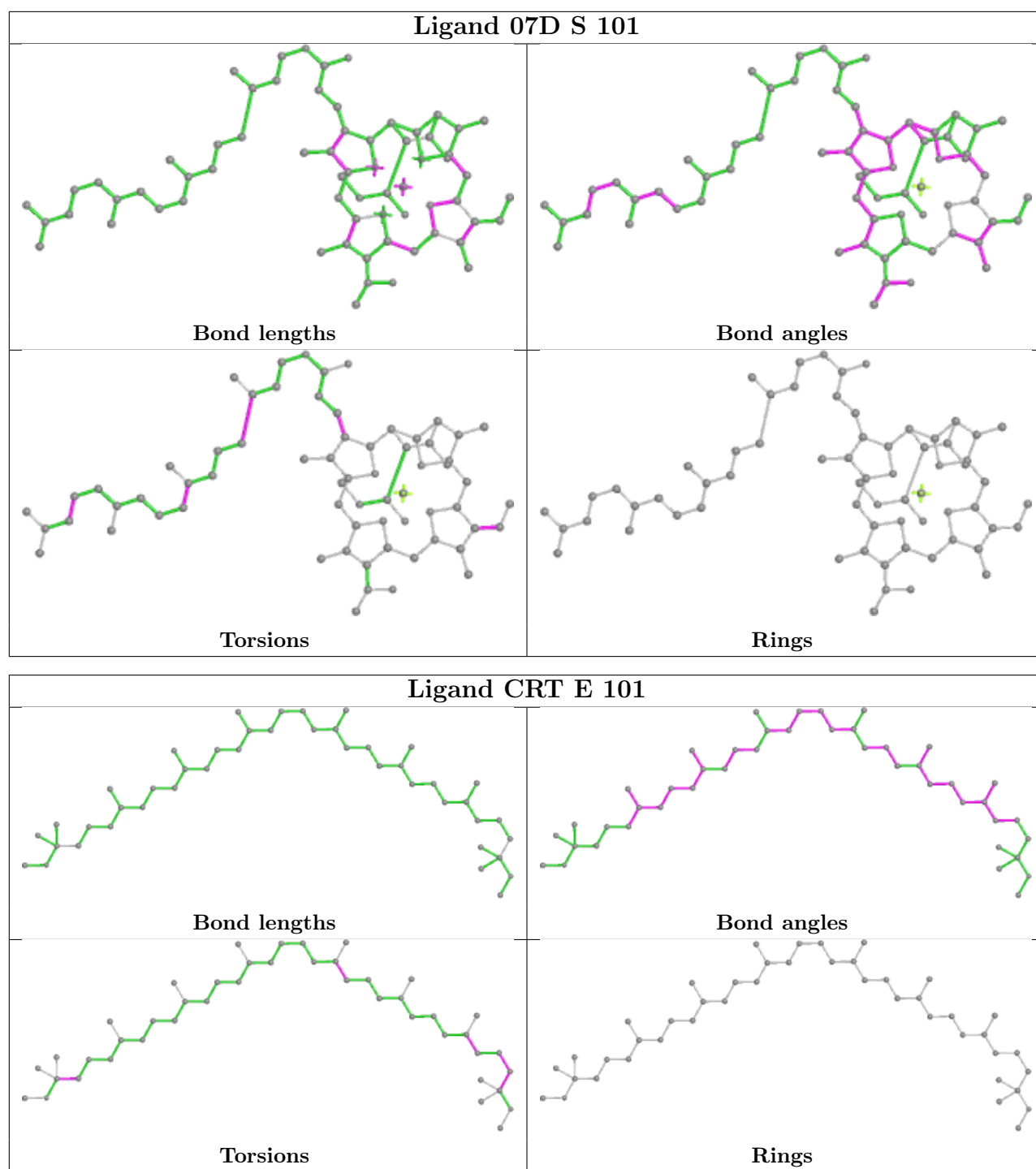




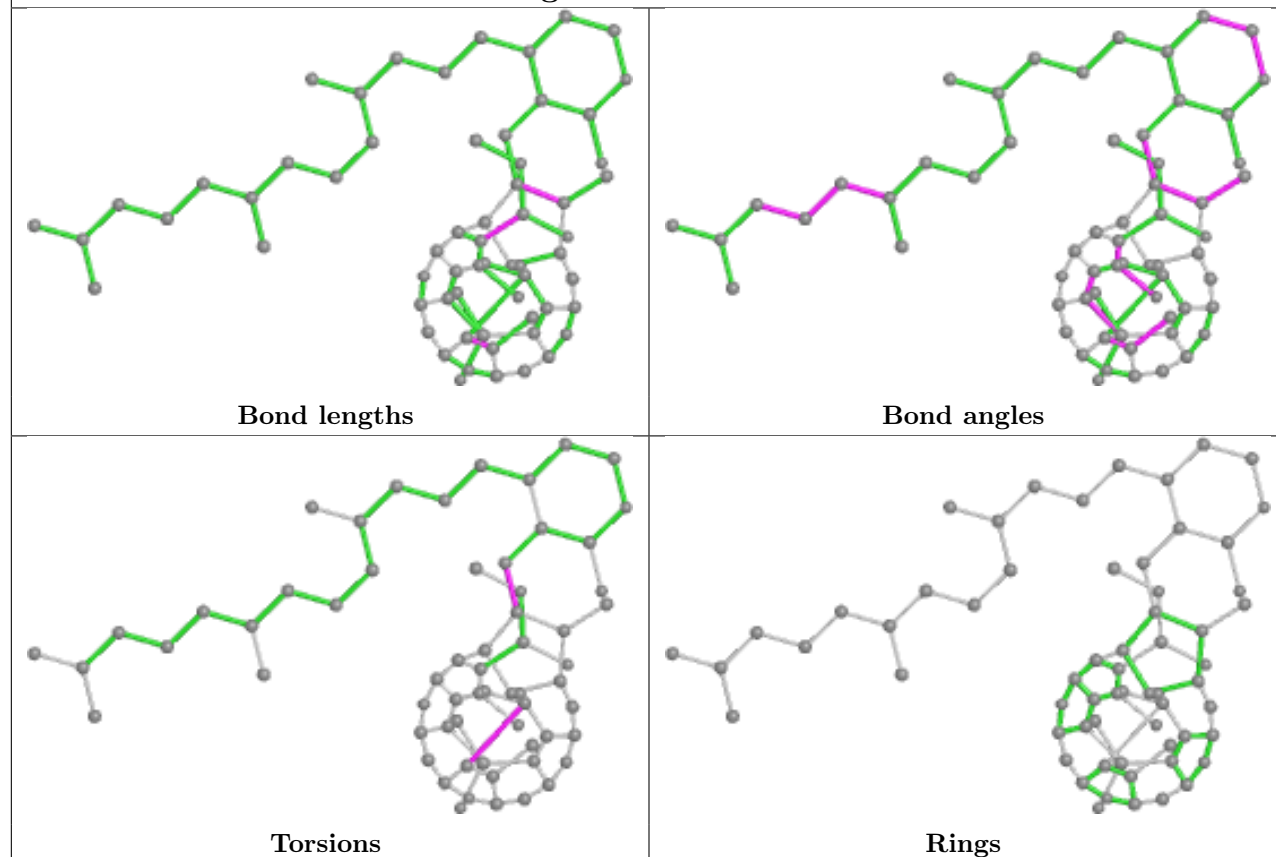




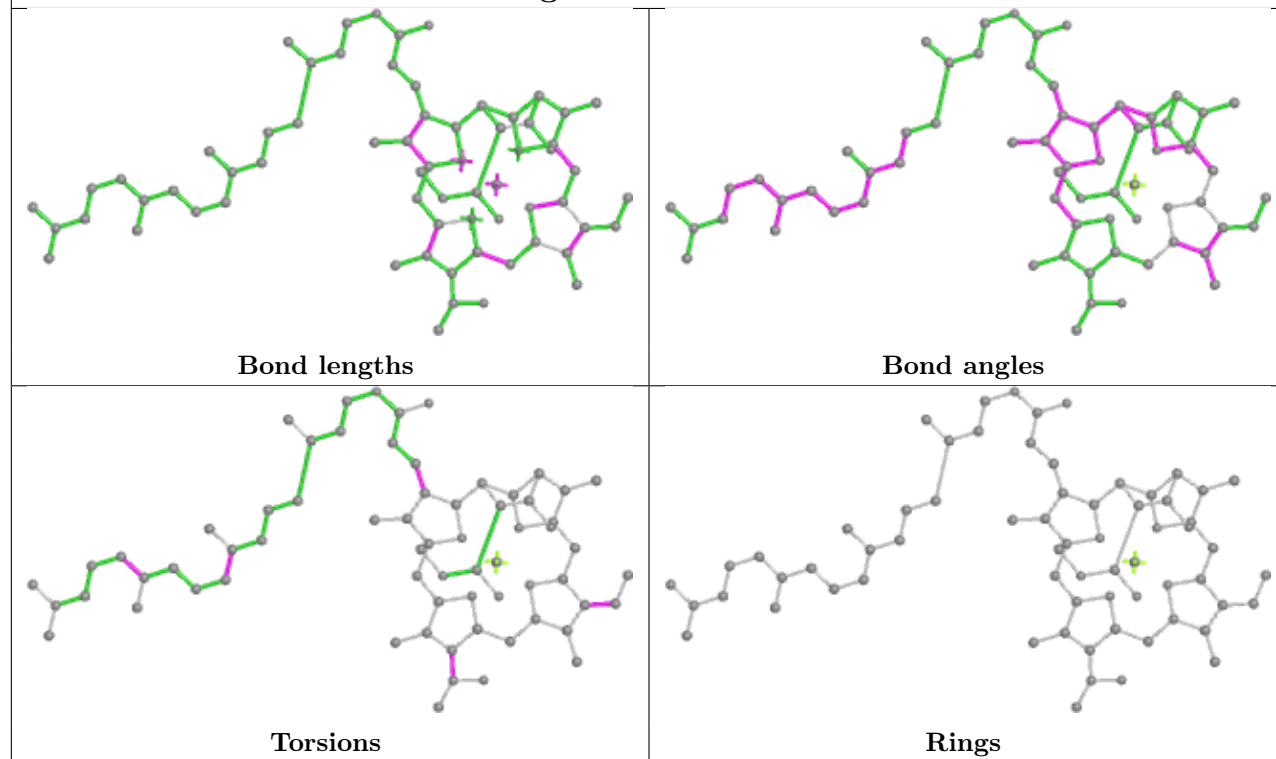


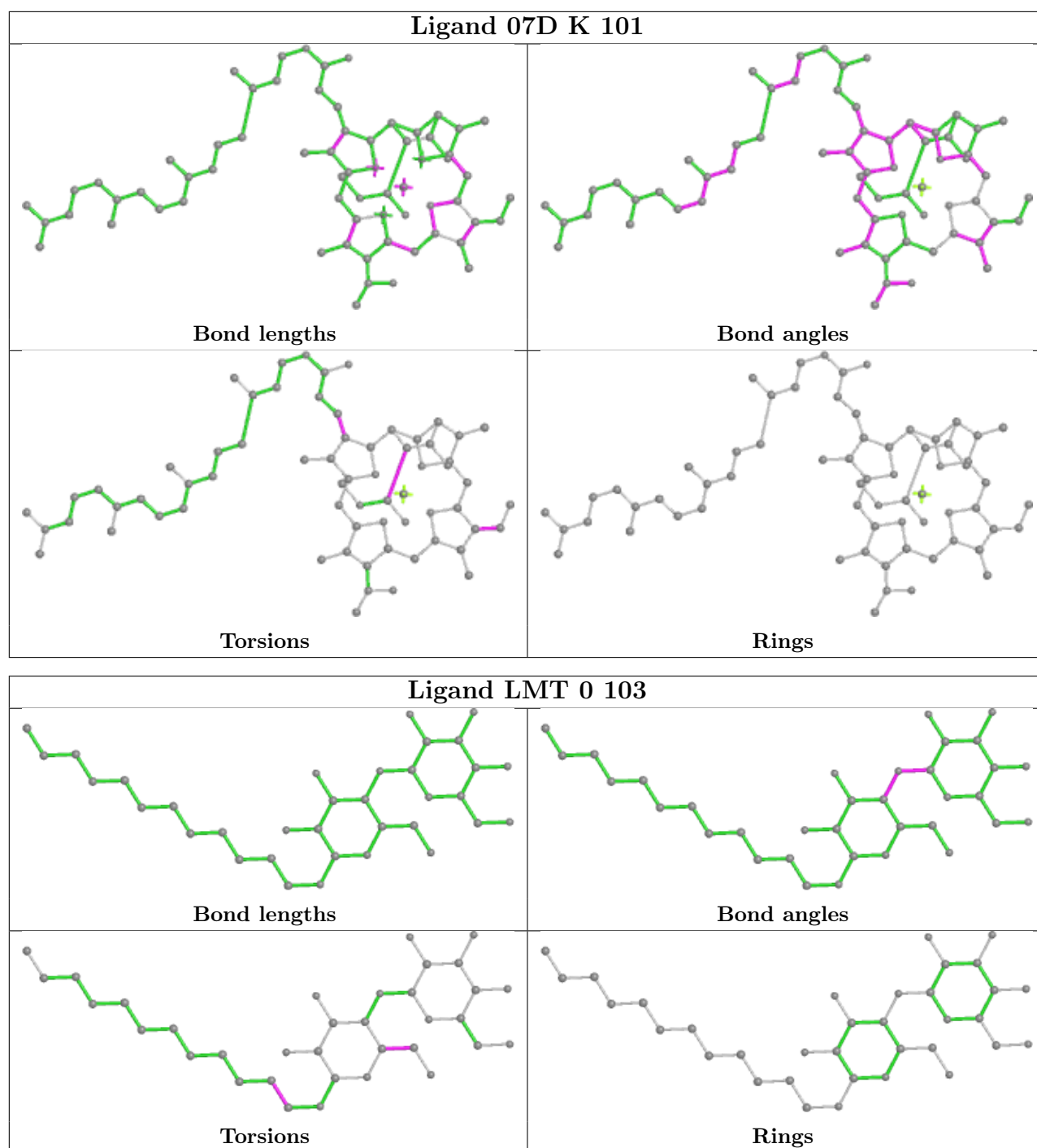


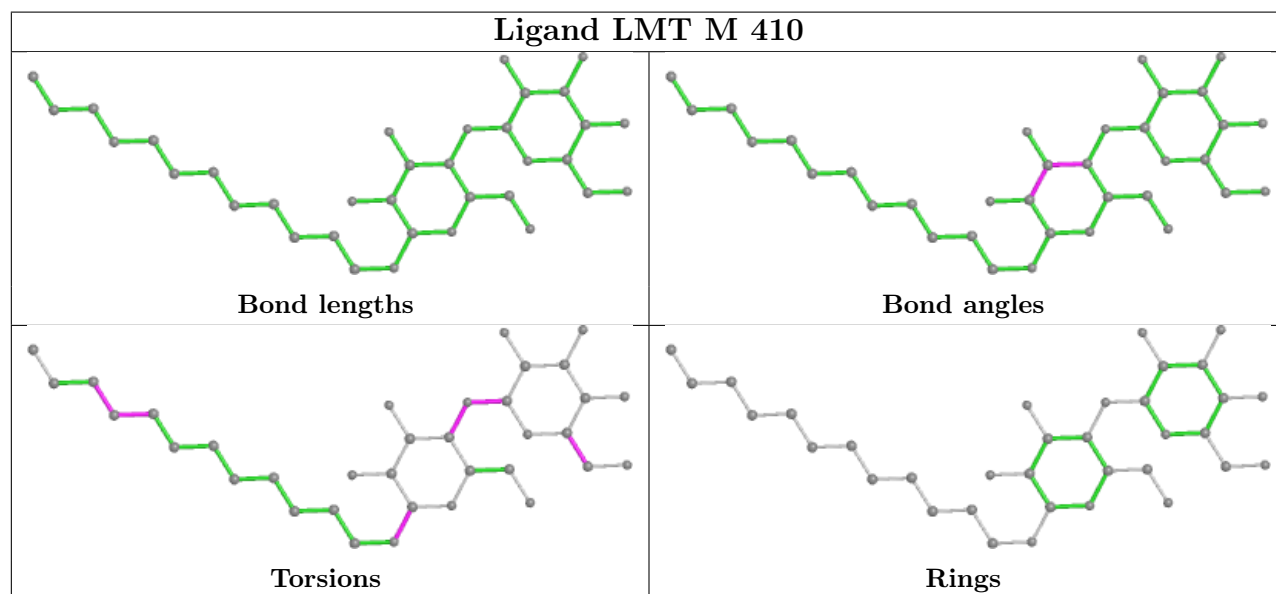
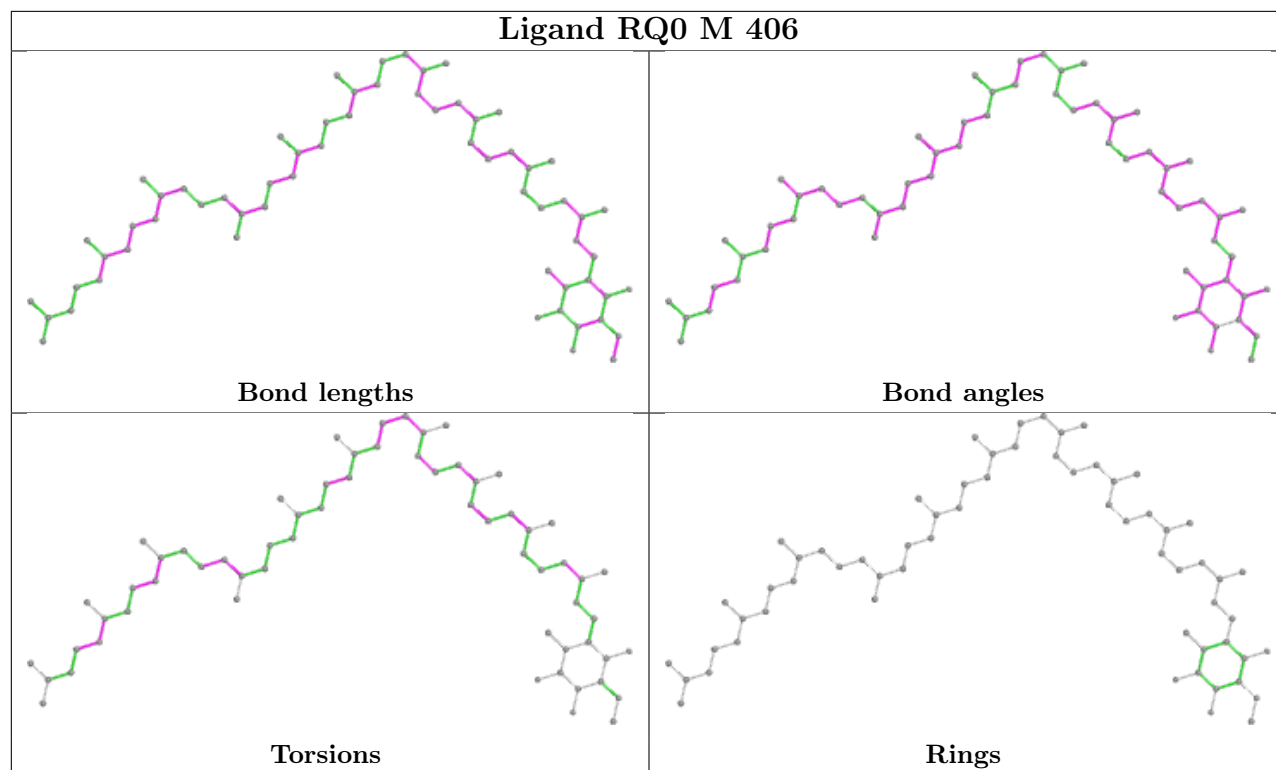
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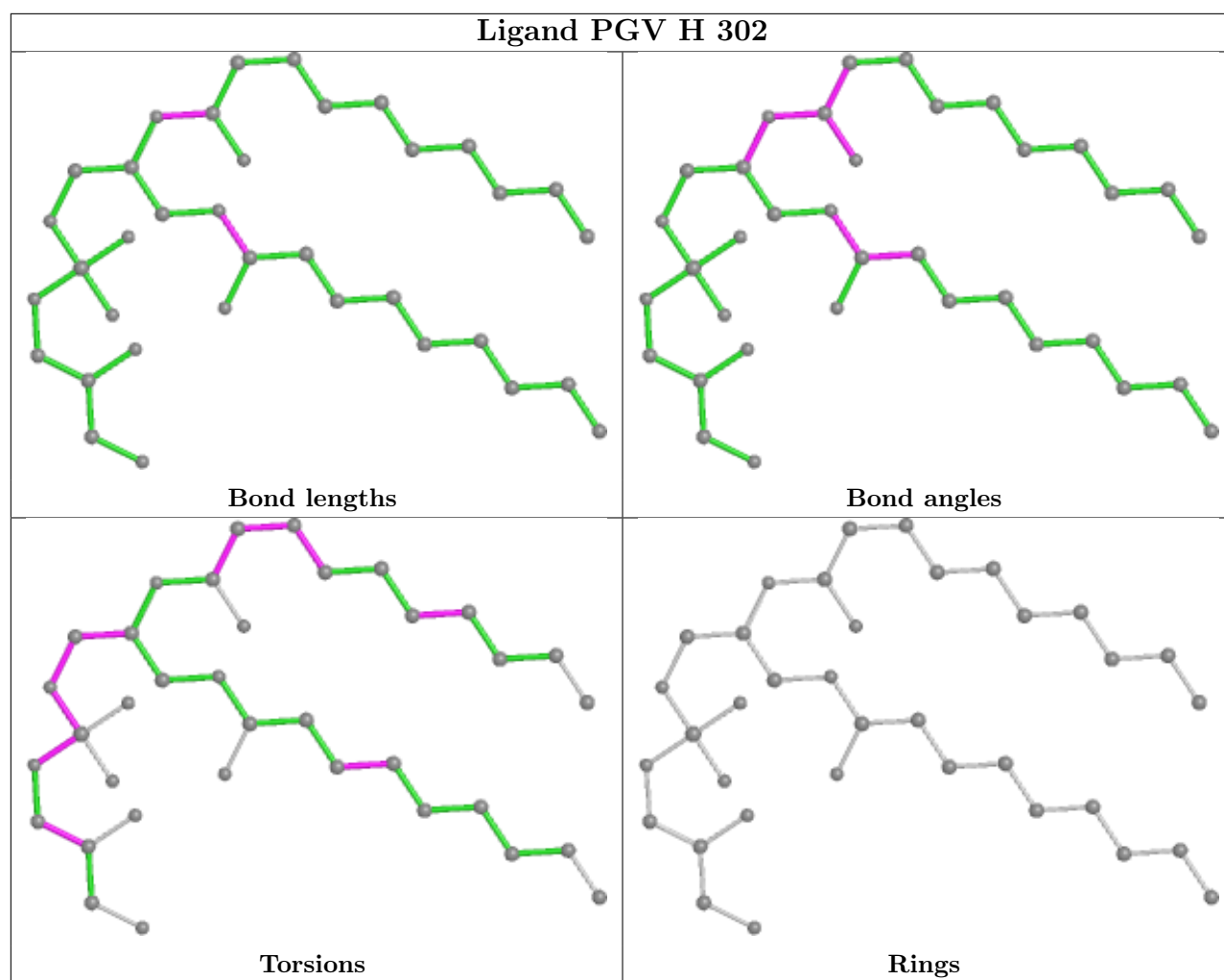


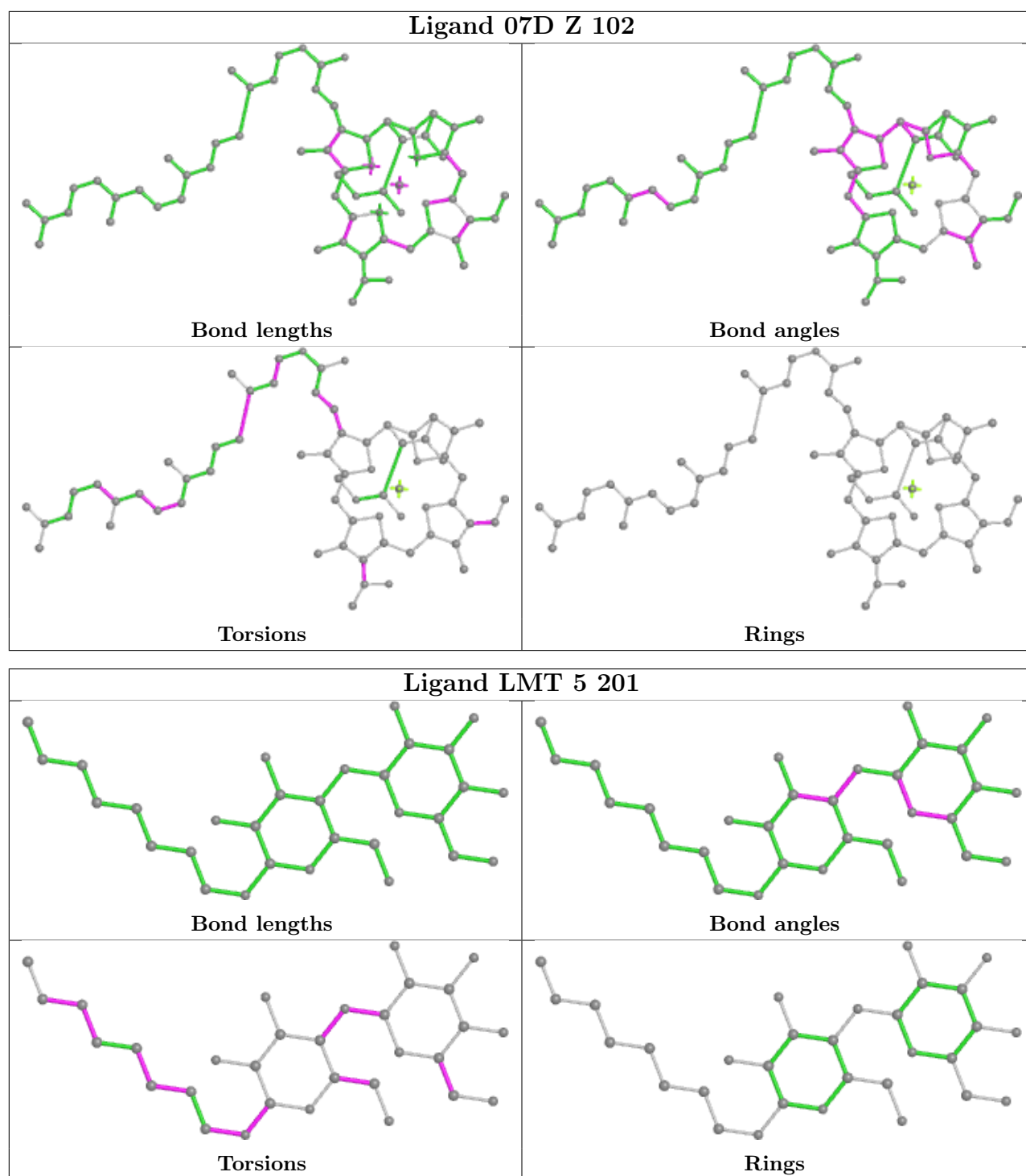
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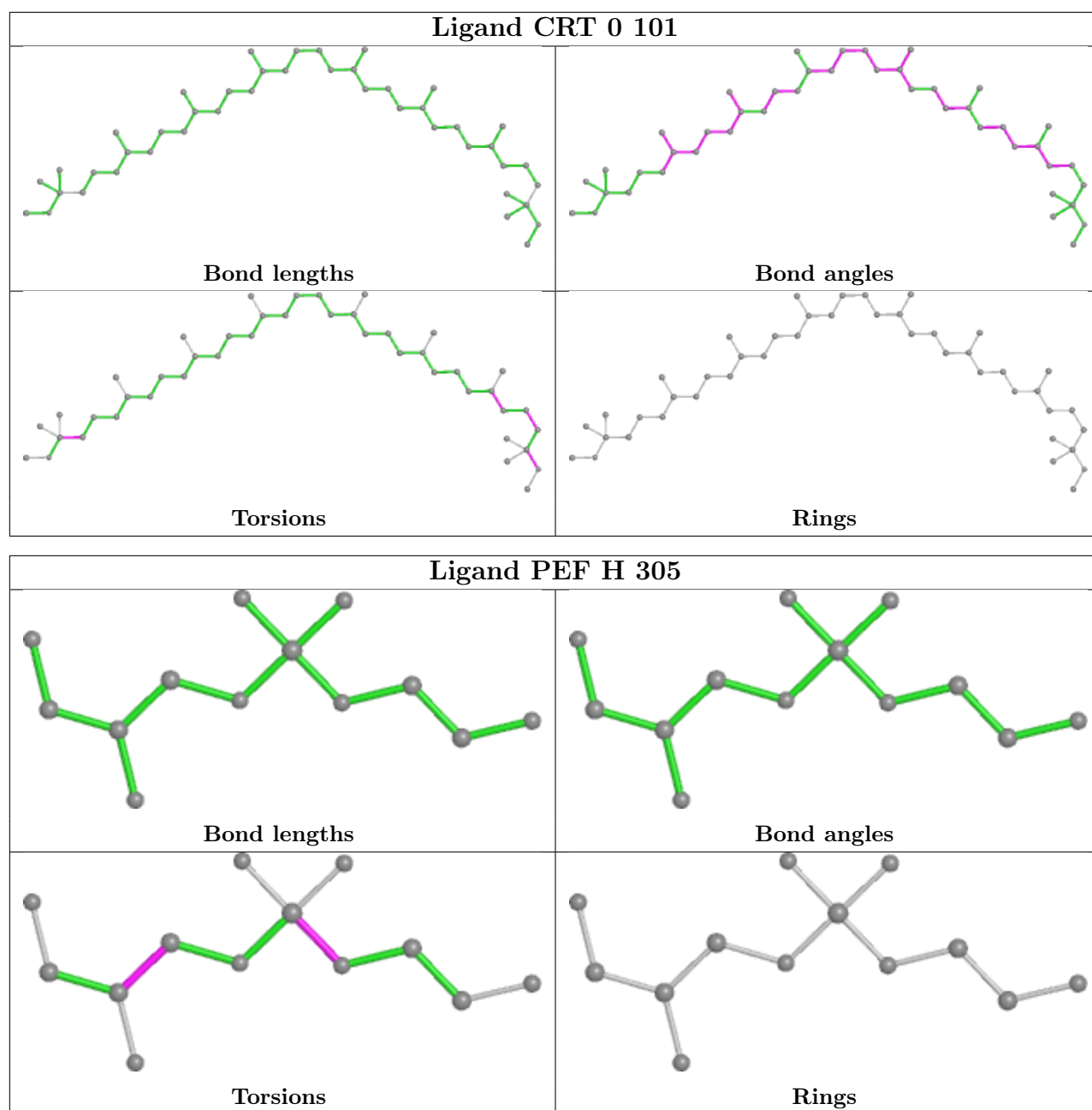


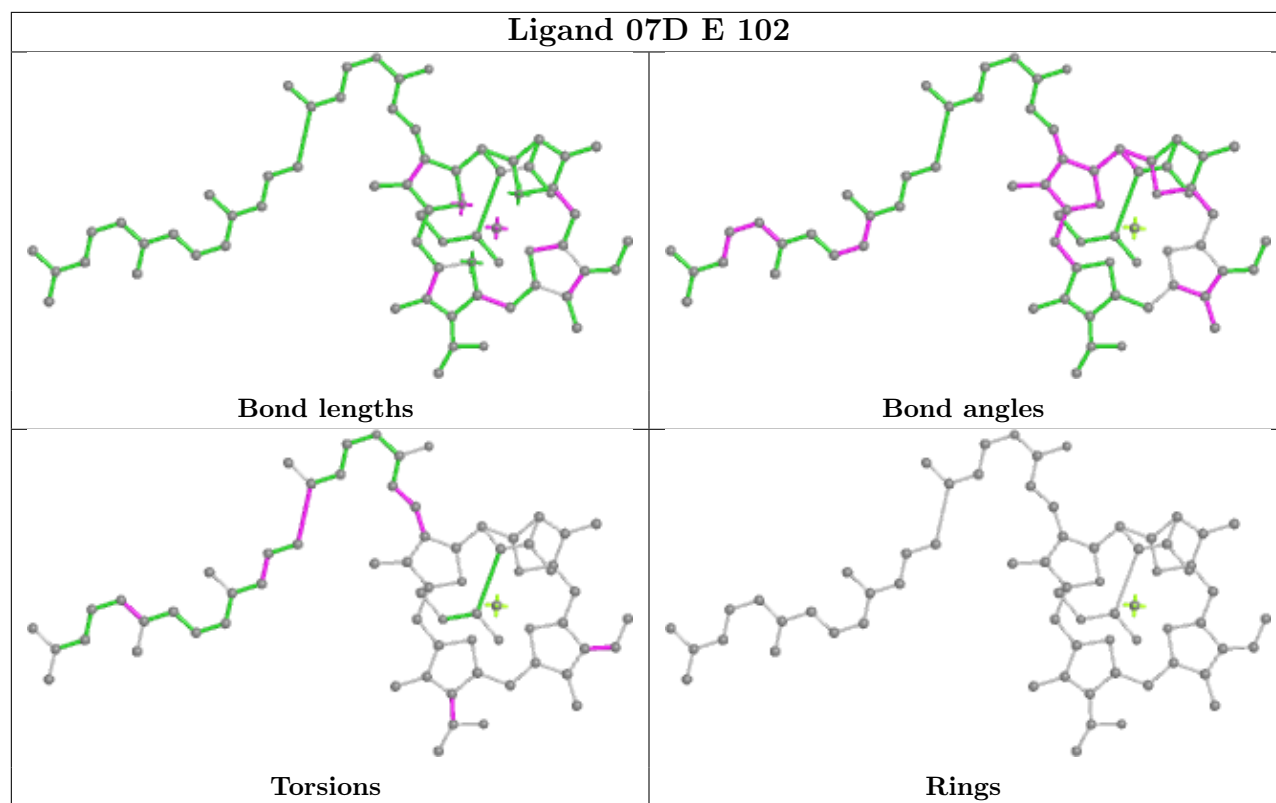
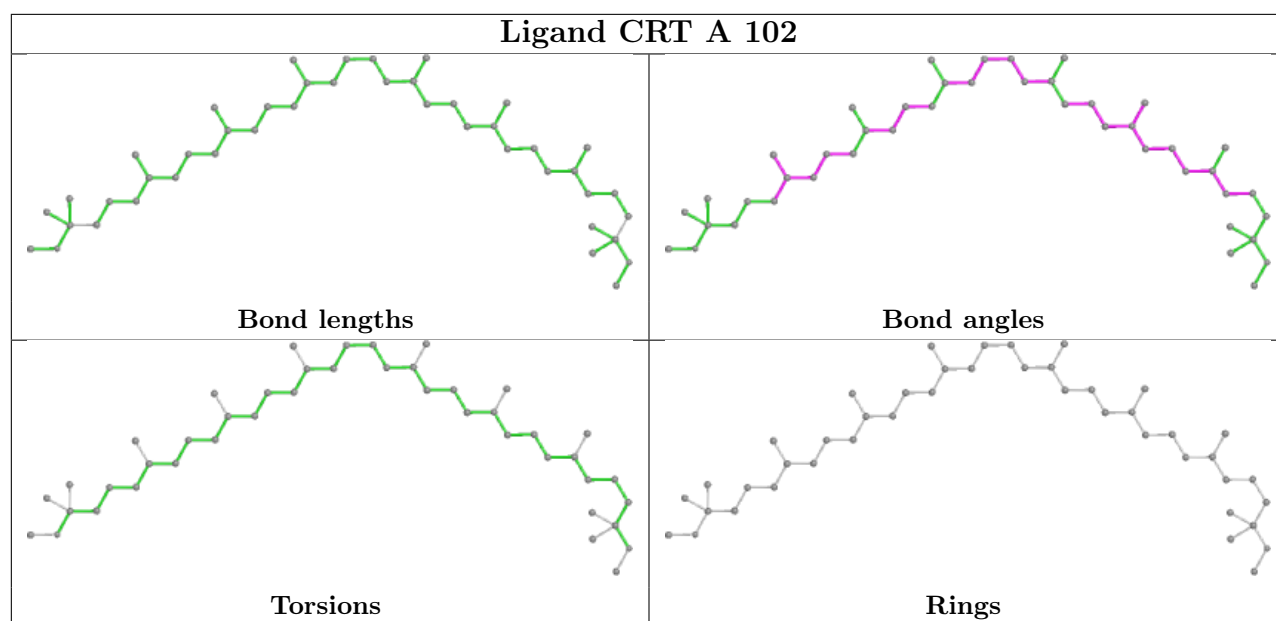


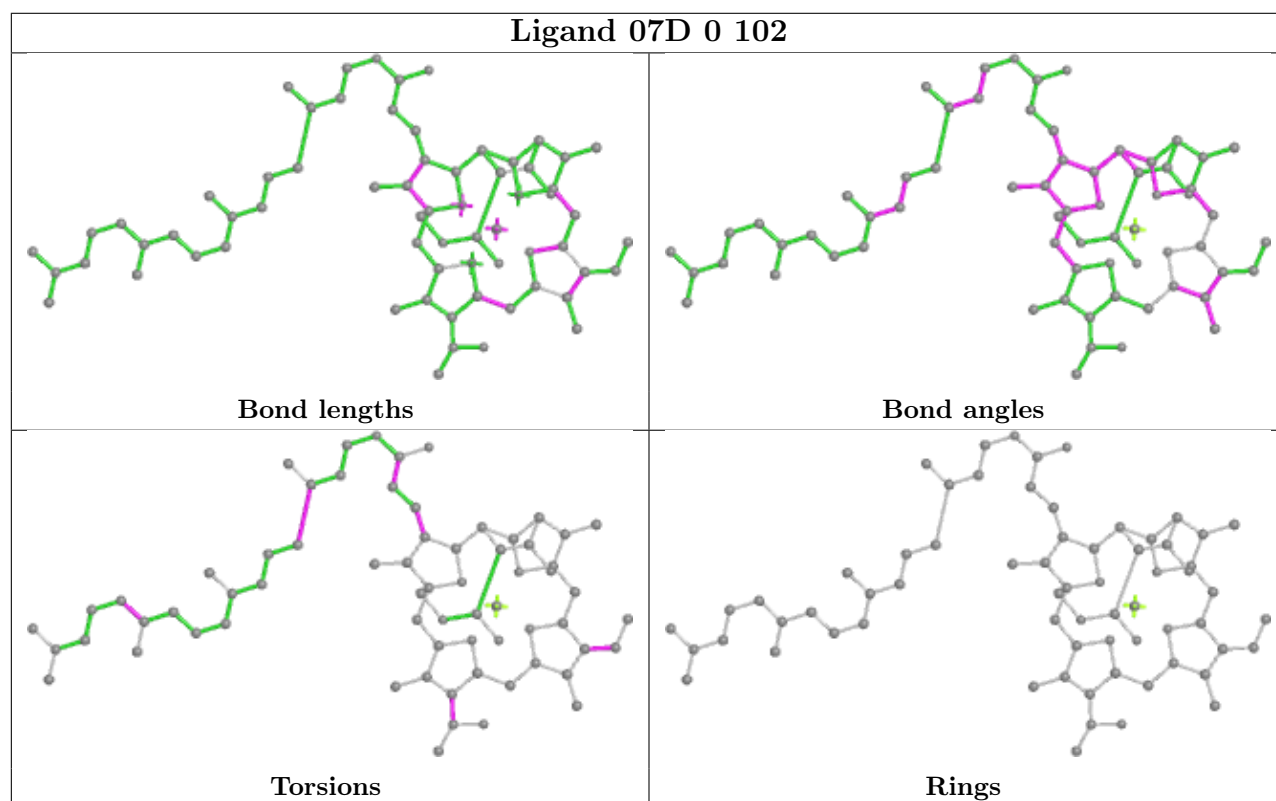
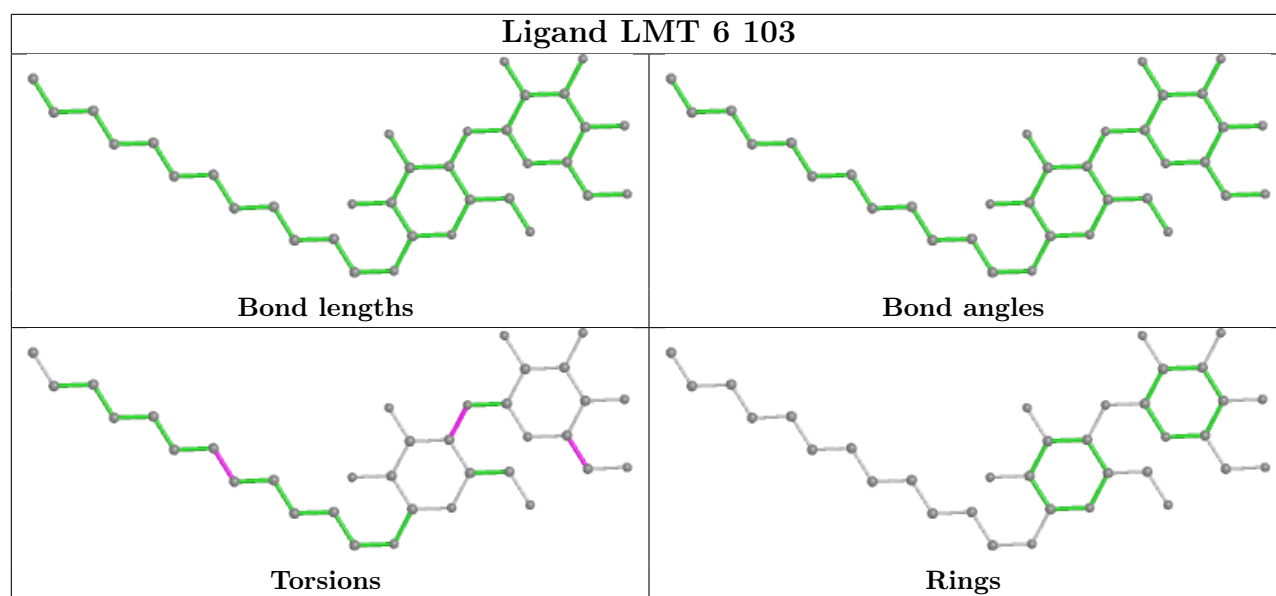


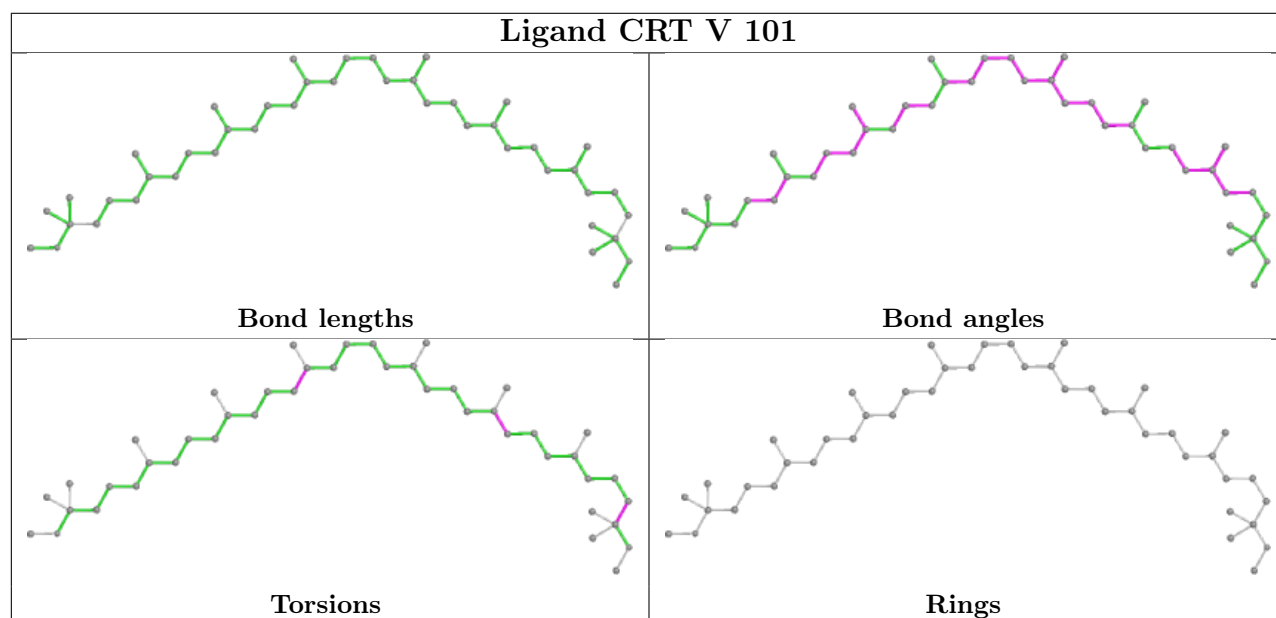
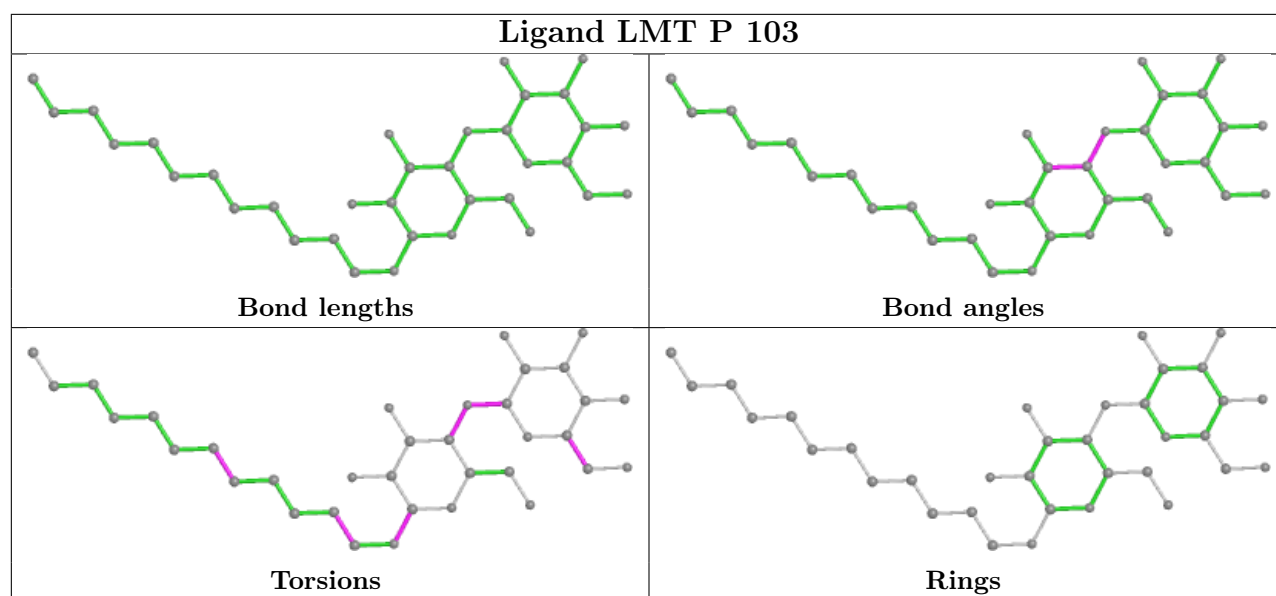


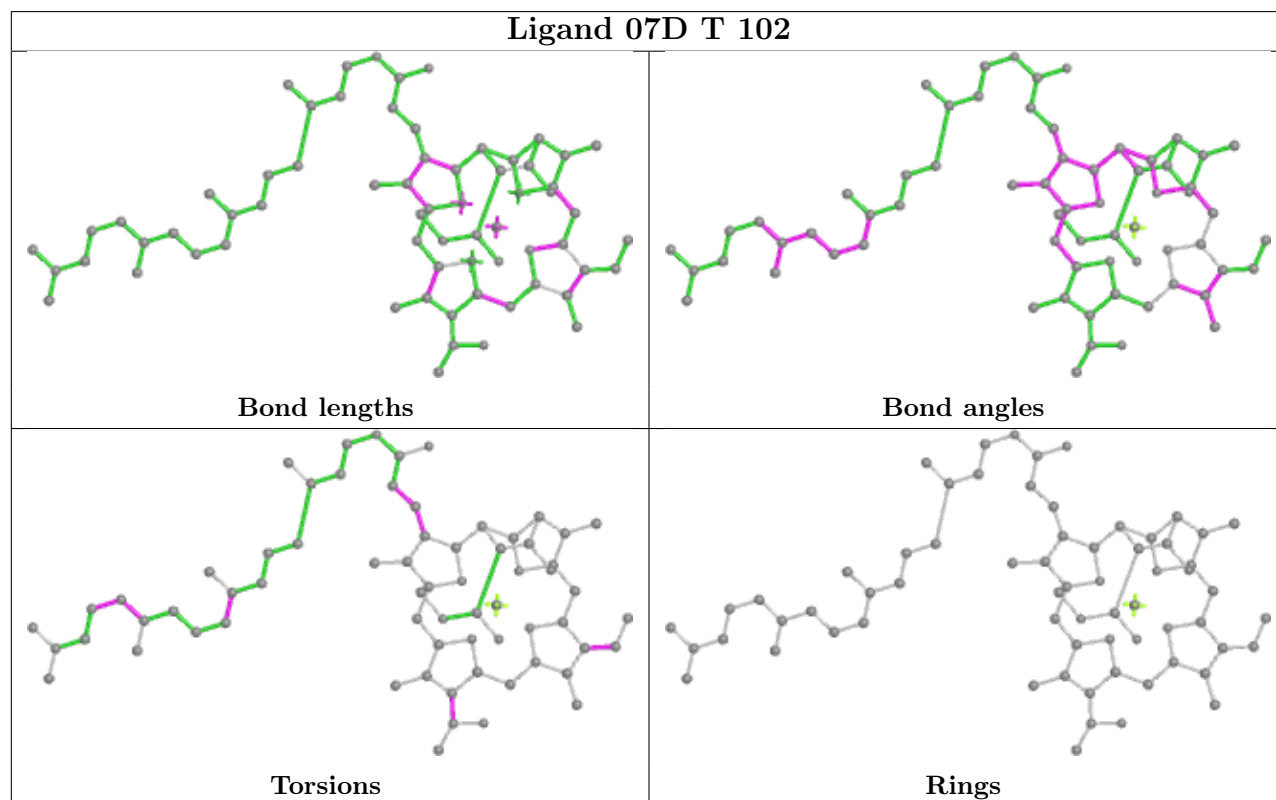
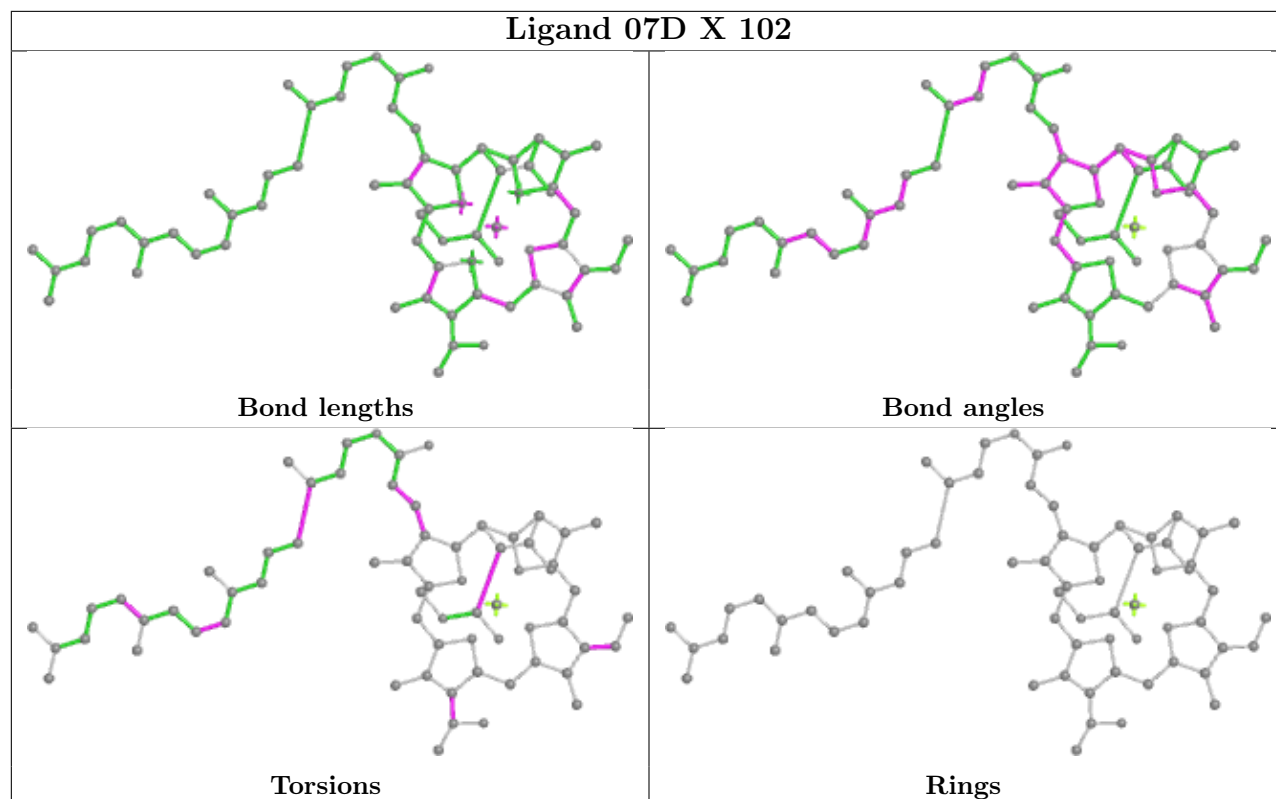


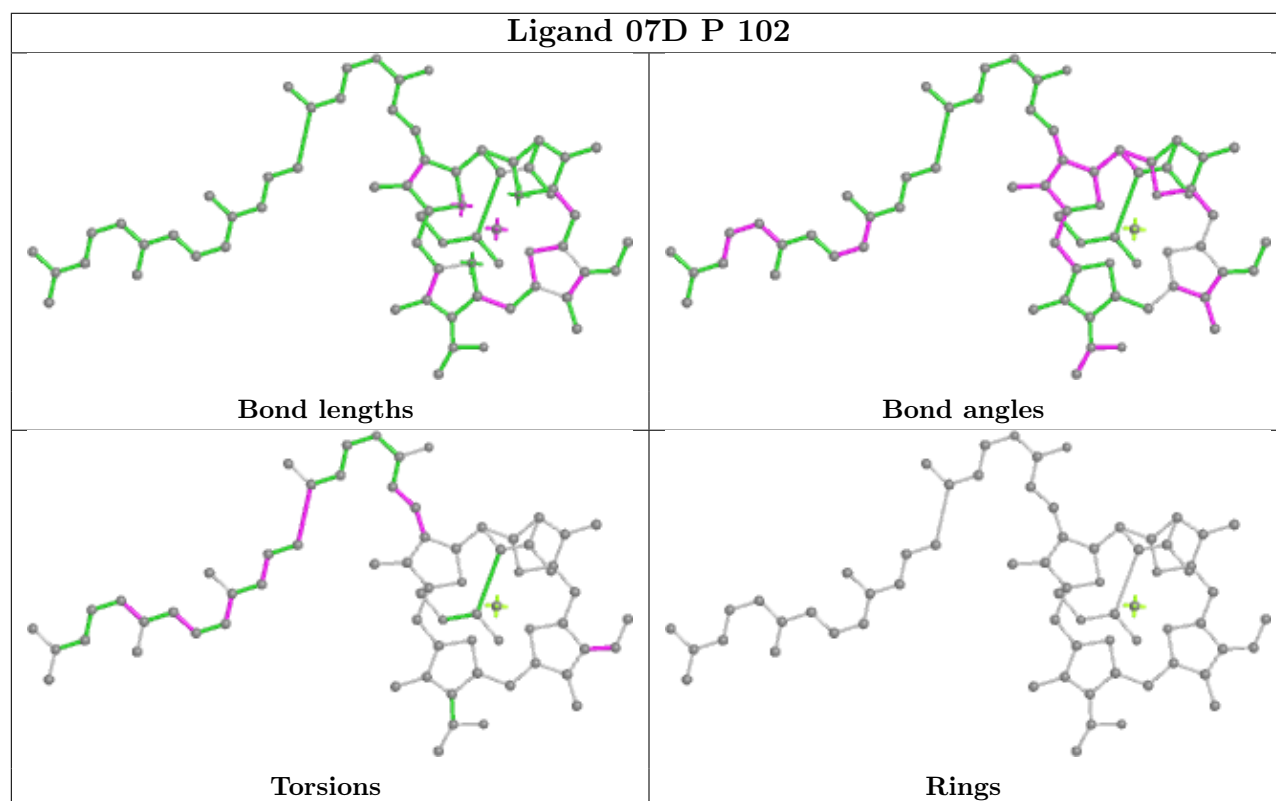
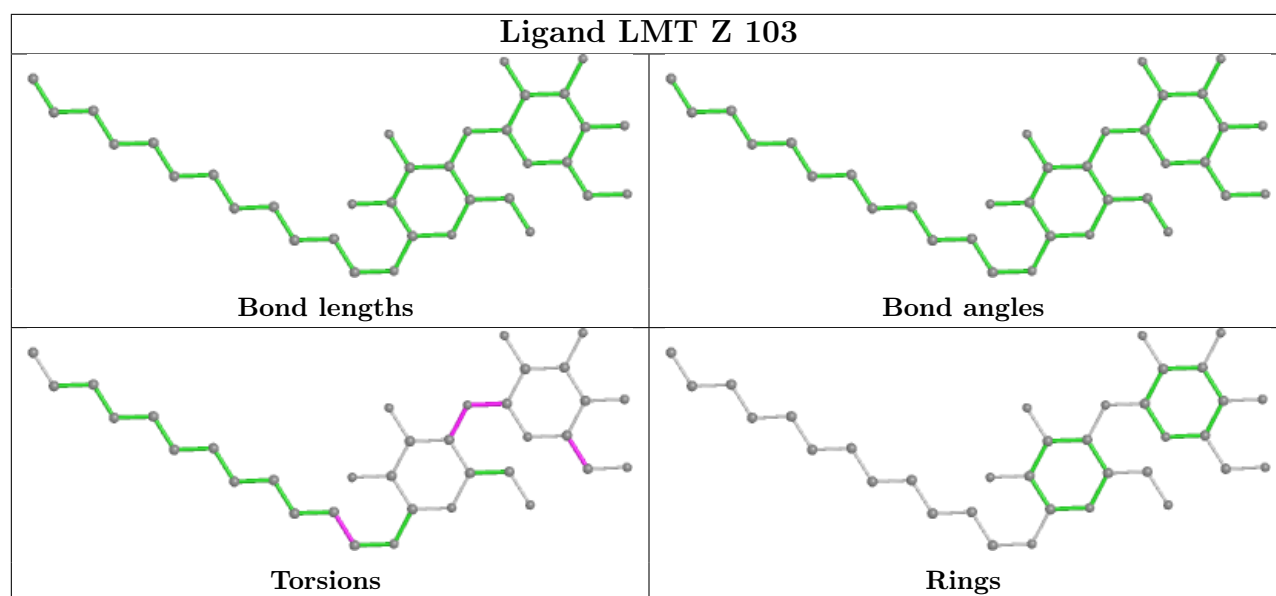


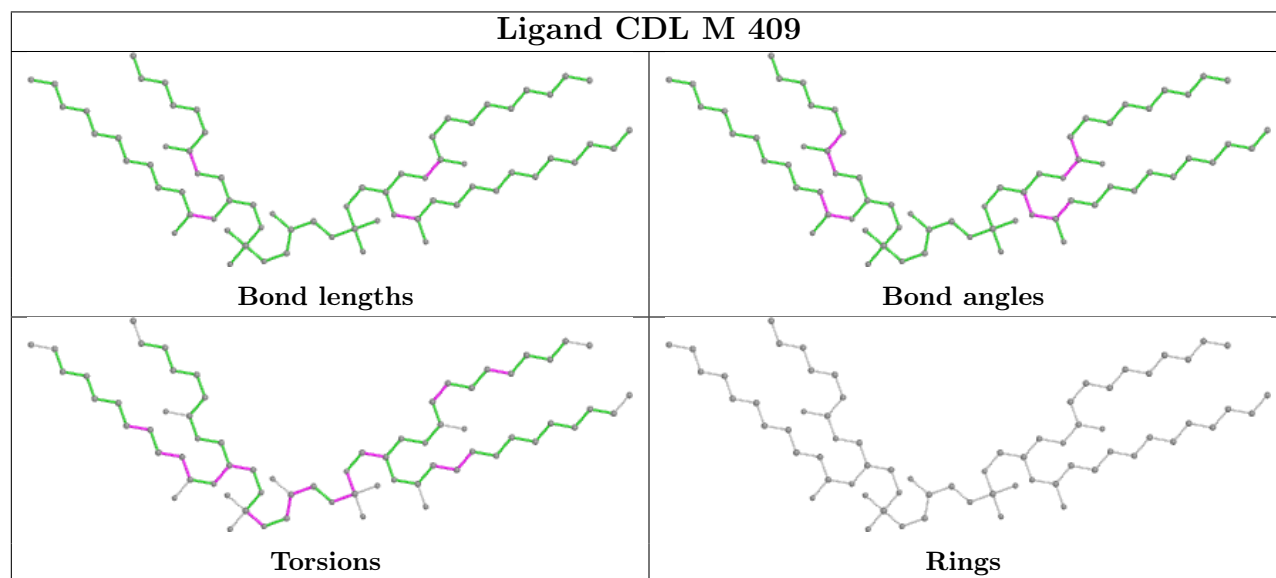
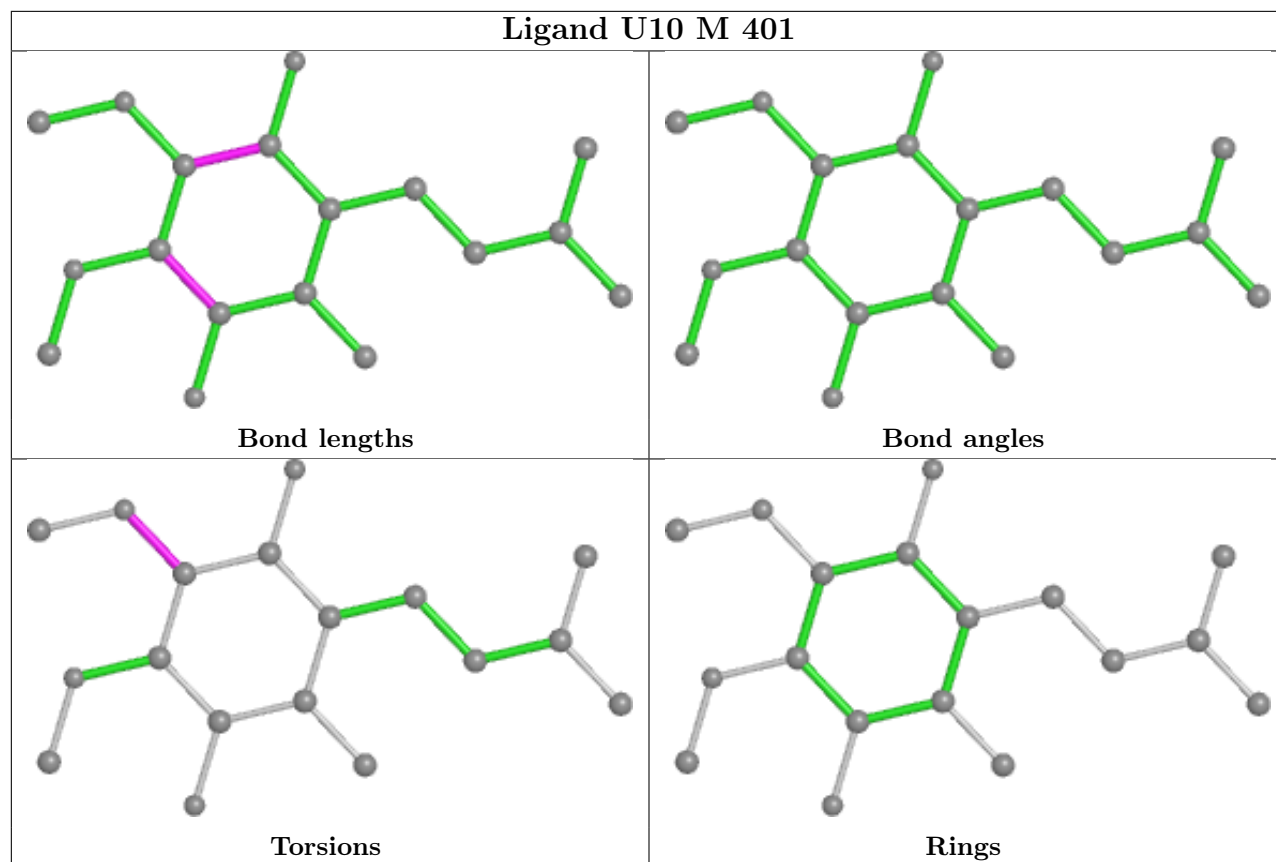


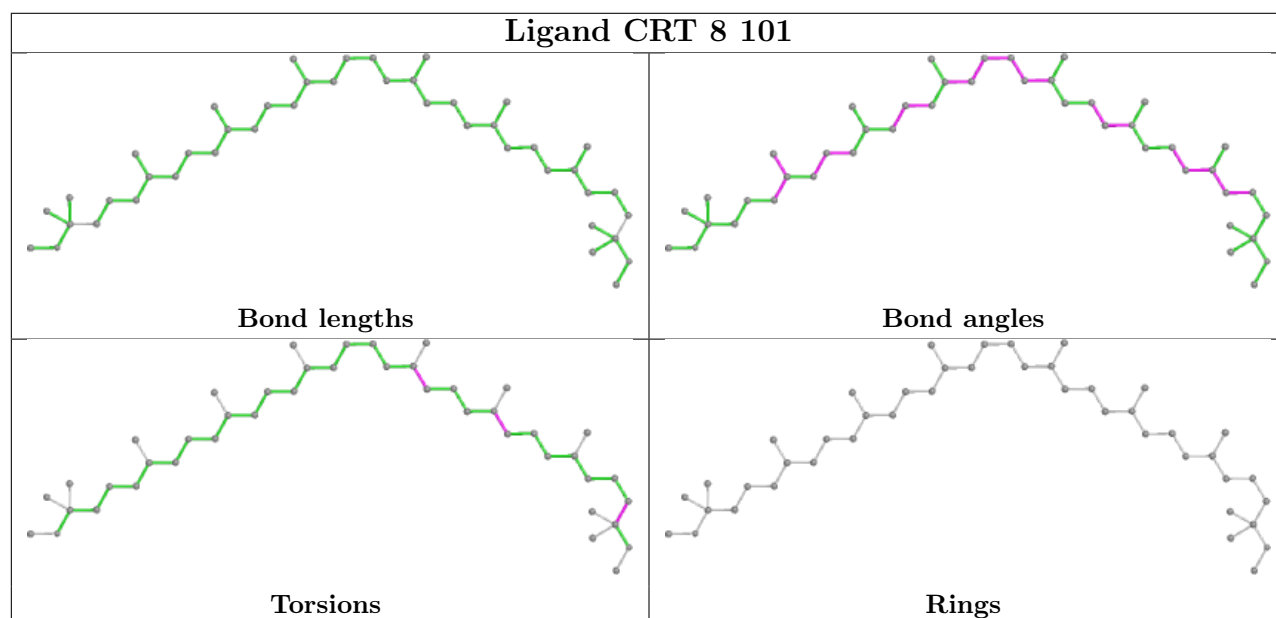
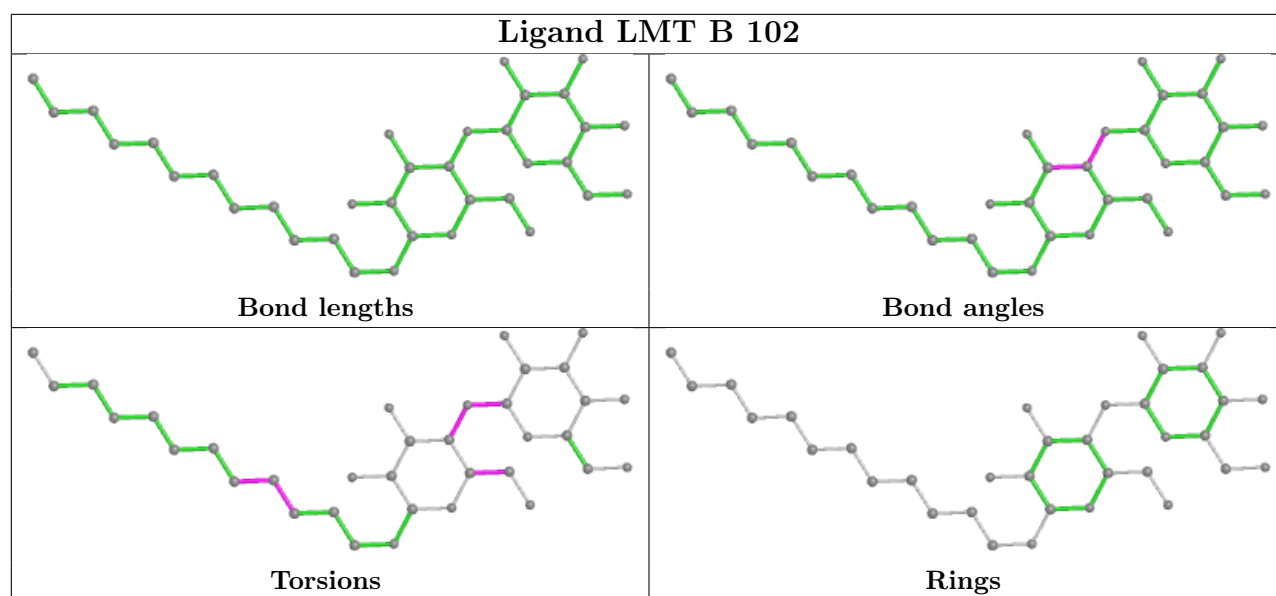


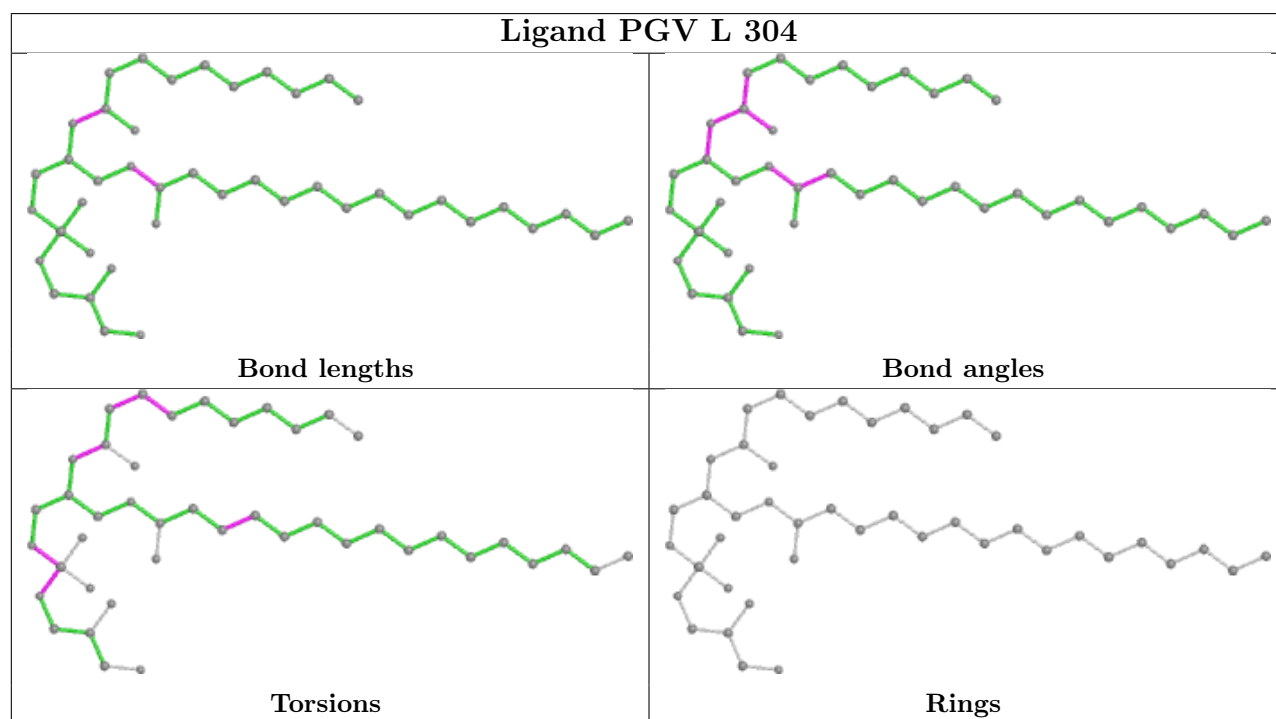
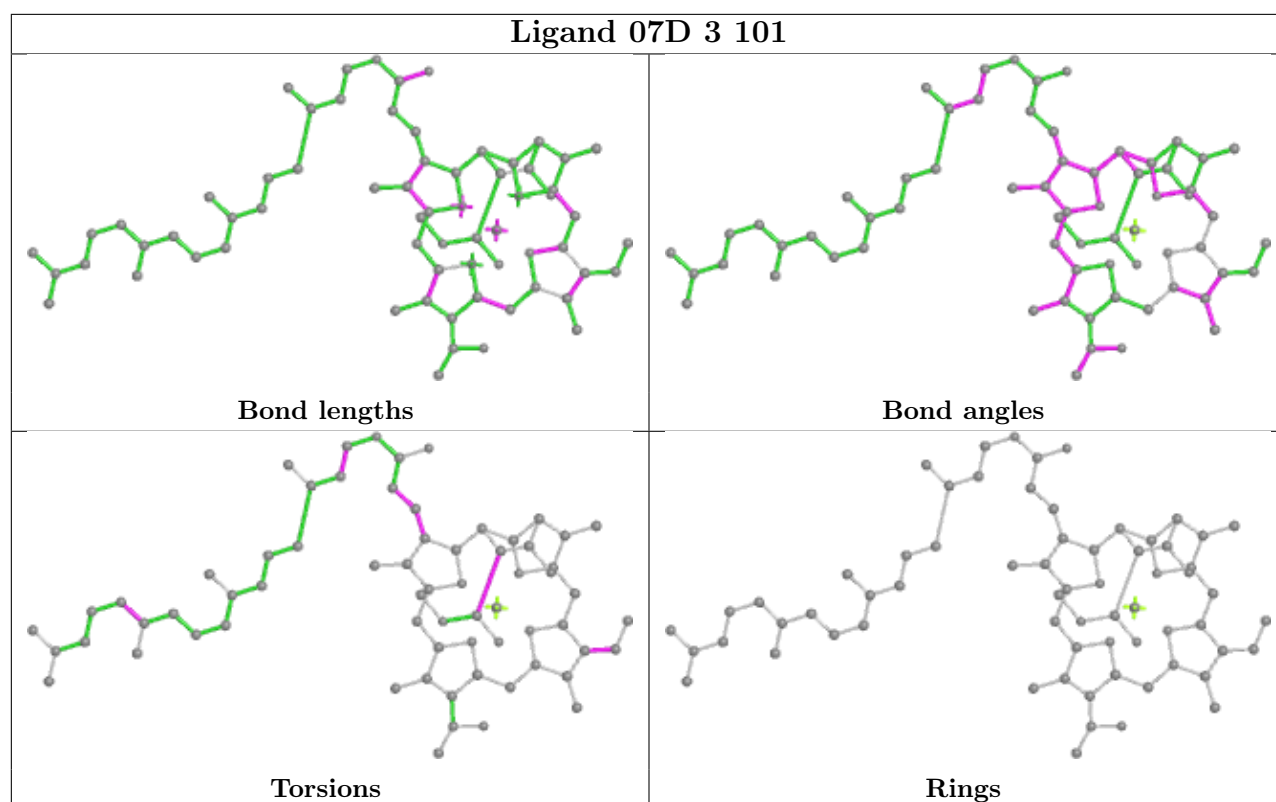


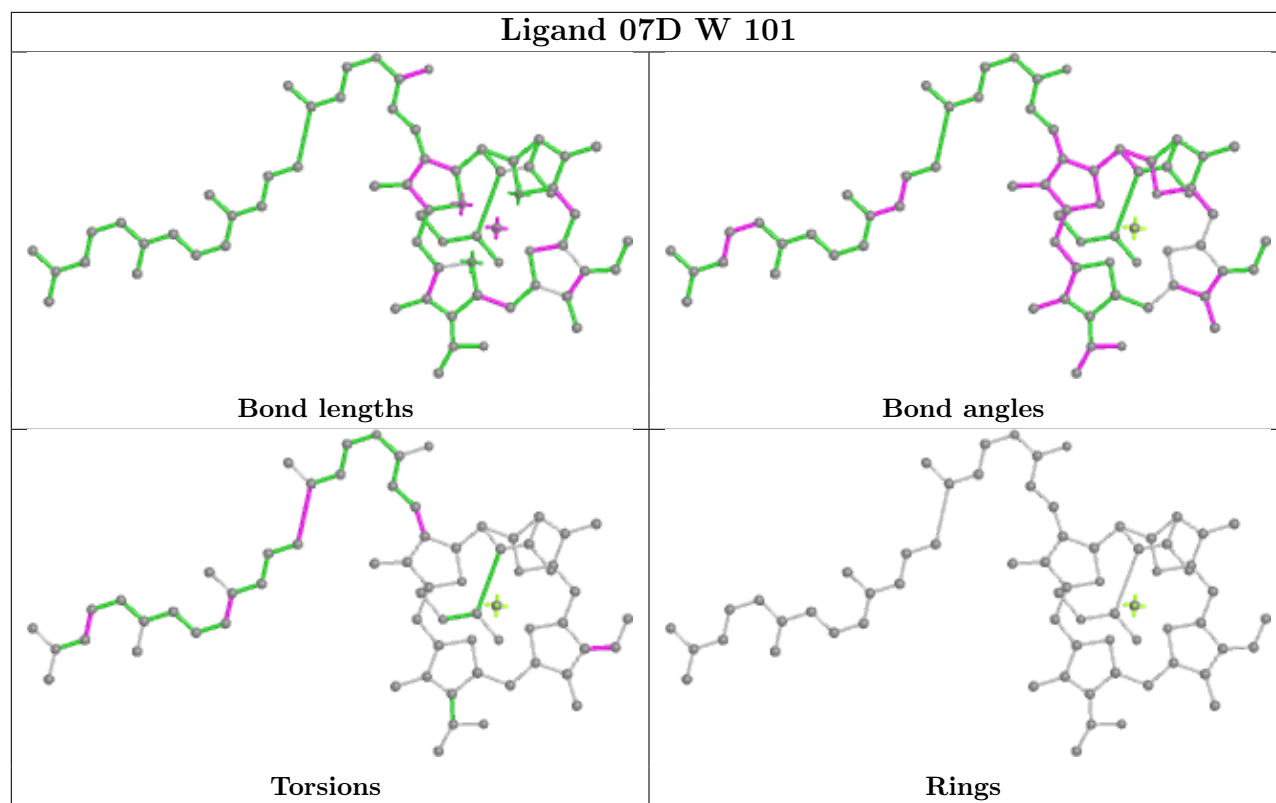
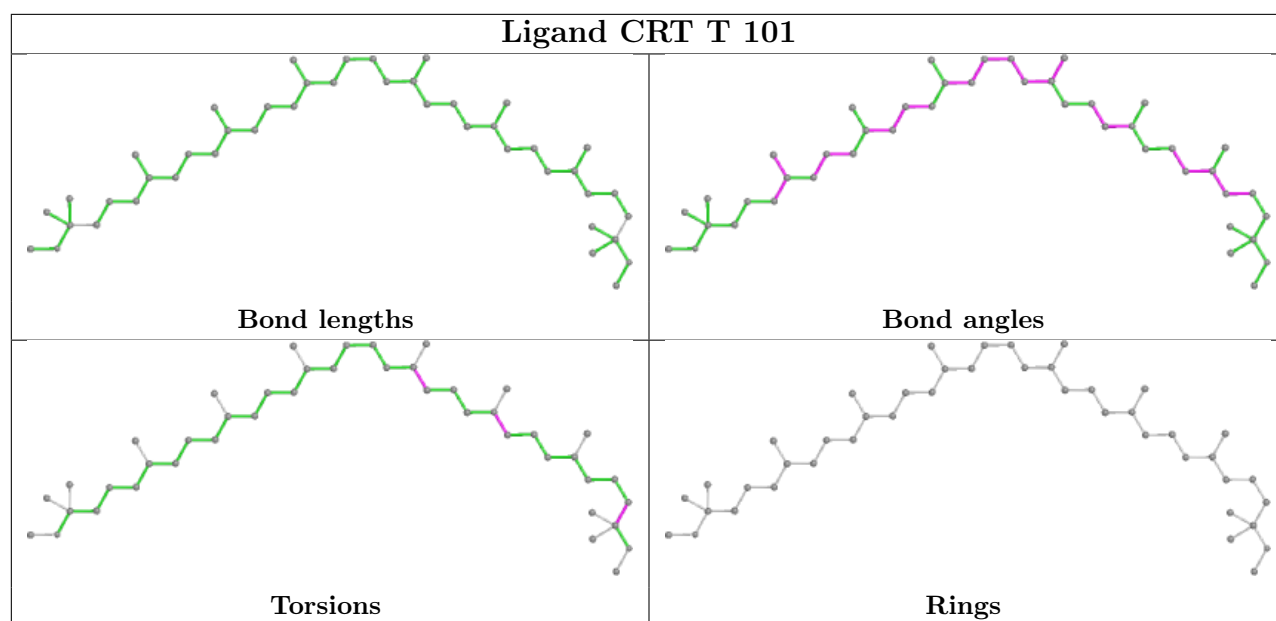


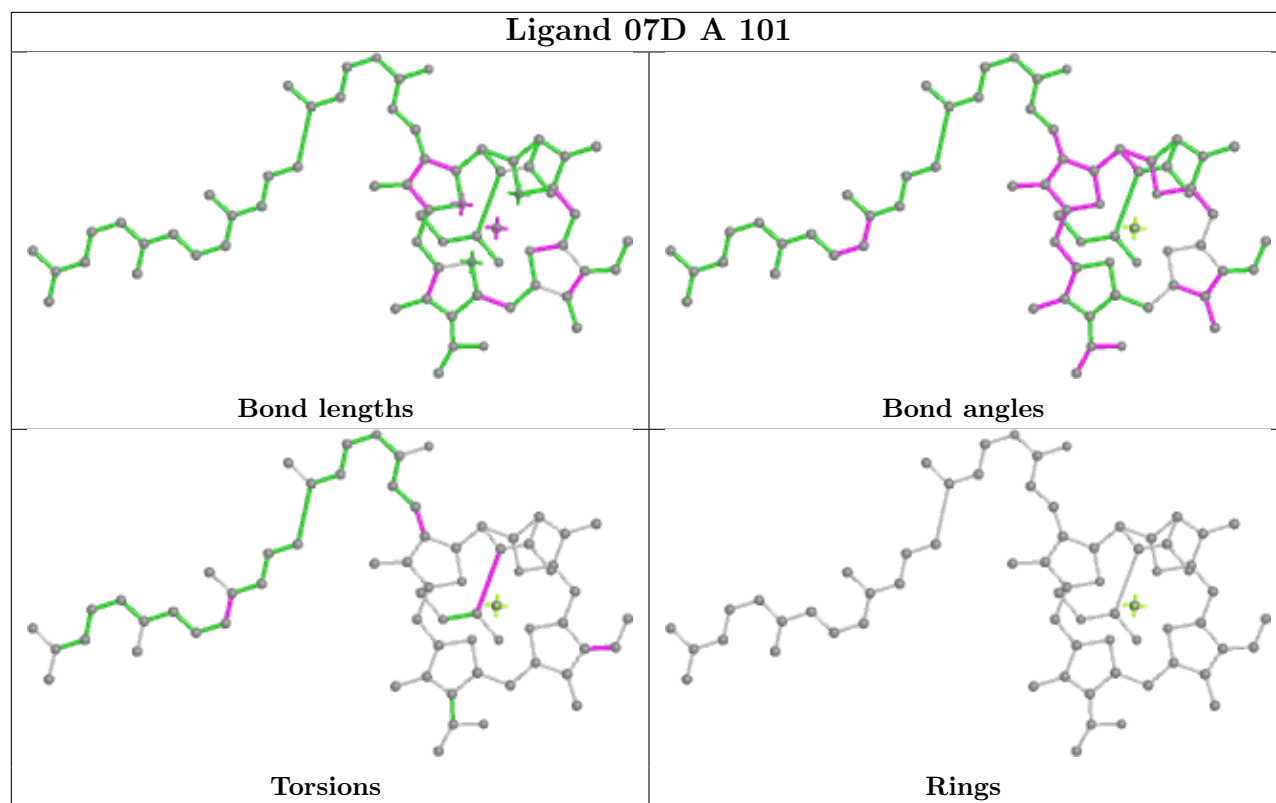
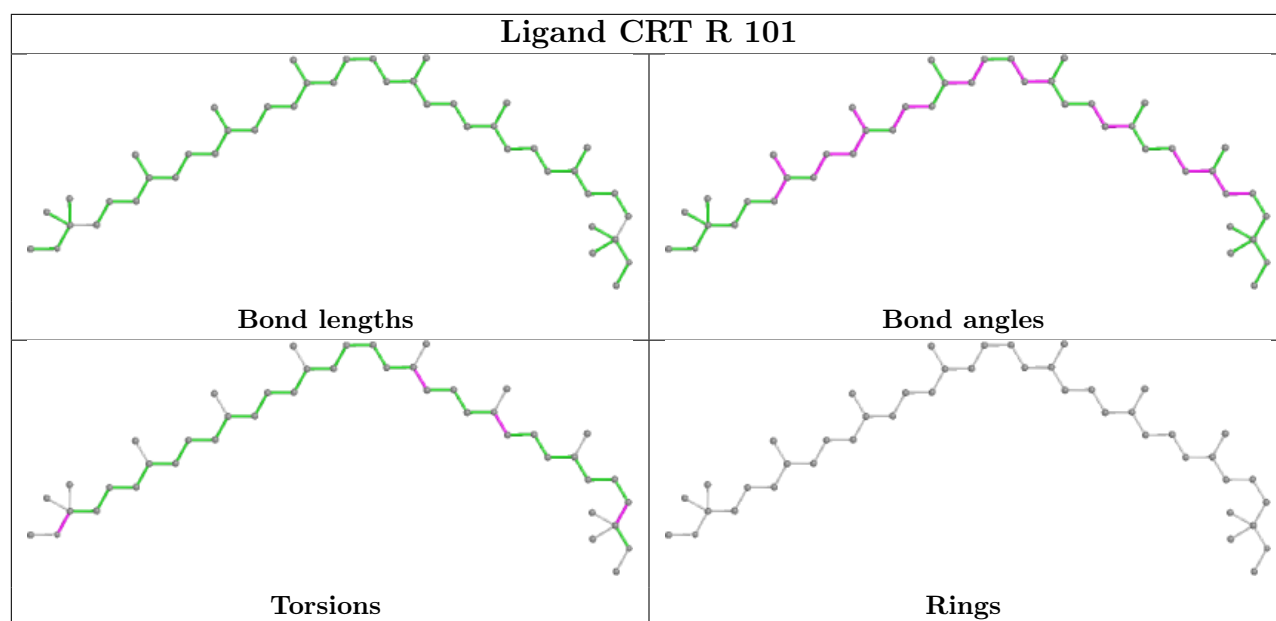


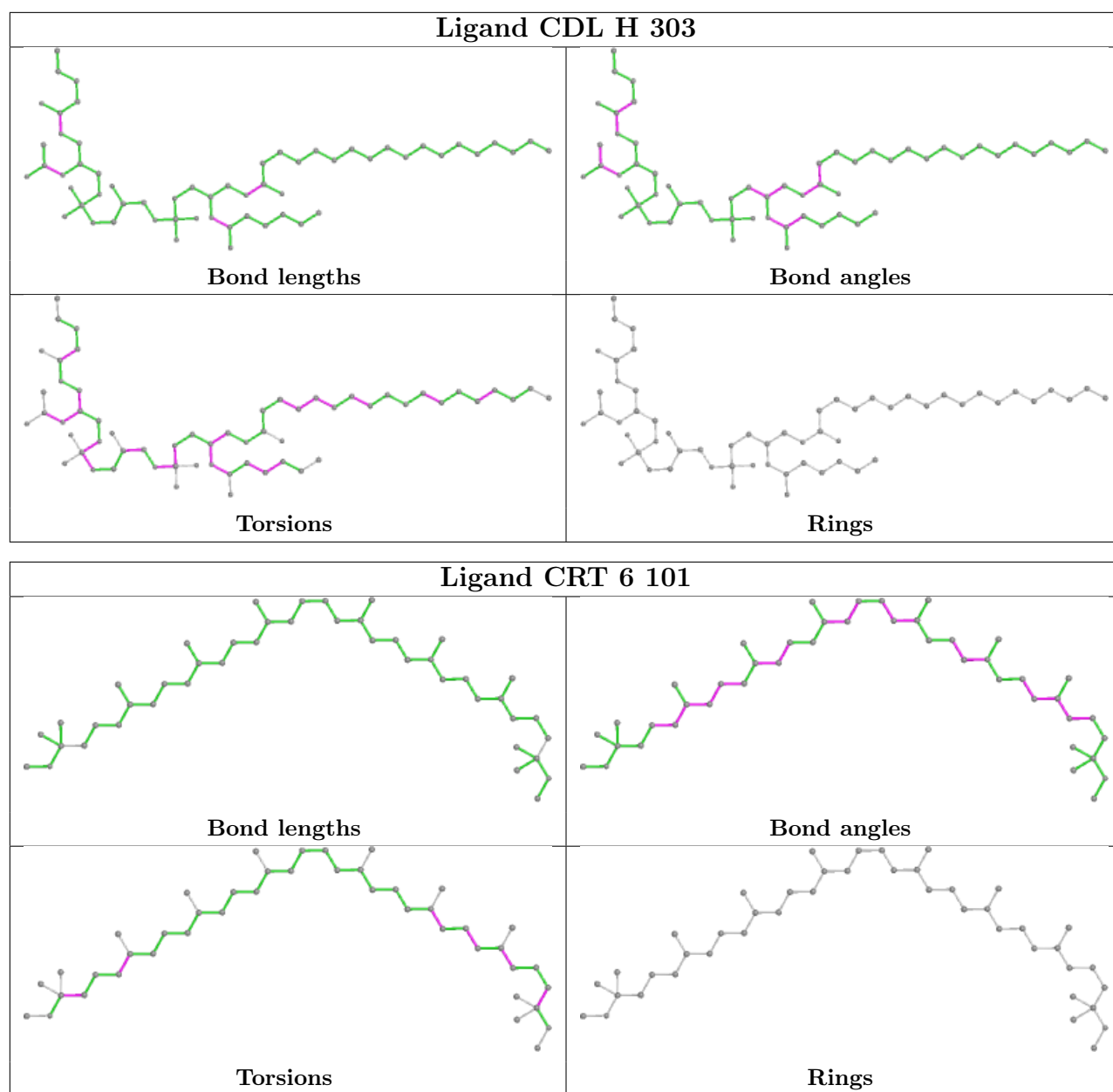




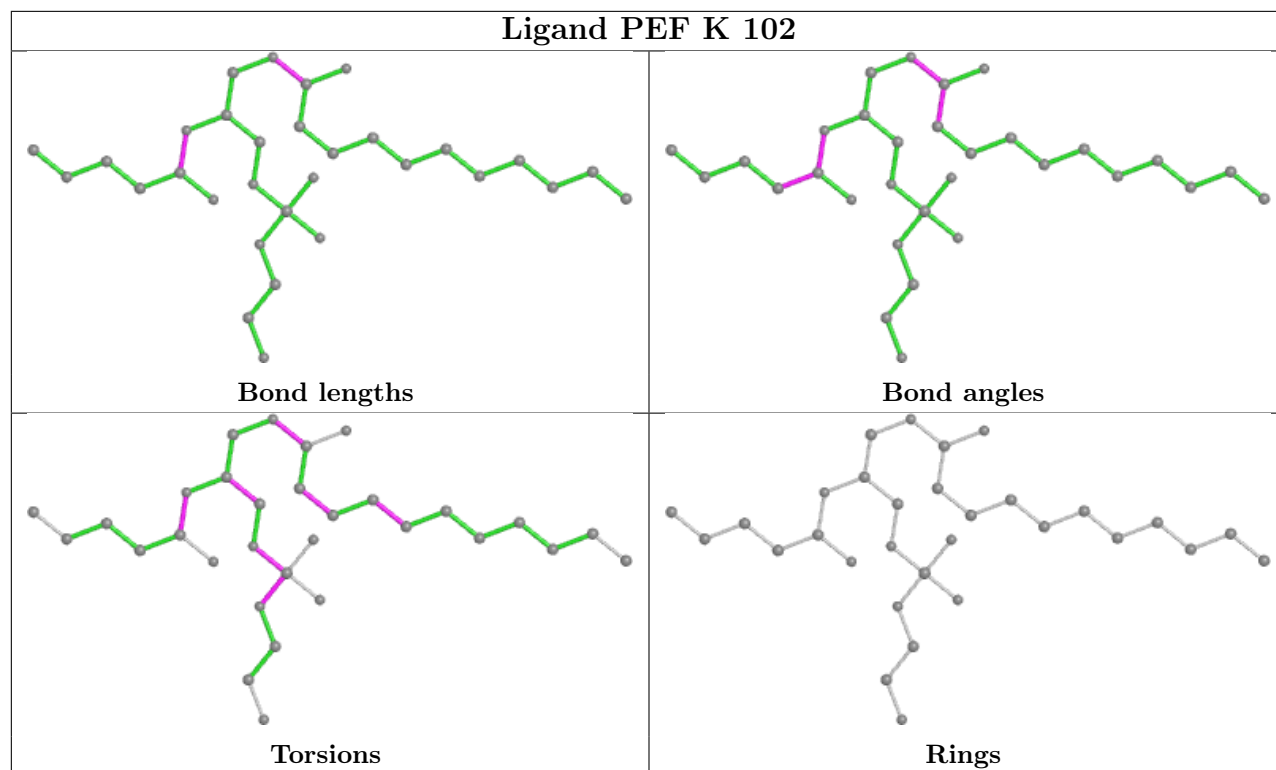




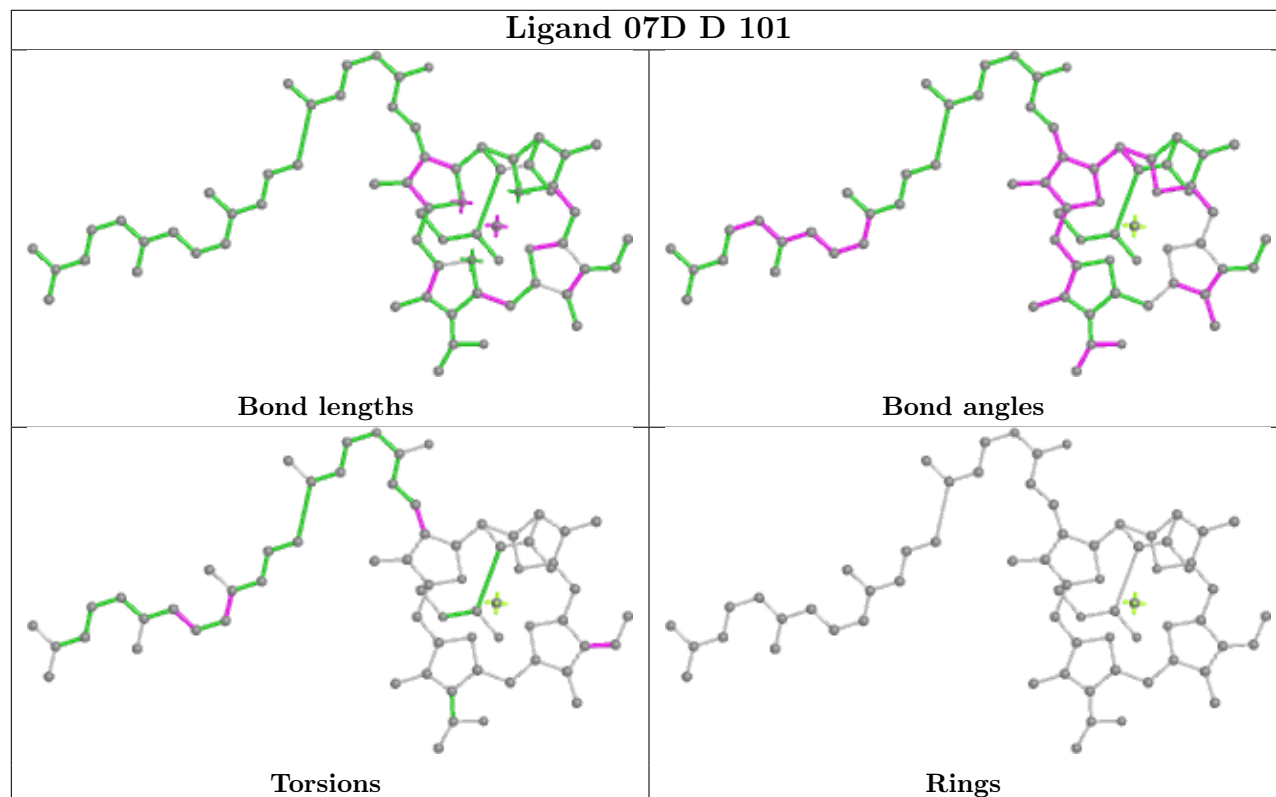


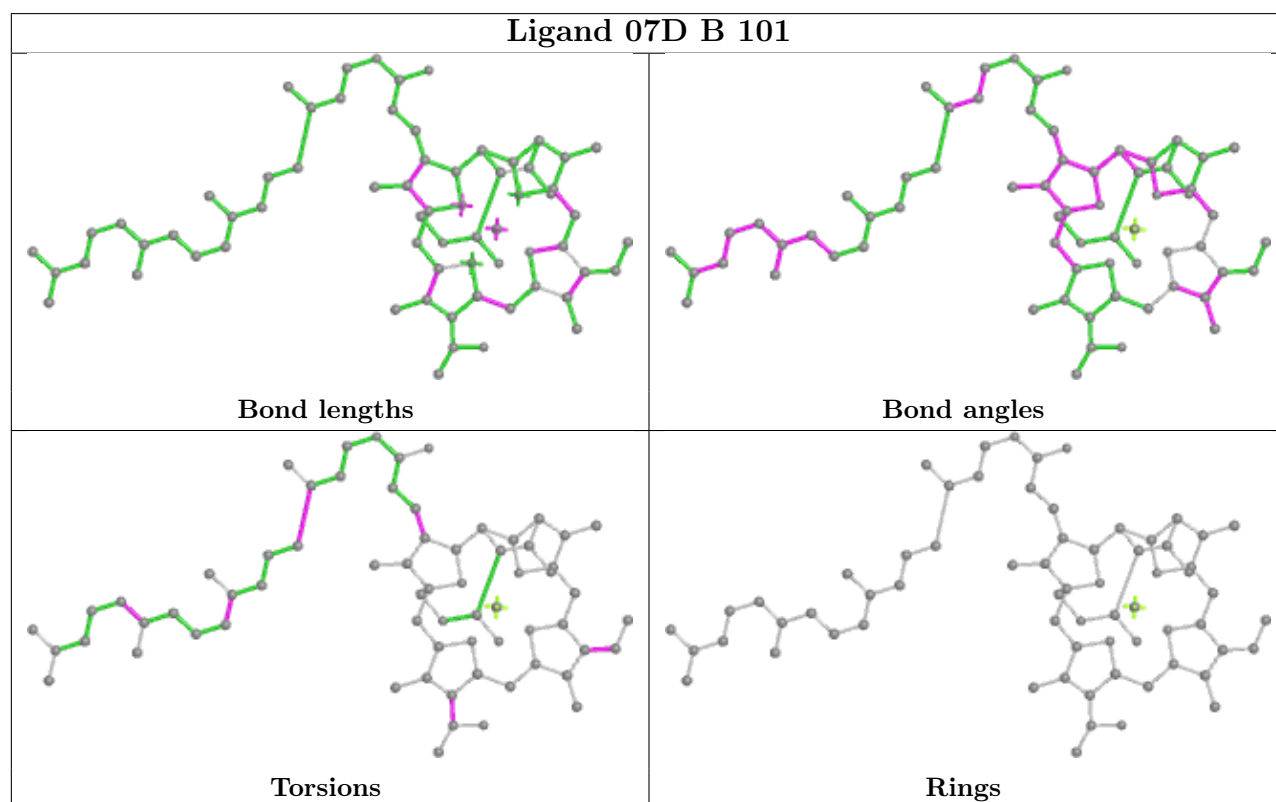
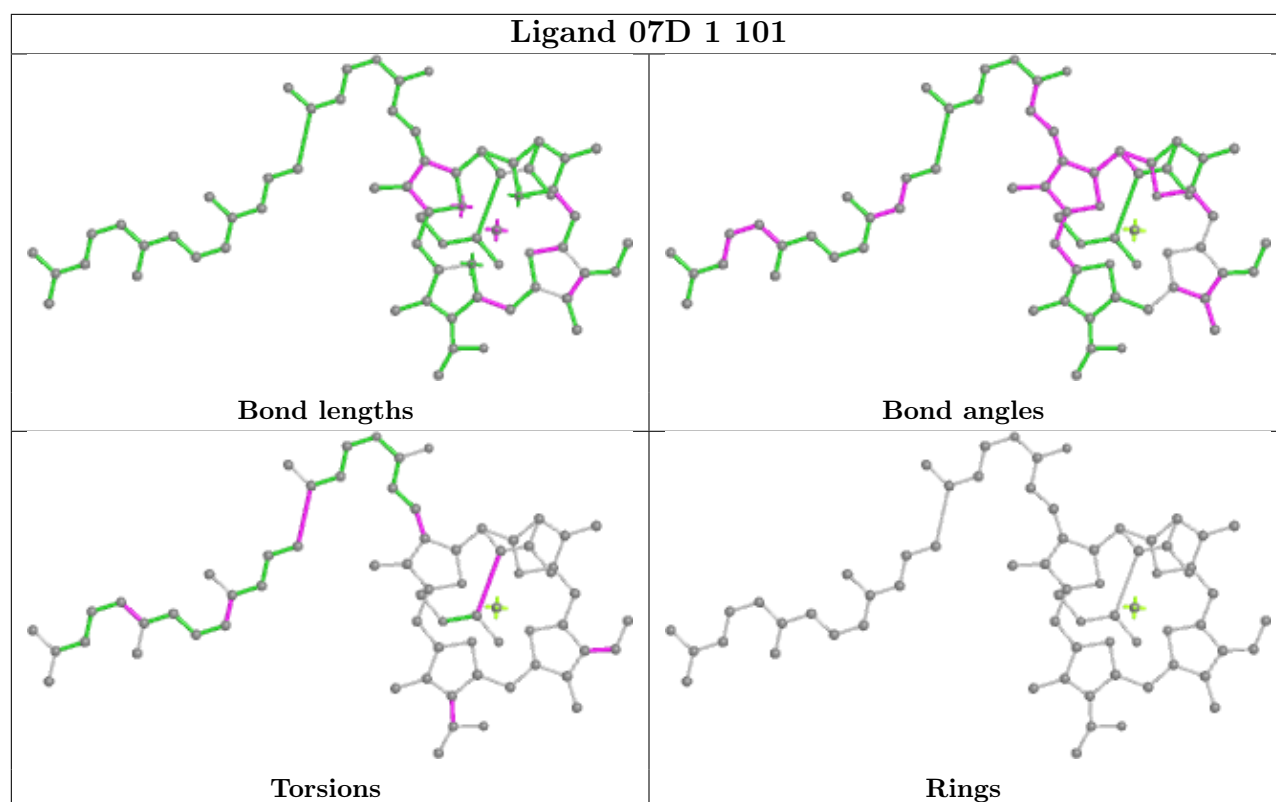


Ligand PEF K 102

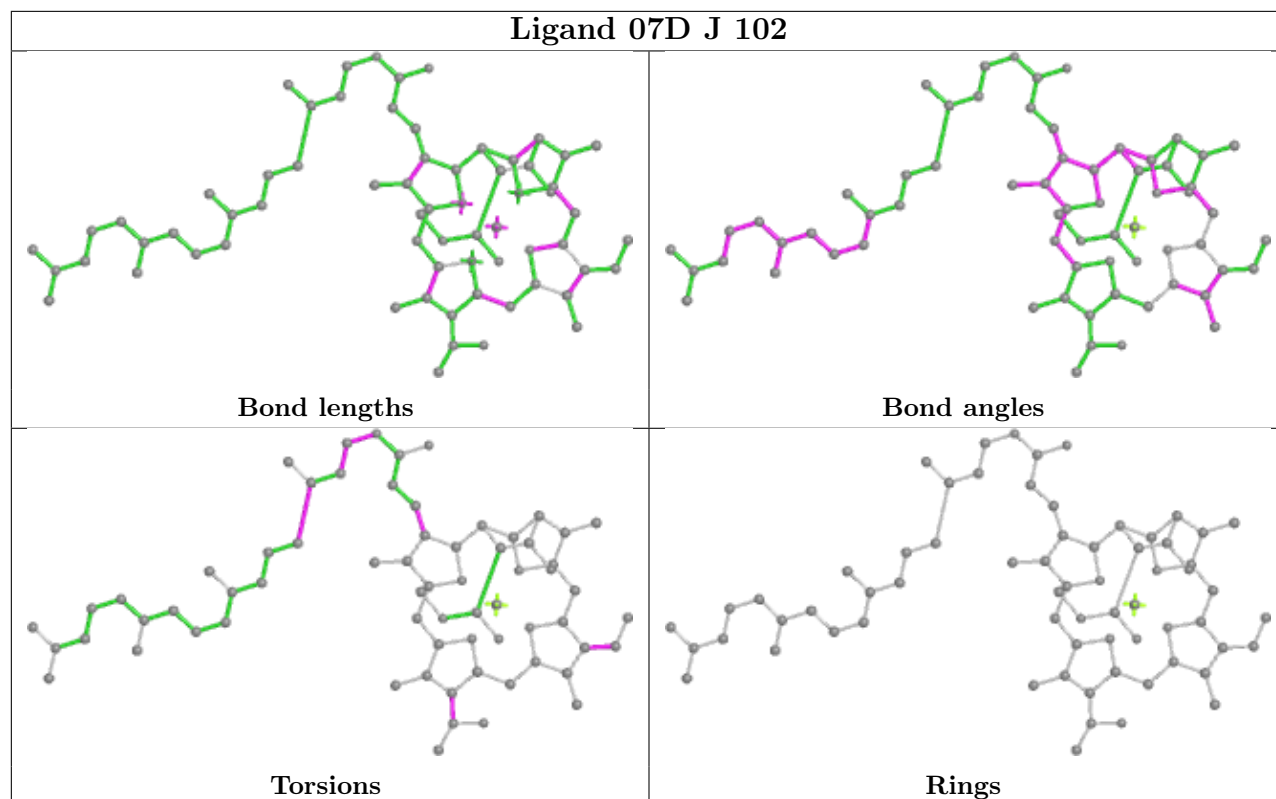


Ligand 07D D 101

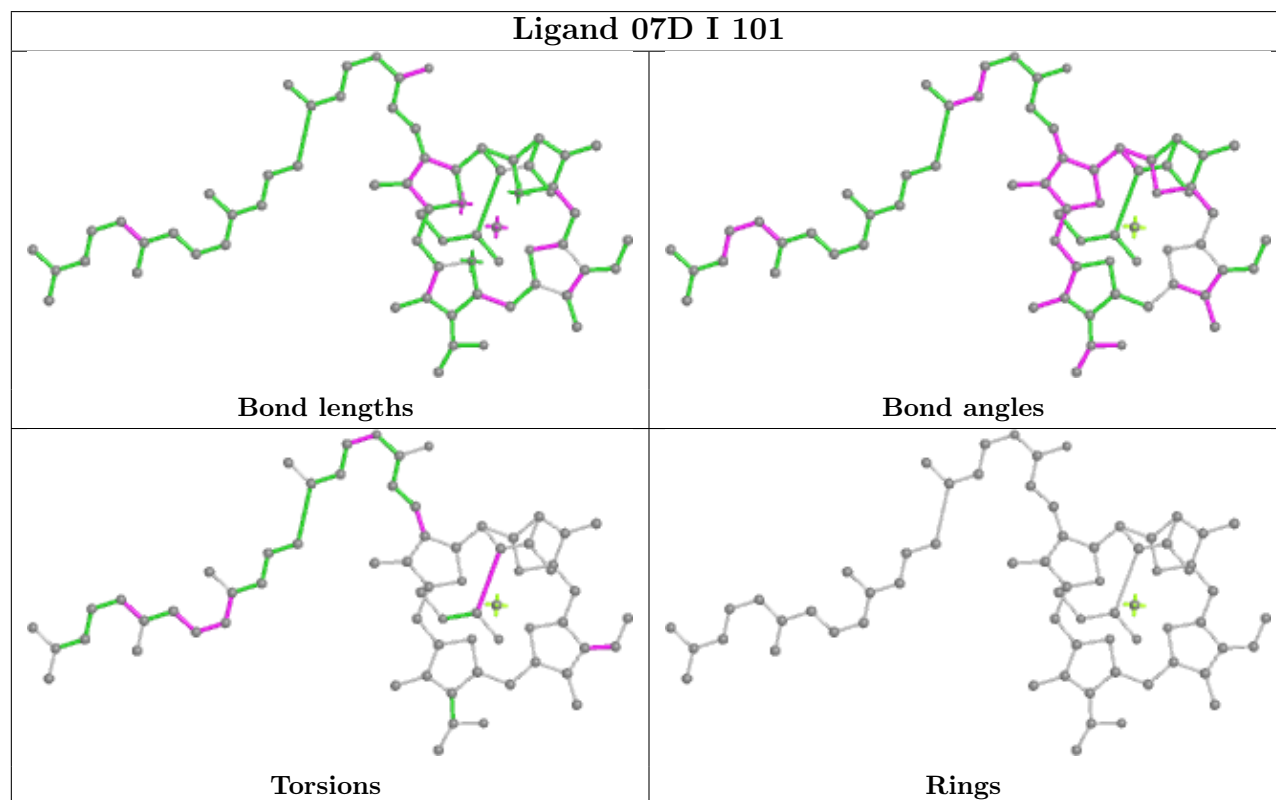


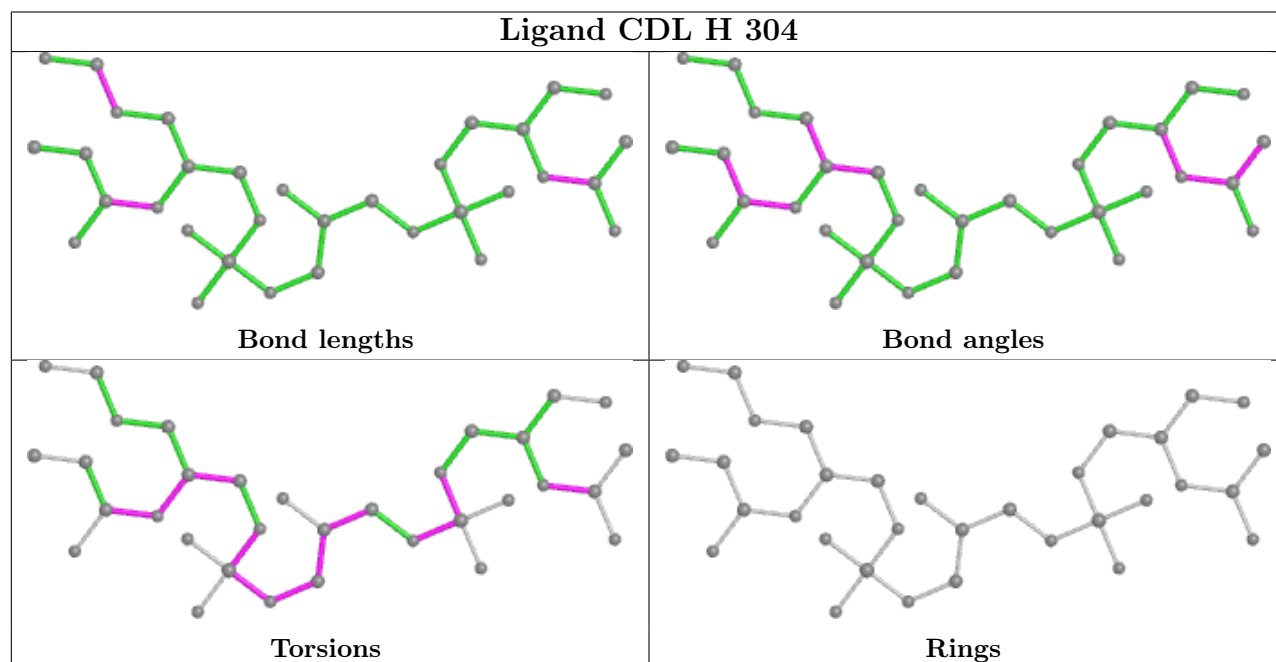
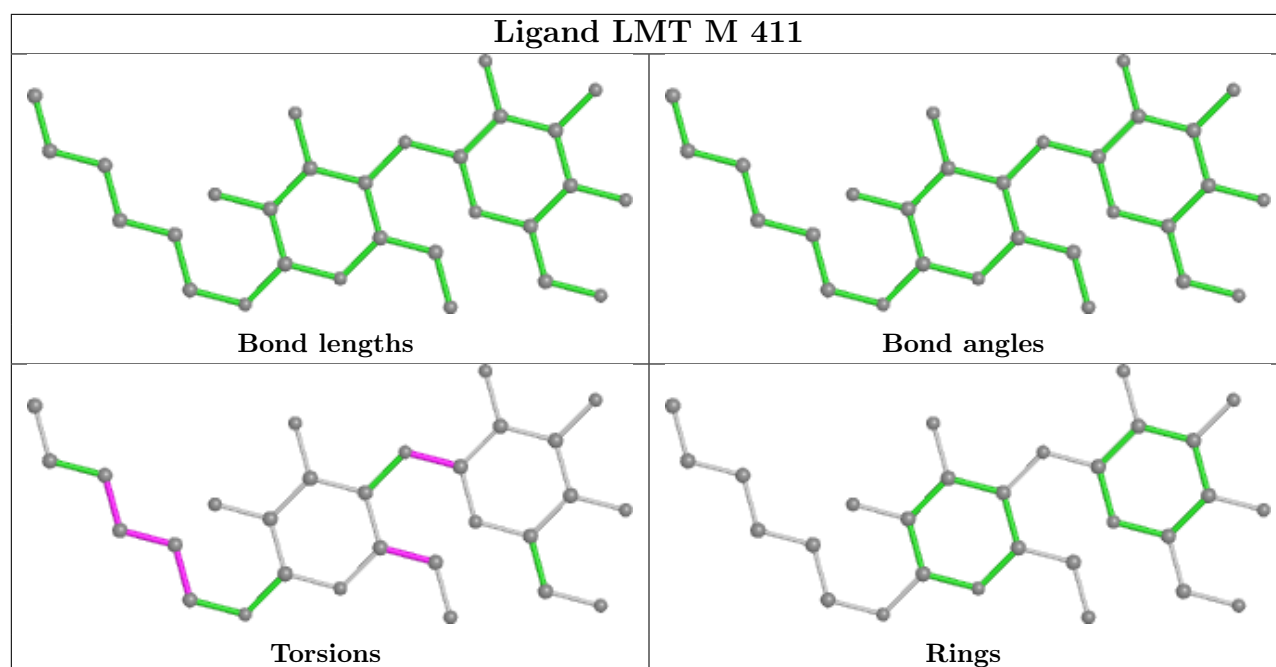


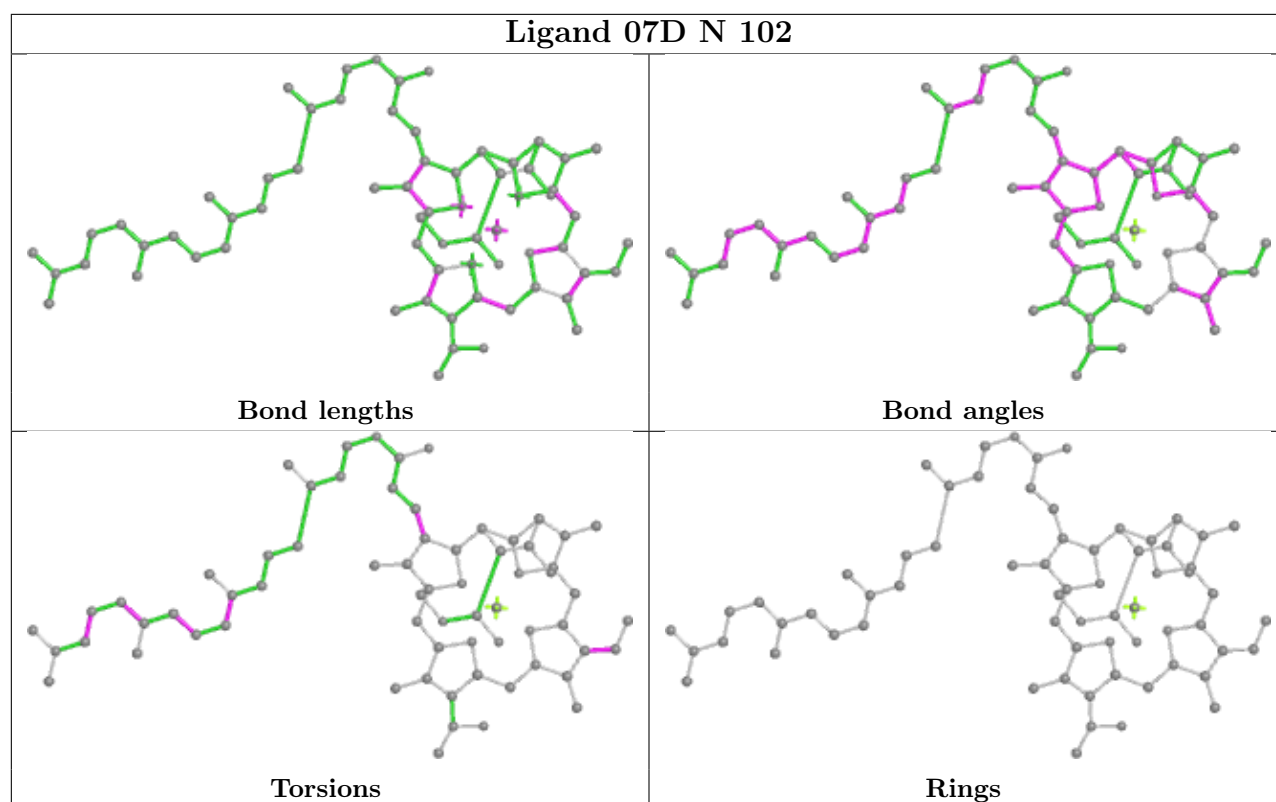
Ligand 07D J 102



Ligand 07D I 101







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

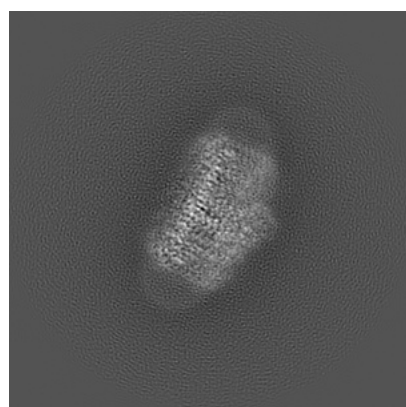
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31258. These allow visual inspection of the internal detail of the map and identification of artifacts.

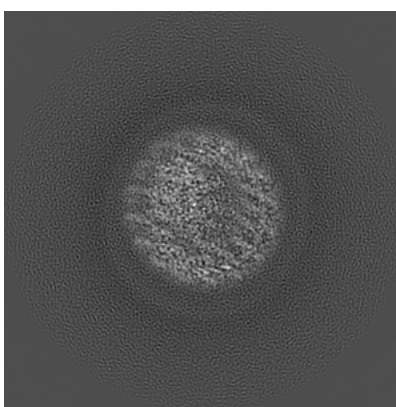
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

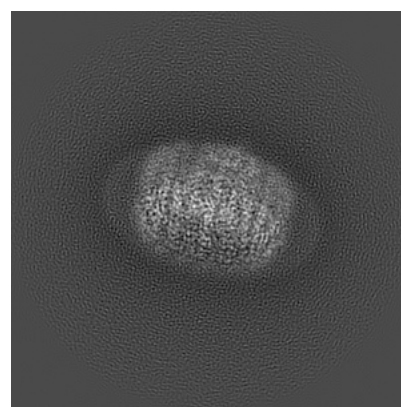
6.1.1 Primary map



X



Y

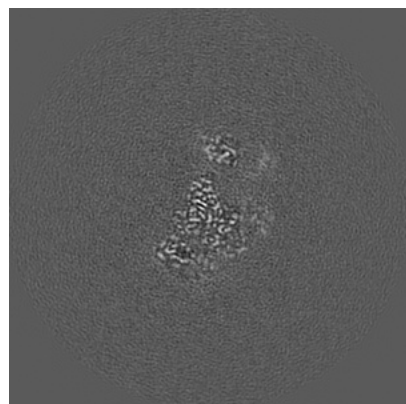


Z

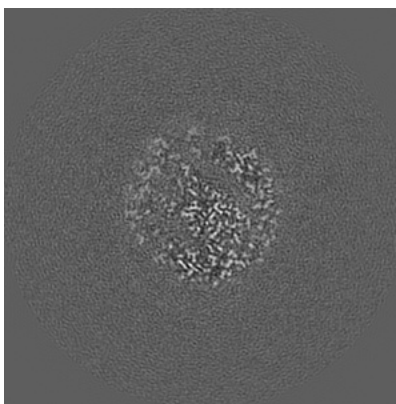
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

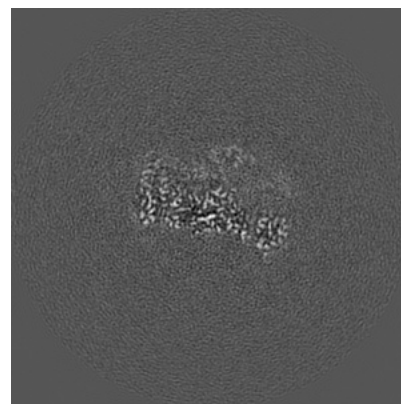
6.2.1 Primary map



X Index: 180



Y Index: 180

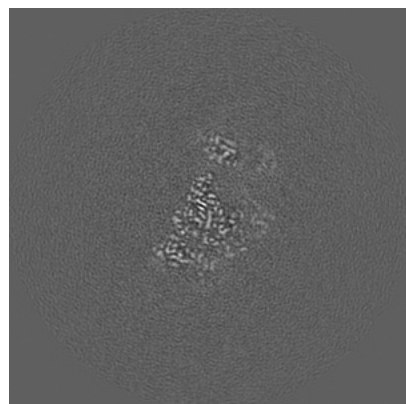


Z Index: 180

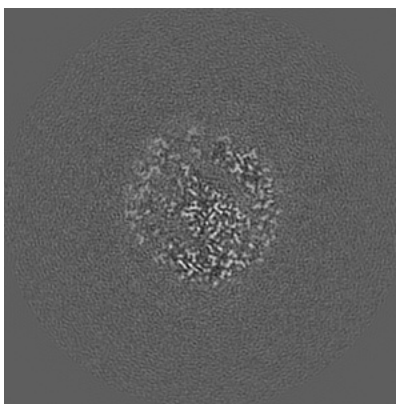
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

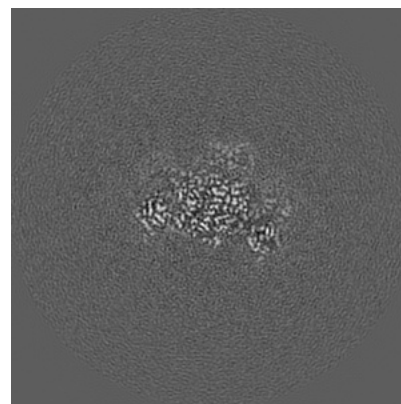
6.3.1 Primary map



X Index: 179



Y Index: 180

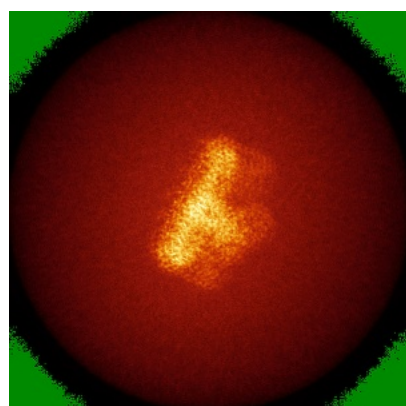


Z Index: 171

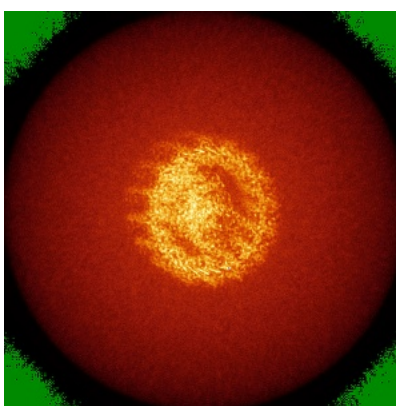
The images above show the largest variance slices of the map in three orthogonal directions.

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

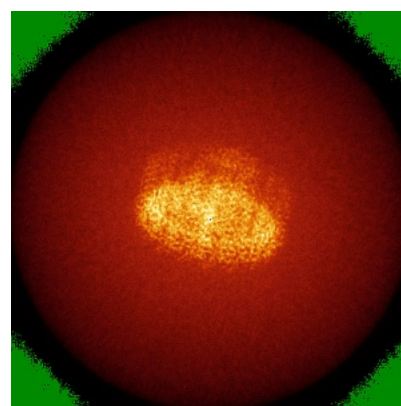
6.4.1 Primary map



X



Y

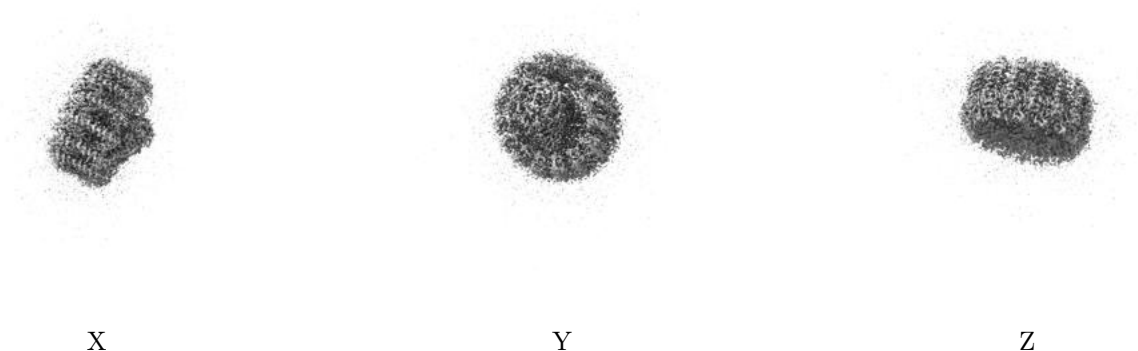


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

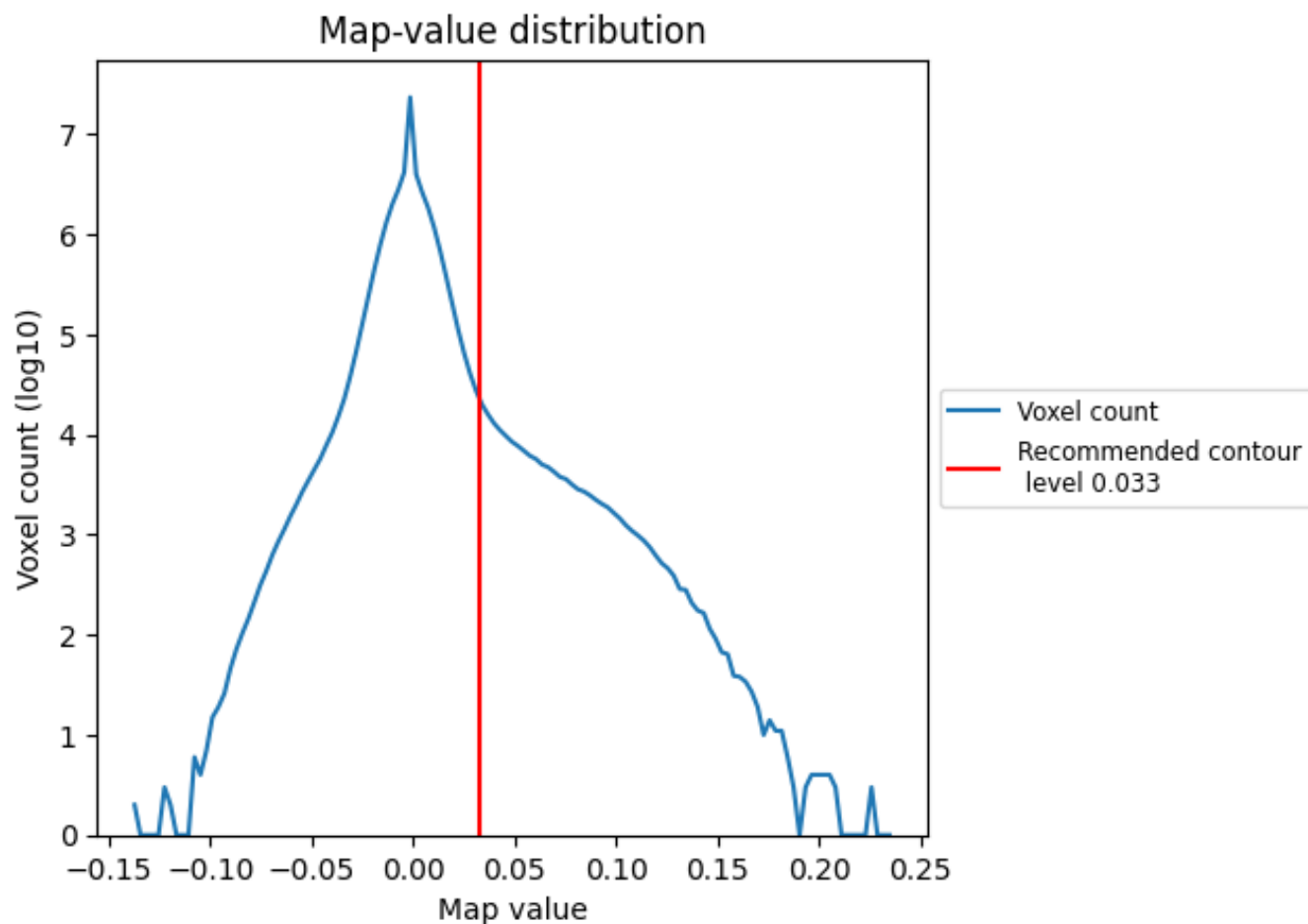
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

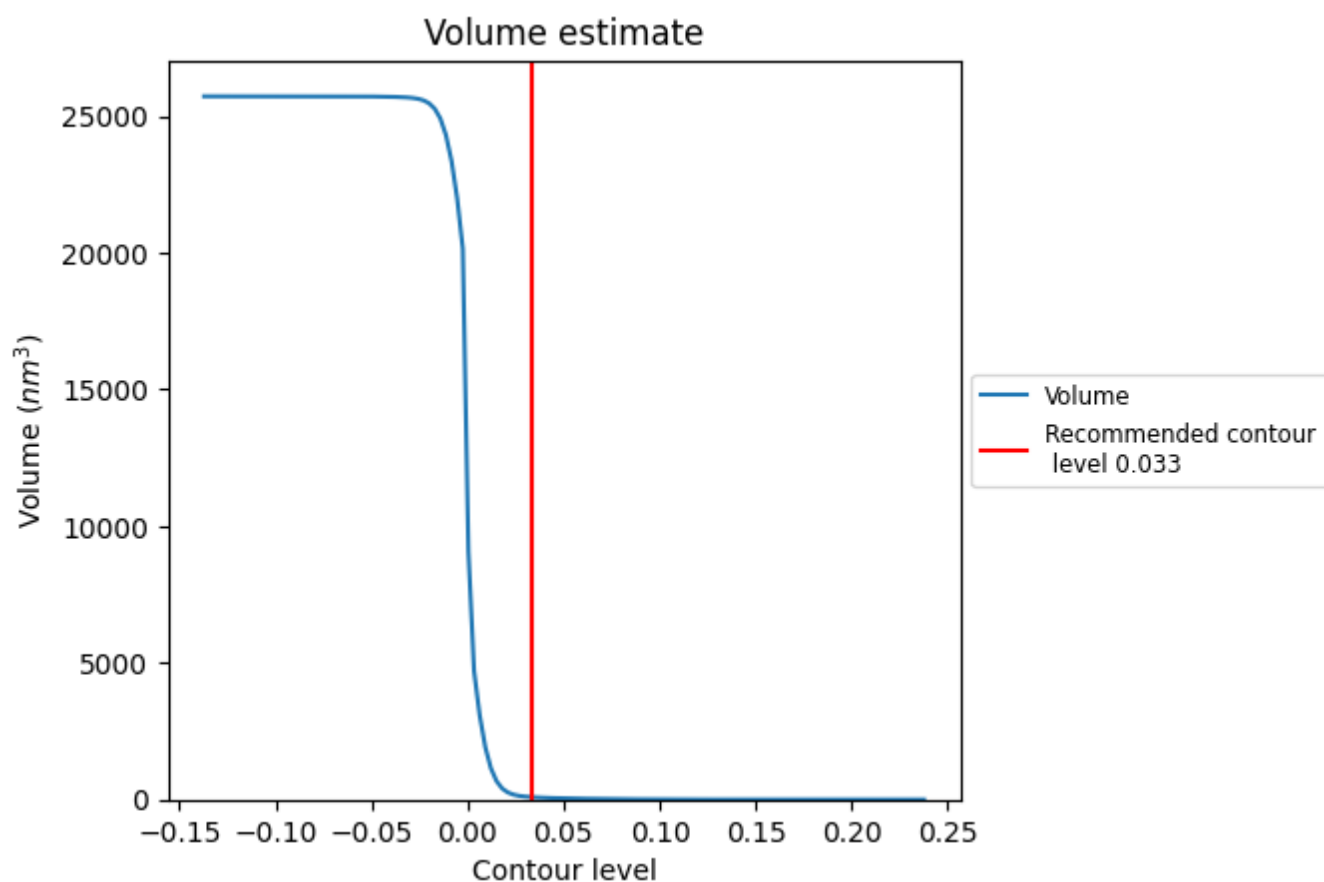
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

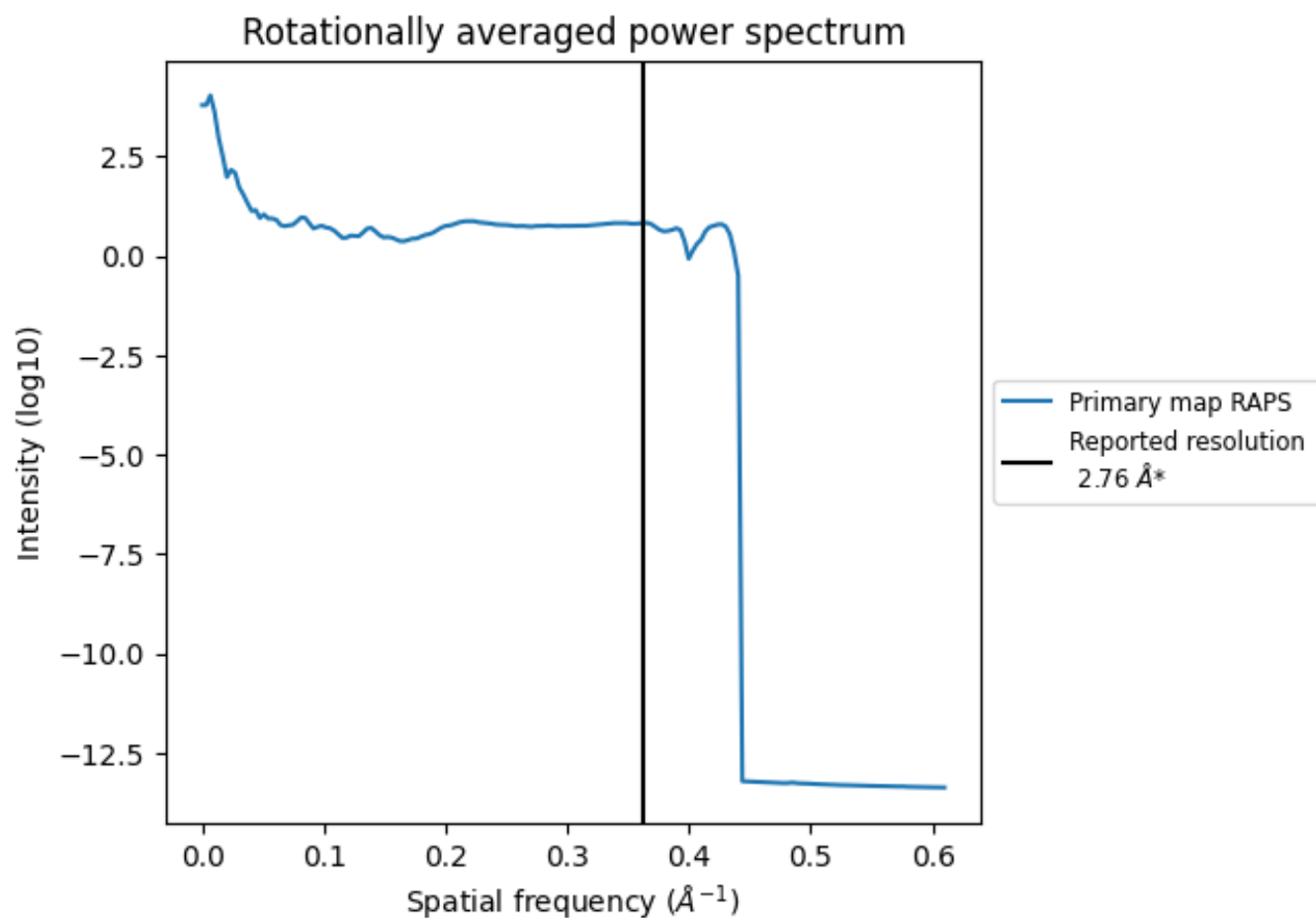
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm³; this corresponds to an approximate mass of 81 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

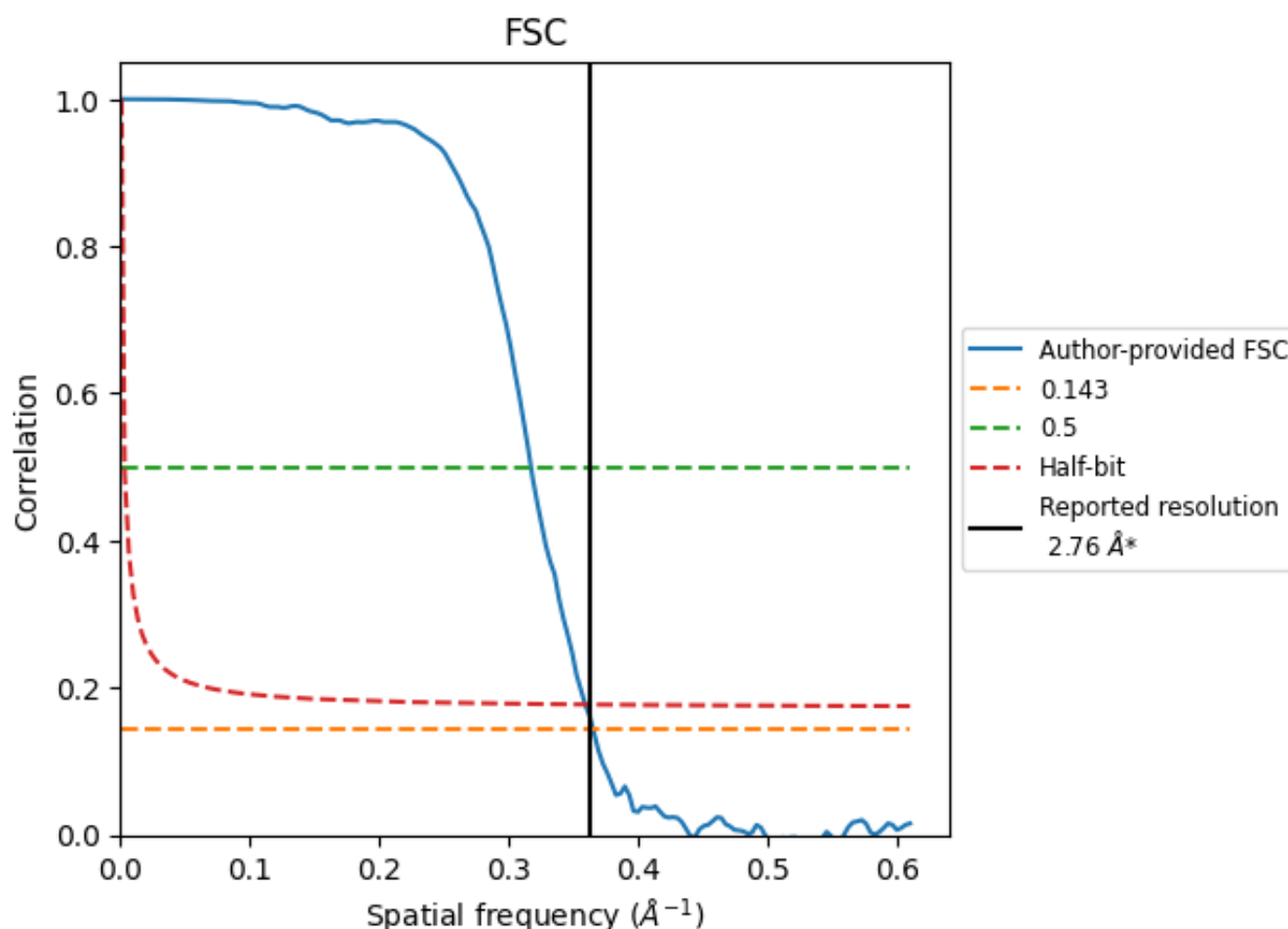


*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

8.2 Resolution estimates [i](#)

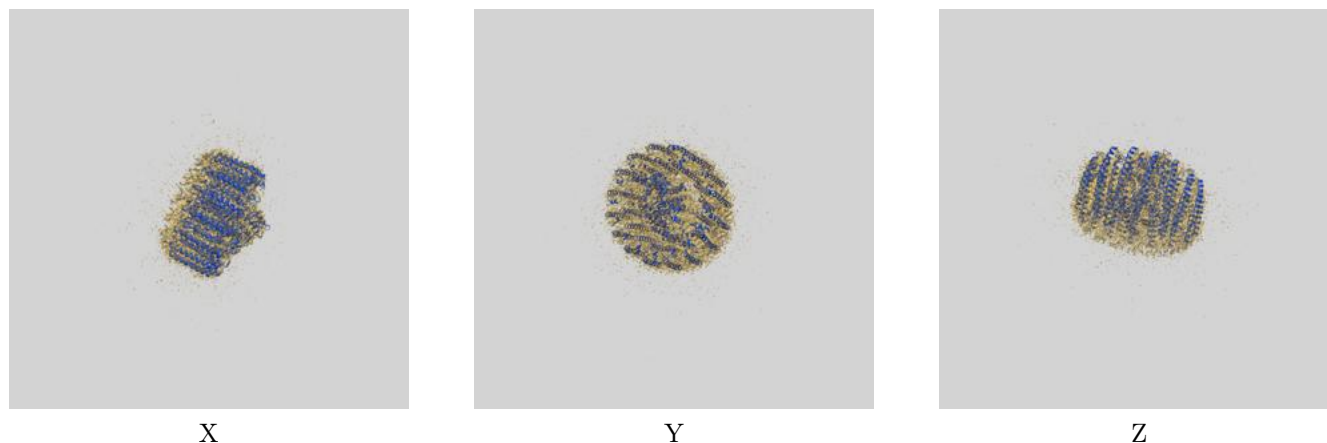
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.74	3.15	2.79
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

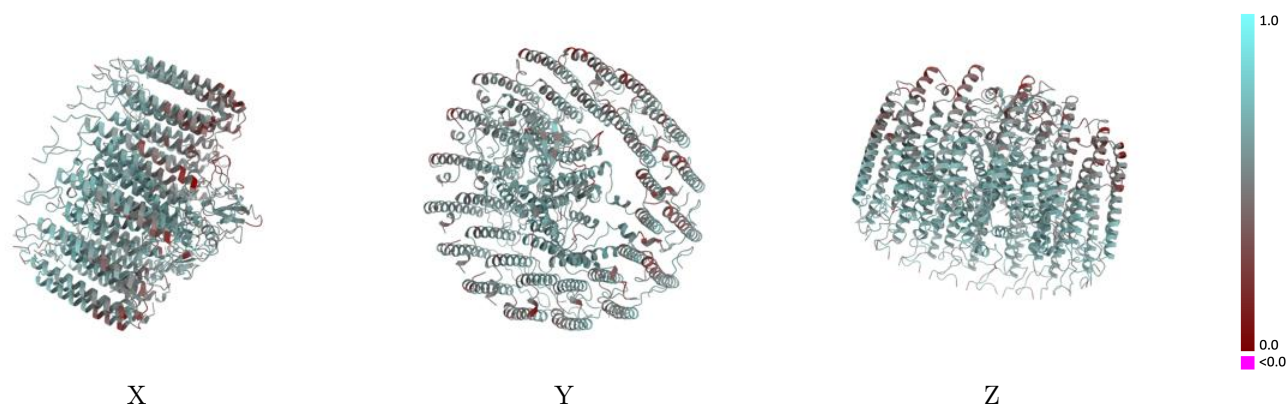
This section contains information regarding the fit between EMDB map EMD-31258 and PDB model 7EQD. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

9.1 Map-model overlay [i](#)



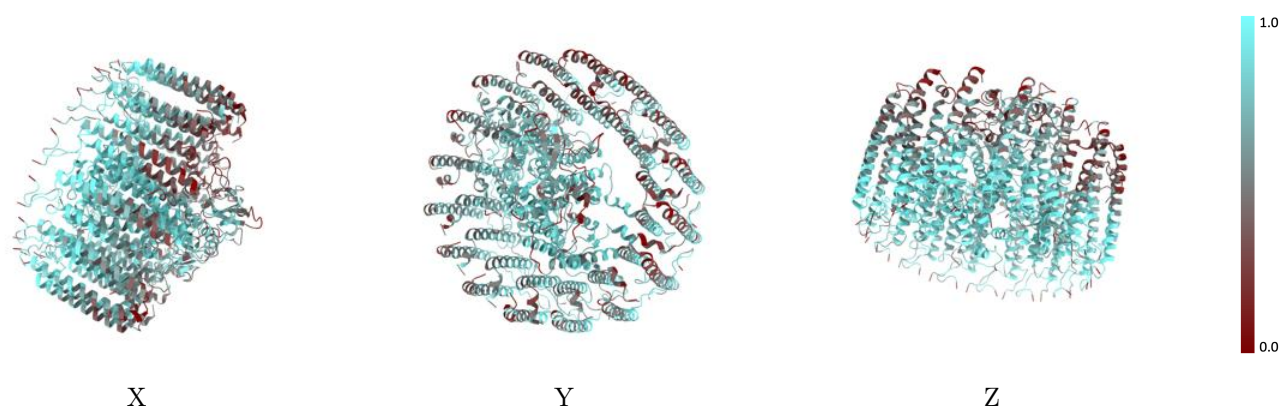
The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



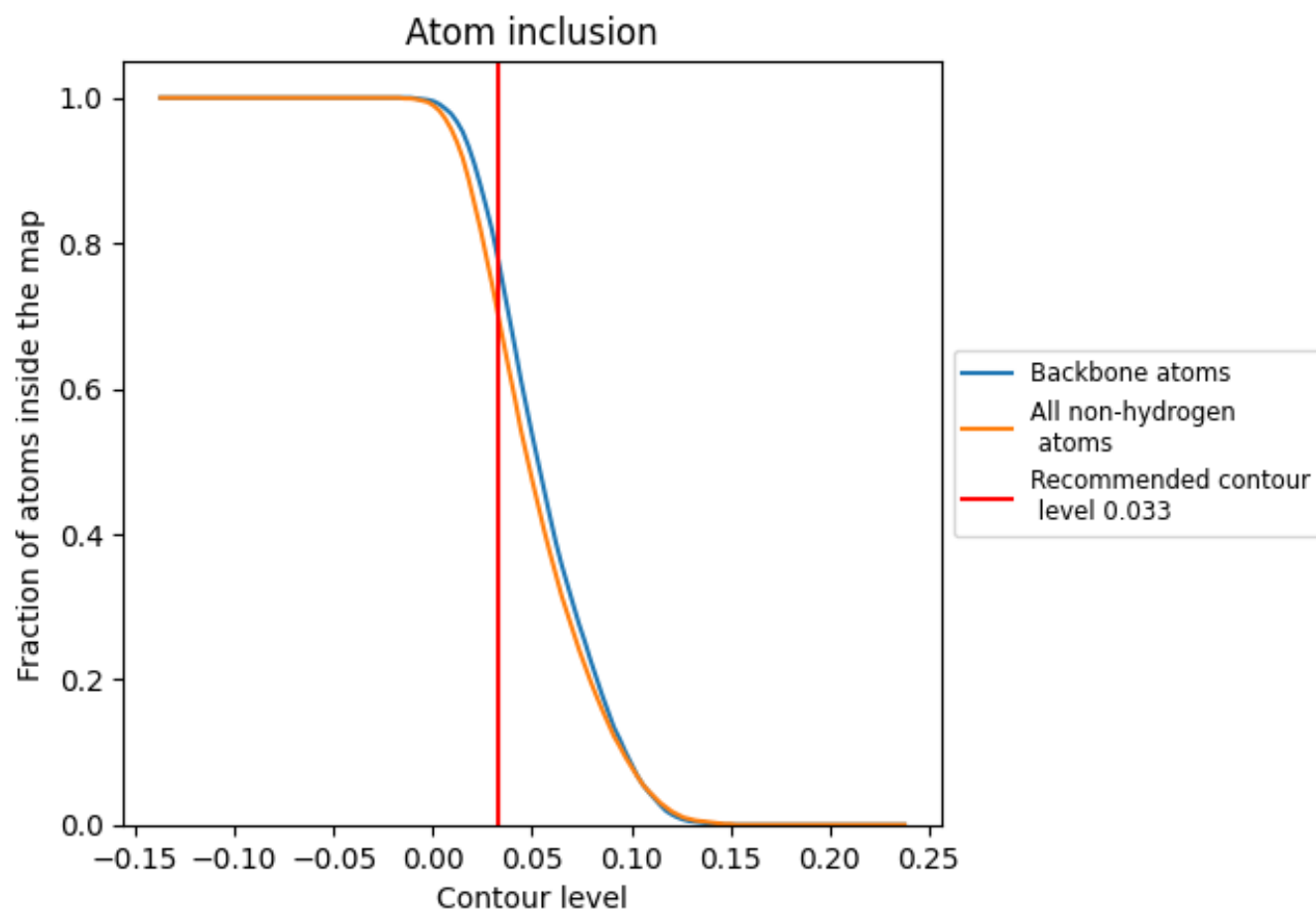
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.033).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7000	 0.5770
0	 0.6870	 0.5780
1	 0.6170	 0.5370
2	 0.5890	 0.5370
3	 0.5810	 0.5370
4	 0.5610	 0.5020
5	 0.5590	 0.5320
6	 0.5610	 0.5080
7	 0.6800	 0.5750
8	 0.6590	 0.5560
9	 0.7380	 0.5940
A	 0.7290	 0.5910
B	 0.6680	 0.5540
D	 0.7530	 0.6020
E	 0.7040	 0.5670
F	 0.7580	 0.5990
G	 0.7430	 0.5960
H	 0.6100	 0.5460
I	 0.7580	 0.5970
J	 0.7070	 0.5900
K	 0.7400	 0.5920
L	 0.8650	 0.6400
M	 0.7990	 0.6240
N	 0.6910	 0.5730
O	 0.7350	 0.5830
P	 0.6270	 0.5550
Q	 0.7280	 0.6010
R	 0.7130	 0.5660
S	 0.6760	 0.5680
T	 0.6560	 0.5560
U	 0.6660	 0.5600
V	 0.5990	 0.5250
W	 0.6690	 0.5650
X	 0.5860	 0.5350
Y	 0.6370	 0.5270
Z	 0.6220	 0.5290

